Electronic Supplementary Material (ESI) for ChemComm.


# Reactivity Prediction in Aza-Michael Additions without Transition State Calculations: The Ames Test for Mutagenicity

# Supporting Information

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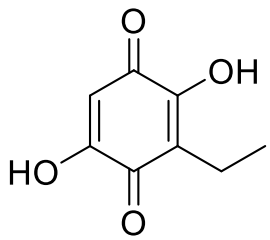
## The supplementary information is split into seven sections:






Embelin (Truncated)

## Full Computational Methods

At the start of this study, the lowest energy transition states from our previous study were optimised to an intermediate structure on the potential energy surface.[1] The activation free energies of the lowest lying transition state were correlated with the energy of their corresponding intermediate structures and a coefficient of determination $R^2 = 0.95$ was obtained (refer to Figure S4). Thus, it was clear that the intermediate states lie close in energy to the transition states, and a predictive approach may exist that utilises the high energy intermediate structure.

To account for molecular flexibility, conformational searches were performed using the MMFF force field, on both the reactants and HEIs of the chosen compounds using Schrödinger's Macromodel (Version 11.3).[2,3] A mixed torsional/low mode sampling approach was adopted for all molecular structures, coupled with the use of the Polak-Ribier Conjugate Gradient (PRCG) minimisation method.[4] Successfully converged conformations were further optimised in Gaussian 16 (Rev. A.03) using both semi-empirical and DFT methods.[5] Semi-empirical optimizations used the Austin Model 1 (AM1) level of theory. DFT structures were optimized using the B3LYP functional with dispersion corrections (D3(BJ)) and the polarized triple zeta valence (def2-TZVPP) basis set to minimise basis set superposition error.[6] Grimme's D3 dispersion-correction term with Becke-Johnson damping was included to improve the accuracy of the model, and better account for weak intermolecular interactions in the toxicant-target systems.[7] Single point energy calculations at the B3LYP-D3(BJ)/def2-TZVPP level of theory were also performed on the AM1 optimized structures. To mimic an aqueous cellular environment where this type of toxicant-target interaction may occur, an implicit solvent model for water was included in all DFT calculations. The integral equation formalism polarizable continuum model (IEF-PCM) was chosen due to extensive use in previous studies of organic chemical reaction mechanisms.[8–10] All structures were verified as stationary points prior to analysis. To account for the poor description of low frequency modes by the rigid rotor harmonic oscillator treatment, temperature and concentration corrected quasi-harmonic free energies were extracted using Goodvibes.[11] All thermochemical data was computed at a temperature of 310.15 K, a concentration of 1 mol $dm^{-3}$, and a vibrational scaling factor of 1.

Prior to conformational searching, a single high energy intermediate for each compound was found using Gaussian 16. Following this, all high energy intermediate structures were imported to Macromodel and the C-N bond length was constrained at 1.5 Å. The Michael acceptor double bond was retrained in the conformational search, and no explicit bond was included between the Michael acceptor β-carbon and methylamine nitrogen. Following DFT optimization, some structures converged to the enol form of the corresponding 1,4 Michael acceptor. These structures are included in the supplementary information, however, they have not be treated as intermediate structures in the thermochemical analysis.

References


1 P. A. Townsend and M. N. Grayson, *J. Chem. Inf. Model.*, 2019, **59**, 5099–5103.
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## Full List of Authors in the Hasselgren Reference (Reference 1)

C. Hasselgren, E. Ahlberg, Y. Akahori, A. Amberg, L. T. Anger, F. Atienzar, S. Auerbach, L. Beilke, P. Bellion, R. Benigni, J. Bercu, E. D. Booth, D. Bower, A. Brigo, Z. Cammerer, M. T. D. Cronin, I. Crooks, K. P. Cross, L. Custer, K. Dobo, T. Doktorova, D. Faulkner, K. A. Ford, M. C. Fortin, M. Frericks, S. E. Gad-mcdonald, N. Gellatly, H. Gerets, V. Gervais, S. Glowienke, J. Van Gompel, J. S. Harvey, J. Hillegass, M. Honma, J. Hsieh, C. Hsu, T. S. Barton-maclaren, C. Johnson, R. Jolly, D. Jones, R. Kemper, M. O. Kenyon, N. L. Kruhlak, S. A. Kulkarni, K. Kümmerer, P. Leavitt, S. Masten, S. Miller, C. Moudgal, W. Muster, A. Paulino, E. Lo, M. Powley, D. P. Quigley, M. V. Reddy, A. Richarz, B. Schilter, R. D. Snyder, L. Stavitskaya, R. Stidl, D. T. Szabo, A. Teasdale, R. R. Tice, A. Trejo-martin, A. Vuorinen, B. A. Wall, P. Watts, A. T. White, J. Wichard, K. L. Witt, A. Woolley, D. Woolley, C. Zwickl and G. J. Myatt, *Regul. Toxicol. Pharmacol.*, 2019, **107**, 104403.

## Full List of Authors in the Gaussian 16 Reference (Reference 22)

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

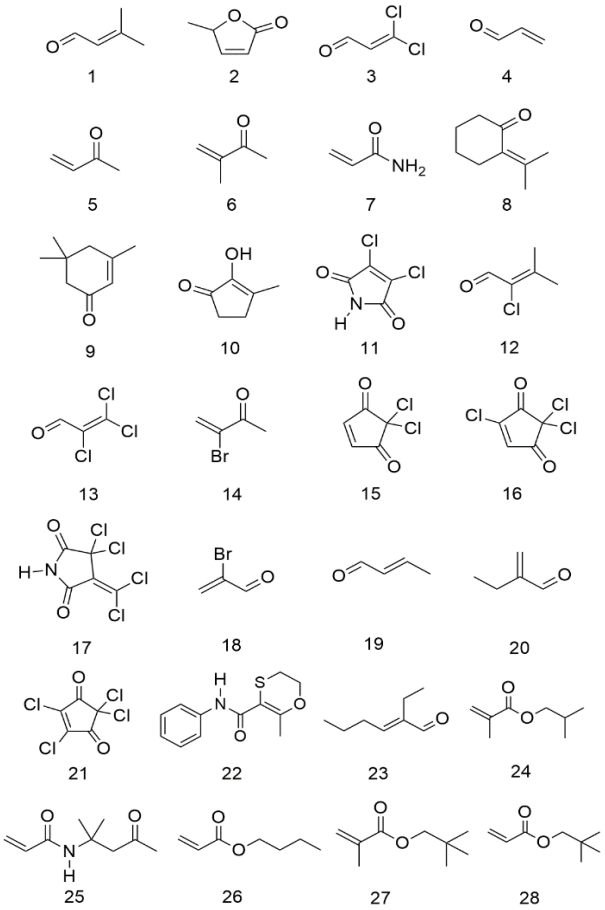


**Figure S1.** Chemical structures of the 28 compounds included in this study.

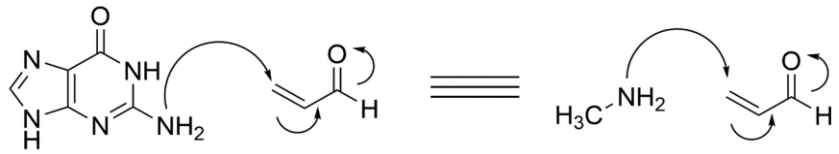

**Figure S2**. Methylamine was chosen as a surrogate nucleophile for a DNA nucleobase such as guanine.

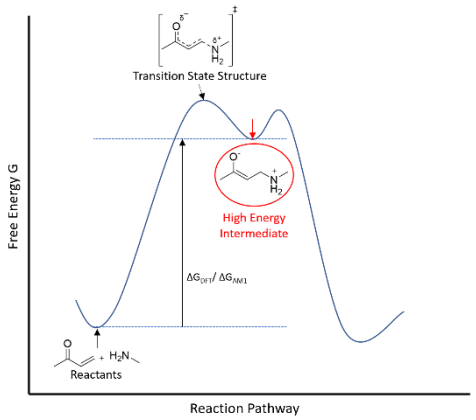


**Figure S3**. Diagram showing reactants, TS and the HEI along the reaction pathway. Intermediate structures are easier to compute than TSs.

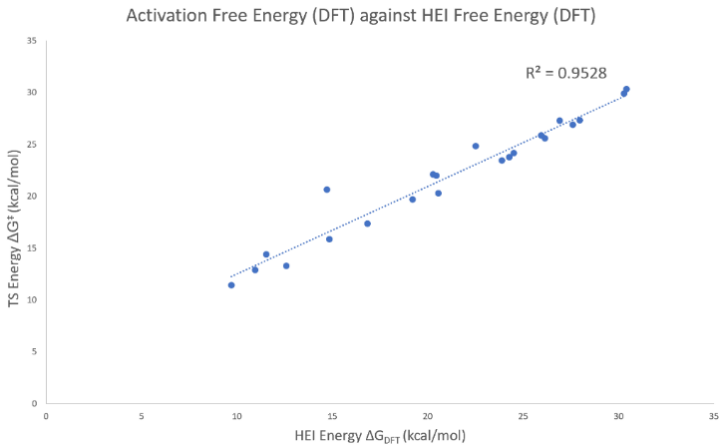


**Figure S4.** Correlation between the activation free energy of the lowest lying TSs (y-axis) and the free energy of the corresponding HEI structure (x-axis).[1] A strong correlation is observed, indicating that HEI structures may be used in Ames test predictions.

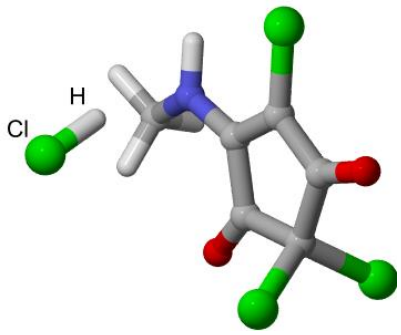


**Figure S5.** In DFT calculations, elimination of hydrogen chloride was apparent in five of the 28 compounds.

1. P. A. Townsend and M. N. Grayson, *J. Chem. Inf. Model.*, 2019, **59**, 5099–5103.

## Formal Protocol (S6)

(i) Structure File Generation The first step involves generating separate structure files that contains 3D atomic coordinates for a chosen 1,4 Michael acceptor and the methylamine nucleophile. It is recommended that structure files (e.g. .xyz, .mol, .mol2, .pdb) be generated through chemical editing software such as ChemDraw or MarvinSketch. Alternatively, the structure may be readily created in the software used for conformational searching e.g. Schrödinger's Maestro.

(ii) Conformational Searches To explore molecular flexibility, a conformational search should be carried out on both the MA reactant and the HEI structure. The bond length between the methylamine nitrogen and the β-carbon of the 1,4 MA in the HEI should be set and constrained to 1.5 Å prior to searching. The MMFF force field should be used in combination with the PRCG minimisation method for energy calculations. Schrödinger's Macromodel was used in this work.[1] All generated conformers of the reactant and HEIs should be saved and imported for DFT calculations.

(iii) DFT Calculations All conformers of the reactant, HEI and methylamine should be treated quantum mechanically using DFT. Permitting availability of DFT functionals, basis sets and solvent models, any *ab initio* quantum chemistry package may be used for this section. Gaussian was used in this study.[2] All structures should be optimised to a minimum at the B3LYP-D3(BJ)/def2tzvpp level of theory. The IEFPCM implicit solvent model for water should be included in all calculations.

(iv) Thermochemical Data Analysis Using GoodVibes by Paton and Funes-Ardoiz, the quasi-harmonic free energy should be calculated at 310.15 K, a concentration of 1 mol $dm^{-3}$ and a vibrational scaling factor of 1.[3] Once thermochemistry has been obtained, $\Delta G_{DFT}$ should be computed according to equation 1. If $\Delta G_{DFT}$ is < 19.0 kcal/mol, the structure should be treated with caution due to possible mutagenic activity. If $\Delta G_{DFT}$ is > 21.0 kcal/mol, the structure likely shows a reduced mutagenic risk and an Ames negative result.

References


1 Macromodel; Schrödinger: New York, NY, 2019.
2 M. J. Frisch *et al*, Gaussian 16 (Rev A.03), Gaussian Inc., Wallingford, CT, 2016
3 Paton, R.; Funes-Ardoiz, I. Goodvibes, ver. 2.0.3. 2019

## Structural Features of Ames Positive/Negative Compounds (S7)

It can be seen in Figure S1 that the Michael acceptor (MA) dataset is structurally diverse. It consists of primarily esters, aldehydes, and ketones, with two amide groups also being included in the study. Our aim in this section is to discuss the structural features that lead to a positive or negative Ames test result. Firstly, it is apparent that all halogen containing Michael acceptors are Ames positive, and should thus be treated with extreme caution in a pharmaceutical/drug development setting. Our DFT results confirm this statement, with no halogen containing structures showing a $\Delta G_{DFT}$ value higher than 14 kcal/mol. Our dataset also shows that not a single ester shows Ames positive behaviour, likely demonstrating that esters are less reactive to nitrogen containing biological nucleophiles. To confirm this, all esters showed calculated $\Delta G_{DFT}$ values higher than 20 kcal/mol. Alongside this key result, all Ames negative compounds showed calculated $\Delta G_{DFT}$ values ranging from 20 – 30 kcal/mol, thus placing all esters into the negative region. Furthermore, upon inspection of structures 5 and 6, it is apparent that methyl substitution at the α-carbon of a simple ketone is sufficient to move from the Ames positive region to the Ames negative region. Parallel to this result, there were no other acyclic Ames positive Michael acceptors with methyl substitution at the α-carbon. Ames positive compounds with α-substitution are plentiful in the dataset; however, all of these structures are substituted with either chlorine or bromine, reconfirming the dangers attached to halogen containing MA's. As described above, it is clear that generalisations can be made in terms of molecular structure through a structure-activity relationship. However, although this SAR-type approach can be powerful and predictive in nature, acquiring a quantum mechanical 'picture' of these systems allows for a physical confirmation of human-derived SARs. The real strength of our model lies in the strong correspondence between the experimental Ames test result (and thus our generalisations discussed above) and the well explored quantum chemical landscape.

## Model Consistency Across Different DFT Methods (S8)

To ensure that our model is consistent across multiple levels of theory, calculations were performed on the AOU of our model with a different DFT functional, a different basis set and a different solvent model. Our chosen functional was the dispersion corrected WB97XD, the 6-31G+(d) basis set and the SMD solvent model (water). Thus, optimizations were performed at: **(1)** B3LYP-D3(BJ)/def2tzvpp-IEFPCM (water), **(2)** WB97XD/def2tzvpp-IEFPCM (water), **(3)** B3LYP-D3(BJ)/6-31G+(d)-IEFPCM (water) and **(4)** B3LYP-D3(BJ)/def2tzvpp-SMD (water) levels of theory. The results of these calculations all show good agreement with our model, and in some cases, the AOU is improved when compared to our chosen level of theory (B3LYP-D3(BJ)/def2tzvpp-IEFPCM (water)). Thus, these results indicate that Ames test predictions are not highly sensitive to the level of theory used. The authors would still recommend that if a prediction on a novel compound were to be made, the level of theory used in our developed model should be chosen. This is suggested because: (i) calculations have been performed at B3LYP-D3(BJ)/def2tzvpp-IEFPCM (water) on a larger dataset of 28 compounds and (ii) our previously published model used this level of theory, and excellent agreement was seen between transition state barriers and the Ames test classification of 1,4 Michael acceptor type compounds.[1]

| | | **$\Delta G_{DFT}$ Level of Theory** | | | |
|---|---|---|---|---|---|
| | **Compound** | **1 (kcal/mol)** | **2 (kcal/mol)** | **3 (kcal/mol)** | **4 (kcal/mol** |
| AP | 12 | 14 | 11.7 | 12.4 | 11.8 |
| AP | 19 | 14.1 | 12.3 | 12.9 | 11.0 |
| AN | 26 | 20.1 | 18.5 | 18.1 | 15.2 |
| AP | 20 | 20.2 | 18.9 | 17.0 | 12.0 |
| AN | 28 | 20.3 | 18.6 | 18.2 | 15.2 |
| AN | 7 | 22.5 | 20.9 | 20.5 | 19.7 |
| AN | 24 | 23.8 | 22.4 | 21.9 | 19.6 |

Table S1. $\Delta G_{DFT}$ values obtained at four different levels of theory. The results show that our model is consistent and relatively insensitive to the chosen level of theory.

1. P. A. Townsend and M. N. Grayson, *J. Chem. Inf. Model.*, 2019, **59**, 5099–5103.

Created using ESIgen v0.0.5

Apart from warfarin and embelin, all atomic coordinates of ground state reactant structures optimised at B3LYP-D3(BJ)/def2tzvpp-IEFPCM (Water) were taken from our previous study: https://doi.org/10.1021/acs.jcim.9b00966. All AM1 structures are newly obtained.

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ESIgen is scientific software, funded by public research grants and published as:

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J Rodriguez-Guerra, P Gomez-Orellana, JD Marechal.
J. Chem. Inf. Model., 2018, 58 (3), pp 561564.
DOI: 10.1021/acs.jcim.7b00714.
```

# Ground State Structures

### Compound_1_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.691523 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.60339 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.     117.0046 cm-1
2.     130.4006 cm-1
3.     189.7685 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.607489        0.249106        0.000001
H          -1.496965        1.344871        0.000004
C          -0.391908       -0.539538       -0.000003
H          -0.542158       -1.613281       -0.000009
C           0.864861       -0.050249       -0.000001
C           1.225977        1.402969       -0.000000
H           1.841935        1.624556        0.874626
H           1.841855        1.624572       -0.874680
H           0.374426        2.074923        0.000045
```

```
C           2.035140       -0.983006        0.000001
H           2.663287       -0.797859        0.875032
H           1.729437       -2.026796       -0.000052
H           2.663353       -0.797786       -0.874966
O          -2.729332       -0.238611        0.000001
```

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### Compound_2_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -344.758331 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -344.683953 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 33)

```
1.     137.9147 cm-1
2.     237.2087 cm-1
3.     247.0046 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.054096       -0.057264        0.456879
C          -0.533352        1.303511        0.123894
C           0.764118        1.233732       -0.158989
C           1.194368       -0.167933       -0.025702
H          -1.375109       -0.103858        1.500369
H          -1.163571        2.179373        0.121159
H           1.436445        2.025197       -0.444187
O           0.111333       -0.909481        0.336262
C          -2.161185       -0.557000       -0.454430
H          -2.434335       -1.576521       -0.188329
H          -3.040218        0.077236       -0.343609
H          -1.839137       -0.532508       -1.494901
O           2.283268       -0.665420       -0.186313
```

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### Compound_3_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1111.261693 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1111.248123 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
1.     127.4861 cm-1
2.     168.1073 cm-1
3.     204.2964 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.065043        0.043270        0.000034
H           2.001054        1.141267        0.000037
C           0.801982       -0.687205        0.000010
H           0.858721       -1.766730        0.000006
C          -0.404644       -0.109798       -0.000007
O           3.144245       -0.517768        0.000048
Cl         -0.668011        1.590880       -0.000004
Cl         -1.848932       -1.044409       -0.000035
```

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### Compound_4_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -192.011509 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -191.974479 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
1.     173.1036 cm-1
2.     326.3352 cm-1
3.     578.9713 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.667203        0.347243        0.000001
O           1.789724       -0.119145        0.000001
```

```
C          -0.559253       -0.450432       -0.000001
H           0.512565        1.442096        0.000001
C          -1.752922        0.142902       -0.000001
H          -2.674251       -0.422187       -0.000002
H          -1.837259        1.222990       -0.000000
H          -0.449008       -1.528013       -0.000001
```

---

### Compound_5_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -231.354696 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.292394 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.     107.4450 cm-1
2.     127.7737 cm-1
3.     290.5998 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.540117       -0.183635       -0.000017
O          -1.438782       -1.012020       -0.000081
C           0.867225       -0.639837       -0.000036
C           1.927339        0.165467        0.000025
H           2.932524       -0.233308        0.000006
H           1.832956        1.242716        0.000096
H           0.987255       -1.716801       -0.000107
C          -0.840233        1.293643        0.000082
H          -0.405810        1.773116        0.878339
H          -0.405796        1.773237       -0.878101
H          -1.916157        1.443372        0.000084
```

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### Compound_6_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.693568 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.604928 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      72.6591 cm-1
2.     140.4953 cm-1
3.     188.0575 cm-1
```

**B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates**

```
C           0.685754       -0.316469        0.000039
C          -0.690363        0.260418       -0.000031
C          -0.881922        1.581766       -0.000155
H          -0.062804        2.285292       -0.000208
H          -1.879521        2.000567       -0.000212
C          -1.822749       -0.723887        0.000040
H          -1.772142       -1.373673       -0.874632
H          -1.772158       -1.373527        0.874822
H          -2.781606       -0.209650       -0.000011
O           0.832696       -1.528995        0.000120
C           1.885351        0.600225       -0.000002
H           2.790003       -0.001062        0.000170
H           1.880188        1.245695       -0.878665
H           1.880045        1.246000        0.878433
```

---

**Compound_7_Ground_State**

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -247.429171 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -247.376667 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      99.5899 cm-1
2.     282.2827 cm-1
3.     286.5705 cm-1
```

**B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates**

```
C           0.480845        0.124324       -0.000014
O           0.529550        1.352529       -0.000010
C          -0.799685       -0.639262        0.000097
C          -1.975230       -0.023167       -0.000046
H          -2.903459       -0.576750       -0.000091
H          -2.029140        1.057456       -0.000168
H          -0.738968       -1.720786        0.000161
N           1.593205       -0.643021        0.000223
H           2.498284       -0.203868       -0.000521
H           1.548870       -1.646509       -0.001081
```

---

### Compound_8_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -426.820066 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -426.643236 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      50.6395 cm-1
  2.      62.8378 cm-1
  3.      98.3380 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.322527       -0.187662        0.142239
C          -0.466157       -1.487184        0.263074
C          -1.976135       -1.298121        0.391438
C          -2.457491       -0.276342       -0.630100
C          -1.886403        1.088311       -0.262921
C          -0.427791        1.088675        0.169811
H          -2.472260       -2.259901        0.257218
H          -0.272238       -2.105326       -0.617590
H          -0.095904       -2.056449        1.118345
H          -2.121627       -0.574278       -1.627220
H          -3.546279       -0.226014       -0.664642
H          -1.965339        1.802669       -1.085665
H          -2.450526        1.520834        0.567711
H          -2.230560       -0.947799        1.396480
O           0.072067        2.150309        0.525787
C           1.662527       -0.209013       -0.048358
C           2.530481        0.993649       -0.278539
```

```
H           3.341034        0.732448       -0.961253
H           1.985002        1.848109       -0.663648
H           2.996078        1.305639        0.660772
C           2.421672       -1.503728       -0.107322
H           1.906149       -2.335184        0.363249
H           2.612408       -1.773488       -1.151062
H           3.398156       -1.385245        0.365067
```

---

### Compound_9_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -426.836444 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -426.659559 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      88.3848 cm-1
2.     126.8658 cm-1
3.     157.8467 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.346439       -0.712952       -0.101500
C          -0.013593       -1.285477       -0.379100
C          -1.185301       -0.369107        0.008764
C          -0.893994        1.039923       -0.529920
C           0.459556        1.579029       -0.125765
C           1.541675        0.611584        0.015949
H          -0.063177       -1.509520       -1.451462
H          -0.109924       -2.249039        0.127101
H          -0.902503        1.014778       -1.625666
H          -1.659437        1.751358       -0.219551
H           2.525691        1.013858        0.223477
O           0.644033        2.781234        0.038217
C          -2.479192       -0.900318       -0.611125
H          -2.691953       -1.909774       -0.254555
H          -3.324883       -0.264469       -0.344166
H          -2.408975       -0.932802       -1.699540
C          -1.340413       -0.325246        1.535417
H          -2.157627        0.340938        1.815588
H          -1.566631       -1.319185        1.923897
H          -0.434306        0.028917        2.026968
C           2.466654       -1.691984        0.022455
```

```
H           3.429231       -1.200856        0.149166
H           2.291810       -2.354393        0.874237
H           2.509438       -2.332404       -0.862284
```

---

### Compound_10_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -384.087946 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -383.988876 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 42)

```
1.      77.1938 cm-1
2.      99.0138 cm-1
3.     136.6279 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.028791       -0.196564       -0.000018
C           0.526345       -1.614794        0.000131
C          -1.004601       -1.496659        0.000165
C          -1.287891       -0.007307        0.000044
C           0.006972        0.680574       -0.000061
H           0.899223       -2.152465        0.874975
H           0.899173       -2.152633       -0.874629
H          -1.465217       -1.952084       -0.876789
H          -1.465170       -1.951933        0.877220
O          -2.385987        0.523088        0.000035
O           0.019225        2.037432       -0.000183
H           0.926036        2.363110       -0.000223
C           2.482817        0.109058       -0.000098
H           2.697816        1.177500       -0.000224
H           2.963850       -0.330654        0.876976
H           2.963794       -0.330849       -0.877104
```

---

### Compound_11_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1278.85912 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1278.841551 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      96.9140 cm-1
2.     147.7482 cm-1
3.     164.5840 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.000270       -0.250470        0.668144
C          -0.000059        1.177529        1.148751
C          -0.000059        1.177529       -1.148751
C          -0.000270       -0.250470       -0.668144
O           0.000345        1.570037       -2.285792
O           0.000345        1.570037        2.285792
Cl         -0.000059       -1.554865       -1.745394
Cl         -0.000059       -1.554865        1.745394
N          -0.000073        1.951437        0.000000
H           0.000939        2.960035        0.000000
```

---

### Compound_12_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -730.31729 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -730.240725 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      53.1612 cm-1
2.     104.2949 cm-1
3.     160.8084 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.082097        1.267915       -0.000016
H          -0.576131        2.242053       -0.000035
C          -0.188033        0.114648        0.000010
C           1.160883        0.167699       -0.000009
C           1.943379        1.444733        0.000034
H           2.597402        1.457232        0.874909
H           2.597426        1.457289       -0.874821
H           1.349325        2.350691        0.000075
C           1.987738       -1.081532       -0.000057
H           1.761152       -1.692366        0.875335
H           1.760320       -1.692966       -0.874798
H           3.049366       -0.848406       -0.000612
O          -2.296406        1.210348       -0.000028
Cl         -1.005814       -1.437476        0.000023
```

---

### Compound_13_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1570.882698 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1570.880265 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
  1.      80.9473 cm-1
  2.     148.8351 cm-1
  3.     187.1120 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.444313        1.297756        0.000002
H          -0.867794        2.230880        0.000005
C          -0.633083        0.065414       -0.000001
C           0.714953        0.071999        0.000001
O          -2.653936        1.299351        0.000001
Cl         -1.510761       -1.418877       -0.000006
Cl          1.636009        1.524648        0.000006
Cl          1.655571       -1.354989       -0.000002
```

---

### Compound_14_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2804.936833 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2804.887333 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.      63.6080 cm-1
2.     154.2358 cm-1
3.     200.8685 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.420971       -0.446065        0.000069
O          -1.171586       -1.633391        0.000013
C          -0.326296        0.572836        0.000047
C          -0.515851        1.887084        0.000118
H           0.305569        2.587192        0.000099
H          -1.516337        2.294736        0.000198
C          -2.840949        0.063604        0.000163
H          -3.030703        0.678227        0.880189
H          -3.030801        0.678264       -0.879817
H          -3.514909       -0.787784        0.000182
Br          1.450979       -0.138522       -0.000095
```

---

### Compound_15_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1262.766943 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1262.739128 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.      45.0478 cm-1
2.     152.0868 cm-1
3.     198.9885 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.000041       -0.268562        0.000000
C          -0.000157        0.691081        1.214461
C          -0.000351        2.062968        0.670264
C          -0.000351        2.062968       -0.670264
C          -0.000157        0.691081       -1.214461
H          -0.000482        2.927947        1.315848
H          -0.000482        2.927947       -1.315848
Cl         -1.472225       -1.265211        0.000000
Cl          1.472774       -1.264539        0.000000
O          -0.000157        0.357040        2.368421
O          -0.000157        0.357040       -2.368421
```

---

### Compound_16_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1722.393109 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1722.377234 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.      16.6344 cm-1
  2.     130.8641 cm-1
  3.     153.9152 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.869846       -0.095273       -0.000004
C          -0.503576       -0.800864       -0.000096
C          -1.520027        0.288040       -0.000075
C          -0.956510        1.508095       -0.000079
C           0.509029        1.409525       -0.000121
H          -1.472469        2.455252       -0.000044
Cl          1.771644       -0.515996       -1.473124
Cl          1.771235       -0.515769        1.473451
O          -0.700893       -1.980630       -0.000169
O           1.302694        2.312626       -0.000215
Cl         -3.174321       -0.084021       -0.000011
```

---

### Compound_17_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2237.436497 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2237.414727 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 33)

```
1.      51.7605 cm-1
2.      70.7526 cm-1
3.     132.6097 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.019660        0.924737       -0.000077
C           1.009550       -0.255928        0.000001
C          -0.335733        0.412293       -0.000017
C          -0.109854        1.883112       -0.000089
N           1.271681        2.067280       -0.000119
H           1.685849        2.989204       -0.000168
O          -0.908545        2.785577       -0.000120
O           3.216718        0.834272       -0.000094
C          -1.533087       -0.191250        0.000026
Cl         -3.018946        0.651832        0.000000
Cl         -1.697620       -1.895549        0.000111
Cl          1.318376       -1.232833       -1.472591
Cl          1.318413       -1.232670        1.472693
```

---

### Compound_18_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2765.594048 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2765.570459 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
  1.     172.0799 cm-1
  2.     191.2543 cm-1
  3.     341.9336 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.801242       -0.283059        0.000089
O          -1.755492       -1.489840        0.000028
C          -0.635360        0.620160        0.000066
C          -0.791268        1.940709        0.000137
H           0.039386        2.629614        0.000122
H          -1.791983        2.353953        0.000214
Br          1.083594       -0.199730       -0.000071
H          -2.762044        0.258829        0.000170
```

---

### Compound_19_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -231.353908 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.29137 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.     129.6644 cm-1
  2.     201.1960 cm-1
  3.     213.3782 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.388291        0.329859        0.000002
O           2.462736       -0.245837       -0.000032
C           0.092605       -0.330122       -0.000014
C          -1.037004        0.388412        0.000026
H           0.080915       -1.414165       -0.000060
H           1.348475        1.435429        0.000049
C          -2.415384       -0.164657        0.000013
H          -2.965821        0.192837        0.873984
H          -2.965823        0.192885       -0.873937
```

```
H          -2.419764       -1.253022       -0.000018
H          -0.950929        1.471782        0.000071
```

---

### Compound_20_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.685085 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.595576 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      82.6639 cm-1
2.     176.2485 cm-1
3.     214.2366 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.590342        0.171310        0.000012
O          -2.108828       -0.927585        0.000031
C          -0.136191        0.411207       -0.000007
H          -2.211795        1.085269        0.000008
C           0.258115        1.688378       -0.000032
H           1.298851        1.977559       -0.000049
H          -0.471859        2.487947       -0.000038
C           0.764338       -0.790743        0.000002
H           0.504980       -1.405548        0.866388
H           0.504976       -1.405564       -0.866372
C           2.257049       -0.490482       -0.000003
H           2.827513       -1.418734        0.000012
H           2.550071        0.080848       -0.881919
H           2.550071        0.080878        0.881892
```

---

### Compound_21_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2182.018774 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2182.013689 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.      34.7040 cm-1
  2.      71.4387 cm-1
  3.     155.4735 cm-1
```

**B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates**

```
C           0.000004       -1.230894        0.000000
C           0.000072       -0.281908        1.216741
C           0.000032        1.097469        0.676170
C           0.000032        1.097469       -0.676170
C           0.000072       -0.281908       -1.216741
Cl         -1.472576       -2.226945        0.000000
Cl          1.472346       -2.227266        0.000000
O           0.000149       -0.606673        2.369322
O           0.000149       -0.606673       -2.369322
Cl          0.000007        2.441970        1.696928
Cl          0.000007        2.441970       -1.696928
```

---

**Compound_22_Ground_State**

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1068.861341 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1068.67063 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 81)

```
  1.      15.5952 cm-1
  2.      32.6761 cm-1
  3.      58.1408 cm-1
```

**B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates**

```
C           0.043355        0.692759       -0.208302
N          -0.898662       -0.244811        0.118805
O          -0.240431        1.837868       -0.547997
C           1.443956        0.193129       -0.135414
C          -2.297442       -0.156675        0.082684
C           2.464810        1.009563        0.217122
S           1.662400       -1.538163       -0.493980
C          -2.998702        0.975687       -0.343026
C          -3.012238       -1.287756        0.496765
C           2.340274        2.428124        0.673265
O           3.768133        0.644403        0.269942
C           3.298850       -1.751741        0.245804
C          -4.389358        0.958226       -0.350525
C          -4.397610       -1.288839        0.485522
C           4.203431       -0.630577       -0.216562
C          -5.098352       -0.163619        0.060471
H          -0.532055       -1.128473        0.441835
H          -2.457326        1.850174       -0.657305
H          -2.473579       -2.167116        0.826250
H           2.991012        2.571276        1.536407
H           2.682589        3.104009       -0.113101
H           1.321475        2.691307        0.926407
H           3.677712       -2.710596       -0.100234
H           3.222537       -1.767801        1.331406
H          -4.920525        1.840340       -0.682575
H          -4.930261       -2.172630        0.809497
H           5.207824       -0.749795        0.184285
H           4.254755       -0.601165       -1.304960
H          -6.179373       -0.163103        0.051763
```

---

### Compound_23_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -388.692935 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -388.524523 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
1.      35.2496 cm-1
2.      45.4134 cm-1
3.      76.0837 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.035810       -1.274071        0.100656
C           0.944752       -0.303055       -0.011939
C          -0.238046       -0.677726        0.505179
C          -1.504922        0.102490        0.527842
C          -2.612503       -0.571195       -0.299023
C          -3.932198        0.189618       -0.224595
C           1.237373        1.024292       -0.653792
C           1.765381        2.054130        0.351988
O           3.173237       -1.101544       -0.300811
H           1.759277       -2.224233        0.594321
H          -0.295936       -1.670584        0.944479
H          -1.349481        1.120711        0.172314
H          -1.846782        0.176311        1.565667
H          -2.752253       -1.595224        0.055709
H          -2.282373       -0.644574       -1.337724
H          -4.702140       -0.298584       -0.822887
H          -4.292699        0.247639        0.804168
H          -3.817210        1.210054       -0.594901
H           1.982529        0.871705       -1.435155
H           0.340795        1.409970       -1.137837
H           2.000833        2.995527       -0.145369
H           1.024389        2.254339        1.126833
H           2.671274        1.692396        0.838975
```

---

### Compound_24_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -463.965638 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.794274 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      26.8506 cm-1
  2.      51.8864 cm-1
  3.      57.6952 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.160553       -0.509745        0.034304
C           2.351244        0.379889       -0.090945
C           3.675552       -0.284263        0.140762
C           2.216777        1.672822       -0.385319
```

```
O           1.241437       -1.688046        0.318420
O          -0.002185        0.110119       -0.193589
C          -1.205145       -0.681021       -0.078029
C          -2.399682        0.228570       -0.302877
C          -3.675600       -0.614242       -0.319338
C          -2.474119        1.332663        0.751105
H           4.487061        0.432219        0.032828
H           3.722652       -0.720941        1.139317
H           3.831088       -1.100362       -0.566299
H           1.247371        2.119763       -0.544909
H           3.083967        2.313625       -0.472134
H          -1.167335       -1.480397       -0.818112
H          -1.234074       -1.133803        0.914444
H          -2.278603        0.691425       -1.286677
H          -3.826190       -1.110114        0.642309
H          -4.545798        0.014250       -0.508956
H          -3.638545       -1.382390       -1.093123
H          -2.599175        0.902668        1.747927
H          -1.570059        1.940354        0.756217
H          -3.323859        1.989079        0.560536
```

---

### Compound_25_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -557.478629 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -557.288535 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      24.7119 cm-1
  2.      41.4442 cm-1
  3.      54.5487 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.588848        0.040772       -0.160334
C          -2.728531       -0.447031        0.671053
C          -3.749804       -1.105013        0.136645
O          -1.539881       -0.128577       -1.380095
N          -0.633109        0.679444        0.547259
C           0.640158        1.201073        0.023016
C           1.444765        0.087843       -0.668553
C           1.748089       -1.166184        0.121956
```

```
C           2.491914       -2.235924       -0.638435
O           1.414475       -1.328210        1.279074
H          -2.696308       -0.247410        1.735609
H          -3.779723       -1.302648       -0.926686
H          -4.572954       -1.458855        0.741117
H          -0.725888        0.666175        1.548630
H           2.399240        0.498805       -1.008371
H           0.922978       -0.226935       -1.574033
H           2.740654       -3.064125        0.019805
H           1.870679       -2.596839       -1.460747
H           3.400051       -1.826541       -1.083322
C           0.362760        2.315738       -0.994355
H           1.304142        2.727102       -1.359079
H          -0.205120        1.937653       -1.840509
H          -0.203214        3.118127       -0.521345
C           1.408655        1.785380        1.210509
H           0.842668        2.602181        1.659832
H           1.599424        1.028393        1.967582
H           2.363427        2.183175        0.869869
```

---

### Compound_26_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -424.625418 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.480034 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      36.9219 cm-1
2.      62.5771 cm-1
3.      85.8048 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.769307        0.202470       -0.000000
C           2.854747       -0.804922       -0.000000
C           4.133630       -0.446655        0.000002
O           1.923142        1.405751        0.000002
O           0.567955       -0.392505       -0.000002
C          -0.592635        0.471790       -0.000003
C          -1.826331       -0.402689        0.000000
C          -3.109359        0.426699       -0.000000
C          -4.365089       -0.440182        0.000002
```

```
H           2.551790       -1.842886       -0.000002
H           4.416977        0.597458        0.000003
H           4.924138       -1.183542        0.000002
H          -0.550518        1.110126        0.882795
H          -0.550520        1.110123       -0.882803
H          -1.806148       -1.052231        0.878606
H          -1.806149       -1.052234       -0.878604
H          -3.116597        1.082066       -0.875234
H          -3.116596        1.082069        0.875231
H          -5.268191        0.170988        0.000002
H          -4.396290       -1.083489       -0.881499
H          -4.396289       -1.083486        0.881506
```

---

### Compound_27_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -503.301511 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -503.103619 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      27.6224 cm-1
  2.      47.2302 cm-1
  3.      56.0104 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           -1.407775       -0.552078       -0.000012
C           -2.554111        0.402164        0.000000
C           -3.914869       -0.227708        0.000048
C           -2.351279        1.719459       -0.000039
O           -1.549249       -1.758633       -0.000050
O           -0.212246        0.045239        0.000023
C            0.952467       -0.805715        0.000001
C            2.205533        0.065082        0.000005
C            3.409990       -0.884610       -0.000010
H           -4.690062        0.535629        0.000042
H           -4.049276       -0.864631       -0.875387
H           -4.049238       -0.864579        0.875528
H           -1.356926        2.139271       -0.000074
H           -3.185560        2.407997       -0.000037
H            0.919027       -1.442760        0.884300
H            0.919015       -1.442735       -0.884316
```

```
H           3.408767       -1.524817        0.883952
H           3.408756       -1.524802       -0.883983
H           4.338797       -0.313225       -0.000011
C           2.239456        0.942808        1.256618
H           1.390472        1.625267        1.283400
H           2.213678        0.331302        2.160578
H           3.153628        1.537572        1.277567
C           2.239445        0.942834       -1.256591
H           3.153613        1.537606       -1.277532
H           1.390456        1.625288       -1.283357
H           2.213669        0.331346       -2.160563
```

---

### Compound_28_Ground_State

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -463.962992 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.791304 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      35.4177 cm-1
  2.      53.7633 cm-1
  3.     102.3162 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.712450        0.318757       -0.000058
C          -2.740263       -0.746918        0.000092
C          -4.037137       -0.460863        0.000059
O          -1.932236        1.511886       -0.000221
O          -0.481887       -0.210017        0.000011
C           0.631004        0.710529       -0.000117
C           1.937512       -0.077860        0.000021
C           2.029718       -0.950945       -1.256791
H          -4.378690        0.565648       -0.000079
H          -4.785134       -1.240862        0.000169
H           0.556114        1.343792       -0.884505
H           0.556093        1.344067        0.884072
H           1.965703       -0.341854       -2.160457
H           2.980683       -1.484915       -1.276497
H           1.227150       -1.687320       -1.285251
C           2.029686       -0.950559        1.257103
H           1.965641       -0.341189        2.160580
```

```
H           1.227121       -1.686929        1.285767
H           2.980654       -1.484517        1.276999
C           3.076804        0.949404       -0.000122
H           4.041081        0.440206       -0.000034
H           3.033462        1.587826       -0.884286
H           3.033442        1.588093        0.883848
H          -2.379585       -1.766269        0.000229
```

### Compound_1_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.677373 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.587558 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      70.6660 cm-1
2.      99.9803 cm-1
3.     123.2068 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.632265       -0.651957       -0.000026
H           2.298014       -1.546896       -0.000073
C           0.204476       -0.958543       -0.000011
H          -0.038130       -2.034129        0.000014
C          -0.783219       -0.041174       -0.000026
C          -0.523714        1.416794       -0.000029
H          -1.473360        2.003905        0.000048
H           0.081453        1.699424        0.899818
H           0.081397        1.699597       -0.899831
C          -2.209893       -0.446842        0.000023
H          -2.721236       -0.034969       -0.906385
H          -2.328777       -1.557743        0.000289
H          -2.721328       -0.034526        0.906178
O           2.112810        0.486959        0.000044
```

---

### Compound_2_Ground_State_AM1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -344.740467 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -344.664228 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 33)

```
1.     117.7445 cm-1
2.     130.6149 cm-1
3.     238.4890 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -1.053981       -0.077510        0.465473
C          -0.571467        1.318923        0.125992
C           0.744558        1.283767       -0.160031
C           1.205998       -0.124732       -0.035440
H          -1.365024       -0.151217        1.542575
H          -1.251977        2.169677        0.135051
H           1.424921        2.086664       -0.440959
O           0.125984       -0.925523        0.331289
C          -2.134388       -0.581222       -0.460409
H          -2.364010       -1.648637       -0.224453
H          -3.056934        0.032214       -0.326299
H          -1.804339       -0.520001       -1.524992
O           2.283147       -0.684985       -0.178094
```

---

### Compound_3_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1111.254024 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1111.238646 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
1.      54.1888 cm-1
2.     166.4849 cm-1
3.     193.3774 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -2.064512        0.065696        0.000121
H          -1.996696        1.176485        0.000334
C          -0.793050       -0.673879       -0.000071
H          -0.890477       -1.775693       -0.000256
C           0.421175       -0.101728       -0.000037
O          -3.150897       -0.515807        0.000052
Cl          0.680092        1.574020        0.000237
Cl          1.832418       -1.045483       -0.000271
```

---

## Compound_4_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -192.003239 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -191.965335 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
  1.      86.8296 cm-1
  2.     348.2673 cm-1
  3.     556.9433 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.118602       -0.761684        0.000000
O          -1.204659       -1.345005       -0.000000
C          -0.000000        0.703693       -0.000000
H           0.841900       -1.326928        0.000000
C           1.177510        1.327432        0.000000
H           1.259654        2.423182       -0.000000
H           2.136911        0.790368        0.000000
H          -0.954638        1.256770       -0.000000
```

---

## Compound_5_Ground_State_AM1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -231.344486 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.280842 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.      41.7853 cm-1
2.     134.0580 cm-1
3.     291.7880 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.549162       -0.173304       -0.000018
O          -1.500200       -0.965567       -0.000091
C           0.842366       -0.664210       -0.000042
C           1.921303        0.116259        0.000023
H           2.938581       -0.300036        0.000001
H           1.870853        1.214164        0.000102
H           0.930453       -1.765621       -0.000122
C          -0.763283        1.306955        0.000098
H          -0.295300        1.758481        0.908453
H          -0.295284        1.758626       -0.908178
H          -1.855052        1.544723        0.000107
```

---

### Compound_6_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.680214 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.59065 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      32.0581 cm-1
2.      87.8132 cm-1
3.     111.7339 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           0.702872       -0.282608        0.053514
C          -0.695898        0.213744        0.025278
C          -0.998558        1.492950        0.269125
H          -0.237368        2.252564        0.491404
H          -2.035200        1.856385        0.268174
C          -1.727107       -0.809916       -0.272322
H          -1.665996       -1.110652       -1.348339
H          -1.549948       -1.721641        0.352883
H          -2.755463       -0.424628       -0.068848
O           0.972405       -1.452422        0.350752
C           1.772767        0.701898       -0.300304
H           2.737455        0.175012       -0.500715
H           1.479551        1.286840       -1.204705
H           1.923274        1.409090        0.552385
```

---

### Compound_7_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -247.414242 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -247.360823 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      48.8453 cm-1
2.     255.4940 cm-1
3.     288.0892 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.467291        0.098888        0.000028
O          -0.507084        1.348696       -0.000142
C           0.811366       -0.658771       -0.000213
C           1.984242       -0.025127        0.000185
H           2.940345       -0.565624       -0.000124
H           2.053215        1.073673        0.000612
H           0.745811       -1.757845       -0.000486
N          -1.642996       -0.614267        0.000054
H          -2.505326       -0.130149        0.000381
H          -1.646309       -1.599693        0.000375
```

### Compound_8_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -426.804648 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -426.62333 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      38.7417 cm-1
2.     101.9930 cm-1
3.     103.8266 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           0.338090       -0.159268        0.182739
C          -0.439036       -1.382047        0.537639
C          -1.739791       -1.485771       -0.235034
C          -2.573299       -0.232811       -0.081142
C          -1.801495        0.989632       -0.525638
C          -0.462474        1.086536        0.157680
H          -1.518193       -1.658223       -1.320902
H           0.164410       -2.309340        0.349416
H          -0.661390       -1.349859        1.639984
H          -3.509697       -0.322061       -0.691435
H          -2.881581       -0.113806        0.991004
H          -1.614807        0.943053       -1.632177
H          -2.396749        1.917516       -0.317980
H          -2.318786       -2.371504        0.135796
O          -0.078386        2.152590        0.653565
C           1.664196       -0.180894       -0.070033
C           2.455316        1.029012       -0.401919
H           3.121136        0.826900       -1.278043
H           1.808887        1.908688       -0.641648
H           3.098215        1.302277        0.473285
C           2.451494       -1.441180       -0.038572
H           2.328515       -1.956975        0.946671
H           2.108680       -2.136860       -0.845342
H           3.540435       -1.239780       -0.191469
```

### Compound_9_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -426.81978 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -426.639503 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      63.4444 cm-1
2.      85.6803 cm-1
3.     113.1326 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.354196       -0.683455       -0.102629
C           0.024097       -1.298849       -0.366079
C          -1.151709       -0.395074        0.010221
C          -0.924143        1.014133       -0.530547
C           0.405651        1.591922       -0.131698
C           1.522921        0.646035       -0.005242
H          -0.035089       -1.543276       -1.462801
H          -0.063810       -2.266857        0.196192
H          -0.958289        0.993463       -1.653629
H          -1.747577        1.690049       -0.178827
H           2.510879        1.096455        0.182144
O           0.552485        2.807466        0.050324
C          -2.424395       -0.959906       -0.607161
H          -2.603401       -1.997421       -0.236158
H          -3.299979       -0.325223       -0.330018
H          -2.343082       -0.987778       -1.720212
C          -1.313896       -0.351116        1.522873
H          -2.171925        0.307093        1.800516
H          -1.507849       -1.375501        1.921877
H          -0.386569        0.050233        1.998286
C           2.483624       -1.634153        0.026033
H           3.465282       -1.102628        0.076649
H           2.362842       -2.243660        0.957090
H           2.500601       -2.331885       -0.848324
```

---

### Compound_10_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -384.078758 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -383.976772 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 42)

```
1.      56.5120 cm-1
2.     107.6840 cm-1
3.     143.0602 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.066379       -0.138564       -0.000002
C           0.630061       -1.578116       -0.000001
C          -0.904763       -1.548798        0.000003
C          -1.285131       -0.085248        0.000001
C          -0.012247        0.687342        0.000001
H           1.023248       -2.105051        0.905086
H           1.023244       -2.105051       -0.905090
H          -1.325552       -2.052017       -0.905327
H          -1.325544       -2.052009        0.905343
O          -2.416060        0.398016       -0.000004
O           0.043125        2.051647        0.000003
H          -0.877157        2.365538       -0.000002
C           2.484538        0.228142       -0.000001
H           2.607363        1.339990        0.000003
H           2.992429       -0.188629        0.906531
H           2.992430       -0.188623       -0.906537
```

---

### Compound_11_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1278.842967 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1278.822232 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      83.9643 cm-1
2.     143.1487 cm-1
```

```
   3.     171.9391 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.000001       -0.274336        0.681092
C           0.000000        1.168658        1.162700
C           0.000000        1.168658       -1.162700
C          -0.000001       -0.274336       -0.681092
O          -0.000000        1.589078       -2.317291
O          -0.000000        1.589078        2.317291
Cl          0.000000       -1.556401       -1.729214
Cl          0.000000       -1.556401        1.729214
N           0.000001        1.971461        0.000000
H           0.000003        2.960287        0.000000
```

---

### Compound_12_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -730.301821 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -730.223261 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
   1.      60.6706 cm-1
   2.      77.9126 cm-1
   3.     124.1695 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           0.628061       -1.555309       -0.000156
H           0.036941       -2.500207       -0.000417
C          -0.170799       -0.321292       -0.000094
C           0.339344        0.933709       -0.000103
C           1.802635        1.164292        0.000130
H           2.268563        0.685595       -0.900277
H           2.050797        2.252825        0.000022
H           2.268210        0.685851        0.900856
C          -0.534740        2.130498       -0.000097
H          -1.194214        2.127145       -0.905461
H          -1.194115        2.127166        0.905323
```

```
H           0.059482        3.076520       -0.000184
O           1.861861       -1.572341        0.000051
Cl         -1.857503       -0.587504        0.000097
```

---

### Compound_13_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1570.868841 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1570.86446 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
  1.      42.3096 cm-1
  2.      87.7173 cm-1
  3.     185.7717 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.508971        1.186921        0.229112
H           1.133007        1.946007        0.952337
C           0.640566       -0.010193        0.100715
C          -0.704175        0.082322        0.019656
O           2.554473        1.336161       -0.395850
Cl          1.427439       -1.506255        0.088686
Cl         -1.492402        1.584233        0.025895
Cl         -1.713916       -1.265601       -0.107666
```

---

### Compound_14_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2804.924419 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2804.873712 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.      24.2083 cm-1
  2.     139.8990 cm-1
  3.     200.0006 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.527520       -0.172560       -0.047969
O           2.578444        0.340097       -0.452192
C           0.298217        0.649577        0.089859
C           0.390924        1.965424        0.314023
H          -0.480970        2.623291        0.434138
H           1.374205        2.458227        0.387494
C           1.452312       -1.612009        0.341068
H           0.931492       -1.726260        1.322430
H           0.888295       -2.185572       -0.435693
H           2.481773       -2.040642        0.421762
Br         -1.366748       -0.195212       -0.076985
```

---

### Compound_15_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1262.753564 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1262.721568 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.      58.1588 cm-1
  2.     158.9451 cm-1
  3.     208.4512 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           0.000002        0.272030        0.000000
C          -0.000001       -0.678986        1.215742
C          -0.000001       -2.065363        0.673206
C          -0.000001       -2.065363       -0.673206
C          -0.000001       -0.678986       -1.215742
H          -0.000004       -2.926294        1.348317
H          -0.000004       -2.926294       -1.348317
```

```
Cl          1.445560        1.255189        0.000000
Cl         -1.445547        1.255203        0.000000
O          -0.000013       -0.345254        2.391035
O          -0.000013       -0.345254       -2.391035
```

---

### Compound_16_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1722.380344 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1722.359491 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.      40.1742 cm-1
2.     142.0408 cm-1
3.     159.9030 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.868843       -0.098255        0.000001
C           0.499985       -0.808642       -0.000006
C           1.533471        0.275565       -0.000000
C           0.961864        1.501796        0.000011
C          -0.519463        1.403864        0.000009
H           1.459836        2.476381        0.000014
Cl         -1.759693       -0.513841        1.445602
Cl         -1.759702       -0.513821       -1.445601
O           0.685061       -2.014272       -0.000013
O          -1.318751        2.327842        0.000003
Cl          3.164548       -0.068274       -0.000002
```

---

### Compound_17_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2237.418313 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2237.392225 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 33)

```
  1.      46.7909 cm-1
  2.      62.6286 cm-1
  3.     130.8217 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           2.056542        0.861694       -0.000076
C           1.013684       -0.295318       -0.000004
C          -0.319496        0.418059       -0.000014
C          -0.041641        1.890392       -0.000086
N           1.356496        2.072802       -0.000116
H           1.792010        2.963345       -0.000165
O          -0.839391        2.830036       -0.000118
O           3.280200        0.747599       -0.000096
C          -1.533696       -0.163695        0.000035
Cl         -2.979552        0.702445        0.000022
Cl         -1.710855       -1.847412        0.000113
Cl          1.231463       -1.261727       -1.445588
Cl          1.231515       -1.261591        1.445663
```

---

### Compound_18_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2765.584173 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2765.559999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 18)

```
  1.      18.2585 cm-1
  2.     212.4741 cm-1
  3.     355.9016 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -1.823744       -0.211277        0.000019
O          -1.854383       -1.439471       -0.000020
C          -0.595220        0.613012        0.000002
```

```
C          -0.692040        1.948094       -0.000011
H           0.181168        2.616120       -0.000025
H          -1.666691        2.459849       -0.000011
Br          1.078579       -0.229999        0.000002
H          -2.763655        0.390773        0.000072
```

---

### Compound_19_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -231.343089 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.279518 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.      75.2332 cm-1
2.     112.0916 cm-1
3.     227.7721 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -1.444840        0.045010        0.000000
O          -2.285611        0.947476        0.000000
C           0.000000        0.300852        0.000000
C           0.901352       -0.688750        0.000000
H           0.298199        1.362597        0.000000
H          -1.750065       -1.027138        0.000000
C           2.360070       -0.472193        0.000000
H           2.815789       -0.946083        0.906153
H           2.815789       -0.946083       -0.906153
H           2.622390        0.614252        0.000000
H           0.583289       -1.746868        0.000000
```

---

### Compound_20_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -270.674523 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.584052 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      28.6251 cm-1
  2.      72.8042 cm-1
  3.     206.7855 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.586127        0.213285       -0.000001
O           2.106682       -0.903586       -0.000002
C           0.123428        0.436975        0.000001
H           2.207174        1.139231       -0.000000
C          -0.358243        1.684926        0.000000
H          -1.433913        1.906485        0.000001
H           0.297955        2.566793       -0.000002
C          -0.709216       -0.795837        0.000004
H          -0.426684       -1.407895       -0.901365
H          -0.426691       -1.407886        0.901382
C          -2.195402       -0.552781       -0.000003
H          -2.737642       -1.529720        0.000001
H          -2.506912        0.021142        0.906166
H          -2.506906        0.021130       -0.906182
```

---

### Compound_21_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2182.007025 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2181.997069 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.      36.4544 cm-1
  2.      69.8193 cm-1
  3.     160.7067 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.000001        1.227919        0.000000
C          -0.000002        0.287025        1.219623
C          -0.000001       -1.106115        0.680284
C          -0.000001       -1.106115       -0.680284
C          -0.000002        0.287025       -1.219623
Cl          1.445694        2.211024        0.000000
Cl         -1.445693        2.211029        0.000000
O           0.000001        0.629351        2.390494
O           0.000001        0.629351       -2.390494
Cl          0.000001       -2.434792        1.681564
Cl          0.000001       -2.434792       -1.681564
```

---

### Compound_22_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1068.836763 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1068.641731 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 81)

```
  1.      15.6247 cm-1
  2.      30.1338 cm-1
  3.      45.5172 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           0.052191        0.570973       -0.196482
N          -0.908728       -0.381295        0.117860
O          -0.233692        1.735539       -0.535873
C           1.467786        0.118826       -0.088128
C          -2.304039       -0.232745        0.077276
C           2.427099        1.012216        0.269833
S           1.749644       -1.511636       -0.471638
C          -2.950441        0.926612       -0.401513
C          -3.102018       -1.311158        0.537301
C           2.186346        2.432683        0.632903
O           3.763184        0.707221        0.399829
C           3.394965       -1.699418        0.125230
C          -4.341181        0.995592       -0.412470
C          -4.488102       -1.219165        0.515440
C           4.231753       -0.492659       -0.222317
C          -5.116608       -0.067998        0.042452
```

```
H          -0.579016       -1.277877        0.412203
H          -2.366475        1.785914       -0.769478
H          -2.632028       -2.231750        0.915379
H           3.090396        2.879908        1.113337
H           1.935807        3.005131       -0.297088
H           1.313939        2.505725        1.328449
H           3.813624       -2.612362       -0.365878
H           3.399826       -1.862184        1.230782
H          -4.828020        1.908300       -0.788855
H          -5.091448       -2.065715        0.876287
H           5.277246       -0.589640        0.181380
H           4.263867       -0.332810       -1.333017
H          -6.213360       -0.002032        0.028897
```

---

### Compound_23_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -388.676024 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -388.505799 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
  1.      35.0189 cm-1
  2.      49.6314 cm-1
  3.      57.1842 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           2.141163       -1.229426        0.168817
C           1.013624       -0.320847       -0.117811
C          -0.246531       -0.758876        0.054771
C          -1.454746        0.051616       -0.218733
C          -2.725484       -0.640339        0.232377
C          -3.939675        0.204620       -0.054642
C           1.352230        1.045397       -0.602853
C           1.479449        2.035023        0.531125
O           3.319719       -0.963572       -0.076179
H           1.858105       -2.204140        0.631511
H          -0.432036       -1.787354        0.413396
H          -1.514731        0.262551       -1.322843
H          -1.365915        1.047861        0.296220
H          -2.665334       -0.853192        1.332389
H          -2.821024       -1.628088       -0.291460
```

```
H          -4.865123       -0.321000        0.283573
H          -3.874905        1.183542        0.479289
H          -4.029528        0.408092       -1.149219
H           2.325432        1.002250       -1.165477
H           0.563095        1.397535       -1.320973
H           1.731362        3.045358        0.127585
H           0.523440        2.109654        1.103390
H           2.289227        1.722507        1.233747
```

---

### Compound_24_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -463.948884 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.775995 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      14.7512 cm-1
2.      32.7907 cm-1
3.      40.3930 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.190109       -0.496330        0.003532
C           2.376382        0.373975       -0.114132
C           3.648169       -0.264396        0.303142
C           2.291916        1.629200       -0.568064
O           1.159237       -1.711105        0.220510
O          -0.003931        0.156727       -0.153274
C          -1.189816       -0.651774       -0.051285
C          -2.372857        0.292621       -0.237023
C          -3.613707       -0.516635       -0.547862
C          -2.577780        1.146553        0.995191
H           4.525093        0.369554        0.026535
H           3.651679       -0.419061        1.411481
H           3.754196       -1.266424       -0.184045
H           1.336129        2.082843       -0.866498
H           3.177792        2.271645       -0.665248
H          -1.157975       -1.434849       -0.853053
H          -1.206262       -1.148783        0.952884
H          -2.147765        0.969499       -1.109221
H          -3.832568       -1.234542        0.279090
H          -4.491597        0.162797       -0.667981
```

```
H          -3.479144       -1.094945       -1.493473
H          -2.848451        0.512714        1.873836
H          -1.638936        1.702506        1.233487
H          -3.399122        1.882776        0.823325
```

---

### Compound_25_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -557.456365 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -557.262103 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      25.1280 cm-1
  2.      32.6737 cm-1
  3.      61.8713 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.652756        0.044696       -0.074706
C           2.744315       -0.653182        0.661166
C           3.808255       -1.132644        0.017066
O           1.694753        0.185524       -1.316934
N           0.625598        0.573641        0.695834
C          -0.586362        1.141003        0.111186
C          -1.371318        0.104938       -0.727817
C          -1.799362       -1.128879        0.008789
C          -2.746894       -2.004554       -0.750559
O          -1.410110       -1.426155        1.144512
H           2.634003       -0.753320        1.752418
H           3.925193       -1.033258       -1.072873
H           4.622557       -1.651225        0.540812
H           0.480263        0.156492        1.590564
H          -0.725530       -0.214722       -1.593414
H          -2.281967        0.606705       -1.147772
H          -2.338924       -2.215557       -1.768656
H          -2.909757       -2.971051       -0.214909
H          -3.729380       -1.483573       -0.860202
C          -1.510571        1.665342        1.226401
H          -2.425160        2.104431        0.762191
H          -1.817202        0.838710        1.912158
H          -0.996564        2.458542        1.819615
C          -0.272580        2.328301       -0.816834
```

```
H          -1.230503        2.755695       -1.197235
H           0.277637        3.121957       -0.258191
H           0.349582        1.999610       -1.684130
```

---

### Compound_26_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -424.610158 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.462974 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      28.5505 cm-1
  2.      40.7403 cm-1
  3.      67.2712 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -1.222793        1.295682        0.000000
C          -1.122009        2.760395        0.000000
C          -2.207086        3.534818        0.000000
O          -2.233261        0.585615        0.000000
O           0.000000        0.679685        0.000000
C          -0.010877       -0.758648        0.000000
C           1.443851       -1.188070        0.000000
C           1.542696       -2.698338        0.000000
C           2.979659       -3.152038        0.000000
H          -0.095311        3.160291        0.000000
H          -3.226418        3.120070        0.000000
H          -2.137326        4.631304        0.000000
H          -0.553261       -1.116589        0.913449
H          -0.553261       -1.116589       -0.913449
H           1.958487       -0.766597        0.902454
H           1.958487       -0.766597       -0.902454
H           1.017379       -3.108555       -0.902975
H           1.017379       -3.108555        0.902975
H           3.032930       -4.267514        0.000000
H           3.513175       -2.772935       -0.905084
H           3.513175       -2.772935        0.905084
```

---

### Compound_27_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -503.284504 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -503.084764 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
1.      17.9737 cm-1
2.      34.4872 cm-1
3.      38.9480 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C           1.425172       -0.545289       -0.080207
C           2.563559        0.391730       -0.007157
C           3.876559       -0.253929        0.232581
C           2.401674        1.710865       -0.157396
O           1.457800       -1.773086       -0.201568
O           0.198908        0.060397       -0.000552
C          -0.945221       -0.806655       -0.085626
C          -2.196903        0.070220        0.030345
C          -3.410538       -0.839815       -0.093919
H           4.713512        0.468812        0.075541
H           3.926689       -0.638355        1.282385
H           4.010653       -1.123422       -0.459364
H           1.414700        2.164510       -0.328372
H           3.249433        2.408287       -0.117048
H          -0.916864       -1.342861       -1.069630
H          -0.895167       -1.552460        0.749688
H          -3.409866       -1.359259       -1.082067
H          -3.406055       -1.609136        0.715024
H          -4.346241       -0.237147       -0.008194
C          -2.212909        1.102143       -1.085361
H          -1.305711        1.750242       -1.017525
H          -2.217321        0.597198       -2.080875
H          -3.122611        1.743668       -1.004580
C          -2.216303        0.769329        1.379723
H          -3.122370        1.415256        1.466514
H          -1.305803        1.406032        1.491868
H          -2.231173        0.018552        2.205704
```

---

### Compound_28_Ground_State_AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -463.947678 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.773836 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      29.1908 cm-1
2.      39.1110 cm-1
3.      70.8737 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -1.723060        0.290306       -0.000063
C          -2.767019       -0.742200        0.000086
C          -4.061946       -0.425558        0.000013
O          -1.845969        1.519224       -0.000263
O          -0.458296       -0.234697        0.000043
C           0.621693        0.715048       -0.000090
C           1.934494       -0.075625        0.000033
C           2.017121       -0.945169       -1.243690
H          -4.412886        0.617475       -0.000161
H          -4.847228       -1.193976        0.000124
H           0.536320        1.355940       -0.915900
H           0.536309        1.356206        0.915533
H           1.977651       -0.312699       -2.162692
H           2.971963       -1.523122       -1.247255
H           1.160643       -1.661379       -1.265554
C           2.017101       -0.944813        1.244007
H           1.977616       -0.312079        2.162828
H           1.160622       -1.661015        1.266063
H           2.971942       -1.522766        1.247753
C           3.077106        0.930138       -0.000101
H           4.055157        0.392050       -0.000017
H           3.026589        1.578605       -0.907413
H           3.026576        1.578864        0.907024
H          -2.400096       -1.781079        0.000260
```

# Structures from Linear Regression Graph

---

### Linear_Regression_1_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.654106 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.515187 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      86.9428 cm-1
2.      98.8877 cm-1
3.     129.6923 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.199553        1.080979       -0.408589
C          -0.557189        0.466053        0.776719
C           0.228801       -0.696589        1.116415
C           1.151938       -0.968799        0.109489
H          -0.469392        1.349545       -1.228285
H          -0.787140        1.188274        1.558557
H           0.118532       -1.289642        2.008302
O           1.066120        0.040750       -0.883467
C           1.013030        2.296390       -0.000647
H           1.617646        2.639932       -0.838869
H           0.354240        3.109461        0.306847
H           1.673752        2.047537        0.830193
O           1.984839       -1.861858       -0.067001
C          -2.162713       -0.908291       -0.788361
H          -1.771634       -0.474885       -1.702537
H          -1.562750       -1.765207       -0.498723
H          -3.199098       -1.198787       -0.929127
N          -2.074176        0.093647        0.299987
H          -2.557491        0.951817        0.038928
H          -2.545640       -0.263173        1.128407
```

---

### Linear_Regression_2_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.920116 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.817563 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      91.9278 cm-1
2.     109.6324 cm-1
3.     205.6559 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.605310        0.158285        0.268789
O           2.731137        0.514092       -0.177409
C           0.694397       -0.725109       -0.283041
H           1.279470        0.585316        1.245302
C          -0.569733       -1.037025        0.376631
H          -0.885624       -2.075448        0.285104
H          -0.587595       -0.747857        1.426432
H           0.922670       -1.218037       -1.222275
C          -1.767924        1.204393        0.010611
H          -1.860461        1.374204        1.078882
H          -2.587324        1.680294       -0.518797
H          -0.814262        1.580886       -0.344687
N          -1.802838       -0.258059       -0.236816
H          -2.668659       -0.652652        0.128938
H          -1.799746       -0.436290       -1.239860
```

---

### Linear_Regression_3_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.589254 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.435787 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      59.2972 cm-1
2.      78.4133 cm-1
3.      88.9406 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.543517       -0.349995        0.022970
C           0.515601        0.542882       -0.265898
C          -0.816801        0.132654       -0.703504
H          -0.873753       -0.844654       -1.170970
H          -1.309524        0.861343       -1.347835
C           0.756634        2.019812       -0.055972
H           0.789683        2.311026        1.001342
H           1.712692        2.332359       -0.483044
H          -0.028769        2.617675       -0.525378
O           2.688682        0.017923        0.441643
C           1.369654       -1.857025       -0.149267
H           2.179298       -2.232725       -0.777982
H           1.473704       -2.339413        0.825239
H           0.424281       -2.178315       -0.581726
C          -3.216067       -0.401423        0.119895
H          -3.613889        0.331972       -0.574714
H          -3.841392       -0.453158        1.005859
H          -3.165820       -1.374559       -0.358932
N          -1.840138        0.007336        0.500686
H          -1.855565        0.905602        0.979581
H          -1.434663       -0.653316        1.161277
```

---

### Linear_Regression_4_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.329224 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.210715 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      95.9915 cm-1
  2.     111.4565 cm-1
  3.     181.0225 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.237253        0.021508        0.079789
O           0.871312        1.014246        0.823350
C           0.425317       -1.056338       -0.199858
C          -0.903787       -1.136457        0.458170
H          -1.570246       -1.853060       -0.017599
H          -0.870110       -1.365304        1.529003
```

```
H           0.709647       -1.809850       -0.917770
C          -2.087152        0.638297       -0.907824
H          -1.280653        0.532094       -1.626712
H          -2.413759        1.673321       -0.864363
H          -2.919546       -0.003206       -1.185435
N          -1.571975        0.234514        0.417315
H          -0.741383        0.844399        0.701851
H          -2.304201        0.296423        1.118972
N           2.546980        0.086897       -0.428430
H           2.724518       -0.516554       -1.217908
H           2.840426        1.035840       -0.610700
```

---

### Linear_Regression_5_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.713022 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.468582 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      41.4538 cm-1
  2.      82.9162 cm-1
  3.     100.2826 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.156185        0.265548       -0.259419
C          -0.949420        1.467233        0.238723
C          -2.461489        1.338972        0.081569
C          -2.933430       -0.019129        0.570523
C          -2.279355       -1.102195       -0.274639
C          -0.761712       -0.972714       -0.467464
H          -2.957692        2.150770        0.618703
H          -0.742003        1.671823        1.302950
H          -0.642739        2.374682       -0.284865
H          -2.646995       -0.144263        1.620206
H          -4.022435       -0.101313        0.528385
H          -2.451883       -2.091790        0.152328
H          -2.736230       -1.117997       -1.270832
H          -2.726599        1.446381       -0.975423
O          -0.191418       -2.061229       -0.819132
C           1.327470        0.454934       -0.342773
C           2.093852       -0.433761       -1.319157
```

```
H           3.169010       -0.259712       -1.234348
H           1.856356       -1.480000       -1.180481
H           1.791145       -0.160318       -2.329476
C           1.771666        1.904296       -0.569791
H           1.440732        2.579768        0.216538
H           2.858592        1.963971       -0.636624
H           1.357964        2.259384       -1.511721
N           1.954983        0.138977        1.112193
H           2.943549        0.387931        1.110604
H           1.498376        0.783750        1.753212
C           1.785772       -1.243978        1.621756
H           2.095600       -1.275037        2.662556
H           0.741011       -1.511280        1.519195
H           2.397684       -1.915002        1.030838
```

---

### Linear_Regression_6_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.723749 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.481239 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      63.2683 cm-1
  2.      68.6861 cm-1
  3.     110.7464 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.985291       -0.417010       -0.513509
C           0.074817       -1.163494        0.310871
C           1.482736       -0.553581        0.243905
C           1.364246        0.925020        0.634792
C           0.333931        1.709707       -0.175499
C          -0.736429        1.009779       -0.707890
H          -0.211073       -1.164896        1.362627
H           0.104544       -2.209549       -0.000643
H           1.101380        0.997282        1.696091
H           2.326585        1.426802        0.516500
H          -1.423848        1.544345       -1.356671
O           0.544195        2.952288       -0.332800
C           2.378876       -1.290010        1.244991
H           2.466307       -2.348180        0.989097
```

```
H           3.382751       -0.861563        1.247970
H           1.978336       -1.218221        2.257878
C           2.095922       -0.691005       -1.155878
H           3.118134       -0.308502       -1.156854
H           2.129354       -1.738033       -1.463306
H           1.528196       -0.133239       -1.898468
C          -1.352610       -1.157682       -1.798248
H          -2.105988       -0.608977       -2.364908
H          -0.463463       -1.240577       -2.419159
H          -1.720263       -2.168077       -1.605526
C          -2.453429        0.172227        1.630733
H          -1.830785       -0.310797        2.375458
H          -3.481860        0.201196        1.978180
H          -2.086538        1.175379        1.432366
N          -2.385308       -0.583700        0.360611
H          -2.562814       -1.573586        0.521908
H          -3.121964       -0.256921       -0.260020
```

---

### Linear_Regression_7_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.974946 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.810322 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
  1.      75.9923 cm-1
  2.     101.8580 cm-1
  3.     120.8171 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.524159        0.059407        0.441743
C           0.181097       -1.412526        0.717663
C          -1.214133       -1.652111        0.109386
C          -1.759054       -0.250885       -0.150932
C          -0.753004        0.648732        0.100912
H           0.162212       -1.554978        1.797225
H           0.941447       -2.090357        0.328528
H          -1.168428       -2.217090       -0.826389
H          -1.863780       -2.212931        0.784021
O          -2.939560        0.006503       -0.550550
O          -0.860533        2.023461       -0.120028
```

```
H          -1.742611        2.147283       -0.496289
C           1.378934        0.751275        1.487150
H           1.634195        1.768051        1.188052
H           0.803080        0.808183        2.409225
H           2.297202        0.204890        1.698785
C           2.862848       -0.328252       -0.916031
H           2.922401       -1.321522       -0.482541
H           3.257848       -0.347731       -1.928529
H           3.434161        0.371311       -0.316656
N           1.443613        0.100852       -0.948470
H           1.374016        1.062799       -1.273636
H           0.918636       -0.457427       -1.617220
```

---

### Linear_Regression_8_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -826.224721 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -826.080063 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      54.2916 cm-1
  2.      80.3442 cm-1
  3.     131.9868 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.449550       -1.223563       -0.154365
H           0.932879       -2.168367       -0.397173
C           0.618931       -0.127105       -0.222962
C          -0.826288       -0.088752       -0.539964
C          -1.428741       -1.454465       -0.858972
H          -2.507621       -1.364548       -0.986095
H          -1.012038       -1.816492       -1.795455
H          -1.228388       -2.194050       -0.089401
C          -1.206011        0.910149       -1.637658
H          -0.841801        1.910109       -1.413141
H          -0.749547        0.585097       -2.570166
H          -2.286676        0.951509       -1.782488
O           2.678366       -1.270606        0.122915
C          -1.466008       -0.365675        1.974150
H          -0.420365       -0.627234        2.101919
H          -2.068267       -1.259838        1.863758
```

```
H          -1.819042        0.216950        2.819040
N          -1.581020        0.458881        0.744873
H          -1.168010        1.374939        0.922614
H          -2.560926        0.618809        0.518376
Cl          1.324789        1.460133        0.191142
```

---

### Linear_Regression_9_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.849846 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.733612 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      60.3829 cm-1
  2.      72.2019 cm-1
  3.     106.2515 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.395136        1.575020       -0.003291
O          -0.392053        2.347024        0.605091
C           0.096410        0.283034       -0.417484
C           0.930510       -0.708942       -1.079366
H           0.421031       -1.269302       -1.862170
H           1.840718       -0.282528       -1.487539
C           2.276381       -1.352510        1.002729
H           3.201615       -0.970773        0.582835
H           2.480116       -2.176132        1.679147
H           1.743430       -0.559433        1.516556
N           1.417007       -1.835732       -0.107983
H           1.902686       -2.552933       -0.644598
H           0.577511       -2.272755        0.272807
C           1.783330        2.133867       -0.312469
H           2.434465        1.490496       -0.898114
H           1.658382        3.076535       -0.846510
H           2.282502        2.356599        0.632111
Br         -1.663305       -0.409961        0.052283
```

---

### Linear_Regression_10_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.682691 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.589001 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      30.8518 cm-1
  2.      85.8174 cm-1
  3.     105.6039 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.797899       -0.062715        0.011871
C           0.366828       -0.799175       -0.643396
C           1.399868        0.231315       -1.080512
C           0.820706        1.511767       -0.688166
C          -0.408133        1.427420       -0.043082
H           1.670458        0.095900       -2.130051
H           1.283158        2.458020       -0.927965
Cl         -1.008771       -0.638998        1.708200
Cl         -2.309588       -0.380869       -0.909480
O           0.483969       -1.987925       -0.775506
O          -1.158751        2.312276        0.401218
C           2.752050       -0.021853        1.117243
H           2.437596        0.981823        1.380981
H           3.752851       -0.220952        1.485502
H           2.053687       -0.747048        1.522275
N           2.760629       -0.134829       -0.365552
H           3.473998        0.480939       -0.752632
H           3.013689       -1.082492       -0.646935
```

---

### Linear_Regression_11_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.314534 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.231692 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      32.6097 cm-1
2.      67.4890 cm-1
3.      83.7810 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.150148       -0.103195        0.001036
C          -0.078716       -1.143604        0.366344
C           1.109804       -0.681098       -0.187553
C           1.048368        0.575298       -0.923427
C          -0.405948        0.996305       -0.747526
H           1.338533        0.550563       -1.977186
Cl         -1.949392        0.573767        1.465643
Cl         -2.405346       -0.817043       -1.078732
O          -0.334713       -2.174511        1.000624
O          -0.849912        2.051858       -1.109668
Cl          2.590981       -1.578598       -0.111497
C           1.866838        1.919134        1.116880
H           2.146120        0.993325        1.606408
H           2.548451        2.717329        1.390319
H           0.849552        2.188959        1.380588
N           1.948206        1.719006       -0.356536
H           1.688847        2.577420       -0.845072
H           2.910725        1.515410       -0.623519
```

---

### Linear_Regression_12_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2333.352866 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2333.266268 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      40.7629 cm-1
2.      49.9035 cm-1
3.      85.1302 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.217357        1.025509       -0.015058
C           1.231209       -0.177822       -0.007541
C          -0.079455        0.401729       -0.266614
C           0.074120        1.807995       -0.475579
N           1.467733        2.094335       -0.357340
H           1.828492        3.032838       -0.431978
O          -0.724690        2.706567       -0.694210
O           3.399829        0.981907        0.229666
C          -1.340556       -0.292976       -0.110869
Cl         -1.291591       -2.050023       -0.602830
Cl         -2.730747        0.463641       -0.941916
C          -1.943798        0.880522        2.105048
H          -2.726413        1.453345        1.623186
H          -1.000450        1.412205        2.071643
H          -2.213028        0.651150        3.130836
N          -1.778640       -0.412869        1.383645
H          -2.635627       -0.965525        1.431357
H          -1.036056       -0.955769        1.835986
Cl          1.403444       -1.047618        1.611280
Cl          1.889779       -1.352825       -1.272718
```

---

### Linear_Regression_13_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.513266 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.422929 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      61.6269 cm-1
  2.      84.3823 cm-1
  3.     136.1281 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.242123        1.833916        0.218570
O           1.227794        2.380095       -0.331552
C          -0.011405        0.501302        0.467870
C          -1.204476       -0.024006        1.115698
H          -1.015598       -0.779424        1.877578
H          -1.798581        0.780594        1.544943
C          -2.739243        0.129007       -0.923175
```

```
H          -3.368818        0.869356       -0.439695
H          -3.323478       -0.473161       -1.611248
H          -1.920393        0.616469       -1.441273
N          -2.161034       -0.753317        0.122909
H          -2.905373       -1.207851        0.649971
H          -1.619784       -1.498095       -0.317209
Br          1.260552       -0.833991       -0.124072
H          -0.584382        2.472955        0.597733
```

---

### Linear_Regression_14_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.267114 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.137844 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.     103.0611 cm-1
  2.     152.2682 cm-1
  3.     191.6318 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.762116       -0.603040        0.334437
O           2.100946        0.405537       -0.415847
C           0.514343       -1.143741        0.405765
C          -0.586264       -0.613652       -0.459612
H          -0.448490       -0.916542       -1.503151
H           0.299792       -1.952157        1.088789
H           2.541230       -1.029893        0.981342
C          -1.985900       -1.003598       -0.021963
H          -2.747902       -0.546872       -0.654404
H          -2.086422       -2.085519       -0.100909
H          -2.174201       -0.727656        1.014930
N          -0.409002        0.901979       -0.543318
H           0.668643        0.957133       -0.673566
H          -0.886405        1.264205       -1.363332
C          -0.787840        1.677533        0.657646
H          -1.865295        1.672370        0.789448
H          -0.304722        1.226840        1.519237
H          -0.439503        2.698926        0.533978
```

### Linear_Regression_15_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.587922 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.432739 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      44.4412 cm-1
2.      67.0419 cm-1
3.      94.8029 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.587464        1.483258        0.355668
O           1.484595        2.211665       -0.163641
C           0.367719        0.128182        0.181820
H          -0.127803        1.969210        1.056029
C          -0.725429       -0.515551        0.906799
H          -0.490485       -1.501587        1.310471
H          -1.139096        0.107268        1.697513
C          -2.665810        0.381451       -0.518873
H          -3.112198        0.897923        0.325453
H          -3.431811        0.089989       -1.230656
H          -1.923577        1.016259       -0.991814
N          -1.973693       -0.830114       -0.015477
H          -2.628687       -1.422817        0.492166
H          -1.634989       -1.381831       -0.801079
C           1.246304       -0.710079       -0.710451
H           0.647055       -1.365747       -1.355672
H           1.783045       -0.039305       -1.383156
C           2.261951       -1.577360        0.046252
H           2.861621       -2.183639       -0.636955
H           2.939232       -0.949995        0.627910
H           1.763592       -2.257661        0.739965
```

---

### Linear_Regression_16_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.754425 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.497666 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      18.8867 cm-1
  2.      30.5457 cm-1
  3.      54.4464 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.187172       -0.537671       -0.164650
N           1.259414        0.305955        0.157198
O           0.409562       -1.647059       -0.692929
C          -1.099581       -0.032917        0.170650
C           2.626287        0.090486        0.071999
C          -2.371182       -0.588150       -0.319957
S          -1.338899        1.525573        0.960554
C           3.467591        1.153493        0.447841
C           3.221787       -1.107411       -0.353575
C          -2.363718       -1.853587       -1.150801
O          -3.187878        0.388479       -1.010436
C          -2.074001        2.490776       -0.435411
C           4.845964        1.025524        0.402138
C           4.607119       -1.218883       -0.393950
C          -2.471891        1.510763       -1.527518
C           5.433225       -0.164662       -0.020660
H           0.984516        1.198905        0.537131
H           3.023565        2.084713        0.777948
H           2.590910       -1.927584       -0.647384
H          -1.812162       -1.662171       -2.066325
H          -1.876813       -2.678890       -0.644123
H          -3.391157       -2.116319       -1.405880
H          -1.364427        3.221547       -0.822973
H          -2.942266        3.013871       -0.038637
H           5.464861        1.862351        0.698716
H           5.043936       -2.152485       -0.725301
H          -3.143741        1.986200       -2.240268
H          -1.587712        1.168035       -2.066593
H           6.509037       -0.265485       -0.057945
N          -3.313295       -0.829212        0.918751
H          -4.268308       -0.940995        0.583798
H          -3.264894        0.068440        1.412611
C          -2.920217       -1.930897        1.825517
H          -3.481539       -1.844367        2.750489
```

```
H          -3.132936       -2.882516        1.351653
H          -1.856112       -1.832166        2.019763
```

---

### Linear_Regression_17_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.591603 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.356371 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
  1.      54.9080 cm-1
  2.      62.0510 cm-1
  3.      75.5897 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.430383       -1.041534       -1.241078
C          -0.641953       -0.558131       -0.209474
C           0.166872        0.641023       -0.458063
C           1.588961        0.659406        0.097993
C           2.465303       -0.418662       -0.534124
C           3.894735       -0.390922       -0.001753
C          -0.601301       -1.263835        1.120838
C          -1.331943       -0.558017        2.274372
O          -2.196998       -2.049968       -1.250371
H          -1.349371       -0.453394       -2.182016
H           0.182017        0.874398       -1.523249
H           1.567880        0.523135        1.182271
H           2.045629        1.636505       -0.084935
H           2.470618       -0.281464       -1.618818
H           2.017874       -1.396720       -0.351869
H           4.371734        0.570700       -0.201343
H           3.912253       -0.551877        1.078076
H           4.503611       -1.168156       -0.464800
H          -1.059049       -2.243342        0.975460
H           0.430585       -1.453284        1.436442
H          -1.360667       -1.184941        3.168438
H          -0.837680        0.372200        2.568446
H          -2.359449       -0.317773        1.996551
N          -0.521477        1.959832        0.147329
H          -0.627370        1.814012        1.148926
H           0.115155        2.746839        0.034195
```

```
C          -1.837393        2.285073       -0.449911
H          -1.690962        2.527686       -1.497909
H          -2.471534        1.409565       -0.359540
H          -2.272347        3.130421        0.074534
```

---

### Linear_Regression_18_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.858993 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.622539 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      27.1035 cm-1
  2.      52.2619 cm-1
  3.      61.6544 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.772970       -1.325042        0.060921
C           2.006404       -0.736723       -0.164094
C           3.283558       -1.471171        0.142961
C           2.074759        0.642809       -0.680067
O           0.485634       -2.476978        0.442636
O          -0.295024       -0.403256       -0.157403
C          -1.616669       -0.932823       -0.172826
C          -2.611674        0.214522       -0.279135
C          -4.015892       -0.346231       -0.507828
C          -2.578916        1.112716        0.956977
H           3.948356       -0.899953        0.801876
H           3.061477       -2.412509        0.644635
H           3.871806       -1.715207       -0.751189
H           1.480824        0.836774       -1.574583
H           3.096890        0.968415       -0.862071
H          -1.728156       -1.610145       -1.024385
H          -1.799902       -1.511868        0.735027
H          -2.333058        0.812924       -1.152202
H          -4.325549       -0.971635        0.333021
H          -4.743512        0.459963       -0.607001
H          -4.060013       -0.954125       -1.412748
H          -3.282812        1.939815        0.855239
H          -2.853845        0.545182        1.849445
H          -1.590571        1.538816        1.126624
```

```
N           1.489300        1.657322        0.334462
H           2.011545        1.573776        1.204020
H           0.550211        1.288106        0.514264
C           1.433271        3.067093       -0.122921
H           0.979636        3.680752        0.649416
H           2.443087        3.409940       -0.327463
H           0.836742        3.110692       -1.028941
```

---

### Linear_Regression_19_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.372153 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.114491 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      34.8714 cm-1
  2.      45.5502 cm-1
  3.      71.0196 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.393257       -1.522587       -0.669619
C          -1.790828       -1.524715       -0.529129
C          -2.516151       -1.090599        0.655101
O           0.210095       -1.780606       -1.749099
N           0.384576       -1.246954        0.475019
C           1.710050       -0.617637        0.405158
C           1.742150        0.581265       -0.571509
C           0.908234        1.790529       -0.247931
C           1.411868        3.098238       -0.793694
O          -0.127883        1.749918        0.398985
H          -2.357610       -1.770125       -1.415836
H          -2.062813       -1.351346        1.612543
H          -3.550671       -1.427502        0.671592
H          -0.146357       -0.885817        1.247823
H           1.389214        0.223186       -1.544906
H           2.772262        0.906739       -0.722810
H           0.662541        3.877349       -0.682644
H           2.316458        3.380342       -0.249271
H           1.696878        2.990257       -1.841105
C           2.064530       -0.158199        1.822351
H           3.045073        0.317402        1.829880
```

```
H           1.335389        0.555206        2.205699
H           2.094983       -1.014441        2.496813
C           2.761378       -1.635063       -0.057793
H           3.758184       -1.191252       -0.036299
H           2.753332       -2.496674        0.610465
H           2.540060       -1.975269       -1.065105
N          -2.650785        0.492498        0.775626
H          -3.043693        0.737093        1.683185
H          -1.697758        0.878526        0.733252
C          -3.457933        1.092879       -0.308928
H          -4.483482        0.744707       -0.222596
H          -3.422352        2.175565       -0.233726
H          -3.034120        0.768077       -1.254596
```

---

### Linear_Regression_20_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529093 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317358 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.3556 cm-1
  2.      46.6080 cm-1
  3.      67.8176 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.732915       -0.603867        0.290990
C           1.516700        0.066144        1.203237
C           2.987950       -0.051337        1.072704
O           1.169095       -1.272441       -0.699852
O          -0.632122       -0.500980        0.478163
C          -1.473874       -0.994159       -0.567648
C          -2.913037       -0.692274       -0.198189
C          -3.240567        0.798185       -0.139573
C          -4.700119        1.066998        0.215464
H           1.086289        0.721374        1.942222
H           3.389935       -1.043896        1.300701
H           3.526597        0.679187        1.671775
H          -1.208575       -0.513079       -1.512744
H          -1.322144       -2.067784       -0.690550
H          -3.140666       -1.159543        0.764540
```

```
H          -3.555430       -1.177532       -0.939059
H          -3.007964        1.251127       -1.108160
H          -2.588717        1.281349        0.590687
H          -5.372434        0.615059       -0.517106
H          -4.948171        0.647896        1.193009
H          -4.913116        2.136381        0.248286
N           3.398492        0.153110       -0.389387
H           4.336004       -0.206126       -0.549019
H           2.705063       -0.469175       -0.873463
C           3.284770        1.543910       -0.882304
H           3.449717        1.557679       -1.955584
H           2.284991        1.898350       -0.651846
H           4.024959        2.162738       -0.382560
```

---

### Linear_Regression_21_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195129 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.932192 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      20.6101 cm-1
  2.      43.4146 cm-1
  3.      68.5416 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.020919       -1.355262       -0.071660
C          -2.204198       -0.697675        0.222495
C          -3.532133       -1.390758        0.077146
C          -2.167281        0.712111        0.649121
O          -0.818618       -2.541584       -0.398771
O           0.098509       -0.474638       -0.011192
C           1.388623       -1.066596       -0.104297
C           2.468586        0.006901        0.049880
C           3.826373       -0.701677       -0.036047
H          -4.022261       -1.606041        1.035891
H          -4.247143       -0.801179       -0.508223
H          -3.403219       -2.344373       -0.434346
H          -1.474347        0.936474        1.461220
H          -3.151222        1.094285        0.912889
H           1.502933       -1.820973        0.678353
```

```
H           1.499333       -1.570934       -1.066946
H           3.947106       -1.206897       -0.996224
H           4.639307        0.018171        0.069255
H           3.932069       -1.446677        0.754674
C           2.337526        0.703280        1.409151
H           1.377433        1.210089        1.499458
H           2.417143       -0.018286        2.224714
H           3.127955        1.444941        1.536709
C           2.366108        1.039198       -1.078777
H           3.184067        1.758547       -1.013475
H           2.416580        0.557157       -2.056799
H           1.433380        1.599871       -1.025975
N          -1.655445        1.634452       -0.488515
H          -2.261519        1.505316       -1.295762
H          -0.748828        1.223006       -0.731008
C          -1.521391        3.070906       -0.144972
H          -2.500648        3.462495        0.113455
H          -0.851301        3.160508        0.704610
H          -1.115600        3.610542       -0.995405
```

---

### Linear_Regression_22_HEI

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.866482 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.628903 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      21.0710 cm-1
  2.      34.2053 cm-1
  3.      81.0076 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.778726       -0.221053       -0.273989
C           1.644715       -1.258798       -0.003988
C           3.090711       -1.014058       -0.212133
O           1.128750        0.949471       -0.625214
O          -0.564077       -0.501057       -0.118883
C          -1.470328        0.598043       -0.192063
C          -2.892638        0.105679        0.080718
C          -3.821895        1.321811       -0.016877
H           3.382752       -0.840937       -1.253068
```

```
H           3.720507       -1.802739        0.192121
H          -1.190064        1.357086        0.542749
H          -1.417513        1.058480       -1.181190
H          -3.776597        1.774324       -1.009339
H          -4.855394        1.026966        0.170749
H          -3.551826        2.084380        0.716219
C          -2.984288       -0.497956        1.486966
H          -2.326932       -1.360913        1.586477
H          -2.699073        0.235443        2.244123
H          -4.005309       -0.820430        1.698355
C          -3.302069       -0.937840       -0.965169
H          -4.329728       -1.264387       -0.796472
H          -3.241722       -0.522486       -1.973303
H          -2.654718       -1.812844       -0.919730
N           3.482678        0.292989        0.475804
H           2.717756        0.927481        0.143943
H           3.363391        0.176010        1.479457
C           4.827254        0.820962        0.156400
H           4.980679        1.756131        0.686935
H           5.579554        0.096673        0.456203
H           4.887213        0.991889       -0.914321
H           1.299761       -2.199106        0.393036
```

---

# HEI Structures - Conformational Searches

### Compound_1_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.569056 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.411177 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      83.1238 cm-1
2.     118.3971 cm-1
3.     168.6251 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.879434        0.062139        0.673910
H           2.652034        0.141774        1.473274
C           0.564836        0.374261        1.036060
H           0.306630        0.550149        2.080705
C          -0.489634        0.514015        0.039995
C          -0.184336        1.600306       -0.999535
H          -0.964233        1.652435       -1.796170
H          -0.158320        2.579229       -0.462773
H           0.820264        1.429337       -1.460229
C          -1.851640        0.791647        0.669382
H          -2.094626        0.033586        1.451771
H          -1.809690        1.795171        1.158909
H          -2.663439        0.803372       -0.096787
O           2.236327       -0.338800       -0.474075
C          -0.955641       -1.984955        0.043019
H          -2.050187       -1.919789        0.274754
H          -0.369717       -1.957820        1.004083
H          -0.742123       -2.941963       -0.500780
N          -0.550179       -0.840723       -0.775607
H          -1.168308       -0.738276       -1.574594
H           0.424233       -0.976218       -1.107310
```

---

### Compound_1_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.565239 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.407636 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      80.1145 cm-1
2.     104.6196 cm-1
3.     160.5883 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.140612        0.074208       -0.330764
H          -3.116605        0.472915       -0.692352
C          -1.009601        0.860913       -0.579329
H          -1.078702        1.739378       -1.221210
C           0.282041        0.557652        0.028964
C           0.234353        0.559743        1.558494
```

```
H           1.209586        0.264670        2.012992
H          -0.007240        1.601110        1.882738
H          -0.576495       -0.117000        1.926297
C           1.377937        1.504250       -0.450263
H           1.514182        1.439952       -1.556072
H           1.068845        2.547847       -0.196976
H           2.350794        1.290748        0.053943
O          -2.121020       -1.061324        0.229468
C           1.946344       -1.424656       -0.134504
H           2.139219       -1.355528        0.968470
H           2.036519       -2.496477       -0.455329
H           2.713761       -0.812542       -0.677550
N           0.608625       -0.919106       -0.432575
H           0.428646       -0.946230       -1.437852
H          -0.117498       -1.497164        0.029590
```

---

### Compound_2_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.604916 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.463984 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      66.9998 cm-1
2.      87.3638 cm-1
3.     124.5903 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.002120        0.994343       -0.337506
C          -0.570537       -0.109306        0.609501
C           0.548467       -0.962453        0.880481
C           1.628985       -0.626281        0.009510
H          -0.610377        1.144079       -1.269178
H          -1.170750        0.287948        1.463125
H           0.620273       -1.695529        1.671447
O           1.277935        0.510980       -0.771138
C           0.158313        2.302972        0.404157
H           0.700087        3.034319       -0.242919
H          -0.842029        2.718169        0.670734
H           0.754138        2.151595        1.336248
O           2.751586       -1.060299       -0.244565
```

```
C          -2.970235       -0.375019       -0.305377
H          -3.404313       -0.212499        0.716228
H          -2.872076        0.618140       -0.818500
H          -3.663889       -1.027958       -0.897923
N          -1.647658       -0.986780       -0.181786
H          -1.260089       -1.181537       -1.107032
H          -1.710782       -1.880249        0.311297
```

---

### Compound_2_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.605632 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.464658 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      44.9513 cm-1
2.      98.6972 cm-1
3.     127.7568 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.452376        1.107398       -0.390669
C          -0.626836        0.287733        0.387934
C           0.038436       -0.929025        0.748256
C           1.294200       -1.009128        0.074747
H           0.103481        1.479060       -1.391142
H          -1.153019        0.874605        1.179140
H          -0.299998       -1.653682        1.475241
O           1.520942        0.188628       -0.659815
C           0.954737        2.259132        0.451822
H           1.821828        2.743755       -0.058513
H           0.144590        3.012265        0.595170
H           1.296396        1.891697        1.449303
O           2.203636       -1.829229       -0.043693
C          -3.024449       -0.502518        0.099011
H          -3.804131       -0.872132       -0.617290
H          -2.746115       -1.329234        0.807443
H          -3.440009        0.356828        0.687238
N          -1.819671       -0.074411       -0.615809
H          -1.474041       -0.850210       -1.189959
H          -2.038693        0.711177       -1.224517
```

### Compound_2_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.600461 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.458498 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      76.0478 cm-1
2.      88.6894 cm-1
3.     135.2760 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.107630        1.036495        0.547599
C           0.460123       -0.413683        0.657930
C          -0.688116       -1.252099        0.451019
C          -1.769465       -0.469432       -0.052992
H          -0.283884        1.394527        1.601041
H           1.080009       -0.573419        1.573756
H          -0.771015       -2.298415        0.708830
O          -1.393932        0.903257       -0.079171
C           0.697443        2.060809       -0.215430
H           0.274258        3.076825       -0.017358
H           1.762868        2.048007        0.114965
H           0.639437        1.891001       -1.317742
O          -2.910532       -0.666547       -0.468471
C           2.900005       -0.697275       -0.131987
H           3.560660       -0.936743       -1.006648
H           3.153436        0.326582        0.250135
H           3.088633       -1.444918        0.683127
N           1.488115       -0.741255       -0.515817
H           1.239689       -1.681160       -0.846489
H           1.320653       -0.096068       -1.288599
```

### Compound_4_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.874617 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.772697 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      45.8059 cm-1
2.      97.2800 cm-1
3.     148.4606 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.825845       -0.219211        0.319305
O          -2.964339       -0.421425       -0.141004
C          -0.846871        0.642079       -0.246742
H          -1.517348       -0.750088        1.257767
C           0.438311        0.781116        0.310806
H           0.974113        1.732255        0.062474
H           0.536148        0.532244        1.399427
H          -1.118412        1.217365       -1.137018
C           2.779725       -0.316440        0.110241
H           2.789821       -0.492499        1.218113
H           3.230344        0.689466       -0.098211
H           3.400807       -1.105394       -0.390096
N           1.400195       -0.335128       -0.368168
H           1.371838       -0.185723       -1.376705
H           0.974114       -1.245590       -0.192210
```

---

### Compound_4_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.875043 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.773177 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      24.7076 cm-1
2.     107.9966 cm-1
3.     169.3064 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.575816       -0.289378        0.255737
O          -2.684104       -0.561730       -0.240052
C          -0.751006        0.808148       -0.116048
H          -1.165262       -0.950149        1.063946
C           0.510700        1.027873        0.462900
H           0.883724        2.082294        0.409162
H           0.677896        0.586284        1.477973
H          -1.129575        1.501909       -0.873361
C           1.959987       -1.077426        0.081343
H           2.469771       -0.983075        1.075551
H           2.626721       -1.643786       -0.620509
H           0.999868       -1.645819        0.218270
N           1.644682        0.252799       -0.436536
H           2.497165        0.799900       -0.508438
H           1.236561        0.161389       -1.370014
```

---

## Compound_4_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.894066 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.790195 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      92.5150 cm-1
  2.     128.1390 cm-1
  3.     170.4672 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.916942       -0.081949       -0.078184
O          -1.532397       -1.256271        0.193629
C          -1.057956        1.025669       -0.146325
H          -2.991671        0.090756       -0.312994
C           0.279215        0.934760        0.382241
H           0.878040        1.874674        0.255237
H           0.325184        0.594142        1.455922
H          -1.395565        1.970194       -0.571282
```

```
C           2.428906       -0.352871        0.043176
H           2.476839       -0.561535        1.144740
H           2.991020        0.593504       -0.172358
H           2.906967       -1.202189       -0.512210
N           1.031444       -0.197265       -0.360083
H           0.960172       -0.022956       -1.363411
H           0.488737       -1.059222       -0.157551
```

---

### Compound_4_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.884632 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.780557 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      44.9693 cm-1
2.     162.5106 cm-1
3.     212.6012 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.744967       -0.196787        0.166722
O           1.285429       -1.321996       -0.156167
C           1.022675        1.012748        0.102553
H           2.787743       -0.130479        0.557189
C          -0.254832        1.061922       -0.536058
H          -0.631321        2.100985       -0.723938
H          -0.322387        0.440657       -1.470522
H           1.449938        1.925222        0.520006
C          -1.781033       -0.908595       -0.050573
H          -2.465200       -1.381163        0.700833
H          -0.870076       -1.561587       -0.203517
H          -2.321132       -0.796600       -1.025817
N          -1.329638        0.407371        0.418509
H          -0.861923        0.292371        1.325729
H          -2.132264        1.019233        0.543944
```

---

### Compound_5_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.210441 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.082186 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      44.1155 cm-1
2.      76.3724 cm-1
3.     110.7220 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.642176       -0.089971       -0.034909
O          -2.708236       -0.555271       -0.490171
C          -0.524548       -0.902726        0.320940
C           0.705656       -0.408918        0.786110
H           1.319014       -1.131773        1.382295
H           0.696620        0.604995        1.262298
H          -0.659341       -1.986185        0.222436
C           3.009772        0.313863       -0.178496
H           3.518295       -0.447095        0.470182
H           3.627390        0.477753       -1.100643
H           2.938044        1.279155        0.388497
N           1.666222       -0.153073       -0.505989
H           1.191213        0.522298       -1.104666
H           1.710166       -1.029646       -1.025040
C          -1.523912        1.400893        0.160531
H          -1.430621        1.630580        1.249008
H          -0.626122        1.798164       -0.369166
H          -2.431086        1.916583       -0.236964
```

---

### Compound_5_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.211788 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.083459 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      40.6074 cm-1
2.      75.9540 cm-1
3.     110.6846 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.521944       -0.253739       -0.006298
O          -2.369418       -1.110452       -0.334785
C          -0.277935       -0.583129        0.611650
C           0.715115        0.347940        0.950111
H           1.429835        0.023607        1.747508
H           0.377246        1.404852        1.107053
H          -0.107882       -1.644870        0.826076
C           2.695647       -0.537894       -0.434963
H           3.280254       -0.479252       -1.390154
H           3.403404       -0.487677        0.433122
H           2.142275       -1.515596       -0.397044
N           1.722325        0.547880       -0.335368
H           2.204718        1.440277       -0.298371
H           1.122242        0.534136       -1.161611
C          -1.820286        1.201914       -0.264106
H          -1.924993        1.741620        0.707511
H          -0.997609        1.674184       -0.851249
H          -2.773999        1.306624       -0.835358
```

---

### Compound_5_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.232573 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.10332 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      49.4301 cm-1
2.      80.6934 cm-1
3.     100.0981 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.414184        0.144319       -0.050155
O          -0.973932        1.307259       -0.296288
C          -0.575995       -0.984931        0.047119
C           0.778710       -0.910994       -0.428375
H           1.350115       -1.868873       -0.312306
H           0.876418       -0.528830       -1.484166
H          -0.948437       -1.923443        0.455473
C           2.950060        0.304069        0.047084
H           3.476377       -0.664674        0.253296
H           3.428133        1.120348        0.649950
H           3.050320        0.547160       -1.043826
N           1.533322        0.174921        0.386046
H           1.414555       -0.030865        1.378666
H           1.024494        1.057528        0.191056
C          -2.880302       -0.058882        0.190199
H          -3.306257       -0.690116       -0.626524
H          -3.040640       -0.582007        1.162970
H          -3.416607        0.919767        0.208159
```

---

### Compound_5_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.23351 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.103912 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      48.1419 cm-1
2.      72.9715 cm-1
3.      91.7184 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.293949        0.106222        0.046100
O           1.030522        1.291386        0.410835
C           0.350660       -0.939085        0.109876
C          -0.854157       -0.766262        0.873116
H          -1.518824       -1.669235        0.873912
H          -0.671476       -0.413868        1.929448
H           0.535019       -1.888670       -0.390832
C          -2.274572        0.102246       -1.008320
H          -1.456915       -0.292832       -1.672457
```

```
H          -2.722105        1.021227       -1.468163
H          -3.064843       -0.684156       -0.893438
N          -1.693882        0.413073        0.301056
H          -1.019009        1.195069        0.206174
H          -2.425370        0.687380        0.951351
C           2.647126       -0.214472       -0.515061
H           3.181496       -0.907028        0.179065
H           2.543080       -0.716663       -1.506278
H           3.253917        0.714290       -0.637121
```

---

### Compound_5_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.223268 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.093813 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      37.9947 cm-1
  2.      59.8323 cm-1
  3.     112.0281 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.278378       -0.163300        0.069984
O          -0.771792       -1.285369        0.341801
C          -0.536776        1.042698        0.051000
C           0.800711        1.067500        0.549449
H           1.218975        2.098387        0.684847
H           0.955728        0.450252        1.476031
H          -0.992703        1.959270       -0.324024
C           2.274135       -0.915940       -0.052267
H           2.873878       -1.408252       -0.861019
H           2.921253       -0.764379        0.849685
H           1.396004       -1.571903        0.225318
N           1.752788        0.377440       -0.509917
H           2.525663        0.987668       -0.763287
H           1.172103        0.223499       -1.343238
C          -2.734335       -0.068040       -0.284055
H          -2.856099        0.429264       -1.275673
H          -3.197770       -1.082508       -0.324637
H          -3.264364        0.542071        0.486337
```

### Compound_6_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.541504 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.386683 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      46.8923 cm-1
2.      64.6118 cm-1
3.      76.3109 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.522169       -0.376299       -0.046858
C          -0.497813        0.574735        0.260164
C           0.777536        0.195347        0.748016
H           0.837426       -0.793115        1.272060
H           1.312602        0.990721        1.330215
C          -0.775015        2.011015        0.067204
H          -0.128925        2.447029       -0.738641
H          -1.843579        2.167067       -0.225187
H          -0.578321        2.590703        1.004817
O          -2.638225       -0.070453       -0.517847
C          -1.235382       -1.832999        0.225545
H          -2.083284       -2.464232       -0.135307
H          -0.303737       -2.159258       -0.293726
H          -1.113781       -1.994728        1.323351
C           3.125332       -0.370938       -0.164210
H           3.567386        0.444086        0.467321
H           3.758781       -0.508260       -1.079850
H           3.125127       -1.324472        0.426728
N           1.750747       -0.019528       -0.513448
H           1.731325        0.845210       -1.055706
H           1.334614       -0.745606       -1.098331
```

### Compound_6_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.539522 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.38458 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      28.1738 cm-1
2.      67.3003 cm-1
3.      77.6578 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.556414       -0.103552       -0.097793
C          -0.328212        0.490747        0.337760
C           0.725772       -0.266765        0.903441
H           0.429816       -1.228942        1.396069
H           1.427310        0.317028        1.552982
C          -0.151307        1.948189        0.193424
H           0.649701        2.188755       -0.553985
H          -1.101754        2.425609       -0.153495
H           0.145093        2.418385        1.165343
O          -2.490061        0.535556       -0.627097
C          -1.728261       -1.589535        0.102446
H          -2.675766       -1.934315       -0.377987
H          -0.875808       -2.151482       -0.346754
H          -1.779020       -1.819397        1.193698
C           2.901349        0.005509       -0.450831
H           3.533515       -0.080939        0.471245
H           2.607162        1.081116       -0.590522
H           3.498971       -0.332379       -1.337917
N           1.688018       -0.796406       -0.291015
H           1.943053       -1.770613       -0.150796
H           1.124531       -0.729988       -1.144682
```

---

### Compound_6_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.559545 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.403878 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      71.8283 cm-1
2.      79.6462 cm-1
3.      99.2738 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.203477       -0.620878        0.069736
C          -0.521064        0.618140        0.153016
C           0.848341        0.605822        0.612345
H           0.996912        0.024434        1.566151
H           1.306108        1.625682        0.705423
C          -1.175670        1.887825       -0.182055
H          -1.481491        1.919413       -1.260439
H          -2.103496        2.031803        0.429978
H          -0.502003        2.760755        0.007153
O          -0.596243       -1.731657        0.123216
C          -2.689644       -0.601159       -0.121309
H          -2.945949       -0.020317       -1.040277
H          -3.087952       -1.639122       -0.219558
H          -3.173069       -0.105990        0.755422
C           3.139904       -0.201077       -0.092814
H           3.536531        0.848056       -0.100062
H           3.701474       -0.814131       -0.845871
H           3.294471       -0.641392        0.927722
N           1.710231       -0.187986       -0.402827
H           1.544315        0.197356       -1.333406
H           1.322141       -1.149426       -0.391691
```

---

### Compound_6_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.559533 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.40387 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      71.6351 cm-1
2.      79.5410 cm-1
3.      99.1972 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.203590       -0.620835       -0.069615
C          -0.520990        0.618067       -0.152923
C           0.848329        0.605543       -0.612420
H           0.996780        0.023912       -1.566096
H           1.306159        1.625346       -0.705850
C          -1.175417        1.887856        0.182101
H          -2.103556        2.031646       -0.429478
H          -1.480610        1.919800        1.260642
H          -0.501874        2.760740       -0.007764
O          -0.596502       -1.731684       -0.122946
C          -2.689794       -0.600895        0.121107
H          -3.088189       -1.638780        0.219843
H          -2.946322       -0.019533        1.039659
H          -3.172956       -0.106251       -0.756060
C           3.139952       -0.201088        0.092682
H           3.536546        0.848050        0.099758
H           3.701622       -0.814043        0.845734
H           3.294401       -0.641511       -0.927818
N           1.710316       -0.187987        0.402878
H           1.544515        0.197558        1.333386
H           1.322343       -1.149440        0.391880
```

---

### Compound_6_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.55079 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.394743 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      49.3037 cm-1
  2.      83.2945 cm-1
  3.      99.3606 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.994689       -0.702277        0.086187
C           0.557821        0.647227        0.186595
C          -0.783830        0.879492        0.647961
```

```
H          -1.074415        0.220604        1.512139
H          -1.013370        1.952781        0.875439
C           1.437214        1.772519       -0.151421
H           2.399606        1.711833        0.419297
H           1.697993        1.777498       -1.242081
H           0.957926        2.754458        0.089081
O           0.202099       -1.678374        0.194961
C           2.447726       -0.953032       -0.186942
H           2.640818       -2.044423       -0.318443
H           2.762009       -0.410029       -1.110722
H           3.057906       -0.576013        0.669313
C          -2.693063       -0.623442       -0.087135
H          -3.366761       -0.908080       -0.936460
H          -3.313180       -0.297239        0.786933
H          -2.061313       -1.511403        0.210180
N          -1.790135        0.462599       -0.487507
H          -2.331155        1.262430       -0.806354
H          -1.205248        0.133462       -1.266937
```

---

### Compound_7_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.276343 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.157342 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      50.8573 cm-1
2.      73.5565 cm-1
3.     104.9382 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.597729       -0.054155       -0.012648
O           2.677567       -0.393980       -0.556094
C           0.532051       -0.970242        0.274578
C          -0.740945       -0.595274        0.745654
H          -1.371664       -1.448242        1.106782
H          -0.800002        0.263429        1.464629
H           0.735541       -2.018724        0.036976
C          -2.960080        0.342101       -0.199855
H          -3.504792       -0.568557        0.163748
H          -3.488499        0.747532       -1.102629
```

```
H          -2.974958        1.118229        0.609897
N          -1.576259       -0.011613       -0.504164
H          -1.066814        0.805628       -0.846242
H          -1.541222       -0.713521       -1.244307
N           1.407349        1.330546        0.245121
H           2.234843        1.871933        0.111998
H           0.966870        1.527022        1.114831
```

---

### Compound_7_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.294983 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.175447 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      77.4045 cm-1
2.      96.9528 cm-1
3.     147.5911 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.440257        0.112454        0.037318
O           1.007267        1.282140        0.297044
C           0.575165       -1.021766       -0.049797
C          -0.754641       -0.898364        0.458020
H          -1.349836       -1.846337        0.402992
H          -0.824983       -0.449091        1.488314
H           0.901062       -1.953122       -0.508679
C          -2.926678        0.332786       -0.042128
H          -2.999278        0.633693        1.036393
H          -3.471647       -0.636861       -0.185735
H          -3.408282        1.123542       -0.675420
N          -1.520725        0.162393       -0.402541
H          -0.996369        1.044323       -0.265635
H          -1.426633       -0.096687       -1.384801
N           2.797547       -0.025309       -0.246220
H           3.194040       -0.926376       -0.153900
H           3.381408        0.739546       -0.009030
```

---

### Compound_7_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.277674 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.158486 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      45.0905 cm-1
2.      71.5863 cm-1
3.     113.3398 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.472484       -0.197831        0.018620
O           2.337618       -1.030178       -0.350075
C           0.285020       -0.556575        0.739515
C          -0.770396        0.325641        1.032504
H          -1.514496       -0.067212        1.771501
H          -0.501602        1.388295        1.273054
H           0.195685       -1.615924        0.999170
C          -2.550137       -0.571064       -0.570517
H          -1.946594       -1.519161       -0.537658
H          -3.040712       -0.477567       -1.574422
H          -3.339669       -0.614415        0.224078
N          -1.654079        0.555545       -0.309858
H          -0.978638        0.627839       -1.075632
H          -2.189012        1.417821       -0.265791
N           1.656424        1.152209       -0.384532
H           1.421907        1.822620        0.311444
H           2.553941        1.323822       -0.785150
```

---

### Compound_7_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.287032 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.167327 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      41.5746 cm-1
2.     104.3721 cm-1
3.     136.6237 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.303713       -0.135727        0.052168
O          -0.768598       -1.257503        0.308807
C          -0.563541        1.091030        0.039857
C           0.770455        1.077784        0.534687
H           1.223279        2.094795        0.657477
H           0.914673        0.459840        1.462202
H          -0.994988        2.008246       -0.358145
C           2.293661       -0.896325       -0.009234
H           2.952134       -0.661779        0.866187
H           2.898982       -1.407469       -0.802141
H           1.454686       -1.575651        0.323769
N           1.698825        0.340103       -0.526567
H           2.430109        0.957139       -0.868736
H           1.077841        0.104251       -1.310869
N          -2.652839       -0.127690       -0.305938
H          -3.143879        0.725302       -0.208172
H          -3.167122       -0.952121       -0.109370
```

---

## Compound_8_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.686865 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.437582 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      61.7895 cm-1
2.      73.6413 cm-1
3.      93.0165 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.290809        0.241383        0.095639
C           1.067439        1.451608       -0.237979
C           2.562355        1.301881       -0.028847
C           3.068920       -0.017112       -0.564258
C           2.388644       -1.162725        0.146570
C           0.884951       -1.042231        0.137754
H           3.094618        2.148630       -0.535765
H           0.880849        1.734678       -1.313588
H           0.732220        2.329801        0.381089
H           2.868301       -0.080027       -1.665733
H           4.178625       -0.088813       -0.420800
H           2.683122       -2.138106       -0.321798
H           2.715163       -1.193766        1.220552
H           2.793125        1.367976        1.067066
O           0.214942       -2.120390        0.150594
C          -1.152741        0.361114        0.332861
C          -1.587688       -0.252799        1.667144
H          -2.694462       -0.211756        1.803983
H          -1.236567       -1.310620        1.755943
H          -1.106815        0.343444        2.480327
C          -1.690425        1.786860        0.256075
H          -2.796854        1.810505        0.409354
H          -1.218430        2.386922        1.072693
H          -1.444265        2.263818       -0.722401
N          -1.821422       -0.499540       -0.824287
H          -1.325041       -0.250706       -1.681354
H          -1.573033       -1.476860       -0.590717
C          -3.264402       -0.365617       -1.007339
H          -3.509580        0.666325       -1.372547
H          -3.631877       -1.115713       -1.757305
H          -3.785858       -0.540002       -0.029458
```

---

### Compound_8_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.693343 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.444016 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      62.3642 cm-1
2.      67.4480 cm-1
3.     102.6716 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.143626       -0.185659        0.148107
C           0.835970       -1.482762        0.023036
C           2.268938       -1.364220       -0.459091
C           2.976993       -0.222971        0.234444
C           2.313567        1.089326       -0.108805
C           0.808772        1.049827       -0.006579
H           2.809579       -2.326456       -0.263269
H           0.837465       -2.012759        1.017804
H           0.282411       -2.154474       -0.692503
H           2.948214       -0.385093        1.343780
H           4.054473       -0.193634       -0.073920
H           2.691599        1.900675        0.567438
H           2.575436        1.385477       -1.159928
H           2.282783       -1.191468       -1.567217
O           0.195942        2.159531       -0.108959
C          -1.278172       -0.185139        0.512378
C          -1.552888        0.617027        1.793876
H          -2.643065        0.668241        2.028259
H          -1.032865        0.092507        2.631592
H          -1.134634        1.650883        1.715533
C          -1.886884       -1.574582        0.687007
H          -1.790284       -2.190449       -0.238524
H          -1.339033       -2.094957        1.510675
H          -2.966446       -1.507242        0.966368
N          -2.061660        0.570635       -0.636187
H          -3.028464        0.710842       -0.358487
H          -1.586634        1.490710       -0.702109
C          -1.994745       -0.113949       -1.928954
H          -2.301802        0.585155       -2.750103
H          -0.934199       -0.452803       -2.098088
H          -2.671498       -1.007232       -1.924835
```

---

### Compound_8_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.680663 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.431842 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      53.0882 cm-1
2.      65.5326 cm-1
```

```
   3.      93.6444 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.276792       -0.198388       -0.163516
C          -1.124796       -1.270465       -0.720299
C          -2.489405       -1.345522       -0.050093
C          -3.066241        0.005896        0.324889
C          -2.340121        1.165510       -0.320376
C          -0.854800        1.092408       -0.069301
H          -3.196395       -1.878660       -0.739497
H          -1.284517       -1.084306       -1.820952
H          -0.643333       -2.280132       -0.639844
H          -4.149866        0.046607        0.037345
H          -3.019755        0.130885        1.439475
H          -2.503208        1.148375       -1.430636
H          -2.741495        2.136295        0.069865
H          -2.405529       -1.972158        0.876729
O          -0.204978        2.156426        0.146081
C           1.099215       -0.409645        0.274620
C           1.335770        0.046132        1.718749
H           2.408536       -0.037376        2.014298
H           0.984488        1.097023        1.868746
H           0.732267       -0.621230        2.380818
C           1.616754       -1.835610        0.123343
H           1.574771       -2.178585       -0.937822
H           2.667625       -1.922384        0.492908
H           0.975125       -2.510176        0.742094
N           1.959257        0.551623       -0.662944
H           1.604526        0.410799       -1.610107
H           1.689557        1.505130       -0.366593
C           3.410544        0.391744       -0.627530
H           3.772438        0.468095        0.431583
H           3.693353       -0.613460       -1.037468
H           3.905682        1.190135       -1.241893
```

---

### Compound_8_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.693342 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.444022 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      62.3478 cm-1
2.      67.4421 cm-1
3.     102.6626 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.143750       -0.185653        0.147925
C           0.835929       -1.482769        0.021994
C           2.269310       -1.364242       -0.458950
C           2.976881       -0.222863        0.234836
C           2.313611        1.089368       -0.108979
C           0.808812        1.049926       -0.006870
H           2.809807       -2.326420       -0.262492
H           0.836537       -2.013827        1.016181
H           0.282676       -2.153544       -0.694665
H           2.947439       -0.384804        1.344175
H           4.054533       -0.193526       -0.072887
H           2.691600        1.900895        0.567052
H           2.575624        1.385115       -1.160168
H           2.284056       -1.191764       -1.567110
O           0.195936        2.159587       -0.109150
C          -1.277953       -0.185206        0.512555
C          -1.552613        0.616581        1.794325
H          -2.642731        0.667326        2.029090
H          -1.032188        0.092059        2.631769
H          -1.134809        1.650618        1.716164
C          -1.886684       -1.574741        0.686730
H          -2.966223       -1.507398        0.966165
H          -1.790218       -2.190273       -0.239029
H          -1.338847       -2.095457        1.510172
N          -2.061741        0.570813       -0.635701
H          -3.028405        0.711013       -0.357451
H          -1.586756        1.490907       -0.701655
C          -1.995537       -0.113642       -1.928581
H          -2.303803        0.585301       -2.749405
H          -0.934944       -0.451784       -2.098833
H          -2.671692       -1.007370       -1.923871
```

---

### Compound_8_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.686867 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.437587 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      61.7965 cm-1
2.      73.5949 cm-1
3.      92.9754 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.290811        0.241386        0.095429
C           1.067480        1.451583       -0.238180
C           2.562367        1.301853       -0.028815
C           3.068983       -0.017143       -0.564161
C           2.388647       -1.162732        0.146652
C           0.884943       -1.042268        0.137692
H           3.094711        2.148600       -0.535642
H           0.881044        1.734559       -1.313837
H           0.732164        2.329834        0.380752
H           2.868458       -0.080085       -1.665650
H           4.178673       -0.088839       -0.420610
H           2.683168       -2.138124       -0.321662
H           2.715071       -1.193718        1.220658
H           2.792976        1.367925        1.067131
O           0.214950       -2.120412        0.150461
C          -1.152704        0.361161        0.332853
C          -1.587546       -0.252841        1.667129
H          -2.694347       -0.212173        1.803868
H          -1.236126       -1.310545        1.756023
H          -1.106921        0.343558        2.480344
C          -1.690375        1.786927        0.256204
H          -2.796748        1.810553        0.409904
H          -1.218043        2.387051        1.072578
H          -1.444642        2.263859       -0.722393
N          -1.821554       -0.499341       -0.824314
H          -1.325267       -0.250448       -1.681431
H          -1.572990       -1.476649       -0.590875
C          -3.264600       -0.365713       -1.007148
H          -3.631977       -1.115675       -1.757294
H          -3.510047        0.666284       -1.372007
H          -3.785912       -0.540550       -0.029278
```

---

## Compound_8_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.69233 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.442742 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      65.7544 cm-1
  2.      69.1634 cm-1
  3.      99.3969 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.137699       -0.202515        0.196840
C           0.840778       -1.474973       -0.060307
C           2.343654       -1.396326        0.129031
C           2.916264       -0.149650       -0.504312
C           2.311375        1.080673        0.128685
C           0.803418        1.043224        0.157746
H           2.581336       -1.395889        1.225382
H           0.460500       -2.288620        0.618206
H           0.629081       -1.818245       -1.114182
H           4.030128       -0.131385       -0.377330
H           2.704413       -0.154134       -1.605495
H           2.663064        1.175378        1.190981
H           2.646015        2.000810       -0.417993
H           2.822765       -2.306024       -0.318246
O           0.195387        2.159000        0.131158
C          -1.303824       -0.227445        0.466382
C          -1.664514        0.468587        1.787109
H          -2.767458        0.491706        1.957377
H          -1.188953       -0.115000        2.612046
H          -1.255433        1.508734        1.815524
C          -1.929528       -1.620683        0.475939
H          -1.537659       -2.178484        1.361623
H          -3.041871       -1.564244        0.565059
H          -1.665775       -2.192031       -0.445995
N          -2.015960        0.624350       -0.667256
H          -2.997646        0.747587       -0.437499
H          -1.539298        1.544167       -0.632815
C          -1.873349        0.040649       -2.002210
H          -2.166509        0.789857       -2.783309
H          -0.797564       -0.257097       -2.149180
H          -2.522340       -0.868795       -2.092040
```

---

## Compound_10_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.927501 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.759441 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
1.      52.7375 cm-1
2.      81.5726 cm-1
3.     116.0675 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.750475        0.171302        0.475770
C           0.249165       -1.065046        1.256975
C          -1.197194       -1.285697        0.819394
C          -1.592610       -0.052298        0.006198
C          -0.427862        0.755211       -0.133112
H           0.293543       -0.833701        2.351441
H           0.875683       -1.973047        1.084419
H          -1.295412       -2.199299        0.183842
H          -1.874521       -1.398889        1.699626
O          -2.750206        0.145591       -0.396276
O          -0.334805        1.919719       -0.855154
H          -0.799969        2.593563       -0.335764
C           1.603477        1.098987        1.322192
H           1.891484        2.011527        0.745440
H           0.984779        1.426651        2.194250
H           2.521123        0.595718        1.710400
C           1.098352       -1.294987       -1.617425
H           0.050157       -0.962964       -1.867591
H           1.694587       -1.405264       -2.560215
H           1.048789       -2.280369       -1.085971
N           1.705240       -0.287522       -0.744339
H           2.599248       -0.617220       -0.392957
H           1.851090        0.568636       -1.285064
```

---

### Compound_10_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.923512 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.754889 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
1.      67.1567 cm-1
2.     112.2065 cm-1
3.     116.5184 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.511121       -0.486351        0.310694
C          -0.378635       -1.743762        0.123252
C          -1.735112       -1.234563       -0.355167
C          -1.717352        0.280102       -0.149827
C          -0.402228        0.638262        0.267191
H          -0.480598       -2.251107        1.115667
H           0.053889       -2.490109       -0.586317
H          -1.904574       -1.467241       -1.434314
H          -2.568902       -1.690463        0.231411
O          -2.721166        0.992257       -0.308191
O           0.028352        1.916125        0.526336
H          -0.361748        2.160668        1.379725
C           1.433305       -0.583265        1.505773
H           1.933874        0.398270        1.693287
H           0.811064       -0.827898        2.402400
H           2.205892       -1.379583        1.383918
C           2.466931        0.671994       -0.903298
H           2.927346        0.875045       -1.905567
H           1.998767        1.616858       -0.504498
H           3.262616        0.327361       -0.193095
N           1.426189       -0.352640       -1.015840
H           0.769120       -0.077582       -1.751882
H           1.844260       -1.247293       -1.256736
```

---

### Compound_11_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1374.727165 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1374.641603 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      51.1909 cm-1
2.      61.3840 cm-1
3.     132.5041 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.542491        0.294643       -0.091735
C          -1.095571       -1.175331       -0.242512
C           1.240447       -1.269462       -0.214565
C           0.892532        0.113887       -0.014935
O           2.320854       -1.866720       -0.261944
O          -2.299522       -1.461097       -0.201760
Cl          1.988637        1.370681        0.076483
Cl         -1.140534        1.305243       -1.436764
N          -0.007411       -2.009812       -0.340463
H          -0.061195       -2.977465       -0.534493
N          -1.128512        0.934148        1.186882
H          -2.147282        0.983158        1.093597
H          -0.749516        1.883675        1.255707
C          -0.769836        0.174909        2.397507
H          -1.114924        0.736074        3.304407
H          -1.262199       -0.833661        2.359483
H           0.347677        0.037836        2.428208
```

---

### Compound_12_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -826.21593 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -826.06864 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      65.2380 cm-1
2.      93.9984 cm-1
3.     175.2587 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.705931        1.718003       -0.110018
H          -1.693588        2.198035       -0.291893
C          -0.690612        0.321954        0.071619
C           0.506210       -0.377344        0.538074
C           1.015128        0.195025        1.870227
H           1.973269       -0.281175        2.187483
H           1.145746        1.303562        1.804027
H           0.236978       -0.018486        2.642659
C           0.355374       -1.887848        0.687953
H           0.008136       -2.362516       -0.260784
H           1.318158       -2.357539        1.003704
H          -0.412930       -2.085396        1.475794
O           0.336748        2.431331       -0.112416
C           1.372846       -0.648178       -1.838286
H           0.305030       -0.423151       -2.115738
H           2.062462       -0.197657       -2.599188
H           1.518971       -1.759122       -1.809259
N           1.644074       -0.074933       -0.517253
H           1.667229        0.959027       -0.582803
H           2.535570       -0.408682       -0.161748
Cl         -2.116802       -0.554276       -0.240563
```

---

### Compound_13_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1666.774226 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1666.703448 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      28.9839 cm-1
2.      87.5604 cm-1
3.     146.7768 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.894964        0.864718       -0.278302
H          -2.958583        0.549389       -0.372236
C          -0.955758       -0.162961       -0.017775
C           0.471140        0.026617       -0.113222
O          -1.602793        2.085583       -0.374955
C           0.607962        1.490132        1.922599
```

```
H          -0.479075        1.248445        2.089972
H           0.819993        2.537126        2.264347
H           1.243193        0.764209        2.494041
N           0.890731        1.391804        0.481190
H           1.881182        1.557696        0.298642
H           0.316058        2.107350       -0.023372
Cl         -1.550950       -1.730933        0.238597
Cl          1.059844        0.122747       -1.842766
Cl          1.455470       -1.244906        0.651234
```

---

### Compound_13_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1666.769742 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1666.699232 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      20.6951 cm-1
2.      84.4262 cm-1
3.     147.3451 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.456482        1.672680        0.123628
H           2.547947        1.876608        0.041737
C           1.071750        0.310915        0.125222
C          -0.298301       -0.136100       -0.016634
O           0.657025        2.639461        0.239532
C          -2.646381        0.461145        0.820868
H          -3.044116        0.399186       -0.227863
H          -3.200700        1.260244        1.381940
H          -2.800691       -0.527108        1.330061
N          -1.219838        0.803278        0.793943
H          -0.836835        0.821251        1.744943
H          -1.080332        1.758818        0.387818
Cl          2.304318       -0.854970        0.121268
Cl         -0.892485       -0.049576       -1.729952
Cl         -0.576769       -1.811894        0.523331
```

---

### Compound_14_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.816605 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.699519 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      73.8853 cm-1
2.      86.9898 cm-1
3.     100.1963 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.154150        1.539827        0.062566
O          -0.904682        2.231478        0.019738
C           0.093456        0.131618        0.232723
C          -1.159778       -0.435107        0.685901
H          -1.120957       -1.535411        0.902772
H          -1.590186        0.118306        1.569354
C          -3.517608       -0.835862       -0.107470
H          -3.909687       -0.408544        0.853384
H          -3.396333       -1.945009        0.009297
H          -4.251802       -0.627536       -0.929683
N          -2.221400       -0.228827       -0.414878
H          -2.310996        0.798564       -0.519750
H          -1.847677       -0.596327       -1.291643
C           1.480929        2.214902       -0.089875
H           1.348871        3.323675       -0.116463
H           2.147466        1.947498        0.765135
H           1.968886        1.886604       -1.039431
Br          1.526937       -0.997261       -0.061709
```

---

### Compound_14_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.818045 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.700493 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      59.4982 cm-1
2.      88.2629 cm-1
3.      97.9319 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.066734        1.576054        0.010243
O           1.164670        2.204474        0.047066
C           0.008311        0.200203        0.354471
C           1.142333       -0.364775        1.054448
H           0.994241       -1.423133        1.396569
H           1.467844        0.284260        1.919585
C           2.307345       -1.340151       -0.940036
H           3.168671       -1.212783       -1.646086
H           1.339032       -1.182557       -1.490902
H           2.318327       -2.377219       -0.514247
N           2.393622       -0.359523        0.148213
H           2.439517        0.598257       -0.245779
H           3.231553       -0.525925        0.701141
C          -1.175719        2.290260       -0.420920
H          -0.965598        3.378040       -0.562627
H          -1.545236        1.865465       -1.385470
H          -1.973703        2.170873        0.350919
Br         -1.446897       -0.881827       -0.008182
```

---

### Compound_14_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.808629 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.691356 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      37.2933 cm-1
2.      81.8626 cm-1
3.      87.9595 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.227857        1.423794       -0.081229
O           1.422103        1.830075       -0.098732
C          -0.071809        0.042484       -0.253160
C           0.999121       -0.810739       -0.709244
H           0.679646       -1.837706       -1.026725
H           1.609539       -0.323409       -1.521484
C           3.375098       -0.598489        0.123844
H           3.746347       -1.190076       -0.752205
H           4.058910       -0.755082        0.998121
H           3.348819        0.497676       -0.144941
N           2.008517       -1.016933        0.462756
H           2.005553       -1.986311        0.771404
H           1.665833       -0.428027        1.234647
C          -0.884625        2.399895        0.143888
H          -0.481576        3.440600        0.188275
H          -1.626038        2.332125       -0.688377
H          -1.405414        2.173007        1.105347
Br         -1.740341       -0.691044        0.058340
```

---

### Compound_14_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.797435 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.680814 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      45.0636 cm-1
  2.      51.6386 cm-1
  3.      89.1481 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.482207        1.630940       -0.049355
O           1.573076        2.017600       -0.509908
C           0.144401        0.272090        0.244866
C          -1.136898       -0.115748        0.729389
H          -1.151459       -1.045332        1.359840
H          -1.723442        0.698192        1.233539
C          -3.397874       -0.913125       -0.159456
H          -3.910753       -0.067287        0.369871
H          -3.356342       -1.798481        0.528612
```

```
H          -3.987992       -1.185981       -1.073736
N          -2.036738       -0.510204       -0.513497
H          -1.559510       -1.267915       -1.006929
H          -2.053111        0.293174       -1.145703
C          -0.580161        2.670288        0.226508
H          -0.230502        3.670537       -0.127772
H          -1.530595        2.420136       -0.300682
H          -0.774934        2.731106        1.323852
Br          1.396604       -1.093834        0.016033
```

---

### Compound_14_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.798835 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.681487 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      46.2100 cm-1
2.      55.2658 cm-1
3.     113.6002 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.451763        1.504393       -0.033125
O           0.176601        2.292448       -0.765779
C          -0.008018        0.195312        0.338835
C          -0.832219       -0.747368        1.012234
H          -0.289876       -1.424323        1.728867
H          -1.744839       -0.316969        1.502487
C          -2.482584       -1.231634       -0.861235
H          -3.366978       -0.983911       -0.217991
H          -2.792394       -1.954390       -1.660437
H          -2.100364       -0.285866       -1.337587
N          -1.415634       -1.798103       -0.030914
H          -1.756436       -2.628188        0.448341
H          -0.636389       -2.068390       -0.637370
C          -1.778839        1.961172        0.526672
H          -1.738536        1.966068        1.641917
H          -2.001510        2.997306        0.173100
H          -2.603941        1.287537        0.193617
Br          1.738527       -0.355228       -0.039789
```

### Compound_14_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.794922 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.678022 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      32.1690 cm-1
2.      53.4788 cm-1
3.      73.0315 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.560742        0.803186       -0.109910
O           2.511857        0.208170       -0.650923
C           0.322587        0.200285        0.280815
C          -0.740014        0.943220        0.868324
H          -1.426242        0.353728        1.532519
H          -0.420796        1.885804        1.389752
C          -2.915884        0.688899       -0.444780
H          -2.632151       -0.386007       -0.614080
H          -3.532928        0.759555        0.488909
H          -3.520781        1.054687       -1.315651
N          -1.693914        1.483305       -0.288661
H          -1.143696        1.429567       -1.153939
H          -1.942480        2.456660       -0.126100
C           1.710065        2.282950        0.159941
H           1.744906        2.465194        1.260644
H           2.661929        2.655048       -0.291378
H           0.860566        2.856688       -0.279447
Br          0.042550       -1.631162        0.051727
```

### Compound_15_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.637946 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.541159 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      49.9832 cm-1
2.      52.4564 cm-1
3.      98.6159 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.814128       -0.071936        0.022590
C           0.311075       -0.924429       -0.552901
C           1.387458        0.020110       -1.106048
C           0.884156        1.347849       -0.923636
C          -0.348973        1.401846       -0.220299
H           1.713124       -0.265202       -2.144463
H           1.338456        2.233475       -1.357397
Cl         -0.968222       -0.408613        1.742483
Cl         -2.310569       -0.402186       -0.819117
O           0.400789       -2.146522       -0.577953
O          -1.019077        2.368321        0.150269
C           2.633840        0.171929        1.113568
H           2.242100        1.226360        1.168560
H           3.640069        0.111861        1.602937
H           1.911317       -0.504528        1.644048
N           2.726946       -0.225919       -0.296954
H           3.454269        0.329096       -0.748510
H           2.977229       -1.212637       -0.361906
```

---

### Compound_15_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.637431 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.540855 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      25.2037 cm-1
2.      74.5393 cm-1
```

```
   3.      99.3713 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.870922       -0.139991        0.008501
C           0.436850       -0.656982       -0.582502
C           1.365154        0.550058       -0.777731
C           0.541575        1.709146       -0.602926
C          -0.750736        1.417093       -0.086592
H           1.989563        0.485497       -1.706290
H           0.829322        2.710764       -0.907445
Cl         -0.922270       -0.639082        1.701163
Cl         -2.250645       -0.740032       -0.869695
O           0.738338       -1.811250       -0.860123
O          -1.674442        2.166117        0.236298
C           3.498715       -0.493775        0.173591
H           4.172954       -0.554121        1.067773
H           4.106632       -0.224289       -0.729862
H           3.015870       -1.494707       -0.001256
N           2.452388        0.511171        0.377969
H           1.967070        0.342277        1.262278
H           2.856461        1.449089        0.430620
```

---

### Compound_16_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.269353 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.183406 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
   1.      44.0431 cm-1
   2.      53.8061 cm-1
   3.      58.0734 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.157028       -0.139600        0.008263
C           0.017829       -1.124671       -0.412876
C          -1.181455       -0.641571        0.178600
```

```
C          -1.033077        0.593303        0.908200
C           0.460614        0.939138        0.827813
H          -1.405055        0.590606        1.972573
Cl          1.892486        0.602017       -1.406872
Cl          2.354285       -0.955292        0.986443
O           0.236175       -2.109332       -1.118416
O           0.948775        1.939417        1.339823
Cl         -2.643570       -1.471446        0.160202
C          -1.600978        1.951308       -1.155228
H          -1.741986        0.974164       -1.696883
H          -2.296988        2.723657       -1.573653
H          -0.536728        2.284978       -1.286107
N          -1.874634        1.747922        0.275568
H          -1.692405        2.611322        0.788698
H          -2.858185        1.491961        0.390353
```

---

### Compound_16_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.264971 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.178919 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      27.7455 cm-1
2.      51.6358 cm-1
3.      75.9986 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.284129       -0.027776       -0.002823
C          -0.330538        1.176872        0.280892
C           0.977467        0.765689       -0.103014
C           1.068049       -0.604951       -0.541776
C          -0.378432       -1.125971       -0.543112
H           1.588798       -0.796501       -1.518947
Cl         -2.493564        0.399368       -1.189124
Cl         -2.026852       -0.592284        1.488541
O          -0.742841        2.241015        0.740772
O          -0.685933       -2.255854       -0.902846
Cl          2.293687        1.808621       -0.184633
C           3.308843       -1.560115        0.132325
H           3.872533       -2.103225        0.935906
```

```
H          3.412682       -2.117182       -0.835772
H          3.732781       -0.525723        0.009362
N          1.888808       -1.454292        0.492911
H          1.485577       -2.389689        0.570499
H          1.802992       -0.978397        1.398872
```

---

### Compound_16_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.266709 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.180885 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      24.5707 cm-1
2.      54.1258 cm-1
3.      80.5518 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C         -1.198249        0.021261       -0.006298
C         -0.341110       -1.257876        0.261884
C          0.994209       -0.941116       -0.115221
C          1.186505        0.423439       -0.541040
C         -0.221919        1.033201       -0.593526
H          1.763968        0.586426       -1.491272
Cl        -1.812063        0.671001        1.512089
Cl        -2.496769       -0.308718       -1.123829
O         -0.834764       -2.292515        0.708415
O         -0.464390        2.150685       -1.032406
Cl         2.244825       -2.062306       -0.178932
C          2.475802        2.515336        0.107721
H          2.992643        3.045863        0.950004
H          3.182209        2.418470       -0.758622
H          1.579571        3.111170       -0.220261
N          2.037290        1.181993        0.534379
H          2.845935        0.586903        0.738988
H          1.484567        1.246777        1.392752
```

---

### Compound_17_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2333.322665 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2333.230884 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      32.2988 cm-1
2.      55.4230 cm-1
3.      87.0876 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           2.310485        0.814113       -0.124755
C           1.234579       -0.313570        0.008813
C          -0.042677        0.433435       -0.035300
C           0.236704        1.855955       -0.107128
N           1.637294        2.042173       -0.168416
H           2.077648        2.920914       -0.269259
O          -0.578022        2.806518       -0.061752
O           3.532924        0.676349       -0.171441
C          -1.366339       -0.095965       -0.145398
Cl         -1.505936       -1.815570        0.248673
Cl         -2.094214        0.115276       -1.796896
C          -2.019082        0.535242        2.206372
H          -0.907403        0.645075        2.353534
H          -2.334280       -0.485950        2.546590
H          -2.559985        1.319073        2.798969
N          -2.330250        0.710504        0.778259
H          -2.198622        1.708790        0.518036
H          -3.296584        0.440487        0.588760
Cl          1.480066       -1.126320        1.566218
Cl          1.432360       -1.470758       -1.297736
```

---

### Compound_17_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2333.318493 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2333.226862 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      32.7136 cm-1
2.      55.2007 cm-1
3.      83.2275 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           2.410020        0.835289       -0.031749
C           1.336568       -0.300226        0.041308
C           0.058763        0.447124        0.073857
C           0.337736        1.870780        0.101115
N           1.736191        2.062735        0.024282
H           2.175120        2.947213       -0.010968
O          -0.475482        2.814932        0.235600
O           3.631343        0.703277       -0.111746
C          -1.269427       -0.078329       -0.051288
Cl         -1.381906       -1.814229        0.278048
Cl         -2.008319        0.207844       -1.673834
C          -3.569046        0.247764        1.056017
H          -4.117353        0.916766        1.771994
H          -3.614678       -0.810888        1.426705
H          -4.058285        0.304314        0.046344
N          -2.173356        0.690535        0.960009
H          -2.132861        1.689617        0.673286
H          -1.708413        0.608841        1.870454
Cl          1.615674       -1.225998        1.526038
Cl          1.506436       -1.356372       -1.353443
```

---

### Compound_18_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.464064 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.373769 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      36.8070 cm-1
2.      72.0130 cm-1
3.     129.4190 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.132564        1.733940        0.271897
O           0.683052        2.505851       -0.255179
C          -0.030637        0.320038        0.416225
C          -1.094731       -0.415703        1.012983
H          -0.782297       -1.346379        1.559612
H          -1.781665        0.202061        1.651543
C          -2.999491        0.004940       -0.608784
H          -3.735511        0.248033        0.201300
H          -3.548637       -0.373756       -1.509937
H          -2.433120        0.938765       -0.880348
N          -2.043804       -0.994741       -0.121322
H          -2.544989       -1.816285        0.208695
H          -1.432666       -1.273091       -0.894956
Br          1.477969       -0.619468       -0.134087
H          -1.083277        2.159113        0.693892
```

---

### Compound_18_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.476823 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.385738 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      78.9527 cm-1
  2.      92.3604 cm-1
  3.     167.3133 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.015848        1.757273        0.009135
O           1.160512        2.283495       -0.037180
C          -0.173291        0.371080        0.209598
C           0.947142       -0.418834        0.675822
H           0.705388       -1.496970        0.872364
H           1.449669        0.033478        1.578740
C           3.215283       -1.212142       -0.076148
H           2.901154       -2.284525        0.023391
H           3.655596       -0.868919        0.897462
```

```
H           3.991016       -1.125797       -0.881945
N           2.050426       -0.386186       -0.400072
H           2.318944        0.611450       -0.489741
H           1.637508       -0.674286       -1.289149
Br         -1.812595       -0.432453       -0.068174
H          -0.885414        2.392496       -0.137528
```

---

### Compound_18_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.478214 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.386671 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      62.8237 cm-1
2.      92.0228 cm-1
3.     165.8987 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.365405        1.713125       -0.265482
O           1.562332        2.109193       -0.269775
C          -0.013954        0.455186        0.254408
C           0.934539       -0.269447        1.072846
H           0.535380       -1.223728        1.507954
H           1.367739        0.379578        1.889566
C           1.910874       -1.683199       -0.749806
H           2.800973       -1.825121       -1.416277
H           1.021923       -1.371244       -1.365156
H           1.671784       -2.646230       -0.227948
N           2.183396       -0.638182        0.244400
H           2.461724        0.237569       -0.236068
H           2.941087       -0.930147        0.857860
Br         -1.695359       -0.247955       -0.049357
H          -0.426647        2.357501       -0.706845
```

---

### Compound_18_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.462623 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.372833 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      47.5008 cm-1
2.      69.8275 cm-1
3.     116.1064 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.549521        1.836530        0.107346
O           1.636850        2.243501       -0.329177
C           0.135758        0.485973        0.297824
C          -1.178801        0.207245        0.773868
H          -1.292297       -0.739287        1.366253
H          -1.666353        1.065068        1.311617
C          -3.519701       -0.259495       -0.135312
H          -3.919449        0.634088        0.412889
H          -3.598091       -1.158252        0.531818
H          -4.136008       -0.430951       -1.056916
N          -2.115527       -0.030944       -0.477917
H          -1.742018       -0.831645       -0.992331
H          -2.022307        0.784379       -1.088312
Br          1.268689       -0.950427       -0.033180
H          -0.234363        2.588630        0.392769
```

---

### Compound_18_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.468348 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.377207 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      28.2034 cm-1
2.     116.0181 cm-1
```

```
  3.     170.7243 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.309432        1.620378       -0.041517
O           1.514666        1.969705       -0.004840
C          -0.115905        0.295466        0.231651
C           0.835789       -0.635041        0.781618
H           0.385223       -1.572130        1.202774
H           1.512006       -0.150785        1.541412
C           3.177621       -0.638711       -0.166237
H           3.598216       -1.078550        0.774602
H           3.162495        0.488175       -0.077906
H           3.813993       -0.942027       -1.037615
N           1.796637       -1.103788       -0.356664
H           1.427312       -0.696640       -1.225960
H           1.782679       -2.117607       -0.444457
Br         -1.861303       -0.233648       -0.077464
H          -0.471728        2.363561       -0.319349
```

---

### Compound_18_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.460501 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.37034 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      36.2005 cm-1
  2.      66.0153 cm-1
  3.     126.9551 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.982524        1.751392        0.011672
O           2.095860        1.804396       -0.532416
C           0.217613        0.588811        0.322825
C          -1.073191        0.727568        0.911340
H          -1.402097       -0.121747        1.565740
H          -1.226385        1.708211        1.439715
```

```
C          -2.837577       -0.515034       -0.447529
H          -3.412580       -0.789636        0.475226
H          -2.061141       -1.304962       -0.642186
H          -3.541190       -0.462916       -1.319456
N          -2.164914        0.771940       -0.244033
H          -1.659283        1.026168       -1.100897
H          -2.861634        1.489666       -0.055616
Br          0.866803       -1.126024        0.014594
H           0.477515        2.710884        0.304382
```

---

### Compound_19_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.231151 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.100758 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      77.4649 cm-1
  2.      96.8769 cm-1
  3.     148.8589 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.111023        0.126636        0.072849
O          -2.041509       -1.083180       -0.289711
C          -0.998992        0.967182        0.230161
C           0.291141        0.583398       -0.299708
H           0.244410        0.257889       -1.382694
H          -1.099193        1.933300        0.724582
H          -3.109069        0.557373        0.316148
C           1.357134        1.646644       -0.118202
H           2.327533        1.341867       -0.578397
H           1.002916        2.578722       -0.623862
H           1.522412        1.876986        0.961481
N           0.698102       -0.762743        0.396546
H           0.703904       -0.607328        1.403938
H          -0.084470       -1.409414        0.180031
C           1.968249       -1.336234       -0.045584
H           1.962955       -1.432385       -1.163565
H           2.815431       -0.667098        0.258374
H           2.119473       -2.351030        0.408737
```

### Compound_19_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.222539 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.091977 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      59.7419 cm-1
2.     114.9504 cm-1
3.     176.6374 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.795441       -0.779897        0.103531
O           2.107750        0.356509       -0.339238
C           0.472791       -1.236520        0.266866
C          -0.621682       -0.475543       -0.270197
H          -0.402572       -0.056557       -1.295693
H           0.273289       -2.177499        0.779789
H           2.605002       -1.479039        0.418693
C          -1.950724       -1.203501       -0.264723
H          -2.778517       -0.558725       -0.646768
H          -1.857270       -2.093329       -0.935208
H          -2.214263       -1.565276        0.758124
N          -0.743539        0.856389        0.605697
H          -0.046014        0.751846        1.352454
H          -1.665842        0.927037        1.027578
C          -0.444659        2.073425       -0.155549
H          -0.502268        2.975572        0.507317
H           0.600399        1.977864       -0.574973
H          -1.176169        2.183528       -0.996859
```

### Compound_20_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.541501 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.38552 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      49.6750 cm-1
  2.      54.6591 cm-1
  3.      93.5777 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.375486       -1.320311       -0.048636
O          -2.545451       -1.317336       -0.473162
C          -0.636033       -0.188642        0.402261
H          -0.818191       -2.293318       -0.008158
C           0.707996       -0.349885        0.833974
H           1.082587        0.454141        1.519184
H           0.972821       -1.368109        1.223449
C           3.085018       -0.347986       -0.151716
H           3.277143       -1.354701        0.304466
H           3.390447        0.444174        0.581532
H           3.703205       -0.243779       -1.081951
N           1.658871       -0.212694       -0.442985
H           1.363778       -0.920790       -1.117779
H           1.464438        0.698812       -0.865645
C          -1.280470        1.139588        0.464648
H          -2.355632        1.033025        0.150149
H          -1.282241        1.514695        1.525554
C          -0.618025        2.182131       -0.407785
H           0.410011        2.419738       -0.037993
H          -0.542913        1.826193       -1.463420
H          -1.211946        3.128098       -0.399675
```

---

### Compound_20_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.540338 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.385053 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      45.3213 cm-1
2.      54.2096 cm-1
3.      84.3719 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.052181        1.445496       -0.288351
O          -2.126873        1.861401        0.181457
C          -0.504977        0.140103       -0.119483
H          -0.425407        2.143221       -0.903879
C           0.768981       -0.170037       -0.662627
H           0.951702       -1.259018       -0.854886
H           1.088780        0.454605       -1.537334
C           3.251751       -0.077759        0.022583
H           3.360409       -1.165760       -0.228252
H           3.983014        0.186298        0.831258
H           3.483967        0.527992       -0.892659
N           1.876382        0.186693        0.440489
H           1.758933        1.172621        0.680500
H           1.650426       -0.350834        1.278646
C          -1.258750       -0.889500        0.627768
H          -0.606067       -1.342170        1.425848
H          -2.125451       -0.397815        1.149846
C          -1.783938       -1.999548       -0.253030
H          -2.468390       -1.585011       -1.031333
H          -0.947696       -2.529186       -0.770223
H          -2.349233       -2.745541        0.356223
```

---

### Compound_20_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.54033 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.385039 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      45.3846 cm-1
2.      54.4126 cm-1
3.      84.4285 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.052520       -1.445491        0.288346
O          -2.127334       -1.861337       -0.181258
C          -0.505228       -0.140179        0.119375
H          -0.425683       -2.143256        0.903776
C           0.768803        0.169955        0.662446
H           0.951485        1.258989        0.854522
H           1.088544       -0.454513        1.537300
C           3.251562        0.077191       -0.022521
H           3.483611       -0.528668        0.892701
H           3.360404        1.165162        0.228398
H           3.982826       -0.186949       -0.831176
N           1.876164       -0.186977       -0.440527
H           1.758519       -1.172855       -0.680654
H           1.650394        0.350685       -1.278652
C          -1.258811        0.889614       -0.627785
H          -0.606347        1.341550       -1.426478
H          -2.126228        0.398389       -1.149105
C          -1.782504        2.000325        0.253066
H          -2.467914        1.586713        1.031031
H          -0.945545        2.528395        0.770725
H          -2.346354        2.747412       -0.356191
```

---

### Compound_20_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.537868 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.382516 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      26.2289 cm-1
2.      50.5816 cm-1
3.      81.3288 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.337944       -1.318433        0.189399
O          -2.393090       -1.452347       -0.456302
C          -0.487605       -0.172861        0.188331
H          -0.991173       -2.163421        0.840189
C           0.725186       -0.188575        0.922933
H           1.112160        0.819062        1.220888
```

```
H           0.753814       -0.904779        1.785201
C           2.849127        0.246677       -0.472659
H           3.382080        0.672960        0.417103
H           2.287262        1.071157       -0.989058
H           3.605083       -0.183490       -1.181098
N           1.895140       -0.771733       -0.032073
H           2.397939       -1.525376        0.430115
H           1.412391       -1.161368       -0.849326
C          -0.866250        1.029079       -0.585565
H          -0.010715        1.343688       -1.247376
H          -1.729049        0.771643       -1.259793
C          -1.258378        2.199584        0.286117
H          -1.536619        3.078488       -0.344252
H          -2.133004        1.930239        0.925331
H          -0.416249        2.499286        0.955673
```

---

### Compound_20_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.537863 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.382511 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      26.0532 cm-1
2.      50.6221 cm-1
3.      81.3558 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.338397       -1.318178        0.189422
O          -2.393546       -1.451802       -0.456343
C          -0.487760       -0.172851        0.188456
H          -0.991901       -2.163278        0.840217
C           0.725061       -0.189009        0.922967
H           1.112327        0.818458        1.221140
H           0.753615       -0.905434        1.785062
C           2.848886        0.246225       -0.472663
H           3.381946        0.672245        0.417167
H           2.287073        1.070891       -0.988837
H           3.604740       -0.183886       -1.181255
N           1.894808       -0.772159       -0.032233
H           2.397505       -1.526003        0.429733
```

```
H           1.412001       -1.161581       -0.849530
C          -0.865992        1.029191       -0.585470
H          -0.010516        1.343155       -1.247687
H          -1.729205        0.772148       -1.259335
C          -1.257079        2.200103        0.286122
H          -2.131722        1.931462        0.925617
H          -0.414568        2.499365        0.955404
H          -1.534891        3.079096       -0.344325
```

---

### Compound_20_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.557396 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.400699 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      45.5780 cm-1
  2.      76.4798 cm-1
  3.      90.5659 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.704631        1.660166       -0.068105
O           0.363416        2.274207       -0.348001
C          -0.736821        0.327812        0.391319
H          -1.680376        2.176388       -0.213533
C           0.499875       -0.277497        0.835928
H           0.374551       -1.324542        1.219209
H           1.060940        0.348095        1.586282
C           2.749202       -0.997378       -0.061654
H           3.257997       -0.455161        0.778863
H           3.417831       -0.988894       -0.962292
H           2.561600       -2.058276        0.250482
N           1.476228       -0.340934       -0.361288
H           0.998086       -0.809155       -1.133362
H           1.627251        0.646329       -0.640765
C          -1.986577       -0.448505        0.449156
H          -2.075096       -0.967952        1.443430
H          -2.865973        0.246865        0.368395
C          -2.085832       -1.488663       -0.645760
H          -3.021017       -2.088368       -0.535026
```

```
H          -2.094349       -1.002313       -1.650417
H          -1.213664       -2.185752       -0.603546
```

---

### Compound_20_HEI_Conformation_7_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.5564 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.399653 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      50.9760 cm-1
  2.      88.0105 cm-1
  3.      95.0029 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.549683        1.640630       -0.011068
O           0.535213        2.232777        0.254117
C          -0.674578        0.239437       -0.085479
H          -1.456611        2.248081       -0.230810
C           0.398761       -0.581892        0.434523
H           0.203624       -1.683052        0.339371
H           0.683779       -0.329779        1.495214
C           2.835476       -1.097338        0.029503
H           2.601154       -2.177101       -0.163802
H           3.044784       -0.960453        1.123481
H           3.745003       -0.804408       -0.558096
N           1.690606       -0.269587       -0.352118
H           1.488674       -0.366534       -1.348349
H           1.883266        0.734444       -0.171172
C          -1.871229       -0.406193       -0.651949
H          -2.508124        0.364685       -1.165595
H          -1.567487       -1.151685       -1.439456
C          -2.712844       -1.118370        0.383308
H          -3.600720       -1.597463       -0.095411
H          -2.117339       -1.911449        0.896614
H          -3.071367       -0.398037        1.156874
```

---

### Compound_21_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2277.90089 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2277.826203 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      29.5689 cm-1
2.      52.2005 cm-1
3.      63.5376 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.399875        0.053139       -0.058257
C          -0.432301       -1.122373       -0.011948
C           0.999414       -0.550563       -0.097434
C           0.856765        0.879385       -0.011827
C          -0.497071        1.325823       -0.001773
Cl         -2.461685       -0.016571        1.339691
Cl         -2.311428        0.003367       -1.548415
O          -0.680974       -2.312807        0.118822
O          -0.968856        2.459938        0.053154
C           1.346929       -0.745976        2.382778
H           1.227511        0.372650        2.436551
H           2.055171       -1.094555        3.178976
H           0.342866       -1.227997        2.526369
N           1.878320       -1.111401        1.059107
H           2.815882       -0.711965        0.946731
H           1.935609       -2.129087        0.970864
Cl          2.181537        1.908322       -0.089392
Cl          1.793351       -1.168229       -1.587667
```

---

### Compound_22_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.709846 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.447607 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
1.      19.9008 cm-1
2.      28.4785 cm-1
3.      41.9880 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C          -0.185033        0.398538       -0.013975
N          -1.246608       -0.512955        0.038068
O          -0.397344        1.632255       -0.153421
C           1.138904       -0.157132        0.136993
C          -2.615935       -0.246475       -0.013333
C           2.308160        0.567803       -0.335032
S           1.402379       -1.568131        0.990450
C          -3.518056       -1.320795        0.208179
C          -3.156593        1.029990       -0.290599
C           2.119073        1.577769       -1.464548
O           3.408510       -0.279463       -0.728084
C           2.457024       -2.464891       -0.113356
C          -4.890463       -1.114557        0.152176
C          -4.534781        1.211887       -0.339019
C           3.028120       -1.574910       -1.191139
C          -5.409607        0.149816       -0.120237
H          -0.993400       -1.465724        0.204142
H          -3.136501       -2.329527        0.426568
H          -2.490360        1.889469       -0.468955
H           1.733746        1.012719       -2.348612
H           1.370579        2.360535       -1.192993
H           3.091641        2.051460       -1.738512
H           1.905631       -3.309897       -0.591033
H           3.271009       -2.900488        0.515873
H          -5.571129       -1.961223        0.326408
H          -4.934678        2.214043       -0.555643
H           3.996198       -1.988472       -1.587940
H           2.291512       -1.455887       -2.031175
H          -6.495819        0.306084       -0.162040
N           2.956104        1.287740        0.929631
H           3.953352        1.417630        0.771733
H           2.823901        0.623934        1.700937
C           2.307066        2.562500        1.248924
H           2.590027        2.886480        2.284198
H           2.626450        3.343766        0.510671
H           1.186701        2.432105        1.177116
```

---

## Compound_22_HEI_Conformation_2_am1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.709853 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.447613 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      19.9300 cm-1
  2.      28.4859 cm-1
  3.      42.0080 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C          -0.185069        0.398404       -0.014481
N          -1.246583       -0.513211        0.036776
O          -0.397460        1.632139       -0.153615
C           1.138864       -0.157194        0.136751
C          -2.615931       -0.246631       -0.013886
C           2.308219        0.567999       -0.334621
S           1.402268       -1.568491        0.989793
C          -3.518041       -1.320606        0.209288
C          -3.156591        1.029591       -0.292255
C           2.119476        1.578368       -1.463811
O           3.408825       -0.278995       -0.727519
C           2.457241       -2.464795       -0.114062
C          -4.890458       -1.114274        0.153813
C          -4.534785        1.211603       -0.340077
C           3.028767       -1.574315       -1.191222
C          -5.409607        0.149867       -0.119660
H          -0.993385       -1.465950        0.203071
H          -3.136473       -2.329143        0.428545
H          -2.490343        1.888785       -0.471914
H           1.734478        1.013643       -2.348221
H           1.370809        2.360956       -1.192195
H           3.092107        2.052225       -1.737254
H           1.906004       -3.309562       -0.592335
H           3.270989       -2.900708        0.515258
H          -5.571123       -1.960675        0.329329
H          -4.934690        2.213569       -0.557560
H           3.997057       -1.987627       -1.587750
H           2.292514       -1.455002       -2.031531
H          -6.495825        0.306214       -0.161021
N           2.955619        1.287569        0.930569
H           3.952910        1.417572        0.773066
H           2.823179        0.623499        1.701608
C           2.306337        2.562177        1.249990
H           2.588752        2.885824        2.285515
```

```
H           2.626018        3.343730        0.512175
H           1.186023        2.431684        1.177574
```

---

### Compound_22_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.707796 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.445908 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      20.2053 cm-1
  2.      30.9469 cm-1
  3.      49.4231 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.264829       -0.323852       -0.068846
N          -1.360137        0.537837       -0.005104
O          -0.405630       -1.581314       -0.086740
C           1.042160        0.281891       -0.161680
C          -2.717541        0.210555        0.021896
C           2.180875       -0.529356        0.257119
S           1.287568        1.759483       -0.879002
C          -3.664483        1.268152       -0.006244
C          -3.201057       -1.116006        0.086748
C           2.010982       -1.268432        1.588354
O           3.429530        0.183521        0.292066
C           2.509623        2.481659        0.172558
C          -5.026418        0.997527        0.029337
C          -4.569902       -1.361538        0.119661
C           3.347317        1.466462        0.915894
C          -5.489737       -0.315490        0.091895
H          -1.143411        1.513485       -0.027243
H          -3.326985        2.314305       -0.056857
H          -2.497232       -1.963652        0.110782
H           1.768541       -0.506674        2.368500
H           1.166508       -1.997502        1.533998
H           2.953747       -1.789126        1.878791
H           2.039642        3.173025        0.913534
H           3.151434        3.098049       -0.505028
H          -5.743333        1.831851        0.006878
H          -4.925800       -2.401728        0.169408
```

```
H           4.426193        1.784629        0.951565
H           2.961144        1.332081        1.962632
H          -6.568037       -0.522139        0.119069
N           2.394089       -1.593050       -0.891406
H           2.483157       -1.057338       -1.756606
H           1.507430       -2.118732       -0.916067
C           3.542538       -2.482509       -0.720551
H           3.690958       -3.106118       -1.641038
H           4.460962       -1.864635       -0.530809
H           3.367971       -3.157068        0.158636
```

---

### Compound_22_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.709859 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.447616 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      19.9283 cm-1
  2.      28.4912 cm-1
  3.      42.0297 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.185070       -0.398484       -0.014471
N          -1.246560        0.513166        0.036807
O          -0.397497       -1.632229       -0.153453
C           1.138855        0.157149        0.136605
C          -2.615924        0.246619       -0.013881
C           2.308258       -0.568011       -0.334715
S           1.402312        1.568344        0.989802
C          -3.156589       -1.029559       -0.292433
C          -3.518022        1.320568        0.209449
C           2.119558       -1.578623       -1.463679
O           3.408743        0.279042       -0.727781
C           2.457144        2.464746       -0.114111
C          -4.534785       -1.211564       -0.340255
C          -4.890441        1.114249        0.153967
C           3.028487        1.574326       -1.191414
C          -5.409598       -0.149855       -0.119670
H          -0.993322        1.465931        0.202896
H          -2.490344       -1.888725       -0.472237
```

```
H          -3.136445        2.329074        0.428835
H           1.370607       -2.360939       -1.192061
H           1.735006       -1.014020       -2.348370
H           3.092124       -2.052836       -1.736737
H           3.270980        2.900643        0.515097
H           1.905816        3.309523       -0.592262
H          -4.934697       -2.213496       -0.557875
H          -5.571101        1.960627        0.329609
H           2.292068        1.454973       -2.031566
H           3.996669        1.987714       -1.588132
H          -6.495817       -0.306194       -0.161029
N           2.955758       -1.287264        0.930613
H           2.823420       -0.622977        1.701490
H           3.953031       -1.417378        0.773089
C           2.306412       -2.561776        1.250284
H           2.588860       -2.885273        2.285843
H           1.186087       -2.431245        1.177894
H           2.626010       -3.343441        0.512559
```

---

### Compound_23_HEI_Conformation_10_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.535477 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.298534 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      31.7611 cm-1
2.      59.6185 cm-1
3.      63.9294 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.302166       -0.021102        0.446465
C          -0.936502       -0.247353        0.095009
C           0.062585        0.632206        0.601343
C           1.452954        0.057509        0.853279
C           2.478631        0.152586       -0.257855
C           3.619431       -0.806154       -0.017348
C          -0.621456       -1.396653       -0.781859
C          -0.727012       -2.722835       -0.063202
O          -3.285420       -0.659070        0.027289
H          -2.476277        0.817977        1.171904
```

```
H          -0.271917        1.192439        1.522905
H           1.298459       -1.028309        1.108950
H           1.880199        0.554306        1.765811
H           2.896166        1.193963       -0.314783
H           2.011175       -0.077308       -1.251214
H           4.091522       -0.615291        0.976539
H           3.254985       -1.861960       -0.036531
H           4.398158       -0.686882       -0.808692
H          -1.347118       -1.405019       -1.642570
H           0.408210       -1.295007       -1.217495
H          -0.521870       -3.565052       -0.766960
H           0.002134       -2.780829        0.779984
H          -1.757615       -2.843362        0.351670
N           0.195995        1.878687       -0.455438
H           1.115897        2.306426       -0.398502
H           0.084222        1.460761       -1.380763
C          -0.832620        2.898803       -0.257529
H          -1.842666        2.404317       -0.272208
H          -0.685280        3.393476        0.737805
H          -0.790049        3.675065       -1.065921
```

---

### Compound_23_HEI_Conformation_14_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.532884 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.295397 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
  1.      28.0999 cm-1
  2.      53.1409 cm-1
  3.      87.7570 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.311185        0.445226       -0.625765
C          -1.046021       -0.192837       -0.442936
C           0.137183        0.561459       -0.695709
C           1.377647       -0.157733       -1.209696
C           2.149156       -1.017891       -0.227585
C           3.512534       -0.459164        0.095287
C          -1.030224       -1.605897       -0.012178
C          -1.049672       -1.771466        1.491818
```

```
O          -3.428580       -0.065762       -0.426946
H          -2.262455        1.507854       -0.984516
H          -0.054351        1.448331       -1.369637
H           2.072643        0.604446       -1.656205
H           1.015505       -0.805168       -2.055532
H           2.283144       -2.041111       -0.674094
H           1.564606       -1.170196        0.718054
H           4.132175       -0.373027       -0.830536
H           3.444634        0.555023        0.557871
H           4.044270       -1.132390        0.811040
H          -1.945507       -2.113322       -0.428827
H          -0.137218       -2.141634       -0.433855
H          -1.948660       -1.265009        1.919239
H          -1.088713       -2.853773        1.764016
H          -0.139131       -1.328825        1.965212
N           0.529524        1.316277        0.703983
H           0.028670        0.796373        1.432230
H           1.528196        1.245171        0.882342
C           0.120744        2.719377        0.736578
H           0.694513        3.298176       -0.033522
H          -0.975732        2.784174        0.498477
H           0.304406        3.170612        1.747033
```

---

### Compound_23_HEI_Conformation_15_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.5346 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.298028 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      43.5875 cm-1
2.      60.0525 cm-1
3.      66.1671 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           2.353588        0.393970       -0.587211
C           1.045315       -0.051134       -0.215659
C          -0.074610        0.522101       -0.869090
C          -1.370164       -0.268436       -0.947115
C          -2.387038       -0.099357        0.160287
C          -3.498388       -1.111943        0.024263
```

```
C           0.933159       -1.088649        0.833633
C           1.259773       -2.471761        0.317357
O           3.426497        0.034733       -0.070238
H           2.381474        1.143806       -1.421901
H           0.176216        0.891149       -1.910553
H          -1.072011       -1.353714       -0.995548
H          -1.874352       -0.020960       -1.921155
H          -2.834853        0.929691        0.128767
H          -1.896056       -0.223734        1.161264
H          -4.260793       -0.958410        0.825552
H          -4.002652       -1.014932       -0.967454
H          -3.096873       -2.150442        0.113480
H           1.652772       -0.842998        1.664189
H          -0.097013       -1.094381        1.279241
H           1.197049       -3.220509        1.143282
H           0.551297       -2.775287       -0.490081
H           2.296288       -2.482686       -0.099666
N          -0.363056        2.023127       -0.212888
H           0.372685        2.621114       -0.585229
H          -1.258292        2.373089       -0.538805
C          -0.303895        2.085746        1.247118
H           0.530451        1.417305        1.603676
H          -0.113544        3.135155        1.594412
H          -1.268813        1.723772        1.687159
```

---

### Compound_23_HEI_Conformation_16_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.549233 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.311034 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      49.3206 cm-1
2.      58.6266 cm-1
3.      82.4632 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.407867        0.503371       -0.508467
C          -1.322982       -0.193653        0.075874
C           0.008085        0.336594       -0.149823
C           1.169630       -0.577976        0.217330
```

```
C           2.369489       -0.388646       -0.688594
C           3.496336       -1.311929       -0.301199
C          -1.585575       -1.403498        0.876858
C          -1.752947       -2.650942        0.037885
O          -2.318391        1.666336       -0.986958
H          -3.394582       -0.013289       -0.512400
H           0.130721        0.711875       -1.211477
H           0.815431       -1.640292        0.107732
H           1.471855       -0.447131        1.289288
H           2.726891        0.673812       -0.649293
H           2.066374       -0.591887       -1.750563
H           3.832906       -1.109616        0.744362
H           3.169827       -2.378360       -0.363052
H           4.366729       -1.169341       -0.986151
H          -0.761436       -1.568194        1.623470
H          -2.527889       -1.255880        1.475609
H          -0.828211       -2.866401       -0.548887
H          -1.973430       -3.532555        0.686992
H          -2.595851       -2.518896       -0.682592
N           0.061024        1.700479        0.648843
H          -0.724082        2.248073        0.257177
H          -0.156633        1.496431        1.623791
C           1.298332        2.472094        0.553032
H           1.546789        2.642668       -0.528055
H           1.182452        3.465621        1.062112
H           2.137095        1.906830        1.038322
```

---

### Compound_23_HEI_Conformation_17_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.553302 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.314967 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      47.2680 cm-1
2.      63.2410 cm-1
3.      74.9372 cm-1
```

### AM1b>

```
C           1.976485        1.082046       -0.755769
C           0.825410        0.703150       -0.020109
```

```
C           0.216158       -0.557811       -0.383615
C          -1.190278       -0.850810        0.125557
C          -2.215131       -0.391340       -0.894864
C          -3.610281       -0.442789       -0.328486
C           0.349558        1.566493        1.075720
C          -0.792784        2.481126        0.696006
O           2.610052        0.298018       -1.512735
H           2.340052        2.126775       -0.626796
H           0.244103       -0.704743       -1.510069
H          -1.365999       -0.327082        1.100968
H          -1.340754       -1.948643        0.310320
H          -2.151974       -1.041478       -1.807272
H          -1.974300        0.656936       -1.218661
H          -3.859943       -1.473621        0.021171
H          -3.707466        0.255821        0.538087
H          -4.353744       -0.144223       -1.106515
H           0.038173        0.941743        1.959036
H           1.204287        2.207274        1.433005
H          -1.725389        1.895682        0.507584
H          -0.997490        3.210444        1.516951
H          -0.543205        3.049441       -0.231592
N           1.209675       -1.717699        0.043029
H           0.905597       -2.606831       -0.344283
H           2.108407       -1.452110       -0.389299
C           1.374061       -1.832417        1.493418
H           0.410896       -2.176092        1.953326
H           2.191167       -2.558277        1.742263
H           1.630243       -0.817167        1.905310
```

---

## Compound_23_HEI_Conformation_18_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.534837 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.298863 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
1.      30.6195 cm-1
2.      44.7536 cm-1
3.      52.5976 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.173994        0.870780        0.592970
C          -1.168754        0.007441        0.057549
C           0.192096        0.249394        0.390293
C           1.132252       -0.943582        0.382328
C           2.550007       -0.614060        0.812390
C           3.564544       -0.910284       -0.263066
C          -1.577338       -1.077404       -0.861495
C          -1.899748       -2.373996       -0.155199
O          -3.391054        0.828463        0.338117
H          -1.798075        1.654670        1.302419
H           0.335649        0.855944        1.327564
H           1.131753       -1.439462       -0.624391
H           0.688605       -1.686383        1.101281
H           2.806109       -1.218509        1.723927
H           2.633438        0.463079        1.117942
H           4.594385       -0.674235        0.099589
H           3.531251       -1.990067       -0.548015
H           3.370265       -0.304534       -1.181258
H          -2.495620       -0.744437       -1.421863
H          -0.773987       -1.265075       -1.625896
H          -2.260789       -3.135913       -0.887652
H          -0.999159       -2.783034        0.362407
H          -2.698265       -2.205332        0.606787
N           0.761146        1.312205       -0.757122
H           0.060652        1.295609       -1.502020
H           1.646606        0.984570       -1.132929
C           0.912315        2.674206       -0.253426
H           1.197799        3.384278       -1.073744
H          -0.062610        3.006048        0.195850
H           1.704119        2.694667        0.540875
```

---

## Compound_23_HEI_Conformation_19_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.554856 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.316708 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
1.      46.7566 cm-1
2.      64.6270 cm-1
3.      76.7441 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           1.812889        0.128872        1.418041
C           0.946903       -0.439514        0.451848
C          -0.217540        0.336177        0.072162
C          -1.305028       -0.392510       -0.708125
C          -2.101418       -1.302348        0.209220
C          -3.189143       -0.567387        0.949739
C           1.262857       -1.752719       -0.136355
C           1.946173       -1.650412       -1.483788
O           1.769673        1.338720        1.768937
H           2.583643       -0.539587        1.865130
H          -0.678048        0.861591        0.963575
H          -0.839778       -0.999581       -1.528729
H          -2.009027        0.338378       -1.188371
H          -1.407239       -1.789422        0.945847
H          -2.561183       -2.118717       -0.408735
H          -2.758000        0.238993        1.591268
H          -3.912652       -0.101662        0.237473
H          -3.750336       -1.274648        1.607470
H           1.939592       -2.318914        0.561960
H           0.333456       -2.375743       -0.250753
H           2.916721       -1.106852       -1.390403
H           2.148538       -2.666941       -1.899051
H           1.305778       -1.095494       -2.212074
N           0.336324        1.569361       -0.748201
H           1.022113        2.002906       -0.107975
H           0.844110        1.205046       -1.553831
C          -0.649154        2.566820       -1.163261
H          -0.137134        3.500665       -1.517527
H          -1.283126        2.163014       -1.995232
H          -1.308318        2.819815       -0.291014
```

---

## Compound_23_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.542566 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.30626 |
| Number of Imaginary Frequencies | 0 |

## Frequencies (Top 3 out of 84)

```
1.      49.7723 cm-1
2.      52.3279 cm-1
3.      57.4917 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.931412       -0.450298       -1.259795
C          -0.900010       -0.424154       -0.271477
C           0.148743        0.532065       -0.404491
C           1.513111        0.180367        0.169812
C           2.185307       -0.857155       -0.708917
C           3.529473       -1.252272       -0.154813
C          -0.957788       -1.382669        0.852024
C          -1.250629       -0.735309        2.187866
O          -2.925177       -1.199612       -1.266273
H          -1.805208        0.284388       -2.097896
H           0.263284        0.939523       -1.448922
H           1.406600       -0.222526        1.211314
H           2.168700        1.090444        0.224224
H           2.308984       -0.447401       -1.746022
H           1.520297       -1.759107       -0.784912
H           4.009877       -2.012458       -0.817155
H           4.207122       -0.367186       -0.084871
H           3.421679       -1.692790        0.865929
H          -1.766349       -2.136109        0.636249
H           0.008356       -1.953347        0.931032
H          -0.389914       -0.111251        2.533438
H          -2.153143       -0.081857        2.118318
H          -1.440698       -1.516424        2.963241
N          -0.385666        1.870131        0.385573
H          -1.403805        1.854013        0.278321
H          -0.182360        1.747730        1.375980
C           0.162302        3.137540       -0.087889
H          -0.106681        3.277863       -1.168171
H          -0.240299        4.003195        0.501739
H           1.280048        3.120572        0.005423
```

---

### Compound_23_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.538913 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.302326 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
  1.      43.2319 cm-1
  2.      56.1780 cm-1
  3.      73.4134 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.197701        0.478924       -1.103200
C          -1.176981       -0.231741       -0.402621
C           0.146321        0.301351       -0.386875
C           1.280703       -0.704375       -0.278980
C           2.653646       -0.078152       -0.400234
C           3.724446       -1.132276       -0.525201
C          -1.513551       -1.500357        0.275759
C          -1.523669       -1.391600        1.784834
O          -3.395966        0.153032       -1.187920
H          -1.856331        1.416267       -1.616409
H           0.350272        1.033113       -1.218714
H           1.131147       -1.437453       -1.119241
H           1.209348       -1.289667        0.675698
H           2.870220        0.560046        0.497464
H           2.684218        0.595056       -1.298068
H           4.731955       -0.655773       -0.594458
H           3.714168       -1.811616        0.361241
H           3.562565       -1.750498       -1.441352
H          -2.534749       -1.829243       -0.065403
H          -0.790763       -2.308625       -0.023663
H          -0.503850       -1.159192        2.179215
H          -2.219999       -0.583322        2.114146
H          -1.859871       -2.353656        2.241520
N           0.216442        1.284294        0.927989
H          -0.746594        1.320555        1.280831
H           0.795187        0.849050        1.642666
C           0.707825        2.631769        0.650995
H           1.741850        2.568721        0.219194
H           0.032045        3.125131       -0.097191
H           0.735577        3.255523        1.583097
```

---

### Compound_23_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.540005 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.30383 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
1.      42.4874 cm-1
2.      57.7121 cm-1
3.      67.3826 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.724374        0.704562        1.196931
C          -0.985941        0.220886        0.071363
C           0.424640        0.398699        0.053208
C           1.274896       -0.615645       -0.696033
C           1.490581       -1.853441        0.156323
C           2.609486       -1.686241        1.151639
C          -1.728767       -0.382877       -1.057162
C          -1.888148       -1.881343       -0.945744
O          -2.962596        0.698281        1.318582
H          -1.102223        1.124799        2.029886
H           0.872905        0.610274        1.064560
H           2.275392       -0.184619       -0.968583
H           0.761884       -0.909588       -1.649650
H           1.725699       -2.716046       -0.522512
H           0.536372       -2.103421        0.694341
H           3.574275       -1.465000        0.633946
H           2.391452       -0.850766        1.860079
H           2.737125       -2.623409        1.746054
H          -2.755502        0.078472       -1.095026
H          -1.222761       -0.138638       -2.031794
H          -2.380714       -2.142892        0.021490
H          -2.518095       -2.268216       -1.782878
H          -0.895832       -2.392882       -0.984983
N           0.659611        1.866885       -0.685198
H           0.665358        1.712617       -1.689845
H          -0.174630        2.414035       -0.460009
C           1.866351        2.580932       -0.282484
H           2.766038        1.946265       -0.497453
H           1.968882        3.556094       -0.828219
H           1.825515        2.785278        0.820088
```

---

### Compound_23_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.541017 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.305159 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
  1.      35.9175 cm-1
  2.      49.9961 cm-1
  3.      52.7218 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           2.224852        0.423562       -1.020003
C           1.142616       -0.019498       -0.198341
C          -0.180888        0.349906       -0.558268
C          -1.314786       -0.518946       -0.051257
C          -2.670197       -0.111530       -0.590518
C          -3.709934       -1.165367       -0.304134
C           1.450800       -0.829212        1.000872
C           1.618816       -2.298765        0.687890
O           3.436295        0.241549       -0.802545
H           1.921418        0.994044       -1.937670
H          -0.309339        0.551950       -1.662349
H          -1.341779       -0.536242        1.069727
H          -1.080444       -1.567920       -0.384753
H          -2.603875        0.056258       -1.698305
H          -2.995059        0.857757       -0.126570
H          -4.708011       -0.839176       -0.684105
H          -3.440702       -2.128863       -0.801052
H          -3.792000       -1.349576        0.794358
H           2.409934       -0.451826        1.453812
H           0.648010       -0.710465        1.778975
H           1.882924       -2.866263        1.612602
H           0.677842       -2.727078        0.266728
H           2.435353       -2.435603       -0.061714
N          -0.418411        1.900519       -0.025313
H           0.409163        2.411367       -0.335780
H          -1.240451        2.304209       -0.464184
C          -0.525441        2.018009        1.427263
H           0.324920        1.449284        1.895182
H          -0.478823        3.090849        1.751421
H          -1.495585        1.572320        1.770204
```

---

### Compound_23_HEI_Conformation_6_am1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.540048 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.302859 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
1.      56.3133 cm-1
2.      61.5244 cm-1
3.      65.6233 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.700323       -0.168002       -1.333695
C          -0.804099       -0.210537       -0.220391
C           0.467131        0.420098       -0.348233
C           1.641753       -0.131866        0.447325
C           2.336543       -1.250413       -0.308208
C           1.564261       -2.543367       -0.277361
C          -1.238948       -0.887452        1.019965
C          -1.409364        0.048109        2.196565
O          -2.853528       -0.634813       -1.366827
H          -1.297120        0.337345       -2.250097
H           0.776761        0.604668       -1.416076
H           1.290329       -0.509171        1.443061
H           2.401676        0.673156        0.642611
H           3.348110       -1.410577        0.152716
H           2.505105       -0.938561       -1.373124
H           1.494183       -2.935493        0.766222
H           0.524949       -2.384302       -0.661002
H           2.070599       -3.310898       -0.910632
H          -2.224628       -1.394883        0.821805
H          -0.508842       -1.695780        1.303300
H          -2.050434        0.918824        1.918153
H          -1.894523       -0.486735        3.048725
H          -0.422830        0.435713        2.551913
N           0.216537        1.973567        0.157295
H          -0.760042        2.173099       -0.075496
H           0.296267        1.986091        1.172081
C           1.101072        2.974340       -0.430184
H           0.967492        2.979294       -1.544299
H           0.879837        4.000634       -0.033937
H           2.167425        2.715651       -0.197077
```

## Compound_23_HEI_Conformation_8_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.53808 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.30049 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 84)

```
1.      36.3935 cm-1
2.      57.2390 cm-1
3.      61.8495 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -2.240983       -0.212378       -0.826820
C          -0.874846       -0.378824       -0.444878
C           0.030328        0.702244       -0.659918
C           1.483902        0.380258       -0.985351
C           2.391773        0.037546        0.177696
C           3.606021       -0.725692       -0.290501
C          -0.462834       -1.675509        0.131397
C          -0.567439       -1.726006        1.640064
O          -3.153805       -1.045598       -0.677491
H          -2.486200        0.770811       -1.310202
H          -0.349705        1.437057       -1.429695
H           1.931530        1.247266       -1.541908
H           1.453814       -0.489948       -1.698079
H           1.836015       -0.578740        0.933814
H           2.733592        0.975121        0.692955
H           3.304484       -1.708784       -0.727473
H           4.159174       -0.148635       -1.070271
H           4.296706       -0.917121        0.565745
H          -1.133921       -2.477185       -0.288444
H           0.586969       -1.933661       -0.176272
H          -1.606414       -1.471182        1.960338
H          -0.323100       -2.750396        2.011959
H           0.136698       -1.007386        2.126945
N           0.007979        1.631591        0.683744
H          -0.163434        0.980446        1.455108
H           0.906959        2.082725        0.829083
C          -1.051370        2.639199        0.655118
H          -0.837031        3.389423       -0.150055
H          -2.028414        2.130468        0.428505
H          -1.130450        3.168337        1.640827
```

## Compound_24_HEI_Conformation_10_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.820995 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.581392 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      23.2089 cm-1
2.      34.2254 cm-1
3.      42.0496 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.138906        0.199974       -0.619403
C          -1.142922        1.055167       -0.101689
C          -0.844352        2.311727        0.591944
C          -2.510505        0.651913       -0.313466
O          -0.291897       -0.993434       -0.990802
O           1.135313        0.720914       -0.689038
C           2.192010       -0.132950       -1.125747
C           3.027721       -0.628013        0.053536
C           3.550781        0.533997        0.868888
C           2.231917       -1.580991        0.917142
H          -1.328000        2.338667        1.603066
H           0.259052        2.434549        0.728447
H          -1.221926        3.196157        0.016996
H          -2.750931        0.369985       -1.376774
H          -3.253483        1.398248        0.072169
H           1.797794       -1.000759       -1.715490
H           2.815399        0.531626       -1.784100
H           3.904187       -1.186697       -0.382891
H           4.215047        1.177912        0.243942
H           2.699154        1.158518        1.234672
H           4.132400        0.165638        1.747362
H           2.846225       -1.938193        1.777404
H           1.320803       -1.066587        1.309705
H           1.899238       -2.461420        0.315939
N          -2.760532       -0.678358        0.451240
H          -2.467199       -0.547255        1.420694
H          -2.116705       -1.366901        0.024856
C          -4.142848       -1.153527        0.386859
H          -4.824260       -0.390408        0.846723
```

```
H          -4.434977       -1.302322       -0.686353
H          -4.252795       -2.125877        0.935299
```

---

## Compound_24_HEI_Conformation_11_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.821466 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.582358 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
  1.      21.3923 cm-1
  2.      30.7460 cm-1
  3.      61.2937 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.373927       -0.119082       -0.256732
C          -1.388865        0.864513       -0.341194
C          -1.133056        2.298372       -0.176202
C          -2.721820        0.395392       -0.627305
O          -0.539360       -1.362197       -0.136040
O           0.930369        0.324983       -0.256348
C           1.936462       -0.686931       -0.122124
C           3.282216        0.032173       -0.159186
C           3.504255        0.822444        1.111735
C           4.387900       -0.979455       -0.368803
H          -0.047707        2.486262        0.016717
H          -1.426709        2.873373       -1.091891
H          -1.718509        2.717530        0.683446
H          -2.787497       -0.303101       -1.508095
H          -3.467642        1.226665       -0.729485
H           1.786635       -1.232059        0.845226
H           1.840224       -1.413491       -0.970402
H           3.270072        0.749381       -1.027975
H           2.655308        1.531693        1.267657
H           3.565216        0.140983        1.994187
H           4.454772        1.404076        1.046952
H           5.379334       -0.466208       -0.384303
H           4.392658       -1.733076        0.455303
H           4.249553       -1.516132       -1.338108
N          -3.196059       -0.502610        0.549422
H          -2.536841       -1.299984        0.570693
```

```
H          -3.070098        0.019485        1.418125
C          -4.575122       -0.974569        0.422466
H          -4.848175       -1.635155        1.286994
H          -5.271833       -0.095984        0.393816
H          -4.682668       -1.555416       -0.531638
```

---

## Compound_24_HEI_Conformation_12_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.815325 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.575799 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      27.6006 cm-1
2.      40.1441 cm-1
3.      48.5505 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.190806        1.118252       -0.179367
C          -1.504653        1.032733        0.355414
C          -2.306834        2.256089        0.494481
C          -2.035308       -0.232499        0.753877
O           0.535797        2.092911       -0.425725
O           0.340430       -0.132998       -0.529441
C           1.707575       -0.184383       -0.921476
C           2.633403       -0.201176        0.292061
C           2.405384       -1.438447        1.131516
C           4.073792       -0.114427       -0.161378
H          -1.684053        3.159260        0.275357
H          -3.178322        2.254242       -0.211031
H          -2.715158        2.355066        1.532486
H          -1.287155       -0.925191        1.228228
H          -2.967312       -0.159435        1.372633
H           1.785498       -1.144745       -1.498314
H           1.954767        0.687441       -1.582892
H           2.387429        0.708825        0.911346
H           1.325832       -1.513864        1.409605
H           2.691386       -2.357715        0.565667
H           3.015472       -1.393335        2.065160
H           4.756586       -0.126470        0.721923
H           4.333071       -0.978508       -0.819672
```

```
H           4.246166        0.830525       -0.730939
N          -2.456221       -1.024132       -0.539628
H          -1.594049       -1.166405       -1.078839
H          -3.062922       -0.417114       -1.093485
C          -3.112142       -2.304416       -0.274697
H          -2.425680       -2.954267        0.329792
H          -4.052610       -2.128010        0.310670
H          -3.367686       -2.831022       -1.231562
```

---

## Compound_24_HEI_Conformation_13_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.813841 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574551 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      19.8434 cm-1
2.      32.0925 cm-1
3.      39.6099 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.460032       -0.031830        0.214174
C           1.457889        0.969932        0.081378
C           1.185464        2.285195       -0.510205
C           2.769078        0.654142        0.567922
O           0.615901       -1.227243        0.560979
O          -0.828836        0.341311       -0.111278
C          -1.830084       -0.673104        0.033618
C          -3.161863       -0.025191       -0.335736
C          -4.198574       -1.102405       -0.569948
C          -3.610490        0.932181        0.746594
H           0.086920        2.437866       -0.651834
H           1.570057        3.110385        0.142444
H           1.680377        2.391889       -1.510983
H           2.772407        0.035224        1.505660
H           3.430780        1.552888        0.677420
H          -1.588220       -1.524697       -0.654414
H          -1.831595       -1.046157        1.090172
H          -3.014734        0.557008       -1.288900
H          -3.890476       -1.767003       -1.412582
H          -4.327909       -1.728788        0.345510
```

```
H          -5.182374       -0.639202       -0.823307
H          -4.543304        1.460690        0.435967
H          -3.813572        0.384071        1.698011
H          -2.810781        1.688798        0.936063
N           3.503100       -0.261034       -0.488581
H           4.417910        0.115483       -0.726054
H           2.915832       -0.242478       -1.331107
C           3.644567       -1.651294       -0.038248
H           4.315017       -1.690418        0.858786
H           2.621921       -2.039345        0.247652
H           4.077407       -2.287274       -0.853343
```

---

## Compound_24_HEI_Conformation_14_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.81389 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574491 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      16.8695 cm-1
2.      35.3357 cm-1
3.      40.0660 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.395668       -0.183236       -0.290731
C           1.263546        0.939573       -0.237162
C           0.808481        2.272627        0.175425
C           2.627817        0.731060       -0.625714
O           0.705686       -1.384156       -0.478130
O          -0.944217        0.071024       -0.075438
C          -1.813504       -1.066250       -0.124970
C          -3.239876       -0.567394        0.086645
C          -3.385743        0.102041        1.435557
C          -3.656421        0.368189       -1.027033
H           1.064698        3.044924       -0.594547
H          -0.299664        2.286480        0.325310
H           1.291734        2.586627        1.137514
H           2.755821        0.014687       -1.481738
H           3.186558        1.685134       -0.813168
H          -1.706569       -1.567193       -1.122312
H          -1.516491       -1.786368        0.681520
```

```
H          -3.902402       -1.479247        0.060905
H          -3.129054       -0.612745        2.253766
H          -2.696970        0.979291        1.502872
H          -4.434294        0.454761        1.584102
H          -4.702211        0.723745       -0.866321
H          -2.974805        1.252911       -1.057740
H          -3.602808       -0.153300       -2.012694
N           3.400438        0.037349        0.563276
H           2.768001        0.081026        1.371534
H           4.251177        0.545860        0.792834
C           3.725561       -1.367998        0.289477
H           2.771838       -1.906597        0.009373
H           4.445411       -1.428245       -0.567199
H           4.182023       -1.849812        1.192643
```

---

## Compound_24_HEI_Conformation_15_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.814553 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574564 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      25.8781 cm-1
2.      39.8078 cm-1
3.      43.0303 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.354363       -0.283164       -0.567401
C           1.534706       -0.993332       -0.221712
C           1.511784       -2.366956        0.294965
C           2.784651       -0.317762       -0.416018
O           0.254808        0.929499       -0.871553
O          -0.821869       -1.007251       -0.536690
C          -2.024751       -0.324532       -0.887224
C          -2.607429        0.426193        0.307512
C          -3.783113        1.266554       -0.139764
C          -3.016488       -0.534354        1.402017
H           0.477333       -2.789492        0.258490
H           2.181716       -3.036288       -0.303494
H           1.864198       -2.406164        1.358963
H           2.815960        0.332390       -1.331838
```

```
H           3.670433       -1.004621       -0.380483
H          -1.839842        0.383904       -1.736253
H          -2.708463       -1.154647       -1.210926
H          -1.799810        1.106295        0.701975
H          -3.459659        2.014964       -0.902739
H          -4.578368        0.623516       -0.588459
H          -4.220291        1.811924        0.730842
H          -3.334083        0.025665        2.313800
H          -3.867540       -1.174440        1.065680
H          -2.157549       -1.198648        1.664527
N           3.011440        0.695628        0.772474
H           3.923451        0.557676        1.201776
H           2.288574        0.477022        1.468794
C           2.867657        2.097913        0.361833
H           3.674684        2.360953       -0.369773
H           1.861255        2.221713       -0.137957
H           2.936122        2.777534        1.250452
```

---

## Compound_24_HEI_Conformation_16_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.809941 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.569792 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      22.2524 cm-1
2.      35.3564 cm-1
3.      55.5752 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.538734       -1.137827       -0.202216
C          -1.861743       -0.616096       -0.170673
C          -2.924575       -1.428404        0.444151
C          -2.177442        0.649984       -0.742683
O          -0.098244       -2.232298        0.186818
O           0.406908       -0.260402       -0.744627
C           1.717228       -0.760357       -0.990248
C           2.728701       -0.220642        0.019981
C           3.047578        1.233898       -0.246202
C           2.245713       -0.421529        1.438762
H          -3.322353       -0.941771        1.372719
```

```
H          -3.785668       -1.564529       -0.258747
H          -2.536010       -2.439670        0.723093
H          -1.489903        0.977606       -1.566153
H          -3.253577        0.750075       -1.047022
H           1.728178       -1.882671       -0.974483
H           1.968829       -0.390998       -2.021831
H           3.673737       -0.819711       -0.122716
H           3.517660        1.353158       -1.252067
H           2.114803        1.847761       -0.221034
H           3.752795        1.625842        0.525487
H           3.063943       -0.207549        2.166261
H           1.387104        0.260443        1.653397
H           1.891503       -1.473496        1.575789
N          -2.020211        1.780814        0.365459
H          -2.081061        1.299334        1.268602
H          -2.778200        2.456942        0.308693
C          -0.734342        2.480008        0.284167
H           0.091714        1.710942        0.284176
H          -0.682265        3.062604       -0.672069
H          -0.603371        3.177396        1.151924
```

---

## Compound_24_HEI_Conformation_18_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.813547 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.573926 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      20.4050 cm-1
2.      31.7623 cm-1
3.      35.9405 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.237985       -0.267249        0.636432
C          -1.261882       -1.103638        0.116491
C          -0.981400       -2.383742       -0.544625
C          -2.615895       -0.662880        0.287412
O          -0.359053        0.903476        1.069236
O           1.034234       -0.804983        0.639284
C           2.107350        0.001823        1.120923
C           2.923008        0.589167       -0.029651
```

```
C           3.444465       -0.505126       -0.934697
C           2.108888        1.596273       -0.810709
H           0.120200       -2.557568       -0.626233
H          -1.425964       -3.240800        0.023681
H          -1.415387       -2.406958       -1.578225
H          -2.812764       -0.158106        1.271699
H          -3.371795       -1.467421        0.090462
H           1.733074        0.820302        1.789283
H           2.739130       -0.719121        1.708247
H           3.800951        1.121872        0.435468
H           4.125396       -1.184939       -0.368419
H           2.593634       -1.111117       -1.331609
H           4.008085       -0.067865       -1.793116
H           2.715524        2.035712       -1.637641
H           1.206876        1.100120       -1.245396
H           1.759573        2.416029       -0.137295
N          -2.927584        0.458287       -0.778336
H          -3.763714        0.232559       -1.312119
H          -2.124851        0.465277       -1.419670
C          -3.069722        1.791658       -0.180443
H          -3.959223        1.806521        0.500889
H          -2.138620        2.013015        0.420973
H          -3.199451        2.568827       -0.977584
```

---

## Compound_24_HEI_Conformation_19_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.813816 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.573956 |
| Number of Imaginary Frequencies | 0 |

## Frequencies (Top 3 out of 87)

```
1.      21.1131 cm-1
2.      33.3155 cm-1
3.      44.2598 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.224663        0.004981       -0.201858
C           1.175897        0.968600        0.229600
C           0.990299        2.409483        0.020080
C           2.344892        0.478454        0.899027
O           0.351888       -1.242472       -0.202067
```

```
O          -0.949656        0.511423       -0.724230
C          -1.957942       -0.410173       -1.135501
C          -3.050948       -0.553099       -0.078107
C          -2.510921       -1.211337        1.171874
C          -3.671395        0.789076        0.241349
H          -0.071423        2.637923       -0.246907
H           1.250102        2.989346        0.942449
H           1.642501        2.789116       -0.809583
H           2.153113       -0.404743        1.566589
H           2.914172        1.277001        1.442988
H          -2.382395        0.059607       -2.064508
H          -1.517964       -1.412808       -1.375897
H          -3.843685       -1.220595       -0.521972
H          -2.088895       -2.216288        0.928128
H          -1.689156       -0.589831        1.605186
H          -3.317940       -1.328747        1.933284
H          -4.449042        0.680985        1.034680
H          -2.885518        1.497640        0.600267
H          -4.147792        1.223764       -0.669994
N           3.359470       -0.076964       -0.176157
H           4.284499        0.327285       -0.049743
H           2.995134        0.225458       -1.087596
C           3.456739       -1.541862       -0.165150
H           3.892095       -1.883200        0.809389
H           2.415983       -1.969341       -0.274323
H           4.104356       -1.900177       -1.006840
```

---

### Compound_24_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.813866 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574866 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      16.4454 cm-1
2.      44.9834 cm-1
3.      52.6347 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.643153       -1.376765       -0.047719
C          -1.850701       -0.682346        0.231879
```

```
C          -3.137220       -1.352047       -0.004287
C          -1.809649        0.653819        0.736334
O          -0.416027       -2.564978       -0.322784
O           0.483020       -0.540006       -0.052316
C           1.745756       -1.184791       -0.218334
C           2.841851       -0.141869       -0.017650
C           2.749755        0.954064       -1.056336
C           2.795755        0.432196        1.381267
H          -3.792099       -1.299121        0.902530
H          -3.695843       -0.874238       -0.850966
H          -2.976510       -2.429735       -0.257941
H          -0.979435        0.854017        1.467751
H          -2.793074        1.018859        1.131960
H           1.841084       -2.012277        0.532914
H           1.793810       -1.621502       -1.250523
H           3.822949       -0.680896       -0.153769
H           2.829061        0.523777       -2.083544
H           1.769640        1.483380       -0.971402
H           3.569915        1.697962       -0.914371
H           3.594351        1.200374        1.515834
H           1.802266        0.907121        1.569463
H           2.945441       -0.376737        2.136197
N          -1.451839        1.622916       -0.450973
H          -2.083607        1.412477       -1.225678
H          -0.503540        1.366510       -0.752646
C          -1.513221        3.043238       -0.107030
H          -2.556133        3.305618        0.211988
H          -0.811482        3.248905        0.743948
H          -1.224905        3.681975       -0.982882
```

---

## Compound_24_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.813889 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574944 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      20.6970 cm-1
2.      42.0194 cm-1
3.      55.5598 cm-1
```

### AM1b>

```
C           0.601115       -1.351839        0.026910
C           1.912420       -0.844833       -0.177925
C           3.068542       -1.662842        0.214549
C           2.101713        0.447075       -0.757778
O           0.190729       -2.477689        0.348167
O          -0.396401       -0.376647       -0.122020
C          -1.744658       -0.832541       -0.005416
C          -2.647878        0.365708       -0.287413
C          -4.068921       -0.112242       -0.493944
C          -2.578075        1.371350        0.841019
H           3.797772       -1.762102       -0.629455
H           3.615747       -1.205858        1.079951
H           2.738232       -2.688764        0.514481
H           1.378180        0.704690       -1.578437
H           3.158032        0.650833       -1.073592
H          -1.921065       -1.654379       -0.747815
H          -1.908783       -1.234922        1.028072
H          -2.287840        0.861174       -1.232628
H          -4.436463       -0.653061        0.411386
H          -4.743382        0.756494       -0.686042
H          -4.124044       -0.806363       -1.366857
H          -3.184515        2.276154        0.596898
H          -2.967950        0.927324        1.788596
H          -1.518096        1.682047        1.008043
N           1.774990        1.534288        0.332389
H           2.306413        1.301735        1.173210
H           0.779421        1.420200        0.560005
C           2.050167        2.908052       -0.087651
H           1.774927        3.637890        0.718443
H           3.141590        3.014951       -0.323555
H           1.455728        3.139313       -1.010722
```

---

## Compound_24_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.82147 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.582363 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      21.3392 cm-1
2.      30.7650 cm-1
3.      61.3532 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C          -0.373940       -0.119101       -0.256665
C          -1.388857        0.864603       -0.341112
C          -1.132907        2.298435       -0.176208
C          -2.721810        0.395552       -0.627251
O          -0.539482       -1.362205       -0.136056
O           0.930360        0.324942       -0.256199
C           1.936393       -0.687020       -0.121810
C           3.282149        0.032045       -0.159284
C           3.504349        0.822604        1.111428
C           4.387809       -0.979614       -0.368835
H          -0.047737        2.486123        0.017930
H          -1.425339        2.873281       -1.092385
H          -1.719292        2.717934        0.682637
H          -2.787503       -0.303007       -1.507990
H          -3.467582        1.226863       -0.729504
H           1.786659       -1.231785        0.845759
H           1.839968       -1.413863       -0.969820
H           3.269866        0.749047       -1.028240
H           2.655221        1.531607        1.267494
H           3.565816        0.141313        1.993975
H           4.454663        1.404523        1.046241
H           5.379242       -0.466369       -0.384508
H           4.392642       -1.733103        0.455391
H           4.249373       -1.516446       -1.338043
N          -3.196134       -0.502373        0.549536
H          -3.070630        0.019929        1.418179
H          -2.536642       -1.299511        0.571156
C          -4.574976       -0.974843        0.422217
H          -4.682008       -1.555867       -0.531836
H          -4.848074       -1.635402        1.286752
H          -5.271995       -0.096514        0.393217
```

---

## Compound_24_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.815324 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.575798 |
| Number of Imaginary Frequencies | 0 |

## Frequencies (Top 3 out of 87)

```
  1.      27.6209 cm-1
  2.      40.1358 cm-1
```

```
   3.      48.5374 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.190607        1.117972       -0.179412
C          -1.504491        1.032796        0.355318
C          -2.306332        2.256385        0.494351
C          -2.035442       -0.232260        0.753891
O           0.536242        2.092440       -0.425793
O           0.340341       -0.133412       -0.529454
C           1.707462       -0.185054       -0.921548
C           2.633392       -0.201146        0.291918
C           2.405499       -1.437969        1.132067
C           4.073740       -0.114569       -0.161678
H          -3.178073        2.254537       -0.210831
H          -2.714229        2.355751        1.532486
H          -1.683428        3.159354        0.274750
H          -1.287469       -0.925125        1.228271
H          -2.967427       -0.158939        1.372645
H           1.785303       -1.145747       -1.497841
H           1.954601        0.686392       -1.583480
H           2.387405        0.709189        0.910711
H           1.325946       -1.513370        1.410152
H           2.691649       -2.357522        0.566755
H           3.015541       -1.392242        2.065710
H           4.756605       -0.126183        0.721573
H           4.332992       -0.978945       -0.819593
H           4.246041        0.830126       -0.731690
N          -2.456542       -1.023887       -0.539580
H          -1.594424       -1.166350       -1.078819
H          -3.063154       -0.416779       -1.093432
C          -3.112705       -2.304018       -0.274537
H          -3.368482       -2.830593       -1.231357
H          -4.053063       -2.127391        0.310939
H          -2.426309       -2.954008        0.329876
```

---

### Compound_24_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.821304 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.582166 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
  1.      21.4591 cm-1
  2.      33.2187 cm-1
  3.      58.7719 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.372435       -0.066415        0.125155
C           1.384320        0.916666        0.005194
C           1.153269        2.241444       -0.577935
C           2.688144        0.566738        0.511663
O           0.539121       -1.289757        0.376266
O          -0.924982        0.336955       -0.104261
C          -1.924437       -0.686010       -0.008233
C          -3.265058       -0.009459       -0.281580
C          -4.311030       -1.063216       -0.574099
C          -3.678639        0.853563        0.890352
H           1.414579        3.056420        0.145169
H           1.779888        2.395354       -1.495123
H           0.079751        2.364899       -0.865171
H           2.680849        0.144743        1.555634
H           3.429706        1.404280        0.432283
H          -1.707495       -1.480725       -0.768680
H          -1.892429       -1.140767        1.015215
H          -3.145107        0.650809       -1.186490
H          -4.030394       -1.654175       -1.478901
H          -4.413953       -1.764720        0.288711
H          -5.300955       -0.580382       -0.757236
H          -4.618869        1.406473        0.653233
H          -3.854875        0.227405        1.797955
H          -2.871689        1.591484        1.118762
N           3.245432       -0.618325       -0.325632
H           2.584666       -1.399544       -0.171281
H           3.189857       -0.363332       -1.313045
C           4.607624       -1.014335        0.032541
H           4.637966       -1.301884        1.116819
H           4.941850       -1.886995       -0.588022
H           5.305760       -0.152508       -0.134795
```

---

### Compound_24_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.814221 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574712 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      23.8271 cm-1
2.      41.6392 cm-1
3.      51.7713 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.166308       -1.245541       -0.312157
C          -1.556037       -1.062347       -0.080448
C          -2.307487       -2.098534        0.641663
C          -2.214144        0.118547       -0.544550
O           0.570311       -2.230934       -0.153408
O           0.469635       -0.077522       -0.762407
C           1.841568       -0.153751       -1.127900
C           2.745457        0.432038       -0.043971
C           2.400711        1.878675        0.231754
C           2.676171       -0.393536        1.221277
H          -3.219144       -2.408117        0.069782
H          -1.670473       -3.004074        0.802083
H          -2.648431       -1.730075        1.644281
H          -1.863721        0.487907       -1.546689
H          -3.333095        0.056863       -0.507304
H           2.141187       -1.213430       -1.343675
H           1.915361        0.465271       -2.063492
H           3.798683        0.387788       -0.444097
H           2.517635        2.491559       -0.694113
H           1.341601        1.962589        0.577501
H           3.066946        2.295649        1.024496
H           3.365330        0.016163        1.997009
H           1.633241       -0.394066        1.622353
H           2.954263       -1.453834        1.004385
N          -1.829450        1.308661        0.408458
H          -0.811706        1.425266        0.322031
H          -2.020021        1.014702        1.367893
C          -2.516873        2.564500        0.108509
H          -2.288977        2.868621       -0.947208
H          -3.624161        2.418345        0.212425
H          -2.186288        3.379601        0.804599
```

---

### Compound_24_HEI_Conformation_8_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.81225 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.572529 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
  1.      24.6654 cm-1
  2.      39.5022 cm-1
  3.      47.9502 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.319652       -1.144630       -0.324439
C           1.722540       -0.988552       -0.162279
C           2.504611       -2.083321        0.429048
C           2.364077        0.222269       -0.568872
O          -0.416195       -2.135231       -0.197573
O          -0.328923        0.058452       -0.642229
C          -1.721561        0.026085       -0.931325
C          -2.513593        0.582939        0.252845
C          -3.803860        1.204809       -0.234971
C          -2.791133       -0.503350        1.269347
H           3.377724       -2.351103       -0.218994
H           2.907800       -1.798129        1.435696
H           1.868929       -2.995293        0.554525
H           1.959711        0.672408       -1.516161
H           3.482649        0.152624       -0.601880
H          -1.835769        0.695009       -1.827668
H          -2.061481       -1.011892       -1.184405
H          -1.889628        1.382865        0.742883
H          -3.594294        2.065797       -0.914302
H          -4.413209        0.453859       -0.793597
H          -4.405146        1.572959        0.630802
H          -3.175989       -0.061594        2.218973
H          -3.552048       -1.220793        0.877474
H          -1.853143       -1.075299        1.479645
N           2.045875        1.334106        0.496954
H           2.293182        0.965378        1.416791
H           1.026005        1.457611        0.482440
C           2.720309        2.609310        0.254802
H           2.428602        2.996456       -0.757134
H           2.438613        3.366837        1.032629
H           3.831061        2.454433        0.277077
```

---

### Compound_24_HEI_Conformation_9_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.814239 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.574748 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      22.2971 cm-1
2.      38.3647 cm-1
3.      50.4704 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.061110        1.156100       -0.320907
C          -1.325806        1.070834        0.321949
C          -2.132501        2.287849        0.488391
C          -1.805306       -0.188105        0.798453
O           0.623686        2.133376       -0.658736
O           0.453965       -0.100922       -0.675591
C           1.791038       -0.175523       -1.154050
C           2.758260       -0.609902       -0.053722
C           2.913131        0.478135        0.985741
C           2.311439       -1.907128        0.583003
H          -2.455034        2.415523        1.553129
H          -1.544124        3.191289        0.189773
H          -3.059245        2.251666       -0.141745
H          -1.011605       -0.857685        1.230512
H          -2.685116       -0.106829        1.488538
H           1.750973       -0.958674       -1.959589
H           2.117272        0.805733       -1.589635
H           3.756796       -0.778883       -0.548996
H           3.337789        1.400114        0.519890
H           1.915710        0.739772        1.417573
H           3.588981        0.142672        1.807682
H           3.026359       -2.216968        1.382300
H           1.298494       -1.780843        1.037641
H           2.257123       -2.718112       -0.182366
N          -2.318189       -1.022416       -0.432887
H          -1.499620       -1.173678       -1.034248
H          -2.973462       -0.437952       -0.954794
C          -2.936858       -2.299626       -0.078481
H          -2.197638       -2.924492        0.489010
H          -3.830220       -2.113569        0.573853
H          -3.261034       -2.857614       -0.995960
```

## Compound_25_HEI_Conformation_11_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.331573 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.071072 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      23.6733 cm-1
2.      35.2636 cm-1
3.      53.2256 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.759568       -0.660448        0.258939
C           1.793254       -0.433581        1.224051
C           3.151800       -0.493356        0.790026
O           0.983662       -0.550000       -0.990891
N          -0.511441       -1.023485        0.724941
C          -1.683201       -1.044895       -0.138866
C          -1.958801        0.321088       -0.813527
C          -2.197742        1.467073        0.119922
C          -2.710318        2.708002       -0.547824
O          -1.995033        1.432371        1.339045
H           1.564550       -0.244055        2.271442
H           3.400324       -1.373786        0.133861
H           3.897837       -0.398843        1.620879
H          -0.713912       -0.741019        1.659722
H          -2.850184        0.215173       -1.485220
H          -1.069554        0.577007       -1.456081
H          -2.679923        3.577458        0.152112
H          -2.094143        2.941170       -1.449032
H          -3.767390        2.543933       -0.870799
C          -1.532371       -2.075133       -1.274231
H          -2.462856       -2.083289       -1.889715
H          -0.662239       -1.814831       -1.924306
H          -1.372934       -3.094510       -0.850139
C          -2.933276       -1.442327        0.669796
H          -3.815332       -1.471422       -0.012530
H          -2.799081       -2.453413        1.122332
H          -3.132153       -0.704317        1.483976
N           3.416882        0.709424       -0.181611
H           3.118945        1.566340        0.284955
H           2.775983        0.553080       -0.977539
C           4.799119        0.822133       -0.642222
```

```
H           5.476435        0.978364        0.237988
H           4.915464        1.681623       -1.353493
H           5.094846       -0.126543       -1.163351
```

---

## Compound_25_HEI_Conformation_12_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.331572 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.071072 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
  1.      23.6528 cm-1
  2.      35.2517 cm-1
  3.      53.2298 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.759600       -0.660440        0.258964
C           1.793277       -0.433487        1.224069
C           3.151814       -0.493277        0.790035
O           0.983695       -0.550040       -0.990867
N          -0.511404       -1.023482        0.724983
C          -1.683155       -1.044917       -0.138830
C          -1.958778        0.321051       -0.813515
C          -2.197788        1.467046        0.119903
C          -2.710693        2.707838       -0.547848
O          -1.994852        1.432480        1.338991
H           1.564570       -0.243857        2.271440
H           3.400340       -1.373754        0.133935
H           3.897863       -0.398679        1.620867
H          -0.713874       -0.740985        1.659756
H          -2.850138        0.215076       -1.485230
H          -1.069525        0.576991       -1.456051
H          -2.680707        3.577268        0.152137
H          -2.094441        2.941261       -1.448938
H          -3.767650        2.543428       -0.871017
C          -1.532312       -2.075171       -1.274179
H          -0.662192       -1.814858       -1.924265
H          -1.372849       -3.094537       -0.850074
H          -2.462802       -2.083358       -1.889655
C          -2.933238       -1.442339        0.669825
H          -2.799068       -2.453439        1.122335
```

```
H          -3.132095       -0.704342        1.484022
H          -3.815295       -1.471392       -0.012500
N           3.416870        0.709430       -0.181724
H           2.776017        0.553013       -0.977671
H           3.118862        1.566356        0.284781
C           4.799133        0.822194       -0.642235
H           5.476371        0.978497        0.238022
H           5.094954       -0.126487       -1.163302
H           4.915493        1.681658       -1.353534
```

---

## Compound_25_HEI_Conformation_13_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.332179 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.071064 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      35.0957 cm-1
2.      38.6635 cm-1
3.      49.2100 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           1.046512       -0.587220       -0.107357
C           2.258934       -1.195868       -0.564879
C           3.357856       -0.345582       -0.899034
O           1.009502        0.633791        0.253650
N          -0.091722       -1.392671        0.009564
C          -1.424139       -0.859612        0.266521
C          -1.830066        0.192690       -0.802265
C          -3.091976        0.932422       -0.461924
C          -2.908416        2.349524       -0.017110
O          -4.216020        0.427641       -0.572446
H           2.363259       -2.276347       -0.645204
H           3.091224        0.531273       -1.553322
H           4.241443       -0.893254       -1.317929
H          -0.078344       -2.236191       -0.515556
H          -1.976062       -0.329081       -1.784664
H          -0.989950        0.931516       -0.912728
H          -3.877110        2.793650        0.315376
H          -2.174702        2.385224        0.825858
H          -2.503726        2.953906       -0.865521
```

```
C          -2.457676       -2.001369        0.227531
H          -2.443834       -2.522983       -0.759236
H          -2.249486       -2.744474        1.033241
H          -3.477888       -1.573997        0.383159
C          -1.501964       -0.205129        1.655774
H          -0.808646        0.669215        1.710243
H          -2.547754        0.138921        1.841974
H          -1.221061       -0.938694        2.448077
N           3.852201        0.366864        0.404331
H           4.022363       -0.347742        1.112532
H           3.045446        0.929789        0.722955
C           5.032876        1.209000        0.221745
H           5.890924        0.580606       -0.134409
H           4.813204        1.993915       -0.549420
H           5.317852        1.710812        1.183669
```

---

## Compound_25_HEI_Conformation_14_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.318324 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.057952 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      22.1897 cm-1
2.      24.0645 cm-1
3.      41.8271 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.554432        0.029713        1.241442
C           1.769847       -0.722496        1.373074
C           2.579239       -1.155505        0.302246
O          -0.127052        0.383542        2.236823
N           0.177483        0.446066       -0.072293
C          -1.097457        1.130594       -0.288701
C          -2.315946        0.298151        0.175441
C          -2.423732       -1.074772       -0.414526
C          -3.577022       -1.879323        0.101301
O          -1.636963       -1.539112       -1.249560
H           2.079186       -0.932198        2.401579
H           2.065072       -1.471753       -0.643609
H           3.353902       -1.912822        0.591588
```

```
H           0.291782       -0.286029       -0.747277
H          -3.252852        0.862648       -0.071185
H          -2.258966        0.191528        1.296050
H          -4.521022       -1.287198        0.034733
H          -3.695451       -2.824266       -0.481670
H          -3.392298       -2.137756        1.173310
C          -1.159576        2.472007        0.463356
H          -1.082278        2.309733        1.565887
H          -0.326616        3.138011        0.136612
H          -2.129692        2.973998        0.235175
C          -1.275052        1.447672       -1.786839
H          -2.239989        1.988206       -1.933561
H          -0.445284        2.099227       -2.149425
H          -1.293435        0.510418       -2.393503
N           3.446289        0.095872       -0.207303
H           3.910682        0.494699        0.609651
H           2.788709        0.799973       -0.548175
C           4.422892       -0.228470       -1.244481
H           4.991536        0.681934       -1.570395
H           5.146156       -0.989333       -0.849311
H           3.890826       -0.663451       -2.131278
```

---

## Compound_25_HEI_Conformation_15_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.332672 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.071637 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      33.6259 cm-1
2.      42.7265 cm-1
3.      55.3451 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.966158       -0.048334       -0.093688
C          -1.823845       -1.173495       -0.318465
C          -3.096302       -1.192025        0.328154
O          -1.405700        1.029470        0.423343
N           0.358758       -0.130987       -0.537542
C           1.365334        0.853160       -0.169421
C           2.753364        0.436477       -0.727133
```

```
C           3.255717       -0.857256       -0.153011
C           4.418147       -0.746100        0.781754
O           2.756507       -1.950040       -0.446346
H          -1.529110       -1.996600       -0.967229
H          -3.074530       -0.923919        1.421454
H          -3.673245       -2.138954        0.166643
H           0.708318       -1.051861       -0.690869
H           3.476110        1.260849       -0.496384
H           2.687244        0.334279       -1.843103
H           4.687988       -1.743781        1.204594
H           5.300476       -0.333313        0.234514
H           4.157921       -0.051250        1.618181
C           1.052140        2.234675       -0.774878
H           1.851699        2.956023       -0.483685
H           1.006182        2.175670       -1.887597
H           0.069813        2.601859       -0.389119
C           1.502048        1.037244        1.352912
H           2.294686        1.790986        1.571114
H           0.531010        1.395632        1.775036
H           1.777427        0.073935        1.844681
N          -3.971733       -0.031892       -0.263137
H          -3.967623       -0.117210       -1.279763
H          -3.459703        0.834119       -0.025149
C          -5.339485        0.016663        0.248866
H          -5.871205       -0.936266       -0.010160
H          -5.900997        0.882763       -0.190229
H          -5.313842        0.125696        1.365295
```

---

## Compound_25_HEI_Conformation_16_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.31309 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.052401 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      27.6671 cm-1
2.      34.2055 cm-1
3.      44.3324 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.929909       -1.205213        0.148675
C           2.345474       -1.447426        0.201555
C           3.330757       -0.488867        0.510481
O           0.115292       -2.081012       -0.235497
N           0.472419        0.108540        0.458090
C          -0.961174        0.396699        0.584907
C          -1.653411        0.247361       -0.792639
C          -3.152822        0.332136       -0.711166
C          -3.881171       -0.962640       -0.885266
O          -3.754423        1.401619       -0.552414
H           2.651268       -2.459874       -0.081334
H           3.086514        0.285737        1.284126
H           4.346160       -0.921694        0.707251
H           0.982477        0.526620        1.207768
H          -1.367405       -0.743187       -1.240954
H          -1.286213        1.062531       -1.470405
H          -4.975752       -0.833966       -0.707843
H          -3.723198       -1.339067       -1.925782
H          -3.475067       -1.720595       -0.170179
C          -1.667982       -0.514508        1.601904
H          -2.740276       -0.217114        1.690743
H          -1.608716       -1.580534        1.270761
H          -1.191262       -0.422029        2.606653
C          -1.147886        1.850808        1.060864
H          -2.237446        2.097523        1.059070
H          -0.752759        1.979851        2.096538
H          -0.625115        2.564900        0.381511
N           3.558928        0.427949       -0.791858
H           2.672304        0.895622       -0.989948
H           3.743410       -0.201204       -1.574386
C           4.632526        1.410086       -0.661311
H           4.742135        2.023631       -1.594148
H           5.599283        0.878869       -0.457598
H           4.407961        2.093083        0.199798
```

---

## Compound_25_HEI_Conformation_18_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.326954 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.065576 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      23.1257 cm-1
2.      33.4845 cm-1
```

```
   3.      45.1533 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.726078       -0.671800       -0.247149
C           1.806577       -0.963636       -1.144449
C           3.134909       -0.937535       -0.631932
O           0.928765       -0.194483        0.911495
N          -0.585131       -0.837867       -0.721931
C          -1.732276       -0.933511        0.173323
C          -2.003800        0.409859        0.894850
C          -2.076430        1.580706       -0.044048
C          -0.907193        2.512219        0.001277
O          -3.045151        1.782849       -0.786091
H           1.629467       -1.192467       -2.194590
H           3.241982       -1.380471        0.395533
H           3.901308       -1.360582       -1.330931
H          -0.667408       -1.403879       -1.536626
H          -1.185137        0.578654        1.645117
H          -2.979696        0.317730        1.439263
H           0.040961        1.917285       -0.020428
H          -0.927057        3.222052       -0.859487
H          -0.939575        3.094835        0.954348
C          -2.996285       -1.317791       -0.618881
H          -3.252209       -0.522317       -1.360467
H          -2.852930       -2.287276       -1.152604
H          -3.850015       -1.427939        0.091022
C          -1.543961       -1.994435        1.275425
H          -2.430298       -1.990554        1.952282
H          -1.443646       -3.009201        0.823095
H          -0.628005       -1.771002        1.874855
N           3.567914        0.574988       -0.413808
H           4.371910        0.813218       -0.988277
H           2.765763        1.135204       -0.728654
C           3.846989        0.896817        0.989532
H           2.924102        0.657111        1.594259
H           4.703487        0.274947        1.356894
H           4.100961        1.982514        1.104654
```

---

### Compound_25_HEI_Conformation_19_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.327419 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.066701 |
| Number of Imaginary Frequencies | 0 |

## Frequencies (Top 3 out of 96)

```
1.      22.5405 cm-1
2.      28.6622 cm-1
3.      37.0659 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.718447        0.199979        0.396305
C           1.674040       -0.293672        1.347644
C           2.862438       -0.902215        0.854874
O           0.981737        0.269957       -0.843754
N          -0.507154        0.661365        0.882128
C          -1.612314        1.070101        0.032211
C          -2.042416       -0.032555       -0.971936
C          -2.295389       -1.364589       -0.325604
C          -1.288043       -2.426832       -0.629231
O          -3.277811       -1.581204        0.394709
H           1.512227       -0.195549        2.420263
H           2.707500       -1.557961       -0.044694
H           3.461957       -1.432898        1.638313
H          -0.755036        0.391338        1.804306
H          -1.231960       -0.136309       -1.742850
H          -2.981337        0.307651       -1.481142
H          -1.463525       -3.336705       -0.007242
H          -1.358311       -2.704728       -1.709273
H          -0.259008       -2.030458       -0.431382
C          -2.837400        1.442080        0.888934
H          -3.232080        0.545193        1.425718
H          -2.575419        2.231359        1.632787
H          -3.640817        1.835205        0.221969
C          -1.249205        2.308052       -0.810974
H          -0.357554        2.095993       -1.449240
H          -2.112954        2.572181       -1.465612
H          -1.022943        3.174761       -0.146373
N           3.826575        0.234992        0.303212
H           4.711362        0.241292        0.803450
H           3.339235        1.119651        0.492975
C           4.072824        0.131611       -1.138741
H           4.584719       -0.838662       -1.366190
H           3.075663        0.161855       -1.667954
H           4.713023        0.980512       -1.493741
```

---

## Compound_25_HEI_Conformation_1_am1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.324629 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.063737 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      28.4663 cm-1
2.      32.5497 cm-1
3.      60.3866 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.353758       -1.530942       -0.636769
C          -1.784605       -1.518197       -0.756370
C          -2.693435       -0.996608        0.186627
O           0.391740       -1.966834       -1.551831
N           0.233161       -1.046463        0.561657
C           1.625369       -0.618568        0.598103
C           1.957788        0.430172       -0.494310
C           1.183143        1.707048       -0.420508
C           1.880506        2.898210       -1.002966
O           0.041195        1.811386        0.054464
H          -2.170396       -1.953129       -1.684201
H          -2.418233       -1.065834        1.271277
H          -3.751171       -1.337653        0.034828
H          -0.348987       -0.434496        1.089470
H           1.749413       -0.039225       -1.499695
H           3.053597        0.660783       -0.444351
H           1.188750        3.771220       -1.079653
H           2.742766        3.178460       -0.349265
H           2.270777        2.649112       -2.019670
C           1.959293        0.006349        1.966524
H           1.344258        0.920761        2.146779
H           1.769762       -0.725902        2.786837
H           3.037822        0.290938        1.986187
C           2.589840       -1.799699        0.388454
H           2.427139       -2.262637       -0.615474
H           3.641658       -1.434789        0.461305
H           2.422095       -2.575245        1.172622
N          -2.789408        0.594943       -0.025765
H          -1.900892        1.007122        0.269819
H          -2.870458        0.758873       -1.030258
C          -3.896013        1.228374        0.687035
H          -3.899146        2.339318        0.531034
H          -4.868067        0.804922        0.321273
H          -3.799205        1.014779        1.783913
```

---

### Compound_25_HEI_Conformation_20_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.317351 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.056723 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      23.9480 cm-1
2.      33.9983 cm-1
3.      47.3179 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.866203        1.566857       -0.382742
C           2.187493        1.195916       -0.808125
C           2.680942       -0.122019       -0.896756
O           0.461770        2.755723       -0.392049
N           0.035786        0.539517        0.149272
C          -1.386732        0.770124        0.385210
C          -2.055425       -0.532085        0.908993
C          -1.936305       -1.693328       -0.035274
C          -3.194548       -2.102764       -0.730939
O          -0.867689       -2.293852       -0.214575
H           2.844341        2.034138       -1.060326
H           1.964032       -0.925854       -1.213025
H           3.637987       -0.211681       -1.474615
H           0.196833       -0.353194       -0.270103
H          -3.136708       -0.307002        1.098066
H          -1.583011       -0.815710        1.886893
H          -2.999025       -2.920378       -1.465957
H          -3.937356       -2.462571        0.022559
H          -3.627943       -1.222326       -1.267306
C          -1.614835        1.834754        1.473197
H          -1.118106        1.538174        2.426635
H          -1.198259        2.816528        1.138007
H          -2.709968        1.945149        1.655611
C          -2.147637        1.221370       -0.873336
H          -2.062450        0.458479       -1.683477
H          -3.226456        1.368299       -0.631715
H          -1.722385        2.188770       -1.239526
N           3.086808       -0.618597        0.574734
```

```
H           3.722506        0.076759        0.966633
H           2.239829       -0.603367        1.146041
C           3.693193       -1.947710        0.612154
H           3.960594       -2.245314        1.660109
H           4.621379       -1.950690       -0.017382
H           2.969275       -2.696303        0.193529
```

---

## Compound_25_HEI_Conformation_21_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.319389 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.058869 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      21.4064 cm-1
2.      23.7681 cm-1
3.      42.3457 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.682888       -0.134117        0.999538
C           1.866299       -0.940575        0.896466
C           2.498932       -1.305300       -0.308311
O           0.164249        0.156758        2.107272
N           0.149197        0.410164       -0.208677
C          -1.108865        1.156960       -0.185579
C          -2.290376        0.331988        0.377041
C          -2.545763       -0.978473       -0.302727
C          -3.658391       -1.779849        0.300055
O          -1.902866       -1.397766       -1.273660
H           2.305915       -1.245496        1.851213
H           1.837325       -1.515324       -1.190881
H           3.267027       -2.113738       -0.197942
H           0.134463       -0.262200       -0.951762
H          -3.223691        0.950194        0.313698
H          -2.083909        0.124523        1.465483
H          -4.573000       -1.149091        0.408862
H          -3.898661       -2.667007       -0.334011
H          -3.346506       -2.134666        1.313412
C          -1.001630        2.428695        0.674677
H          -0.781003        2.167734        1.738202
H          -0.190478        3.089940        0.288754
```

```
H          -1.968487        2.983844        0.627855
C          -1.476105        1.610290       -1.612502
H          -2.424793        2.196375       -1.576391
H          -0.673817        2.260386       -2.034659
H          -1.623364        0.731038       -2.284865
N           3.344750       -0.048352       -0.868886
H           2.771068        0.779556       -0.685108
H           3.499851       -0.119923       -1.870568
C           4.626419        0.099044       -0.178186
H           4.434679        0.097384        0.929543
H           5.292553       -0.765698       -0.433533
H           5.135682        1.055574       -0.466093
```

---

## Compound_25_HEI_Conformation_22_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.314789 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.053843 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      27.0911 cm-1
2.      36.7056 cm-1
3.      40.0384 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.989708       -0.908076       -0.226609
C           2.340225       -1.062481       -0.691372
C           3.181504       -0.017163       -1.119281
O           0.331872       -1.865589        0.251522
N           0.432603        0.404635       -0.243823
C          -0.966670        0.634832        0.125584
C          -1.944124       -0.172525       -0.770004
C          -3.365606       -0.137328       -0.284318
C          -3.864067       -1.401741        0.340159
O          -4.093384        0.854163       -0.419002
H           2.736278       -2.081248       -0.629607
H           2.708973        0.822924       -1.694898
H           4.116404       -0.360395       -1.633053
H           0.671973        0.911689       -1.070053
H          -1.597586       -1.241646       -0.808121
H          -1.912619        0.247864       -1.809758
```

```
H          -3.163291       -1.720933        1.151184
H          -4.886350       -1.262378        0.766364
H          -3.899398       -2.207669       -0.433520
C          -1.218297        0.264320        1.595258
H          -1.056948       -0.830003        1.754159
H          -0.530284        0.832129        2.265231
H          -2.270734        0.524853        1.862951
C          -1.298371        2.130676       -0.041860
H          -0.673524        2.749321        0.644465
H          -1.125092        2.467010       -1.091948
H          -2.375854        2.294291        0.203853
N           3.726927        0.787497        0.171010
H           2.931711        0.860885        0.811702
H           4.034460        1.724481       -0.073839
C           4.812018        0.069090        0.840972
H           5.079021        0.554795        1.815642
H           4.474978       -0.986776        1.030174
H           5.715360        0.049662        0.177428
```

---

## Compound_25_HEI_Conformation_23_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.3239 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.062641 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      26.3845 cm-1
2.      36.8001 cm-1
3.      44.5179 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.150472       -0.654420        0.046243
C          -2.414243       -1.326743       -0.058373
C          -3.576447       -0.655861        0.416354
O          -1.069132        0.572163        0.361525
N           0.002779       -1.374508       -0.298109
C           1.348132       -0.921254        0.044814
C           1.709277        0.338288       -0.785194
C           2.985155        0.995165       -0.339020
C           2.820293        2.286054        0.400365
O           4.104136        0.532398       -0.592561
```

```
H          -2.496649       -2.319512       -0.498876
H          -3.422115       -0.082581        1.370599
H          -4.484172       -1.308766        0.484479
H          -0.099326       -2.363644       -0.304162
H           0.867005        1.078061       -0.704317
H           1.816805        0.039588       -1.861371
H           3.801465        2.657891        0.781413
H           2.382871        3.052170       -0.285510
H           2.120293        2.137953        1.259613
C           1.495184       -0.587959        1.539633
H           0.805040        0.246188        1.816680
H           1.252074       -1.479993        2.164333
H           2.547081       -0.281654        1.753380
C           2.369206       -2.025784       -0.288229
H           2.286920       -2.337431       -1.356642
H           3.400248       -1.632835       -0.114267
H           2.209419       -2.917721        0.363149
N          -3.968247        0.481910       -0.622188
H          -4.897781        0.327714       -1.003323
H          -3.285566        0.399027       -1.385845
C          -3.881885        1.831872       -0.055937
H          -4.606022        1.932746        0.792991
H          -2.831114        1.984031        0.328597
H          -4.113422        2.604325       -0.834506
```

---

## Compound_25_HEI_Conformation_24_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.324491 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.063225 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      25.1106 cm-1
2.      35.3569 cm-1
3.      47.4016 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.124657        0.578800       -0.165320
C          -2.324760        1.206620       -0.639973
C          -3.425486        0.375866       -0.993372
O          -1.081355       -0.658393        0.113890
```

```
N          -0.006690        1.394650        0.058155
C           1.325895        0.861926        0.317659
C           1.784605       -0.098621       -0.814247
C           3.046768       -0.844637       -0.488759
C           2.872433       -2.294624       -0.161965
O           4.165087       -0.316618       -0.520555
H          -2.409734        2.289904       -0.715010
H          -3.138924       -0.565368       -1.536529
H          -4.248153        0.913143       -1.531354
H          -0.012300        2.267843       -0.416943
H           1.954386        0.499677       -1.748014
H           0.961339       -0.838567       -1.010405
H           3.837095       -2.749773        0.167345
H           2.112534       -2.406503        0.650580
H           2.505548       -2.836403       -1.067917
C           2.340831        2.017917        0.401420
H           2.350949        2.613520       -0.542578
H           2.093453        2.693928        1.253771
H           3.362412        1.594547        0.559005
C           1.369565        0.103518        1.654503
H           0.690306       -0.782730        1.618570
H           2.414596       -0.238204        1.849189
H           1.050299        0.769613        2.490650
N          -4.097152       -0.172759        0.338381
H          -5.066694        0.123718        0.410243
H          -3.567383        0.257670        1.106778
C          -4.013447       -1.631243        0.466461
H          -4.567105       -2.117287       -0.377586
H          -2.924253       -1.925354        0.418292
H          -4.451810       -1.969661        1.441039
```

---

## Compound_25_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.318323 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.057949 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      22.2227 cm-1
2.      24.0830 cm-1
3.      41.8872 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.554449        0.029691        1.241414
C          -1.769855       -0.722535        1.373034
C          -2.579241       -1.155541        0.302201
O           0.127014        0.383533        2.236806
N          -0.177489        0.446064       -0.072319
C           1.097461        1.130589       -0.288692
C           2.315943        0.298150        0.175479
C           2.423774       -1.074754       -0.414517
C           3.577106       -1.879264        0.101280
O           1.637006       -1.539121       -1.249538
H          -2.079197       -0.932246        2.401538
H          -2.065077       -1.471796       -0.643652
H          -3.353915       -1.912847        0.591540
H          -0.291713       -0.286052       -0.747294
H           2.258906        0.191490        1.296084
H           3.252848        0.862679       -0.071077
H           3.695569       -2.824194       -0.481709
H           4.521080       -1.287096        0.034712
H           3.392405       -2.137726        1.173287
C           1.275097        1.447673       -1.786824
H           1.293493        0.510420       -2.393491
H           0.445341        2.099235       -2.149427
H           2.240042        1.988203       -1.933515
C           1.159559        2.471996        0.463375
H           1.082259        2.309704        1.565905
H           2.129672        2.973999        0.235202
H           0.326591        3.137992        0.136634
N          -3.446272        0.095872       -0.207353
H          -2.788660        0.799875       -0.548362
H          -3.910513        0.494794        0.609641
C          -4.423039       -0.228434       -1.244393
H          -4.991567        0.682027       -1.570360
H          -3.891135       -0.663611       -2.131192
H          -5.146393       -0.989129       -0.849059
```

---

## Compound_25_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.319737 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.058324 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
  1.      31.2474 cm-1
  2.      46.8960 cm-1
  3.      50.7983 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.636491       -1.781487        0.232035
C           2.058957       -1.654175        0.144508
C           2.737164       -0.615666       -0.545670
O           0.052853       -2.731600        0.809004
N          -0.122937       -0.692718       -0.293804
C          -1.577209       -0.649491       -0.234083
C          -2.059550        0.716631       -0.805762
C          -1.359746        1.888206       -0.178704
C          -2.170888        2.688487        0.789899
O          -0.191660        2.199125       -0.455172
H           2.637618       -2.404537        0.689066
H           2.351468       -0.347216       -1.567065
H           3.846901       -0.776476       -0.594143
H           0.210234       -0.369614       -1.177832
H          -3.163836        0.792192       -0.635813
H          -1.876899        0.738017       -1.912964
H          -1.551238        3.478152        1.278719
H          -3.018360        3.177136        0.249069
H          -2.591841        2.012494        1.575057
C          -2.259053       -1.744101       -1.073520
H          -3.367046       -1.645792       -0.996480
H          -1.965946       -1.664437       -2.146922
H          -1.953160       -2.748102       -0.687329
C          -2.099729       -0.778380        1.205148
H          -1.840137       -1.786445        1.614199
H          -1.649295        0.001639        1.863478
H          -3.208822       -0.656606        1.207483
N           2.547054        0.748437        0.237694
H           1.673036        1.187468       -0.070284
H           2.431535        0.505491        1.225704
C           3.651576        1.692106        0.066282
H           3.443797        2.655249        0.602728
H           4.596312        1.242902        0.470837
H           3.789241        1.905464       -1.026189
```

---

## Compound_25_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.324636 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.063743 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      28.4711 cm-1
2.      32.6672 cm-1
3.      60.4240 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.353893       -1.530912       -0.636835
C          -1.784742       -1.518123       -0.756519
C          -2.693588       -0.996460        0.186398
O           0.391652       -1.966823       -1.551850
N           0.232955       -1.046469        0.561626
C           1.625192       -0.618680        0.598206
C           1.957846        0.429986       -0.494201
C           1.183410        1.706994       -0.420542
C           1.880981        2.897977       -1.003118
O           0.041483        1.811585        0.054423
H          -2.170487       -1.953044       -1.684375
H          -2.418418       -1.065563        1.271062
H          -3.751338       -1.337446        0.034589
H          -0.349215       -0.434518        1.089432
H           1.749476       -0.039404       -1.499593
H           3.053688        0.660427       -0.444171
H           1.189348        3.771071       -1.079966
H           2.743230        3.178196       -0.349388
H           2.271288        2.648698       -2.019762
C           1.959022        0.006232        1.966650
H           3.037570        0.290747        1.986417
H           1.344031        0.920688        2.146832
H           1.769359       -0.725995        2.786955
C           2.589561       -1.799919        0.388685
H           3.641411       -1.435120        0.461634
H           2.421654       -2.575432        1.172851
H           2.426909       -2.262857       -0.615252
N          -2.789528        0.595139       -0.026094
H          -1.900763        1.007216        0.268898
H          -2.871218        0.759022       -1.030532
C          -3.895597        1.228667        0.687444
H          -3.798034        1.015105        1.784263
H          -3.898784        2.339607        0.531411
H          -4.867927        0.805249        0.322379
```

## Compound_25_HEI_Conformation_7_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.317352 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.056724 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      23.9459 cm-1
2.      34.0020 cm-1
3.      47.3278 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.866212       -1.566673        0.382654
C          -2.187312       -1.195565        0.808563
C          -2.680742        0.122336        0.897024
O          -0.461966       -2.755611        0.391907
N          -0.035849       -0.539596       -0.149760
C           1.386734       -0.770144       -0.385249
C           2.055588        0.531987       -0.908999
C           1.936481        1.693259        0.035232
C           3.194757        2.102660        0.730858
O           0.867864        2.293756        0.214627
H          -2.844063       -2.033753        1.061161
H          -1.963713        0.926421        1.212354
H          -3.637447        0.212273        1.475381
H          -0.197251        0.353454        0.268682
H           1.583272        0.815615       -1.886950
H           3.136870        0.306812       -1.097980
H           2.999289        2.920354        1.465806
H           3.628040        1.222216        1.267321
H           3.937603        2.462349       -0.022661
C           2.147297       -1.221211        0.873569
H           2.061772       -0.458247        1.683610
H           1.722050       -2.188628        1.239724
H           3.226208       -1.368045        0.632280
C           1.615142       -1.834940       -1.473018
H           1.118989       -1.538324       -2.426748
H           2.710343       -1.945630       -1.654845
H           1.198139       -2.816582       -1.137959
N          -3.087612        0.618199       -0.574581
H          -3.724189       -0.076908       -0.965459
H          -2.241155        0.601838       -1.146625
```

```
C          -3.693023        1.947735       -0.612512
H          -2.968117        2.696145       -0.195267
H          -3.961299        2.244657       -1.660440
H          -4.620555        1.951945        0.017986
```

---

## Compound_25_HEI_Conformation_9_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.33466 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.073664 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      30.4009 cm-1
2.      42.6588 cm-1
3.      45.9715 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.684141       -0.290218        0.361585
C           1.759245       -0.276859        1.307138
C           2.942903        0.453510        0.977774
O           0.866311        0.026221       -0.859604
N          -0.589802       -0.644457        0.808611
C          -1.675354       -1.032141       -0.078771
C          -2.135686        0.150336       -0.968364
C          -2.442494        1.395063       -0.183314
C          -1.439681        2.496115       -0.307521
O          -3.467717        1.513162        0.499269
H           1.685737       -0.785952        2.266256
H           2.759893        1.489086        0.574920
H           3.699814        0.482613        1.803935
H          -0.653152       -0.998243        1.734051
H          -3.057500       -0.170634       -1.519707
H          -1.323630        0.367049       -1.713549
H          -1.621856        3.291875        0.453315
H          -0.408989        2.077695       -0.176012
H          -1.511789        2.945148       -1.328331
C          -1.278941       -2.172844       -1.037330
H          -2.132584       -2.399637       -1.718297
H          -0.395354       -1.872137       -1.650813
H          -1.026403       -3.093938       -0.461115
C          -2.886609       -1.521954        0.737000
```

```
H          -3.685738       -1.857376        0.034304
H          -2.605831       -2.381825        1.390462
H          -3.295190       -0.695695        1.368561
N           3.637751       -0.244368       -0.238054
H           3.760193       -1.231543       -0.011430
H           2.949021       -0.188265       -1.007838
C           4.909080        0.359099       -0.633572
H           5.635181        0.298422        0.219123
H           4.743044        1.438169       -0.892710
H           5.341104       -0.168742       -1.524099
```

---

## Compound_26_HEI_Conformation_10_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482441 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.26948 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      18.0878 cm-1
2.      34.8097 cm-1
3.      55.3418 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.971642        1.618807       -0.135450
C          -2.164746        0.971476       -0.537621
C          -2.196883       -0.416138       -0.837737
O          -0.697314        2.820275        0.008884
O           0.056443        0.727950        0.206662
C           1.318828        1.314030        0.526640
C           2.309776        0.178905        0.713229
C           2.687332       -0.462753       -0.604177
C           3.627894       -1.623190       -0.408993
H          -3.062333        1.586100       -0.619229
H          -1.292772       -0.810093       -1.377638
H          -3.141488       -0.756336       -1.335004
H           1.630471        2.002724       -0.301664
H           1.208400        1.911197        1.470163
H           1.869416       -0.593815        1.395740
H           3.225321        0.592160        1.211543
H           3.166779        0.304138       -1.268551
H           1.753308       -0.807954       -1.122154
```

```
H           3.156075       -2.413348        0.223866
H           3.897410       -2.075088       -1.393989
H           4.567518       -1.288981        0.094100
N          -2.133522       -1.219857        0.524156
H          -2.861667       -0.852872        1.138616
H          -1.229731       -0.982226        0.949286
C          -2.264998       -2.668310        0.376560
H          -3.258496       -2.907562       -0.085935
H          -2.188341       -3.184329        1.369591
H          -1.451614       -3.047478       -0.296904
```

---

## Compound_26_HEI_Conformation_11_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489632 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.276276 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      24.0035 cm-1
2.      25.1794 cm-1
3.      64.8388 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.610532       -0.379732        0.128065
C           1.681122       -1.180280       -0.325698
C           3.000906       -0.869759        0.135026
O           0.680891        0.746077        0.687545
O          -0.655254       -0.861526       -0.128504
C          -1.740885       -0.027486        0.293843
C          -3.011601       -0.761422       -0.096514
C          -4.245062       -0.000148        0.338379
C          -4.525729        1.198103       -0.531782
H           1.500525       -2.023095       -0.989391
H           3.097714       -0.753208        1.251197
H           3.785177       -1.570462       -0.252484
H          -1.676181        0.127994        1.402122
H          -1.661863        0.967634       -0.216098
H          -3.005551       -1.775673        0.382450
H          -3.024212       -0.918981       -1.206195
H          -4.126868        0.329344        1.404758
H          -5.126676       -0.694582        0.302920
```

```
H          -5.454562        1.715740       -0.190254
H          -3.679954        1.926349       -0.487439
H          -4.665239        0.888805       -1.595934
N           3.375848        0.559753       -0.371398
H           3.229884        0.587193       -1.381546
H           2.679191        1.192960        0.056397
C           4.734645        0.979718       -0.031164
H           5.472848        0.275057       -0.496535
H           4.862752        0.956266        1.083409
H           4.933411        2.020013       -0.400849
```

---

## Compound_26_HEI_Conformation_12_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.483543 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.26977 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      28.2667 cm-1
2.      39.9318 cm-1
3.      58.4113 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.526477       -1.578044       -0.254203
C          -1.857360       -1.252813       -0.610256
C          -2.602901       -0.274273        0.100111
O           0.229475       -2.479600       -0.648510
O           0.033239       -0.683108        0.670780
C           1.354661       -0.946547        1.129167
C           2.392216       -0.348220        0.195329
C           2.340860        1.163655        0.183971
C           3.308705        1.747254       -0.812040
H          -2.293884       -1.790572       -1.453037
H          -2.450476       -0.271591        1.213890
H          -3.693675       -0.254098       -0.155273
H           1.391919       -0.459920        2.140968
H           1.519091       -2.052330        1.225710
H           2.213264       -0.746628       -0.838606
H           3.408738       -0.689283        0.521956
H           2.571821        1.555172        1.209952
H           1.295661        1.490661       -0.064492
```

```
H           3.073744        1.392254       -1.844698
H           3.256740        2.862640       -0.800738
H           4.354769        1.440764       -0.568169
N          -2.055793        1.153950       -0.304499
H          -2.069264        1.218091       -1.323291
H          -1.070839        1.171886       -0.012697
C          -2.787527        2.270233        0.291882
H          -3.858685        2.233451       -0.038915
H          -2.342386        3.253724       -0.012856
H          -2.750758        2.182325        1.409862
```

---

## Compound_26_HEI_Conformation_13_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.48331 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.269772 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      22.4642 cm-1
2.      36.8898 cm-1
3.      57.9064 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.380031        1.458623       -0.248236
C          -1.551878        1.125780       -0.970159
C          -2.046538       -0.204485       -1.017000
O           0.296089        2.498528       -0.221682
O           0.039103        0.442991        0.624900
C           1.285816        0.617111        1.290267
C           2.454255        0.248660        0.394080
C           2.464537       -1.224652        0.051221
C           3.585073       -1.567027       -0.895702
H          -2.055877        1.933136       -1.503294
H          -1.258770       -1.004964       -1.073004
H          -2.844728       -0.371227       -1.785326
H           1.389892        1.678094        1.640952
H           1.216374       -0.076462        2.171246
H           3.407336        0.524221        0.915701
H           2.388589        0.859096       -0.545707
H           1.478015       -1.496748       -0.410685
H           2.567353       -1.828304        0.991582
```

```
H           4.574279       -1.310982       -0.444639
H           3.576708       -2.658554       -1.131126
H           3.479630       -0.998653       -1.851472
N          -2.736033       -0.526796        0.370689
H          -3.410209        0.214802        0.565363
H          -1.994481       -0.455262        1.076792
C          -3.379450       -1.837957        0.434563
H          -4.186974       -1.895447       -0.341825
H          -2.618105       -2.634912        0.224445
H          -3.829033       -2.018735        1.446223
```

---

## Compound_26_HEI_Conformation_14_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489359 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.275248 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.3345 cm-1
2.      37.5317 cm-1
3.      53.0947 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.536908       -0.635811        0.190653
C           1.664116       -1.264790       -0.381526
C           2.964555       -0.841583        0.043082
O           0.514037        0.439592        0.844690
O          -0.676051       -1.248128       -0.046046
C          -1.843621       -0.621630        0.484754
C          -2.331103        0.480157       -0.439508
C          -3.642702        1.069537        0.030203
C          -4.819922        0.173139       -0.257217
H           1.542560       -2.065853       -1.107534
H           3.109787       -0.805966        1.159519
H           3.799427       -1.412505       -0.439923
H          -2.584941       -1.463862        0.540186
H          -1.640118       -0.216538        1.509963
H          -2.440474        0.074102       -1.478498
H          -1.546189        1.282048       -0.470297
H          -3.799628        2.056116       -0.482322
H          -3.586853        1.276156        1.132001
```

```
H          -5.767092        0.654452        0.087079
H          -4.904407       -0.028029       -1.352648
H          -4.711103       -0.805747        0.269539
N           3.148695        0.658171       -0.353430
H           2.411027        1.169316        0.159946
H           2.944189        0.750697       -1.349461
C           4.469119        1.203663       -0.041253
H           4.529522        2.286674       -0.327314
H           5.254005        0.629679       -0.600338
H           4.661437        1.104257        1.059828
```

---

### Compound_26_HEI_Conformation_15_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489843 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.275689 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.2878 cm-1
2.      37.3669 cm-1
3.      51.7502 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.522495       -0.457232       -0.081652
C           1.639798       -1.269263        0.210945
C           2.823221       -0.637926        0.712613
O           0.502849        0.795394       -0.207185
O          -0.659167       -1.126515       -0.322128
C          -1.801768       -0.341103       -0.661773
C          -2.451191        0.233135        0.584568
C          -3.734435        0.966900        0.263969
C          -4.881336        0.034099       -0.030195
H           1.590768       -2.347994        0.078659
H           2.656121        0.058026        1.582388
H           3.649595       -1.358810        0.944313
H          -1.516656        0.478165       -1.371803
H          -2.478271       -1.078901       -1.171601
H          -1.720831        0.938623        1.063873
H          -2.650908       -0.593446        1.314818
H          -3.567882        1.647175       -0.613068
H          -4.005988        1.617233        1.138052
```

```
H          -5.811222        0.616232       -0.239396
H          -4.657078       -0.602274       -0.920271
H          -5.074922       -0.639250        0.839704
N           3.362617        0.337815       -0.381517
H           3.462561       -0.185661       -1.252412
H           2.608998        1.031109       -0.525153
C           4.616462        1.002142       -0.027843
H           5.416631        0.232663        0.132497
H           4.474561        1.582247        0.922200
H           4.937279        1.704618       -0.841478
```

---

## Compound_26_HEI_Conformation_16_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.484127 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270664 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      21.4994 cm-1
2.      37.2111 cm-1
3.      55.5186 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.781856       -0.244535        0.258651
C          -1.773688       -1.234235        0.054369
C          -3.114676       -0.972741        0.449678
O          -0.920988        0.948161        0.616912
O           0.509200       -0.652493       -0.018275
C           1.533174        0.328264        0.178623
C           2.846972       -0.359529       -0.146140
C           4.002641        0.600651        0.032310
C           5.319717       -0.059298       -0.284594
H          -1.491328       -2.194866       -0.376233
H          -3.218966       -0.356851        1.383175
H          -3.755522       -1.891074        0.500187
H           1.344287        1.199864       -0.500747
H           1.504933        0.685850        1.240747
H           2.819118       -0.739536       -1.200275
H           2.976673       -1.249646        0.522773
H           4.015055        0.979245        1.088739
H           3.856640        1.490933       -0.635186
```

```
H           6.159519        0.663748       -0.147069
H           5.493583       -0.934466        0.387247
H           5.335027       -0.421608       -1.340996
N          -3.814167       -0.071139       -0.657985
H          -4.738025       -0.425084       -0.893154
H          -3.218097       -0.138023       -1.490558
C          -3.914650        1.337030       -0.257210
H          -4.288989        1.965011       -1.106730
H          -4.616902        1.432174        0.610960
H          -2.889336        1.693317        0.059808
```

---

## Compound_26_HEI_Conformation_17_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489494 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.275026 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      24.2414 cm-1
2.      34.8834 cm-1
3.      59.7834 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.480963       -0.963738        0.070426
C           1.683924       -0.974478       -0.668968
C           2.898857       -0.639803        0.008715
O           0.289620       -0.449612        1.203395
O          -0.605871       -1.538056       -0.554224
C          -1.860258       -1.528571        0.127453
C          -2.738704       -0.400079       -0.388339
C          -2.564592        0.865845        0.422362
C          -3.280366        2.032954       -0.205361
H           1.684476       -1.253702       -1.720527
H           3.057438       -1.195497        0.977078
H           3.807358       -0.716185       -0.642919
H          -2.308977       -2.524190       -0.140232
H          -1.717988       -1.459373        1.236922
H          -3.809839       -0.728520       -0.345826
H          -2.488433       -0.200900       -1.463431
H          -1.467151        1.087286        0.518405
H          -2.953209        0.698969        1.461800
```

```
H          -4.372522        1.820178       -0.303301
H          -3.154996        2.948857        0.421095
H          -2.874071        2.244380       -1.224106
N           2.837144        0.838593        0.522511
H           3.581604        1.023521        1.189571
H           1.928356        0.915831        1.009296
C           2.889904        1.810805       -0.573129
H           2.667499        2.842888       -0.196781
H           3.907361        1.793286       -1.042918
H           2.124735        1.516748       -1.344028
```

---

## Compound_26_HEI_Conformation_18_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489888 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.275336 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      24.9900 cm-1
2.      39.0569 cm-1
3.      53.5977 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.425185        0.365692       -0.171403
C           1.510477        0.269229       -1.069519
C           2.392559       -0.850936       -0.948550
O           0.265739       -0.277136        0.899270
O          -0.517896        1.323280       -0.479126
C          -1.626018        1.489639        0.405753
C          -2.840889        0.738017       -0.113345
C          -2.911030       -0.669579        0.437922
C          -3.999620       -1.472930       -0.223891
H           1.654692        1.017970       -1.845633
H           1.869789       -1.848749       -0.895979
H           3.198293       -0.868776       -1.727219
H          -1.363994        1.169082        1.447137
H          -1.813554        2.598022        0.380888
H          -2.801439        0.705453       -1.233931
H          -3.765047        1.302491        0.176986
H          -3.091955       -0.627864        1.544595
H          -1.914285       -1.167716        0.290056
```

```
H          -3.809757       -1.566489       -1.320630
H          -4.045584       -2.499134        0.214094
H          -4.994018       -0.984293       -0.082304
N           3.111852       -0.819933        0.442411
H           2.355906       -0.673044        1.132335
H           3.564374       -1.708930        0.638094
C           4.084143        0.272425        0.541433
H           3.580072        1.224950        0.217661
H           4.451384        0.380301        1.594897
H           4.950577        0.067762       -0.139471
```

---

## Compound_26_HEI_Conformation_19_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.484249 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270119 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      31.1927 cm-1
2.      38.3721 cm-1
3.      49.3935 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.705336       -0.804756        0.173019
C          -1.911321       -1.178383       -0.468522
C          -3.142914       -0.625534       -0.020746
O          -0.514802        0.094127        1.024638
O           0.407367       -1.517548       -0.234187
C           1.654971       -1.196129        0.377895
C           2.304055       -0.008441       -0.309905
C           3.696501        0.230661        0.229745
C           4.353645        1.409664       -0.440143
H          -1.883770       -1.907985       -1.277822
H          -3.207215       -0.454713        1.087540
H          -4.045037       -1.175216       -0.395763
H           1.515632       -0.991624        1.471287
H           2.263336       -2.129362        0.232692
H           1.663622        0.897443       -0.143278
H           2.346333       -0.193068       -1.414655
H           4.322363       -0.687713        0.073097
H           3.641917        0.408701        1.336520
```

```
H           5.379193        1.569399       -0.028164
H           4.437827        1.241103       -1.541039
H           3.757513        2.339342       -0.273463
N          -3.301991        0.838026       -0.622001
H          -4.232577        0.980372       -1.006536
H          -2.620451        0.902052       -1.386417
C          -3.011571        1.886390        0.363031
H          -3.003384        2.896001       -0.123590
H          -3.789169        1.870654        1.169911
H          -2.000893        1.674969        0.823831
```

---

## Compound_26_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.490988 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277796 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      21.0198 cm-1
2.      39.3134 cm-1
3.      65.0826 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.687378       -0.222391       -0.154929
C           1.690595       -1.197261        0.034372
C           3.023891       -0.886656       -0.385827
O           0.846997        1.000125       -0.410590
O          -0.611354       -0.649409        0.022704
C          -1.625662        0.350694       -0.127112
C          -2.950631       -0.353022        0.104592
C          -4.097586        0.623858       -0.035224
C          -5.425559       -0.051490        0.190740
H           1.448181       -2.165405        0.467246
H           3.109447       -0.494371       -1.438250
H           3.749707       -1.725044       -0.222913
H          -1.453949        1.166330        0.622508
H          -1.563826        0.788077       -1.157348
H          -2.955908       -0.812034        1.127187
H          -3.062387       -1.189215       -0.633573
H          -4.076755        1.081575       -1.059714
H          -3.969496        1.460153        0.702117
```

```
H          -5.473999       -0.492833        1.215611
H          -6.258763        0.684172        0.083315
H          -5.581318       -0.872276       -0.550587
N           3.534331        0.328240        0.452993
H           2.888971        1.104919        0.230319
H           3.410626        0.105839        1.441784
C           4.918479        0.709809        0.175446
H           5.599570       -0.148703        0.414467
H           5.022768        0.964440       -0.912452
H           5.216242        1.599734        0.790065
```

---

### Compound_26_HEI_Conformation_20_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.481895 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268057 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      25.6563 cm-1
2.      33.8814 cm-1
3.      59.8298 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.453190       -1.536089       -0.040953
C           1.710374       -1.286447       -0.642937
C           2.155540        0.033065       -0.920860
O          -0.177516       -2.591313        0.126886
O          -0.137852       -0.385839        0.503701
C          -1.463495       -0.501470        1.010653
C          -2.495421       -0.453309       -0.102263
C          -2.534434        0.881028       -0.815061
C          -3.278517        1.935499       -0.036705
H           2.322348       -2.152697       -0.898212
H           1.356963        0.742237       -1.272665
H           3.058293        0.083736       -1.582451
H          -1.570428       -1.455978        1.591216
H          -1.563243        0.382251        1.696924
H          -3.501922       -0.683263        0.334195
H          -2.246874       -1.263285       -0.839594
H          -3.027232        0.747012       -1.814624
H          -1.481732        1.222018       -1.005527
```

```
H          -2.801633        2.104426        0.959094
H          -3.278971        2.902770       -0.594974
H          -4.338610        1.626746        0.132553
N           2.604100        0.702694        0.441223
H           3.266779        0.073489        0.896557
H           1.763394        0.734649        1.029286
C           3.178681        2.039101        0.296046
H           3.455337        2.470687        1.293770
H           4.096043        1.982922       -0.346965
H           2.430213        2.712379       -0.199363
```

---

## Compound_26_HEI_Conformation_21_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.484612 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270439 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.9668 cm-1
2.      42.7328 cm-1
3.      49.4521 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.634148       -0.485255        0.033519
C          -1.765742       -1.177786       -0.461982
C          -2.842964       -0.442750       -1.029752
O          -0.477891        0.747081        0.196936
O           0.410995       -1.299597        0.428902
C           1.584203       -0.665372        0.935143
C           2.469982       -0.181446       -0.198424
C           3.780811        0.353353        0.333418
C           4.670340        0.840635       -0.781048
H          -1.784105       -2.267098       -0.428831
H          -2.537456        0.474546       -1.601458
H          -3.550543       -1.072798       -1.628898
H           1.309386        0.184832        1.612158
H           2.086122       -1.481150        1.522212
H           1.924156        0.620015       -0.763255
H           2.659316       -1.025682       -0.911061
H           4.308300       -0.451489        0.911035
H           3.578159        1.194541        1.048215
```

```
H           4.170672        1.659475       -1.353186
H           5.631216        1.232835       -0.368937
H           4.903201        0.010349       -1.490888
N          -3.743010        0.144771        0.142203
H          -3.479345       -0.376704        0.985709
H          -4.731685       -0.010998       -0.037705
C          -3.504698        1.574280        0.373190
H          -3.851300        2.162182       -0.515729
H          -4.052952        1.924996        1.285658
H          -2.393614        1.734919        0.508452
```

---

## Compound_26_HEI_Conformation_22_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.481397 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.267729 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.6906 cm-1
2.      37.7414 cm-1
3.      59.2864 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.617647        1.444079       -0.025140
C           2.028195        1.386144        0.080816
C           2.775885        0.307417       -0.461698
O          -0.185093        2.354893        0.230954
O           0.042456        0.235956       -0.448061
C          -1.361131        0.221133       -0.685023
C          -2.120340       -0.044388        0.603667
C          -3.607131       -0.183429        0.363040
C          -3.978494       -1.510358       -0.247848
H           2.523924        2.213944        0.589946
H           2.407091       -0.081788       -1.449733
H           3.882107        0.483587       -0.487857
H          -1.690412        1.192028       -1.140058
H          -1.502277       -0.616256       -1.420386
H          -1.928652        0.814265        1.301903
H          -1.721777       -0.971869        1.090268
H          -3.956637        0.649266       -0.303547
H          -4.143512       -0.067862        1.342662
```

```
H          -3.489821       -1.639953       -1.243775
H          -3.656853       -2.352687        0.411365
H          -5.084550       -1.576204       -0.388397
N           2.579389       -0.952402        0.475054
H           2.799830       -0.669888        1.431046
H           1.576463       -1.170070        0.446864
C           3.368302       -2.120684        0.087818
H           3.170386       -2.986823        0.772578
H           3.103030       -2.415585       -0.961755
H           4.459430       -1.863572        0.126562
```

---

## Compound_26_HEI_Conformation_23_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.481409 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.267823 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      28.6360 cm-1
2.      33.3447 cm-1
3.      56.2703 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.561009        1.374588       -0.111257
C          -1.902256        1.375979        0.342703
C          -2.528590        0.199088        0.831466
O           0.199487        2.307267       -0.413241
O          -0.040045        0.085400       -0.299940
C           1.334996       -0.025927       -0.652140
C           2.218698        0.099814        0.576223
C           3.679177       -0.110446        0.243934
C           4.022344       -1.559626        0.011514
H          -2.436917        2.326540        0.313026
H          -1.870170       -0.474227        1.445276
H          -3.507697        0.380012        1.345307
H           1.412232       -1.050703       -1.105741
H           1.605544        0.752686       -1.413142
H           1.889564       -0.638759        1.352165
H           2.072392        1.127777        1.004522
H           4.301617        0.282013        1.092055
H           3.946112        0.490644       -0.665594
```

```
H           5.112342       -1.669928       -0.205640
H           3.779043       -2.172452        0.913074
H           3.448696       -1.969730       -0.854613
N          -2.875454       -0.727854       -0.403555
H          -3.398060       -0.167995       -1.078695
H          -1.976452       -0.965558       -0.838180
C          -3.614212       -1.941240       -0.058404
H          -3.810408       -2.567519       -0.968095
H          -3.017217       -2.541681        0.677811
H          -4.592862       -1.660857        0.412556
```

---

## Compound_26_HEI_Conformation_24_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.484417 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270056 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      24.8196 cm-1
2.      37.6011 cm-1
3.      62.1064 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.555571       -0.865278        0.033643
C           1.552155       -0.872096       -0.972557
C           2.896615       -0.560512       -0.628378
O           0.639296       -0.467044        1.218641
O          -0.678666       -1.335016       -0.375961
C          -1.728146       -1.356626        0.590663
C          -2.412806       -0.006524        0.705392
C          -3.153745        0.361745       -0.561023
C          -3.761773        1.737029       -0.470166
H           1.281876       -1.145526       -1.992453
H           3.218455       -0.920161        0.385874
H           3.640981       -0.853469       -1.413684
H          -2.431898       -2.134889        0.189169
H          -1.328716       -1.671940        1.590134
H          -1.636619        0.770401        0.934679
H          -3.128041       -0.039827        1.567938
H          -3.959705       -0.394347       -0.756139
H          -2.440954        0.313609       -1.426977
```

```
H          -2.970117        2.508341       -0.309445
H          -4.308409        1.984017       -1.412078
H          -4.482392        1.794643        0.381302
N           3.049749        1.018317       -0.517514
H           3.881550        1.343868       -1.003575
H           2.224946        1.412822       -0.983398
C           3.078942        1.485284        0.873450
H           4.010850        1.116460        1.374915
H           2.180083        1.061137        1.412638
H           3.053946        2.604988        0.916116
```

---

## Compound_26_HEI_Conformation_25_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482647 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268888 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      21.7506 cm-1
2.      29.7361 cm-1
3.      59.4604 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.808871        1.472674        0.256931
C          -2.125685        0.995105        0.052297
C          -2.411067       -0.028429       -0.888285
O          -0.377299        2.441448        0.901402
O           0.173135        0.666657       -0.337432
C           1.521726        1.120142       -0.213971
C           2.399539        0.131372       -0.961072
C           2.506870       -1.207640       -0.262385
C           3.448433       -1.176215        0.913895
H          -2.918526        1.451312        0.646874
H          -1.822356        0.036004       -1.845221
H          -3.503013       -0.171022       -1.093087
H           1.603878        2.146249       -0.659862
H           1.791539        1.176511        0.873214
H           3.418505        0.586007       -1.072196
H           1.978346       -0.022887       -1.989147
H           2.862953       -1.977128       -0.998047
H           1.484954       -1.521231        0.081201
```

```
H           4.479076       -0.897142        0.585840
H           3.109310       -0.430284        1.673171
H           3.494154       -2.179864        1.401553
N          -1.911212       -1.428042       -0.329151
H          -1.876168       -2.127191       -1.066186
H          -0.955298       -1.259857        0.009367
C          -2.740611       -1.909335        0.778009
H          -2.277878       -2.806346        1.265567
H          -2.840342       -1.080647        1.532119
H          -3.759348       -2.177085        0.394628
```

---

## Compound_26_HEI_Conformation_26_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.484773 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270369 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      25.8481 cm-1
2.      35.3090 cm-1
3.      61.5707 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.486121       -0.027680       -0.341644
C          -1.380583        1.013424       -0.690689
C          -2.488044        1.297763        0.155322
O          -0.596664       -0.885729        0.564761
O           0.629876       -0.123456       -1.152134
C           1.575833       -1.148723       -0.850691
C           2.510513       -0.738207        0.272457
C           3.413258        0.405939       -0.133073
C           4.282313        0.859865        1.010637
H          -1.192678        1.602877       -1.588043
H          -2.287621        1.167843        1.252855
H          -2.968357        2.289392       -0.051031
H           1.043970       -2.098661       -0.581327
H           2.133284       -1.275289       -1.817834
H           3.129480       -1.625452        0.566076
H           1.892699       -0.441588        1.161220
H           2.778887        1.258903       -0.494358
H           4.058790        0.087059       -0.993803
```

```
H           4.926403        0.022770        1.373938
H           4.943973        1.699187        0.687009
H           3.655549        1.214068        1.864612
N          -3.641463        0.240690       -0.129126
H          -4.545612        0.696626       -0.222630
H          -3.403789       -0.198290       -1.025656
C          -3.719771       -0.799211        0.903386
H          -4.044236       -0.342406        1.873947
H          -2.691424       -1.250294        1.036076
H          -4.449170       -1.597126        0.607595
```

---

## Compound_26_HEI_Conformation_27_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482062 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268882 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      20.3554 cm-1
2.      26.5524 cm-1
3.      59.0917 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.820799        1.366485        0.093865
C          -2.184491        1.096610       -0.173973
C          -2.586185       -0.015780       -0.957637
O          -0.265508        2.348325        0.611251
O           0.034369        0.306819       -0.242738
C           1.432190        0.550292       -0.079040
C           2.153151       -0.668495       -0.628504
C           3.655394       -0.514284       -0.526915
C           4.165370       -0.703884        0.878630
H          -2.919253        1.786031        0.244619
H          -1.917454       -0.238004       -1.834945
H          -3.663493        0.003167       -1.263504
H           1.715576        1.481224       -0.636466
H           1.649652        0.703517        1.010495
H           1.861980       -0.809480       -1.702376
H           1.822086       -1.582423       -0.070573
H           3.953561        0.501140       -0.900912
H           4.141307       -1.270377       -1.199869
```

```
H           3.897308       -1.717706        1.263045
H           5.277166       -0.600438        0.903485
H           3.725425        0.058898        1.565950
N          -2.421700       -1.352305       -0.115125
H          -1.490602       -1.288303        0.314112
H          -2.447229       -2.172055       -0.715640
C          -3.433639       -1.471274        0.937065
H          -4.441747       -1.626398        0.472118
H          -3.202635       -2.328695        1.621159
H          -3.446577       -0.513135        1.526125
```

---

## Compound_26_HEI_Conformation_28_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.479942 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.26637 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      17.7248 cm-1
2.      44.3874 cm-1
3.      49.3882 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.442462        1.705150        0.175685
C          -1.744450        1.329318        0.585749
C          -2.092979       -0.029274        0.808294
O           0.102949        2.816247        0.088739
O           0.339393        0.622163       -0.252746
C           1.697633        0.915595       -0.583185
C           2.379632       -0.396635       -0.933178
C           2.931451       -1.126211        0.273435
C           1.849317       -1.776711        1.096111
H          -2.470804        2.129209        0.735895
H          -1.291481       -0.655525        1.288691
H          -3.077744       -0.172533        1.322922
H           1.707456        1.617227       -1.459527
H           2.188742        1.423316        0.287580
H           3.223520       -0.164421       -1.635483
H           1.656472       -1.059632       -1.475906
H           3.506524       -0.406017        0.914155
H           3.655965       -1.909950       -0.074734
```

```
H           1.066087       -1.024991        1.366461
H           1.360619       -2.600786        0.522016
H           2.276836       -2.205962        2.033822
N          -2.253858       -0.737034       -0.597969
H          -2.891099       -0.172709       -1.161764
H          -1.330325       -0.689007       -1.044076
C          -2.716599       -2.121936       -0.526950
H          -2.790481       -2.576268       -1.549880
H          -1.996019       -2.722110        0.089158
H          -3.725248       -2.153669       -0.037267
```

---

## Compound_26_HEI_Conformation_29_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.483314 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.269775 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      22.4718 cm-1
2.      36.8943 cm-1
3.      57.8859 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.379935        1.458473       -0.248213
C          -1.551702        1.125808       -0.970356
C          -2.046564       -0.204409       -1.017151
O           0.296369        2.498251       -0.221511
O           0.038844        0.442744        0.625009
C           1.285485        0.616646        1.290569
C           2.454047        0.248616        0.394369
C           2.464504       -1.224577        0.051002
C           3.585215       -1.566535       -0.895866
H          -2.055468        1.933195       -1.503653
H          -1.258892       -1.004987       -1.073148
H          -2.844768       -0.371054       -1.785482
H           1.389463        1.677499        1.641677
H           1.215971       -0.077281        2.171262
H           3.407051        0.524095        0.916171
H           2.388394        0.859380       -0.545208
H           1.478079       -1.496600       -0.411157
H           2.567221       -1.828547        0.991169
```

```
H           4.574330       -1.310570       -0.444559
H           3.576974       -2.657980       -1.131672
H           3.479878       -0.997836       -1.851453
N          -2.736032       -0.526577        0.370514
H          -3.410276        0.214980        0.565126
H          -1.994472       -0.454890        1.076605
C          -3.379291       -1.837798        0.434588
H          -4.186918       -1.895453       -0.341680
H          -2.617882       -2.634682        0.224440
H          -3.828713       -2.018538        1.446326
```

---

## Compound_26_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491157 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277649 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      19.0987 cm-1
2.      41.0507 cm-1
3.      56.8223 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.570521        0.153310        0.354163
C          -1.409140       -0.951603        0.616196
C          -2.816254       -0.718038        0.743765
O          -0.914658        1.296972       -0.044971
O           0.782875       -0.068165        0.493673
C           1.634678        1.041707        0.183892
C           3.061322        0.578027        0.414810
C           3.536382       -0.352144       -0.680116
C           4.941390       -0.833716       -0.427781
H          -0.990748       -1.948089        0.740230
H          -3.096225        0.111166        1.452889
H          -3.402858       -1.644144        0.977166
H           1.464085        1.351259       -0.879894
H           1.373539        1.899294        0.857680
H           3.125637        0.055546        1.405016
H           3.720364        1.483967        0.459227
H           3.490892        0.177636       -1.668232
H           2.836430       -1.227652       -0.740356
```

```
H           4.998372       -1.394135        0.536720
H           5.272867       -1.512852       -1.249902
H           5.650833        0.027332       -0.374079
N          -3.350322       -0.170743       -0.618300
H          -3.062766       -0.816759       -1.354800
H          -2.843456        0.717067       -0.774049
C          -4.796149        0.045874       -0.652546
H          -5.325677       -0.926318       -0.472247
H          -5.082532        0.770834        0.154708
H          -5.112482        0.460107       -1.645892
```

---

## Compound_26_HEI_Conformation_30_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482778 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.269143 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      22.7696 cm-1
2.      25.1803 cm-1
3.      53.9174 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.711035       -0.407933        0.222992
C           1.783040       -1.223849       -0.213265
C           3.106798       -0.926333        0.213111
O           0.751342        0.682176        0.839659
O          -0.545288       -0.869275       -0.120972
C          -1.648872       -0.063277        0.306563
C          -2.902284       -0.783999       -0.157571
C          -4.153402       -0.048973        0.272039
C          -4.413627        1.186529       -0.551106
H           1.576438       -2.086637       -0.846395
H           3.185952       -0.527823        1.260270
H           3.832063       -1.764540        0.045928
H          -1.620371        0.040595        1.422489
H          -1.560881        0.955286       -0.153387
H          -2.905527       -1.819146        0.274378
H          -2.878791       -0.890377       -1.273125
H          -4.070867        0.231977        1.355534
H          -5.029305       -0.745030        0.176989
```

```
H          -3.574191        1.915948       -0.446535
H          -4.517464        0.925665       -1.632174
H          -5.355974        1.683643       -0.216166
N           3.679846        0.265318       -0.670852
H           4.623728        0.065955       -0.992437
H           3.063579        0.328252       -1.488903
C           3.662867        1.550711        0.036979
H           3.947460        2.386837       -0.653008
H           2.620535        1.724154        0.439474
H           4.382925        1.517551        0.895082
```

---

## Compound_26_HEI_Conformation_31_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.488553 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.274139 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      20.9665 cm-1
2.      45.1392 cm-1
3.      50.3046 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.297623       -0.530102        0.476866
C          -1.222747        0.233206        1.221987
C          -2.618025        0.062283        0.948677
O          -0.515520       -1.163535       -0.588955
O           0.997999       -0.531216        0.949901
C           1.971457       -1.259037        0.200383
C           2.523243       -0.447567       -0.959597
C           3.599851        0.535227       -0.551890
C           3.044742        1.722769        0.191275
H          -0.881232        0.914047        1.998720
H          -2.970860       -1.007401        0.938787
H          -3.280629        0.684509        1.604474
H           2.767796       -1.479247        0.961597
H           1.524937       -2.215398       -0.180174
H           1.674567        0.094986       -1.452919
H           2.951498       -1.162984       -1.710593
H           4.135886        0.889758       -1.472507
H           4.358541        0.013375        0.090047
```

```
H           3.872802        2.375537        0.558088
H           2.385126        2.329746       -0.474785
H           2.437266        1.381621        1.066251
N          -2.889514        0.504585       -0.524575
H          -2.515182        1.446514       -0.647505
H          -2.320934       -0.130271       -1.109990
C          -4.296938        0.449387       -0.917901
H          -4.422241        0.755172       -1.989902
H          -4.678104       -0.598118       -0.788726
H          -4.896233        1.137073       -0.265210
```

---

### Compound_26_HEI_Conformation_32_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.489049 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.274935 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      19.9492 cm-1
2.      27.1789 cm-1
3.      63.4560 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.511910       -0.596830        0.212239
C           1.431112        0.065805        1.053864
C           2.810345       -0.307772        0.976930
O           0.771570       -1.306323       -0.795092
O          -0.822318       -0.390137        0.492222
C          -1.754310       -1.033777       -0.386112
C          -3.146543       -0.731718        0.141608
C          -3.731468        0.548578       -0.416559
C          -3.100424        1.775058        0.190761
H           1.091550        0.823150        1.757201
H           2.993703       -1.418681        1.040617
H           3.461083        0.241117        1.705710
H          -1.603711       -0.645332       -1.426674
H          -1.552226       -2.137353       -0.380485
H          -3.112631       -0.673163        1.261356
H          -3.811820       -1.590550       -0.138526
H          -4.836277        0.560410       -0.217736
H          -3.597084        0.568237       -1.530634
```

```
H          -3.358601        1.853562        1.274501
H          -1.986977        1.718995        0.103699
H          -3.459496        2.696686       -0.326667
N           3.372061        0.003132       -0.451488
H           4.269101       -0.452459       -0.596799
H           2.682576       -0.404442       -1.105713
C           3.492258        1.442464       -0.700876
H           2.515300        1.930950       -0.430529
H           4.304699        1.869287       -0.057468
H           3.725095        1.638484       -1.779608
```

---

## Compound_26_HEI_Conformation_33_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.488918 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.274445 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      22.8948 cm-1
2.      41.2396 cm-1
3.      51.3910 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.291875       -0.092073        0.370652
C           1.193457        0.950504        0.677055
C           2.381986        1.072102       -0.112515
O           0.512117       -1.103572       -0.345936
O          -0.940778       -0.019621        0.985031
C          -1.864319       -1.079365        0.732931
C          -2.599001       -0.897700       -0.584165
C          -3.763970        0.064875       -0.497998
C          -3.318104        1.500768       -0.397143
H           0.976186        1.653694        1.478191
H           2.212778        1.068918       -1.226145
H           3.025418        1.941748        0.180731
H          -1.325750       -2.063635        0.737174
H          -2.567088       -1.018142        1.607268
H          -2.981201       -1.901281       -0.909562
H          -1.865426       -0.546086       -1.356953
H          -4.398567       -0.193890        0.391010
H          -4.407320       -0.061707       -1.409410
```

```
H          -4.196416        2.172104       -0.241591
H          -2.609351        1.626486        0.458837
H          -2.793164        1.815479       -1.331280
N           3.240125       -0.217768        0.086565
H           2.649691       -0.994626       -0.255699
H           3.374320       -0.358304        1.088921
C           4.524848       -0.197600       -0.611761
H           5.144706        0.656882       -0.232657
H           5.080877       -1.158148       -0.448722
H           4.348090       -0.058632       -1.711165
```

---

## Compound_26_HEI_Conformation_34_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.476544 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.263489 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      16.1464 cm-1
2.      31.7697 cm-1
3.      38.4233 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.942881        1.477744       -0.065718
C           2.295098        1.225689        0.275589
C           2.701059       -0.017786        0.825974
O           0.366585        2.519256       -0.416510
O           0.141910        0.328512       -0.047757
C          -1.249780        0.523883       -0.301238
C          -1.913459       -0.829294       -0.109365
C          -3.396775       -0.765396       -0.402479
C          -4.176483       -0.093482        0.698569
H           3.010329        2.032468        0.109405
H           1.962192       -0.481173        1.533555
H           3.729896       -0.011579        1.268371
H          -1.655181        1.288656        0.411422
H          -1.381299        0.902706       -1.348625
H          -1.741653       -1.182009        0.940702
H          -1.427194       -1.573574       -0.793572
H          -3.782132       -1.810774       -0.541475
H          -3.564906       -0.219683       -1.368781
```

```
H          -3.837564        0.961987        0.836385
H          -5.265421       -0.084415        0.450655
H          -4.039508       -0.634058        1.666295
N           2.778456       -1.090476       -0.355021
H           2.414338       -0.604625       -1.184628
H           3.742162       -1.356249       -0.539415
C           1.972327       -2.288538       -0.108517
H           0.897789       -1.973370        0.020995
H           2.047872       -3.006078       -0.966788
H           2.323924       -2.793970        0.827886
```

---

## Compound_26_HEI_Conformation_35_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.483836 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270342 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      21.0386 cm-1
2.      39.7431 cm-1
3.      57.3570 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.075479       -1.464913        0.117842
C          -2.262119       -0.758289       -0.192512
C          -2.250380        0.393043       -1.022181
O          -0.891637       -2.556715        0.678366
O           0.091890       -0.769207       -0.229680
C           1.325808       -1.449118        0.002649
C           2.441010       -0.527231       -0.457512
C           2.612539        0.657593        0.468169
C           3.686854        1.594836       -0.018438
H          -3.193199       -1.139487        0.229394
H          -1.542295        0.335162       -1.894991
H          -3.266805        0.733744       -1.346976
H           1.413263       -1.690309        1.094582
H           1.329246       -2.407416       -0.580316
H           2.221925       -0.165808       -1.495887
H           3.391957       -1.120126       -0.494759
H           2.866022        0.293711        1.498981
H           1.634660        1.203998        0.544373
```

```
H           3.436860        1.991447       -1.032196
H           3.797936        2.458065        0.681200
H           4.668788        1.066354       -0.083861
N          -1.638259        1.623873       -0.228015
H          -0.777263        1.266982        0.205581
H          -1.393441        2.382910       -0.858275
C          -2.541469        2.112341        0.816491
H          -2.871186        1.234921        1.438409
H          -3.442544        2.582265        0.343491
H          -2.028726        2.864273        1.470822
```

---

## Compound_26_HEI_Conformation_36_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.483464 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.270165 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      18.0101 cm-1
2.      35.6893 cm-1
3.      54.0314 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.914089        1.434408       -0.208706
C          -2.037588        0.754648       -0.737690
C          -1.975382       -0.614308       -1.105828
O          -0.716080        2.637545        0.022167
O           0.131301        0.576250        0.163069
C           1.334479        1.203873        0.608049
C           2.370900        0.110967        0.799440
C           2.866980       -0.433893       -0.522244
C           3.853859       -1.555198       -0.327057
H          -2.956824        1.329877       -0.857421
H          -1.006514       -0.927022       -1.585752
H          -2.855966       -0.970889       -1.699009
H           1.665245        1.957879       -0.153293
H           1.126002        1.734522        1.574470
H           1.929876       -0.720959        1.407808
H           3.228620        0.540425        1.380172
H           3.346548        0.393086       -1.110027
H           1.988366       -0.794940       -1.120235
```

```
H           3.385010       -2.403237        0.228358
H           4.210628       -1.935337       -1.314621
H           4.739519       -1.204123        0.256073
N          -1.964308       -1.520559        0.198324
H          -1.663554       -2.468083       -0.013905
H          -1.271976       -1.088130        0.822059
C          -3.268183       -1.546963        0.865048
H          -4.006724       -2.093747        0.223093
H          -3.198018       -2.050339        1.864149
H          -3.617704       -0.486629        1.001863
```

---

## Compound_26_HEI_Conformation_37_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.483203 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268865 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.1108 cm-1
2.      31.4144 cm-1
3.      49.2600 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.573638       -0.543559        0.056246
C          -1.775575       -1.267897       -0.135147
C          -2.881228       -0.634945       -0.767349
O          -0.357942        0.678281       -0.117904
O           0.478650       -1.294669        0.545946
C           1.721386       -0.627010        0.759879
C           2.497323       -0.503480       -0.539264
C           3.904101        0.003129       -0.310617
C           3.945438        1.473037        0.020318
H          -1.828321       -2.310534        0.178173
H          -2.607221        0.089027       -1.581211
H          -3.670607       -1.350901       -1.115017
H           1.550180        0.381789        1.217734
H           2.252610       -1.297950        1.487788
H           1.939793        0.189007       -1.223992
H           2.536905       -1.508693       -1.035307
H           4.508903       -0.181393       -1.238473
H           4.385125       -0.582330        0.517461
```

```
H           3.383848        1.682200        0.962854
H           5.001206        1.811049        0.155593
H           3.483165        2.073964       -0.799894
N          -3.629480        0.281988        0.295071
H          -4.636591        0.146844        0.255524
H          -3.295412       -0.026155        1.215059
C          -3.317798        1.706338        0.128742
H          -3.737081        2.072372       -0.843963
H          -3.752196        2.307781        0.968827
H          -2.193673        1.827438        0.112163
```

---

## Compound_26_HEI_Conformation_38_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482589 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268188 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      27.5403 cm-1
2.      37.1899 cm-1
3.      43.6322 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.649809       -0.657647        0.263841
C           1.796515       -1.287364       -0.278643
C           3.089979       -0.845924        0.114991
O           0.580769        0.379831        0.962846
O          -0.548417       -1.265868       -0.061486
C          -1.743473       -0.687190        0.460320
C          -2.212392        0.462200       -0.414461
C          -3.549267        1.005596        0.039172
C          -4.701510        0.113417       -0.345949
H           1.673154       -2.122647       -0.967951
H           3.169332       -0.515922        1.185700
H           3.909101       -1.565404       -0.145764
H          -2.474775       -1.539671        0.437809
H          -1.584437       -0.341432        1.514847
H          -2.276994        0.118083       -1.479211
H          -1.438984        1.274427       -0.367249
H          -3.701590        2.019239       -0.419054
H          -3.537612        1.146119        1.152678
```

```
H          -4.742097       -0.022543       -1.453843
H          -4.598014       -0.893927        0.125298
H          -5.667884        0.561265       -0.009956
N           3.456866        0.471156       -0.697272
H           2.797026        0.508729       -1.482205
H           4.401216        0.423446       -1.071498
C           3.308148        1.689158        0.107700
H           2.274523        1.691584        0.566144
H           4.070059        1.692613        0.929551
H           3.444248        2.602777       -0.527091
```

---

## Compound_26_HEI_Conformation_39_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.48155 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268014 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      24.0984 cm-1
2.      30.8958 cm-1
3.      58.9464 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.387701        1.218473       -0.067775
C           1.722833        1.445734        0.345707
C           2.555494        0.389992        0.802046
O          -0.529359        2.009748       -0.336414
O           0.088210       -0.139552       -0.254968
C          -1.257982       -0.482560       -0.566917
C          -2.106444       -0.532990        0.691329
C          -3.493649       -1.069427        0.415487
C          -4.369858       -0.071765       -0.297844
H           2.086617        2.473720        0.310776
H           2.041003       -0.389649        1.427408
H           3.505125        0.732066        1.288455
H          -1.684908        0.248170       -1.303236
H          -1.172642       -1.498695       -1.038489
H          -2.167287        0.502197        1.120924
H          -1.597222       -1.183193        1.449938
H          -3.973293       -1.347163        1.392005
H          -3.420102       -2.009101       -0.193960
```

```
H          -3.937196        0.195905       -1.292170
H          -5.389909       -0.496888       -0.458848
H          -4.466798        0.865752        0.301645
N           3.016347       -0.456491       -0.453397
H           2.157764       -0.841169       -0.863831
H           3.414696        0.188517       -1.137245
C           3.961209       -1.528381       -0.144436
H           3.498134       -2.226863        0.601635
H           4.233141       -2.105833       -1.066861
H           4.891825       -1.088354        0.301110
```

---

## Compound_26_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491158 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277614 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      19.2164 cm-1
2.      38.4328 cm-1
3.      57.6370 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.557969        0.035299       -0.012276
C           1.390121       -1.068076        0.275655
C           2.712679       -1.079777       -0.273358
O           0.903329        1.152167       -0.480245
O          -0.772967       -0.109134        0.316318
C          -1.608245        1.026949        0.061514
C          -3.014245        0.641614        0.483954
C          -3.656095       -0.312147       -0.500026
C          -5.037628       -0.718585       -0.057651
H           1.024602       -1.895196        0.880389
H           2.767686       -0.877977       -1.380185
H           3.294051       -2.003075       -0.016886
H          -1.230271        1.897172        0.659534
H          -1.556219        1.285574       -1.027908
H          -3.624863        1.578676        0.562072
H          -2.980117        0.166357        1.499049
H          -3.003561       -1.219885       -0.602427
H          -3.710615        0.172510       -1.510586
```

```
H          -4.998566       -1.234820        0.932065
H          -5.700594        0.175007        0.040202
H          -5.493684       -1.416165       -0.800892
N           3.501033        0.133859        0.314605
H           2.982371        0.973049        0.004629
H           3.432136        0.094186        1.332516
C           4.898895        0.203547       -0.109215
H           5.401689        1.106751        0.326460
H           5.439879       -0.719169        0.228418
H           4.945251        0.262785       -1.228849
```

---

### Compound_26_HEI_Conformation_40_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.481898 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.268059 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      25.6532 cm-1
2.      33.8835 cm-1
3.      59.8330 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.453314        1.536190       -0.040924
C          -1.710510        1.286437       -0.642863
C          -2.155564       -0.033122       -0.920806
O           0.177248        2.591486        0.126989
O           0.137888        0.385940        0.503588
C           1.463542        0.501630        1.010488
C           2.495440        0.453330       -0.102450
C           2.534458       -0.881106       -0.815066
C           3.278460       -1.935491       -0.036516
H          -2.322576        2.152633       -0.898102
H          -1.356954       -0.742182       -1.272766
H          -3.058391       -0.083842       -1.582293
H           1.570504        1.456200        1.590946
H           1.563313       -0.382019        1.696853
H           3.501946        0.683349        0.333968
H           2.246887        1.263205       -0.839888
H           3.027319       -0.747241       -1.814618
H           1.481760       -1.222097       -1.005554
```

```
H           2.801489       -2.104271        0.959268
H           3.278938       -2.902837       -0.594655
H           4.338545       -1.626735        0.132787
N          -2.603883       -0.702882        0.441255
H          -1.763068       -0.734913        1.029164
H          -3.266464       -0.073705        0.896775
C          -3.178514       -2.039259        0.296029
H          -2.430121       -2.712515       -0.199526
H          -3.455065       -2.470924        1.293750
H          -4.095952       -1.983000       -0.346868
```

---

## Compound_26_HEI_Conformation_41_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.480193 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.266105 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      19.5477 cm-1
2.      43.6503 cm-1
3.      59.7535 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.217068       -1.284538        0.057481
C          -1.566103       -1.527588       -0.296504
C          -2.628557       -0.733125        0.211872
O           0.812055       -1.945504       -0.151664
O          -0.032364       -0.056791        0.710186
C           1.262805        0.263927        1.205626
C           1.928038        1.296850        0.308024
C           2.700306        0.664654       -0.831371
C           4.086503        0.241583       -0.417717
H          -1.761223       -2.361256       -0.972573
H          -2.522630       -0.424197        1.287588
H          -3.648881       -1.151785        0.013860
H           1.069374        0.700586        2.223569
H           1.898804       -0.655079        1.301587
H           2.616104        1.923307        0.933591
H           1.138766        1.976183       -0.108840
H           2.775458        1.397286       -1.677721
H           2.132081       -0.232119       -1.203472
```

```
H           4.036877       -0.502527        0.414082
H           4.618339       -0.230392       -1.278832
H           4.684546        1.118954       -0.071124
N          -2.601709        0.663051       -0.529885
H          -1.697123        1.088888       -0.294895
H          -2.598825        0.484499       -1.535096
C          -3.699224        1.558754       -0.168578
H          -3.676150        1.745724        0.937539
H          -4.676821        1.076926       -0.433768
H          -3.614459        2.538891       -0.707479
```

---

## Compound_26_HEI_Conformation_42_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.480413 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.266425 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      17.9453 cm-1
2.      43.6191 cm-1
3.      55.1461 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.135890       -1.514922        0.206917
C          -1.388087       -1.317018        0.838063
C          -1.989795       -0.033401        0.918529
O           0.615571       -2.501702        0.175849
O           0.280714       -0.413553       -0.556273
C           1.578395       -0.466948       -1.140303
C           2.669402       -0.101628       -0.148222
C           2.834137        1.389462        0.052532
C           1.739193        1.981832        0.901695
H          -1.870607       -2.193146        1.273673
H          -1.276569        0.818274        1.095430
H          -2.863447        0.021670        1.617717
H           1.767096       -1.494827       -1.551221
H           1.522569        0.277936       -1.979396
H           3.637200       -0.524372       -0.527768
H           2.442341       -0.599833        0.831412
H           2.855042        1.903000       -0.945336
H           3.825870        1.582670        0.542344
```

```
H           1.780351        1.569492        1.938906
H           1.843860        3.091981        0.956791
H           0.738351        1.733085        0.469504
N          -2.577455        0.328981       -0.505820
H          -3.168593       -0.446805       -0.807653
H          -1.772474        0.362076       -1.141819
C          -3.317639        1.588861       -0.550528
H          -4.193102        1.532161        0.148419
H          -2.645701        2.425151       -0.221756
H          -3.688582        1.803227       -1.587209
```

---

## Compound_26_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491014 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277188 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      31.6609 cm-1
2.      45.5394 cm-1
3.      48.3981 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.574927       -0.797671        0.104034
C          -1.748195       -1.179974       -0.582034
C          -3.003264       -0.677111       -0.110222
O          -0.447334        0.142514        0.931306
O           0.564698       -1.505622       -0.216494
C           1.779316       -1.122537        0.427390
C           2.428188        0.044566       -0.294710
C           3.791790        0.345506        0.286077
C           4.448172        1.505124       -0.417551
H          -1.697416       -1.857891       -1.431391
H          -3.181766       -0.810362        0.993940
H          -3.882664       -1.053001       -0.694712
H           1.590954       -0.867129        1.502436
H           2.413422       -2.046949        0.353670
H           1.760785        0.941320       -0.200324
H           2.519158       -0.194533       -1.386022
H           4.444439       -0.563657        0.201622
H           3.688527        0.577906        1.379209
```

```
H           3.824625        2.426865       -0.322521
H           5.452367        1.711098        0.025339
H           4.580390        1.283158       -1.504165
N          -2.994575        0.878729       -0.249535
H          -2.219807        1.203022        0.353432
H          -2.746130        1.109921       -1.212501
C          -4.251138        1.522354        0.131722
H          -5.078627        1.149960       -0.527564
H          -4.491904        1.265524        1.197232
H          -4.172885        2.636977        0.032324
```

---

## Compound_26_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491476 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277599 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      30.7906 cm-1
2.      45.1025 cm-1
3.      50.1128 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.543952        0.590607       -0.017165
C          -1.698174        1.159182        0.563972
C          -2.776867        0.287171        0.920168
O          -0.427563       -0.562031       -0.510024
O           0.551943        1.422774       -0.112216
C           1.725168        0.895618       -0.730746
C           2.526840        0.062614        0.252621
C           3.843454       -0.367686       -0.354431
C           4.649922       -1.198676        0.609830
H          -1.752965        2.228740        0.755286
H          -2.478348       -0.608701        1.534245
H          -3.639680        0.817779        1.400039
H           1.453725        0.288726       -1.633244
H           2.290499        1.816446       -1.038126
H           1.919315       -0.836090        0.539887
H           2.708895        0.657732        1.184895
H           4.433250        0.539009       -0.653945
H           3.648370       -0.958514       -1.288482
```

```
H           4.087756       -2.118745        0.901265
H           5.616309       -1.507837        0.143508
H           4.874958       -0.618433        1.537275
N          -3.320288       -0.381851       -0.382501
H          -2.524778       -0.919686       -0.766099
H          -3.537172        0.357453       -1.052482
C          -4.478690       -1.249527       -0.173199
H          -5.325514       -0.649030        0.251494
H          -4.805185       -1.716474       -1.139507
H          -4.208664       -2.061182        0.553116
```

---

## Compound_26_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482407 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.269798 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      23.3983 cm-1
2.      39.4167 cm-1
3.      49.9967 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.000554        1.580233       -0.007774
C          -2.335191        1.165423        0.217663
C          -2.643450       -0.132138        0.705067
O          -0.520008        2.694544       -0.266440
O          -0.076735        0.524727        0.017433
C           1.297651        0.887742       -0.116500
C           2.105948       -0.382393        0.081838
C           3.584697       -0.093559       -0.057944
C           4.410355       -1.339254        0.134136
H          -3.123529        1.890697        0.010902
H          -1.936503       -0.532720        1.481849
H          -3.708649       -0.259540        1.028336
H           1.461451        1.324605       -1.136455
H           1.555447        1.662843        0.651803
H           1.792103       -1.149106       -0.673096
H           1.891314       -0.807734        1.096426
H           3.886650        0.679669        0.697420
H           3.786745        0.340739       -1.072870
```

```
H           4.240278       -1.772795        1.149331
H           4.141688       -2.112358       -0.625847
H           5.496981       -1.104200        0.028725
N          -2.443184       -1.166038       -0.476388
H          -2.973827       -0.829090       -1.280933
H          -1.448878       -1.117582       -0.727212
C          -2.822132       -2.539029       -0.147191
H          -2.636059       -3.228187       -1.012465
H          -2.222054       -2.887781        0.734394
H          -3.910877       -2.571513        0.120693
```

---

## Compound_26_HEI_Conformation_7_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.482667 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.269501 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      20.6588 cm-1
2.      41.6179 cm-1
3.      59.0290 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -1.140885       -1.582757       -0.109368
C          -2.346981       -0.845828       -0.029218
C          -2.400195        0.438027        0.575604
O          -0.915812       -2.757446       -0.439655
O          -0.002841       -0.819709        0.190786
C           1.243325       -1.516866        0.190184
C           2.316716       -0.521581        0.593227
C           2.585046        0.493077       -0.496967
C           3.619964        1.503625       -0.076030
H          -3.242951       -1.309932       -0.443870
H          -1.769126        0.559764        1.497913
H          -3.439313        0.820310        0.747537
H           1.187438       -2.366274        0.920719
H           1.429677       -1.933532       -0.834369
H           3.255199       -1.091957        0.819404
H           2.002687        0.006656        1.530873
H           1.624287        1.014423       -0.753127
H           2.928392       -0.036302       -1.424912
```

```
H           3.282286        2.062084        0.830368
H           4.586244        0.998360        0.166355
H           3.803587        2.238953       -0.896113
N          -1.732874        1.480457       -0.410138
H          -0.749649        1.196478       -0.499357
H          -2.164846        1.363742       -1.327934
C          -1.825793        2.871254        0.030519
H          -1.342426        2.973770        1.037843
H          -1.314226        3.559282       -0.692771
H          -2.905101        3.164506        0.115645
```

---

## Compound_26_HEI_Conformation_8_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491237 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277179 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      25.4856 cm-1
2.      45.9014 cm-1
3.      61.8900 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.424246       -0.813567       -0.036572
C          -1.399311       -0.743598       -1.055320
C          -2.763192       -0.530603       -0.674290
O          -0.548935       -0.455560        1.163910
O           0.815443       -1.278014       -0.423759
C           1.840129       -1.322270        0.569483
C           2.518969        0.025359        0.734893
C           3.291043        0.425919       -0.502806
C           3.894864        1.798829       -0.361941
H          -1.120625       -0.872629       -2.098968
H          -3.143381       -1.221308        0.130186
H          -3.472051       -0.516944       -1.542395
H           1.415504       -1.663059        1.549863
H           2.554770       -2.089545        0.166143
H           3.211958       -0.028217        1.614405
H           1.735523        0.795271        0.963150
H           2.600087        0.399414       -1.387253
H           4.102558       -0.324534       -0.696616
```

```
H           3.098297        2.565366       -0.202637
H           4.593335        1.835672        0.508910
H           4.465128        2.069535       -1.283100
N          -2.868299        0.863618        0.022190
H          -2.260529        0.799284        0.856154
H          -2.456564        1.561012       -0.599582
C          -4.228506        1.243965        0.401310
H          -4.233576        2.240604        0.916163
H          -4.872215        1.298658       -0.515599
H          -4.650685        0.470487        1.096102
```

---

## Compound_26_HEI_Conformation_9_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.491642 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.277533 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 78)

```
1.      26.7818 cm-1
2.      42.2183 cm-1
3.      61.6320 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.400369       -0.413321       -0.270809
C           1.348526        0.025551       -1.220445
C           2.461614        0.799232       -0.758627
O           0.531450       -0.438707        0.981175
O          -0.768010       -0.934529       -0.786062
C          -1.735652       -1.422192        0.143849
C          -2.577869       -0.297915        0.718384
C          -3.453263        0.346919       -0.333447
C          -4.226895        1.512201        0.225988
H           1.220883       -0.201229       -2.276765
H           2.190591        1.673247       -0.101792
H           3.147893        1.128821       -1.581221
H          -2.358517       -2.120305       -0.478047
H          -1.228221       -1.984677        0.970724
H          -1.891948        0.468328        1.167759
H          -3.215351       -0.712447        1.541981
H          -4.165745       -0.415210       -0.746703
H          -2.806151        0.689563       -1.184556
```

```
H          -4.882878        1.183318        1.068064
H          -3.532079        2.297455        0.610902
H          -4.870123        1.967705       -0.565068
N           3.306475       -0.084486        0.213559
H           2.670419       -0.315929        0.995311
H           3.529313       -0.958692       -0.264539
C           4.521560        0.561188        0.708767
H           5.069434       -0.113659        1.417857
H           5.191941        0.811943       -0.154821
H           4.247360        1.509085        1.243129
```

---

## Compound_27_HEI_Conformation_11_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.149525 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.883202 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      20.2466 cm-1
2.      28.4079 cm-1
3.      35.0227 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.575963       -0.272956        0.629705
C          -1.676924       -1.052086        0.183546
C          -1.515667       -2.384604       -0.410510
C          -2.987038       -0.497443        0.365105
O          -0.591582        0.926223        0.995751
O           0.648696       -0.912150        0.634387
C           1.798392       -0.169004        1.031642
C           2.640398        0.241959       -0.185908
C           3.910840        0.907235        0.321322
H          -0.433598       -2.630900       -0.549051
H          -1.970385       -3.176967        0.237971
H          -2.017731       -2.442393       -1.411290
H          -3.115232        0.070416        1.326097
H          -3.808524       -1.248693        0.230102
H           1.516415        0.735978        1.629527
H           2.379014       -0.890195        1.668781
H           3.661642        1.814474        0.922287
H           4.490926        0.201674        0.963226
```

```
H           4.551899        1.214192       -0.539363
C           1.860038        1.222716       -1.044413
H           0.908194        0.747578       -1.385514
H           1.601587        2.133027       -0.451441
H           2.458609        1.524633       -1.936103
C           2.997345       -0.988473       -1.003138
H           2.065364       -1.527251       -1.302187
H           3.560443       -0.696386       -1.921240
H           3.629897       -1.683146       -0.400284
N          -3.241157        0.589630       -0.749826
H          -4.105857        0.402386       -1.252037
H          -2.457479        0.502793       -1.408730
C          -3.266055        1.958277       -0.218999
H          -4.132240        2.075109        0.482218
H          -2.304179        2.137899        0.346832
H          -3.359773        2.702044       -1.052240
```

---

## Compound_27_HEI_Conformation_12_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.149836 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.883344 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      19.6648 cm-1
2.      29.3498 cm-1
3.      41.2760 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.557033        0.046373       -0.167833
C           1.593446        0.960123        0.164678
C           1.508671        2.393072       -0.142048
C           2.745664        0.427401        0.830511
O           0.587474       -1.203930       -0.079935
O          -0.591174        0.607096       -0.693684
C          -1.683958       -0.254799       -1.002677
C          -2.766552       -0.193534        0.085183
C          -3.944873       -1.038818       -0.374371
H           0.453159        2.688554       -0.364772
H           1.870168        3.013054        0.717780
H           2.134725        2.658326       -1.033919
```

```
H           2.512101       -0.390756        1.564387
H           3.392942        1.214348        1.298930
H          -2.088520        0.159563       -1.965953
H          -1.343467       -1.312559       -1.148175
H          -4.351419       -0.650816       -1.338998
H          -3.629340       -2.099716       -0.520124
H          -4.756905       -1.010382        0.390987
C          -3.214763        1.244737        0.284249
H          -2.334437        1.882422        0.541966
H          -3.677706        1.639604       -0.651625
H          -3.963904        1.307798        1.108965
C          -2.218488       -0.748056        1.389120
H          -1.330662       -0.149698        1.709088
H          -2.995554       -0.706384        2.188410
H          -1.891782       -1.806940        1.251009
N           3.675989       -0.277112       -0.233477
H           4.633218        0.060358       -0.163357
H           3.303967       -0.008676       -1.152404
C           3.660842       -1.741084       -0.123415
H           4.103837       -2.049633        0.858591
H           2.587093       -2.091377       -0.170133
H           4.248035       -2.205130       -0.957740
```

---

## Compound_27_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.149612 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.884059 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      14.5222 cm-1
2.      37.8919 cm-1
3.      49.5029 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.843453       -1.390343       -0.051200
C          -2.110248       -0.811155        0.228848
C          -3.328508       -1.601168        0.002650
C          -2.193836        0.526555        0.723552
O          -0.506538       -2.553656       -0.319746
O           0.198533       -0.450659       -0.065879
```

```
C           1.516634       -0.974454       -0.223267
C           2.515484        0.160938        0.037903
C           3.918954       -0.402664       -0.131168
H          -3.982251       -1.603846        0.911820
H          -3.932767       -1.184424       -0.844945
H          -3.067485       -2.660623       -0.244305
H          -1.381542        0.810721        1.447370
H          -3.204964        0.799403        1.123575
H           1.675255       -1.815170        0.501838
H           1.625156       -1.365986       -1.268548
H           4.059012       -0.794216       -1.167177
H           4.676796        0.395308        0.055399
H           4.092188       -1.236032        0.591227
C           2.343069        0.686753        1.453298
H           1.294221        1.040634        1.602260
H           2.550971       -0.122690        2.193485
H           3.043959        1.534490        1.642003
C           2.297704        1.285901       -0.960278
H           3.023707        2.114021       -0.778743
H           2.433526        0.910673       -2.002831
H           1.260732        1.688102       -0.859788
N          -1.938020        1.515917       -0.473566
H          -2.554120        1.241983       -1.240976
H          -0.972671        1.346183       -0.782193
C          -2.127960        2.927009       -0.138733
H          -3.187448        3.093618        0.189876
H          -1.439696        3.203803        0.703037
H          -1.909434        3.582922       -1.022049
```

---

## Compound_27_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.157199 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.89128 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      18.6323 cm-1
2.      33.9374 cm-1
3.      65.9307 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.633649       -0.145905       -0.205139
C          -1.612028        0.877471       -0.180338
C          -1.314457        2.261556        0.199808
C          -2.947583        0.505807       -0.575963
O          -0.843000       -1.386404       -0.269626
O           0.682710        0.247002       -0.097560
C           1.650434       -0.808991       -0.068388
C           3.035843       -0.161588        0.053237
C           4.068694       -1.276823        0.119056
H          -1.545760        2.972883       -0.634362
H          -1.923471        2.577419        1.086755
H          -0.232826        2.375162        0.461204
H          -3.002348       -0.055093       -1.550845
H          -3.661169        1.370957       -0.580641
H           1.441626       -1.473819        0.809546
H           1.569842       -1.407446       -1.012551
H           3.884303       -1.927602        1.007137
H           4.020981       -1.906924       -0.801237
H           5.093613       -0.842417        0.201591
C           3.105049        0.677863        1.318282
H           2.316635        1.469004        1.290066
H           2.936379        0.038128        2.217268
H           4.105608        1.164216        1.406728
C           3.303336        0.714484       -1.159578
H           2.515546        1.502475       -1.237423
H           4.301705        1.205290       -1.070726
H           3.287060        0.100758       -2.091816
N          -3.495961       -0.534073        0.440899
H          -3.386932       -0.147875        1.380081
H          -2.864337       -1.350525        0.368166
C          -4.883678       -0.930340        0.200260
H          -5.549816       -0.031100        0.276215
H          -4.972949       -1.363135       -0.831238
H          -5.211407       -1.697838        0.949853
```

---

## Compound_27_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.150062 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.88387 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      21.0313 cm-1
2.      40.6684 cm-1
```

```
   3.      49.5203 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.533692       -1.254918       -0.289524
C           1.924222       -1.019653       -0.117485
C           2.745853       -2.030953        0.562287
C           2.516078        0.188167       -0.601103
O          -0.156058       -2.270108       -0.109894
O          -0.166767       -0.108002       -0.697412
C          -1.544676       -0.237565       -1.019757
C          -2.439342        0.314017        0.101146
C          -2.237982       -0.499677        1.368171
H           3.642490       -2.301417       -0.051634
H           3.116464       -1.656309        1.552003
H           2.151577       -2.961391        0.742965
H           2.106470        0.550789       -1.583064
H           3.637089        0.168019       -0.615662
H          -1.675810        0.380974       -1.949074
H          -1.812110       -1.307176       -1.227329
H          -1.172856       -0.430461        1.697642
H          -2.900522       -0.125706        2.183835
H          -2.464185       -1.576236        1.172766
C          -3.886942        0.200867       -0.353496
H          -4.047158        0.778831       -1.295060
H          -4.151078       -0.867723       -0.540196
H          -4.568579        0.604266        0.433016
C          -2.104627        1.772493        0.364149
H          -2.732900        2.172695        1.195350
H          -1.029043        1.870493        0.648572
H          -2.286805        2.385191       -0.551042
N           2.132203        1.356594        0.378413
H           2.377837        1.063758        1.325599
H           1.107924        1.435528        0.339912
C           2.757879        2.639259        0.057478
H           2.429903        3.436799        0.774823
H           3.873459        2.534022        0.108985
H           2.470081        2.941554       -0.984040
```

---

### Compound_27_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.150257 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.88416 |
| Number of Imaginary Frequencies | 0 |

## Frequencies (Top 3 out of 96)

```
1.      20.6699 cm-1
2.      31.6606 cm-1
3.      48.3727 cm-1
```

## AM1 Geometry in Cartesian Coordinates

```
C           0.474900        1.191963       -0.305555
C           1.757821        1.007504        0.277475
C           2.674524        2.151747        0.377446
C           2.149649       -0.279890        0.758311
O          -0.137954        2.219243       -0.632722
O          -0.164733       -0.021728       -0.605702
C          -1.522741        0.011595       -1.023212
C          -2.473048       -0.348488        0.129190
C          -3.880691       -0.458778       -0.436985
H           3.059645        2.269967        1.422287
H           3.562009        2.022733       -0.295570
H           2.152739        3.097822        0.087203
H           1.323550       -0.868953        1.243707
H           3.066871       -0.263565        1.402778
H          -1.792999        1.016086       -1.443170
H          -1.585983       -0.771487       -1.826997
H          -3.929758       -1.262466       -1.210250
H          -4.602616       -0.704312        0.378193
H          -4.187103        0.507244       -0.905370
C          -2.432111        0.741929        1.186764
H          -1.382726        0.882575        1.544594
H          -2.784274        1.710396        0.756488
H          -3.081566        0.471072        2.052395
C          -2.065351       -1.676974        0.743447
H          -2.741699       -1.937029        1.592284
H          -2.118814       -2.490216       -0.019335
H          -1.016894       -1.611740        1.123527
N           2.525125       -1.178374       -0.477189
H           3.201116       -0.663225       -1.043797
H           1.667014       -1.268562       -1.034089
C           3.048261       -2.498049       -0.124404
H           3.986274       -2.378842        0.479058
H           2.287497       -3.045298        0.492618
H           3.276049       -3.099048       -1.043707
```

---

## Compound_27_HEI_Conformation_6_am1

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.156979 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.890701 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      22.4358 cm-1
2.      30.1152 cm-1
3.      39.3996 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.482212        0.220653       -0.609072
C          -1.558267        1.029904       -0.167905
C          -1.368622        2.345765        0.450018
C          -2.887410        0.515084       -0.382713
O          -0.538585       -1.001637       -0.905821
O           0.751818        0.830431       -0.686543
C           1.880187        0.033111       -1.039971
C           2.738244       -0.285847        0.193826
C           3.996533       -0.998882       -0.277399
H          -1.784867        3.163611       -0.192783
H          -1.887119        2.403297        1.442387
H          -0.281137        2.553086        0.610671
H          -3.079587        0.151717       -1.431026
H          -3.691776        1.227154       -0.060662
H           1.570524       -0.914524       -1.551555
H           2.460044        0.685510       -1.747920
H           4.574237       -0.348832       -0.977435
H           4.645909       -1.246242        0.596147
H           3.732322       -1.946343       -0.805457
C           1.964581       -1.189124        1.139117
H           1.014627       -0.686480        1.444290
H           1.704195       -2.148034        0.629615
H           2.569477       -1.412247        2.049575
C           3.115104        1.002974        0.905338
H           3.737528        1.645535        0.237673
H           2.190707        1.567689        1.179602
H           3.695405        0.780794        1.832245
N          -3.060600       -0.780523        0.458755
H          -2.802588       -0.569079        1.424054
H          -2.358124       -1.444835        0.090448
C          -4.403046       -1.358931        0.395060
H          -4.655905       -1.594373       -0.672599
H          -4.456846       -2.301226        1.001301
H          -5.149241       -0.621115        0.791252
```

---

### Compound_27_HEI_Conformation_7_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.157188 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.890847 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      26.6304 cm-1
2.      30.2373 cm-1
3.      42.2842 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.469872        0.118002       -0.268066
C           1.543396        0.961004        0.111296
C           1.526754        2.415794       -0.067879
C           2.685016        0.320548        0.715743
O           0.508278       -1.136303       -0.374521
O          -0.711596        0.740163       -0.612490
C          -1.809489       -0.075035       -1.018203
C          -2.826297       -0.250132        0.119387
C          -2.187957       -1.011098        1.268915
H           1.707303        2.947600        0.901594
H           2.325037        2.745448       -0.783227
H           0.539375        2.753520       -0.469392
H           2.428526       -0.386447        1.553786
H           3.474586        1.046789        1.042634
H          -2.276416        0.505143       -1.860056
H          -1.462619       -1.076659       -1.382004
H          -1.827650       -2.008206        0.917986
H          -1.307761       -0.441041        1.654718
H          -2.921806       -1.156468        2.096376
C          -4.007816       -1.040277       -0.422917
H          -4.477516       -0.501429       -1.280443
H          -3.675230       -2.047157       -0.772018
H          -4.775793       -1.175651        0.375744
C          -3.298976        1.111208        0.601456
H          -3.825496        1.652474       -0.220685
H          -4.000512        0.996542        1.461750
H          -2.422157        1.722656        0.925532
N           3.338904       -0.623375       -0.332017
```

```
H           3.511694       -0.083528       -1.181626
H           2.616184       -1.328700       -0.556407
C           4.566936       -1.270297        0.130816
H           5.333873       -0.489162        0.375344
H           4.346970       -1.866310        1.055830
H           4.974995       -1.954970       -0.658523
```

---

## Compound_27_HEI_Conformation_8_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.149697 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.883712 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      16.3499 cm-1
2.      30.8237 cm-1
3.      39.2664 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.714667       -0.106680       -0.293627
C          -1.678972        0.934112       -0.232161
C          -1.343158        2.300038        0.187230
C          -3.020104        0.607395       -0.619718
O          -0.916459       -1.329366       -0.487065
O           0.597498        0.265993       -0.079161
C           1.565070       -0.788109       -0.134530
C           2.947745       -0.157541        0.075309
C           3.980614       -1.274194        0.042521
H          -0.240779        2.409949        0.340541
H          -1.663731        3.050360       -0.580364
H          -1.854622        2.566432        1.149080
H          -3.085835       -0.112730       -1.479629
H          -3.661685        1.509167       -0.800788
H           1.339834       -1.533659        0.671655
H           1.503723       -1.293960       -1.132884
H           3.949390       -1.805165       -0.938981
H           5.003494       -0.851430        0.187336
H           3.781715       -2.013660        0.854818
C           2.995890        0.547060        1.421028
H           2.208953        1.339031        1.460733
H           2.811203       -0.181277        2.246436
```

```
H           3.995209        1.019089        1.576169
C           3.233591        0.838872       -1.036193
H           3.232118        0.324772       -2.026982
H           2.446402        1.631362       -1.044375
H           4.230091        1.316976       -0.881585
N          -3.725644       -0.158770        0.566439
H          -4.618090        0.270411        0.799651
H          -3.098372       -0.062933        1.374222
C          -3.924264       -1.586117        0.285518
H          -4.637388       -1.706022       -0.570514
H          -2.926721       -2.035813        0.001246
H          -4.334176       -2.111545        1.186689
```

---

## Compound_27_HEI_Conformation_9_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.146389 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.879372 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 96)

```
1.      23.1018 cm-1
2.      37.2630 cm-1
3.      54.4206 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.739123       -1.131490       -0.174186
C           2.108718       -0.747003       -0.182497
C           3.097196       -1.654535        0.423577
C           2.540684        0.467558       -0.788439
O           0.200300       -2.168094        0.248041
O          -0.126109       -0.174843       -0.717449
C          -1.478119       -0.554184       -0.949105
C          -2.432831        0.109122        0.055623
C          -3.809509       -0.515706       -0.122538
H           3.922431       -1.890281       -0.295827
H           3.565500       -1.196655        1.333740
H           2.613732       -2.615582        0.730329
H           1.860894        0.860651       -1.589321
H           3.608288        0.441585       -1.136135
H          -1.701409       -0.183621       -1.986483
H          -1.598050       -1.669202       -0.906805
```

```
H          -4.147141       -0.417601       -1.182061
H          -3.780252       -1.599186        0.145302
H          -4.551197       -0.004981        0.536990
C          -2.519424        1.601380       -0.218571
H          -1.497199        2.050965       -0.220676
H          -2.988715        1.787695       -1.214430
H          -3.133463        2.105645        0.565341
C          -1.946508       -0.132174        1.474281
H          -0.998372        0.430626        1.652818
H          -2.711539        0.203481        2.213427
H          -1.735805       -1.219977        1.624121
N           2.562578        1.625131        0.302564
H           3.353730        2.248441        0.159567
H           2.675531        1.157787        1.207503
C           1.321635        2.405266        0.322378
H           1.220139        2.976306       -0.636915
H           0.452168        1.690981        0.408871
H           1.313358        3.121100        1.184827
```

---

## Compound_28_HEI_Conformation_1_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.829054 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.589156 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      19.8402 cm-1
2.      38.3979 cm-1
3.      68.5755 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.739637       -0.088454       -0.178244
C           1.674011       -1.125329        0.033840
C           3.026315       -0.914013       -0.387347
O           0.983072        1.115098       -0.456467
O          -0.585614       -0.424213        0.001912
C          -1.527554        0.640691       -0.170219
C          -2.930489        0.063181        0.055734
C          -3.934511        1.192434       -0.123740
H           3.140679       -0.549374       -1.446959
H           3.693233       -1.796272       -0.205415
```

```
H          -1.305319        1.450362        0.572512
H          -1.428676        1.054404       -1.207298
H          -3.862116        1.618374       -1.153089
H          -4.971177        0.808905        0.031789
H          -3.740934        2.007443        0.614143
C          -3.038306       -0.499170        1.463450
H          -2.272601       -1.298784        1.610664
H          -2.863054        0.305844        2.216583
H          -4.053142       -0.932233        1.631285
C          -3.206771       -1.034264       -0.958673
H          -4.220174       -1.470775       -0.791290
H          -3.159763       -0.623579       -1.995553
H          -2.441354       -1.841654       -0.859972
N           3.616021        0.279808        0.429338
H           3.025349        1.093912        0.189117
H           3.475232        0.085949        1.421837
C           5.023520        0.561109        0.149433
H           5.379511        1.440788        0.747623
H           5.644260       -0.336691        0.407692
H           5.147364        0.786555       -0.942849
H           1.365766       -2.066023        0.484852
```

---

## Compound_28_HEI_Conformation_2_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.820206 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.580778 |
| Number of Imaginary Frequencies | 0 |

### Frequencies (Top 3 out of 87)

```
1.      15.4584 cm-1
2.      40.9403 cm-1
3.      50.0618 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.799170        1.721653       -0.056634
C           2.153586        1.410751        0.214113
C           2.541728        0.139073        0.713236
O           0.241019        2.794842       -0.332215
O          -0.037059        0.594861       -0.061146
C          -1.432083        0.845707       -0.223259
C          -2.187043       -0.464257        0.039665
```

| | | | |
|---|---|---|---|
| C | -1.746081 | -1.527302 | -0.952737 |
| H | 1.837607 | -0.315566 | 1.463014 |
| H | 3.600662 | 0.092505 | 1.076186 |
| H | -1.756416 | 1.640508 | 0.498446 |
| H | -1.613788 | 1.204805 | -1.270077 |
| H | -2.292612 | -2.482963 | -0.768835 |
| H | -1.950999 | -1.191121 | -1.997312 |
| H | -0.649963 | -1.713730 | -0.848169 |
| C | -3.673749 | -0.191179 | -0.136493 |
| H | -4.011931 | 0.593823 | 0.581673 |
| H | -3.884523 | 0.161058 | -1.174637 |
| H | -4.258904 | -1.123016 | 0.051018 |
| C | -1.919482 | -0.940232 | 1.457898 |
| H | -2.286112 | -0.185064 | 2.193823 |
| H | -2.439682 | -1.909072 | 1.648349 |
| H | -0.821998 | -1.079226 | 1.611444 |
| N | 2.464362 | -0.904921 | -0.473477 |
| H | 2.977076 | -0.515605 | -1.266112 |
| H | 1.474745 | -0.950887 | -0.745226 |
| C | 2.965561 | -2.236786 | -0.138791 |
| H | 2.861207 | -2.938077 | -1.008028 |
| H | 4.047499 | -2.167086 | 0.148853 |
| H | 2.385264 | -2.643097 | 0.731286 |
| H | 2.891006 | 2.194060 | 0.033537 |

### Compound_28_HEI_Conformation_3_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.828721 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.588428 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.8451 cm-1
2.      30.3754 cm-1
3.      47.7062 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.576881       -0.621276       -0.376019
C          -1.617925       -1.274614        0.319990
C          -2.969596       -0.928146       -0.001688
O          -0.666002        0.426449       -1.067527
O           0.676046       -1.180448       -0.230747
C           1.777805       -0.541106       -0.870718
C           2.618305        0.261434        0.133891
C           3.820144        0.830307       -0.605195
H          -3.213639       -0.944368       -1.101221
H          -3.730044       -1.516362        0.574523
H           2.385677       -1.394191       -1.277981
H           1.435895        0.124529       -1.705167
H           4.463428        1.410035        0.099119
H           4.430201        0.007344       -1.048930
H           3.486366        1.510044       -1.425481
C           3.090877       -0.649767        1.254297
H           3.754875       -1.450122        0.848489
H           3.658605       -0.065946        2.017368
H           2.211626       -1.133097        1.745017
C           1.789223        1.397403        0.708298
H           1.426729        2.062276       -0.112556
H           0.897979        0.980724        1.237585
H           2.394165        1.998554        1.427425
N          -3.191435        0.576328        0.355272
H          -2.526968        1.099535       -0.239393
H          -2.906248        0.718051        1.325336
C          -4.559058        1.048169        0.141687
H          -4.647291        2.137863        0.393038
H          -4.840912        0.896220       -0.933821
H          -5.263568        0.461797        0.788148
H          -1.394548       -2.039616        1.060529
```

---

### Compound_28_HEI_Conformation_4_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.828871 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.588508 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      29.5894 cm-1
2.      29.9682 cm-1
3.      46.1465 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.579889        0.306750       -0.294364
C          -1.601532        1.237736       -0.003529
C          -2.790712        0.760799        0.635803
O          -0.674562       -0.948280       -0.297918
O           0.625133        0.852354       -0.686753
C           1.689633       -0.034889       -1.021450
C           2.702175       -0.152233        0.127474
C           3.227398        1.225862        0.493497
H          -2.615010        0.130356        1.552543
H          -3.533923        1.570227        0.856546
H           1.303266       -1.049900       -1.298380
H           2.176913        0.452172       -1.909456
H           2.375314        1.894898        0.765484
H           3.927304        1.157379        1.360020
H           3.770782        1.676113       -0.371437
C           3.851495       -1.029678       -0.345216
H           3.479837       -2.048658       -0.609507
H           4.339935       -0.582775       -1.244121
H           4.615205       -1.127344        0.462981
C           2.037961       -0.788757        1.336463
H           2.766616       -0.888539        2.175191
H           1.178725       -0.156907        1.669710
H           1.642334       -1.798935        1.071510
N          -3.492994       -0.253329       -0.322760
H          -2.813783       -1.021726       -0.453335
H          -3.615901        0.199686       -1.229495
C          -4.766949       -0.768410        0.177571
H          -4.601019       -1.274521        1.165276
```

```
H          -5.484944        0.081306        0.320911
H          -5.207598       -1.506768       -0.542881
H          -1.475129        2.291566       -0.242382
```

### Compound_28_HEI_Conformation_5_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.820629 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.58057 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      21.5424 cm-1
2.      43.5677 cm-1
3.      56.3569 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.520772        1.556312       -0.046934
C          -1.919525        1.531158        0.169660
C          -2.747658        0.524380       -0.395319
O           0.330333        2.419839        0.215565
O          -0.031120        0.368589       -0.614291
C           1.340718        0.308891       -0.978445
C           2.155951       -0.513533        0.031712
C           2.126148        0.164847        1.390728
H          -2.474354        0.211015       -1.439823
H          -3.845074        0.736317       -0.314998
H           1.345613       -0.205264       -1.977934
H           1.778780        1.337570       -1.071620
H           2.732560       -0.410104        2.129527
H           2.529807        1.203510        1.310023
H           1.072601        0.236901        1.755010
C           3.590341       -0.588242       -0.470127
H           4.027035        0.436444       -0.546436
H           4.212682       -1.189252        0.235167
H           3.627519       -1.068869       -1.477039
C           1.584835       -1.917149        0.141345
H           0.515175       -1.868540        0.458942
H           1.638708       -2.437674       -0.844712
H           2.155421       -2.512487        0.893522
N          -2.523730       -0.814955        0.413770
H          -2.653792       -0.608134        1.405066
H          -1.534804       -1.061948        0.282608
```

```
C          -3.387290       -1.919813        0.000254
H          -3.167463       -2.847106        0.591928
H          -4.460612       -1.632144        0.153197
H          -3.221155       -2.132336       -1.088869
H          -2.342715        2.328259        0.782616
```

---

### Compound_28_HEI_Conformation_6_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.822182 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.581997 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      19.2643 cm-1
2.      35.6412 cm-1
3.      56.5084 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C          -0.821849        0.123327       -0.289367
C          -1.737368        1.181305       -0.070623
C          -3.094606        1.024296       -0.466099
O          -1.050479       -1.051414       -0.660603
O           0.496610        0.432396       -0.011874
C           1.442619       -0.620933       -0.221893
C           2.838208       -0.064337        0.087091
C           3.150802        1.093368       -0.846566
H          -3.245003        0.430337       -1.407509
H          -3.666219        1.987865       -0.503104
H           1.195052       -1.475820        0.459810
H           1.378443       -0.967827       -1.285987
H           4.158486        1.514924       -0.617629
H           3.138852        0.748466       -1.908125
H           2.383629        1.895745       -0.723824
C           3.845668       -1.184098       -0.128959
H           3.807087       -1.544624       -1.184785
H           4.877231       -0.815127        0.084809
H           3.625895       -2.042849        0.549589
C           2.899467        0.408217        1.530149
H           2.131489        1.200827        1.701200
H           2.696340       -0.441527        2.224879
H           3.909187        0.824905        1.759195
```

```
N          -3.856775        0.161770        0.630973
H          -3.255073        0.171478        1.462144
H          -4.750731        0.580727        0.874735
C          -4.064024       -1.228909        0.210526
H          -4.772882       -1.258289       -0.656989
H          -3.069057       -1.657045       -0.114186
H          -4.483351       -1.838892        1.052114
H          -1.384491        2.113052        0.371122
```

---

### Compound_28_HEI_Conformation_8_am1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.82194 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.581341 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      25.3333 cm-1
  2.      31.2509 cm-1
  3.      43.4904 cm-1
```

### AM1 Geometry in Cartesian Coordinates

```
C           0.675607       -0.656046       -0.444572
C           1.738084       -1.326461        0.210241
C           3.080910       -0.949413       -0.068723
O           0.721320        0.373118       -1.157045
O          -0.570202       -1.216427       -0.227983
C          -1.699762       -0.611206       -0.850596
C          -2.507781        0.228675        0.150253
C          -2.932788       -0.637079        1.324436
H           3.272341       -0.641750       -1.131907
H           3.839009       -1.700153        0.275246
H          -1.394749        0.020792       -1.724747
H          -2.317088       -1.483625       -1.198539
H          -3.474769       -0.024422        2.083623
H          -3.607033       -1.456326        0.977467
H          -2.033143       -1.096154        1.801173
C          -3.739868        0.759996       -0.566694
H          -4.359990       -0.083904       -0.953497
H          -4.360973        1.364804        0.136435
H          -3.441015        1.407093       -1.425927
C          -1.665754        1.392094        0.645333
```

```
H          -0.753919        1.002846        1.160141
H          -1.335479        2.021824       -0.215909
H          -2.248476        2.021486        1.358599
N           3.432136        0.363535        0.756519
H           2.703832        0.445892        1.474692
H           4.333631        0.278664        1.219389
C           3.418617        1.572548       -0.075208
H           4.252740        1.525008       -0.822157
H           2.433283        1.615877       -0.628090
H           3.539805        2.489921        0.557204
H           1.514506       -2.144804        0.894571
```

---

### Compound_1_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.603958 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.448671 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.     101.0448 cm-1
2.     150.0224 cm-1
3.     200.5206 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.777681       -0.535384        0.629857
H          -2.551248       -0.827811        1.352702
C          -0.480943       -0.764876        0.968998
H          -0.234650       -1.213868        1.919827
C           0.643687       -0.416327        0.030261
C           0.806391       -1.459692       -1.083119
H           1.591815       -1.175734       -1.788618
H           1.078250       -2.414414       -0.637629
H          -0.128882       -1.589276       -1.626076
C           1.968275       -0.205061        0.751984
H           1.880375        0.520970        1.557999
H           2.277920       -1.152215        1.191971
H           2.750391        0.119612        0.064420
O          -2.182616        0.035488       -0.471286
C           0.276794        2.127858        0.075869
H           1.308166        2.419682        0.246270
H          -0.229741        1.975754        1.024264
```

```
H          -0.232906        2.902443       -0.490566
N           0.209004        0.867092       -0.692214
H           0.717740        0.960913       -1.566451
H          -0.848470        0.641284       -0.875428
```

---

### Compound_1_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.602596 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.44727 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      90.6165 cm-1
  2.     163.0829 cm-1
  3.     206.4267 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.092265        0.225459       -0.164811
H          -3.085532        0.643539       -0.378242
C          -1.024929        1.063097       -0.270032
H          -1.166542        2.098112       -0.544704
C           0.375950        0.591121        0.029591
C           0.646699        0.546605        1.537103
H           1.659796        0.217960        1.772015
H           0.520788        1.552965        1.931500
H          -0.067119       -0.105775        2.038195
C           1.430464        1.426470       -0.686203
H           1.264525        1.424846       -1.764076
H           1.363998        2.456739       -0.338832
H           2.439913        1.069947       -0.482010
O          -2.034947       -1.041564        0.138849
C           1.528981       -1.730540       -0.107081
H           1.442701       -1.953976        0.950629
H           1.451837       -2.654104       -0.674155
H           2.489072       -1.263553       -0.307972
N           0.420885       -0.842522       -0.514730
H           0.393164       -0.771705       -1.529126
H          -0.562625       -1.218107       -0.212305
```

---

### Compound_2_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.654266 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.515324 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      74.2553 cm-1
2.     103.3827 cm-1
3.     130.4003 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.049223        0.965056       -0.315624
C          -0.546066       -0.157228        0.609866
C           0.647404       -0.945171        0.853251
C           1.660988       -0.577667       -0.026070
H          -0.708594        1.109620       -1.173371
H          -1.109696        0.212703        1.465919
H           0.746044       -1.710052        1.604761
O           1.212119        0.507772       -0.823975
C           0.123914        2.281430        0.419804
H           0.575906        3.021746       -0.238685
H          -0.842851        2.659432        0.754657
H           0.767073        2.146545        1.289919
O           2.808364       -0.986050       -0.227585
C          -2.994655       -0.361200       -0.299648
H          -3.373825       -0.125173        0.689969
H          -2.879243        0.550150       -0.877252
H          -3.676358       -1.035678       -0.808572
N          -1.668097       -1.011453       -0.151174
H          -1.282493       -1.273469       -1.057257
H          -1.757325       -1.880741        0.371150
```

---

### Compound_2_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.65466 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.515439 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      76.0888 cm-1
2.     111.4140 cm-1
3.     136.0709 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.487575        1.112153       -0.368111
C          -0.605254        0.358355        0.408165
C           0.032559       -0.900426        0.749009
C           1.215951       -1.053264        0.032369
H           0.099467        1.555356       -1.287790
H          -1.044994        0.952563        1.208939
H          -0.327382       -1.613786        1.469600
O           1.443888        0.111769       -0.746312
C           1.153788        2.185606        0.473181
H           1.987968        2.624384       -0.072439
H           0.442680        2.976922        0.713425
H           1.529180        1.757775        1.403195
O           2.057098       -1.953206       -0.044642
C          -2.984672       -0.560390        0.091201
H          -3.788078       -0.703531       -0.624525
H          -2.613370       -1.520154        0.435972
H          -3.334430        0.030314        0.932778
N          -1.863049        0.160610       -0.557734
H          -1.534570       -0.371378       -1.362326
H          -2.182695        1.066556       -0.899936
```

---

### Compound_2_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -440.650831 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -440.511565 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      78.8012 cm-1
2.     104.4925 cm-1
3.     144.5787 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.047737        1.009985        0.520002
C           0.399035       -0.453808        0.675922
C          -0.851848       -1.177591        0.522344
C          -1.813877       -0.361760       -0.065890
H          -0.274988        1.351153        1.534624
H           0.993818       -0.617670        1.572394
H          -0.995763       -2.222320        0.742300
O          -1.280286        0.946726       -0.209095
C           0.878528        2.010728       -0.137560
H           0.377163        2.975637       -0.196888
H           1.786285        2.142922        0.450063
H           1.150892        1.723960       -1.154404
O          -2.969310       -0.545879       -0.459374
C           2.889082       -0.702642       -0.180805
H           3.478912       -1.089998       -1.006273
H           3.094040        0.352390       -0.044225
H           3.125011       -1.244861        0.729868
N           1.444875       -0.890638       -0.473499
H           1.246611       -1.875824       -0.633760
H           1.181562       -0.417169       -1.335540
```

---

### Compound_3_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1207.211609 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1207.135781 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      27.8632 cm-1
2.      64.3690 cm-1
3.     108.8959 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.827631       -0.478362       -0.017824
H           2.806598       -0.431590        1.080537
C           1.591326       -0.117168       -0.715453
H           1.616120       -0.167309       -1.796441
C           0.466264        0.262385       -0.109537
O           3.831403       -0.812769       -0.612049
Cl          0.255080        0.405693        1.584766
Cl         -2.923216       -1.202151       -0.093065
C          -1.265288        1.952035       -0.711291
H          -1.538374        2.112649        0.324766
H          -0.506496        2.660581       -1.026457
H          -2.145214        2.022667       -1.341413
N          -0.733795        0.558627       -0.855239
H          -0.558403        0.366149       -1.840659
H          -1.550187       -0.144932       -0.551563
```

---

### Compound_4_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.920346 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.81794 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      68.9323 cm-1
  2.      93.3253 cm-1
  3.     195.3077 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.875457       -0.215112        0.272202
O          -3.062309       -0.363572       -0.131194
C          -0.882751        0.606267       -0.231398
H          -1.556207       -0.804734        1.163303
C           0.452585        0.633945        0.364719
H           0.937583        1.609333        0.362010
H           0.474747        0.226814        1.374725
H          -1.085423        1.243267       -1.085721
C           2.857565       -0.275685        0.125890
H           2.825921       -0.644148        1.146460
H           3.240337        0.739892        0.109657
H           3.482125       -0.920056       -0.484948
```

```
N           1.473236       -0.267574       -0.415854
H           1.472398        0.043427       -1.386123
H           1.082689       -1.208695       -0.427314
```

---

### Compound_4_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.920116 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.817565 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      91.8836 cm-1
2.     109.5308 cm-1
3.     205.4439 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.605254       -0.158255        0.268832
O          -2.730994       -0.514205       -0.177465
C          -0.694421        0.725244       -0.282955
H          -1.279474       -0.585195        1.245401
C           0.569739        1.037151        0.376600
H           0.885790        2.075504        0.284931
H           0.587623        0.748143        1.426426
H          -0.922747        1.218120       -1.222201
C           1.767827       -1.204438        0.010680
H           1.860737       -1.374263        1.078907
H           2.586990       -1.680420       -0.518996
H           0.814025       -1.580882       -0.344264
N           1.802781        0.257981       -0.236869
H           2.668746        0.652530        0.128589
H           1.799442        0.436026       -1.239938
```

---

### Compound_4_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.929513 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.826822 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.     109.6722 cm-1
2.     157.9225 cm-1
3.     208.8140 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.810928       -0.216545       -0.045661
O          -1.211639       -1.349739        0.182805
C          -1.200521        1.001550       -0.053707
H          -2.885010       -0.252830       -0.275751
C           0.258811        1.086169        0.257984
H           0.728259        2.002816       -0.093144
H           0.481046        0.982039        1.324467
H          -1.748999        1.900173       -0.290864
C           2.312888       -0.376747        0.096845
H           2.259120       -0.623598        1.153403
H           2.947203        0.495267       -0.043766
H           2.718673       -1.220436       -0.454023
N           0.949481       -0.088784       -0.391321
H           0.950053        0.049084       -1.398839
H           0.234900       -0.879676       -0.177442
```

---

### Compound_4_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -287.921272 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -287.817887 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      75.1502 cm-1
2.     123.8351 cm-1
3.     208.1202 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.728989        0.025577       -0.317802
O          -1.811661       -0.977067        0.451277
C          -0.733102        0.983706       -0.372328
H          -2.549824        0.184340       -1.048368
C           0.403114        0.983201        0.556085
H           0.766174        1.977815        0.809072
H           0.194000        0.424906        1.466856
H          -0.820021        1.790597       -1.088135
C           1.488616       -1.181376       -0.249242
H           2.361238       -1.574636       -0.761637
H           0.592044       -1.321005       -0.842530
H           1.369476       -1.658314        0.718082
N           1.665835        0.278675       -0.031522
H           1.874579        0.730303       -0.920292
H           2.466940        0.445157        0.577112
```

---

## Compound_5_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.257055 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.128865 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      72.6179 cm-1
  2.      79.4635 cm-1
  3.      96.1592 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.664172       -0.108891       -0.017826
O          -2.774800       -0.578507       -0.413441
C          -0.550624       -0.890705        0.274589
C           0.757842       -0.408273        0.710657
H           1.310503       -1.132030        1.307506
H           0.751658        0.543182        1.236127
H          -0.655793       -1.962108        0.141117
C           3.097585        0.320487       -0.121254
```

```
H           3.556549       -0.436141        0.507533
H           3.691196        0.471757       -1.017496
H           3.006350        1.252612        0.427804
N           1.736153       -0.140397       -0.497181
H           1.280194        0.539026       -1.103803
H           1.784174       -1.002973       -1.036932
C          -1.607984        1.410038        0.130816
H          -2.441038        1.732131        0.757900
H          -0.685585        1.801649        0.556647
H          -1.748766        1.867804       -0.850503
```

---

### Compound_5_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.256662 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.12825 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      55.8860 cm-1
2.      98.8367 cm-1
3.     105.1736 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.498835       -0.242641        0.020042
O          -2.399083       -1.093787       -0.253216
C          -0.289826       -0.560083        0.633050
C           0.778685        0.377719        0.964874
H           1.410003        0.042389        1.785912
H           0.452768        1.394382        1.168229
H          -0.123410       -1.604877        0.868826
C           2.566701       -0.649973       -0.568341
H           3.203311       -0.455331       -1.425724
H           3.166995       -0.950742        0.285183
H           1.838848       -1.420010       -0.803049
N           1.825601        0.584254       -0.209970
H           2.479736        1.324807        0.041361
H           1.299788        0.913222       -1.017634
C          -1.814320        1.199249       -0.372699
H          -2.783824        1.474744        0.045684
H          -1.080277        1.938335       -0.055483
H          -1.904911        1.257973       -1.459346
```

### Compound_5_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.270597 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.143035 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      75.5186 cm-1
2.     147.4477 cm-1
3.     161.0070 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.328284       -0.093640        0.067478
O          -0.730520       -1.241386        0.279882
C          -0.649459        1.089709        0.013465
C           0.826403        1.100734        0.252696
H           1.320982        1.990625       -0.132364
H           1.094385        1.000477        1.309479
H          -1.153607        2.018353       -0.203943
C           2.781707       -0.479948        0.034245
H           3.465890        0.348568       -0.136111
H           3.116456       -1.351945       -0.520708
H           2.752274       -0.714922        1.094768
N           1.422981       -0.115562       -0.407211
H           1.393447        0.010588       -1.415324
H           0.645268       -0.860334       -0.141656
C          -2.821000       -0.145308       -0.144537
H          -3.303361       -0.583435        0.732519
H          -3.247039        0.841843       -0.320402
H          -3.057605       -0.789078       -0.994915
```

### Compound_5_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.261156 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.132445 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      59.3240 cm-1
2.     104.2354 cm-1
3.     108.6134 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.297065       -0.046616       -0.128183
O           1.130445       -1.063506       -0.871931
C           0.364968        0.963151        0.075245
C          -0.924685        0.967401       -0.618201
H          -1.305850        1.963084       -0.839461
H          -0.909603        0.364843       -1.524627
H           0.605262        1.799548        0.716956
C          -1.906066       -1.130442        0.460574
H          -2.671543       -1.475454        1.148889
H          -1.996696       -1.638048       -0.493996
H          -0.913709       -1.287999        0.867427
N          -2.075071        0.328284        0.230006
H          -2.973805        0.508557       -0.217011
H          -2.088339        0.812721        1.125882
C           2.634653        0.068607        0.591883
H           2.712421        0.964572        1.207726
H           2.783378       -0.807988        1.226702
H           3.444816        0.073625       -0.140988
```

---

### Compound_6_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.589254 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.43578 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      59.3175 cm-1
2.      78.4194 cm-1
3.      89.0695 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.543548       -0.349961       -0.022966
C          -0.515576        0.542870        0.265843
C           0.816798        0.132596        0.703473
H           0.873704       -0.844648        1.171076
H           1.309601        0.861325        1.347686
C          -0.756605        2.019803        0.055952
H          -0.790683        2.310822       -1.001375
H          -1.712177        2.332608        0.483946
H           0.029356        2.617620        0.524473
O          -2.688707        0.018035       -0.441576
C          -1.369756       -1.856993        0.149257
H          -1.474128       -2.339398       -0.825205
H          -0.424262       -2.178322        0.581421
H          -2.179234       -2.232621        0.778227
C           3.216178       -0.401212       -0.119823
H           3.613839        0.332573        0.574464
H           3.841486       -0.453155       -1.005787
H           3.166196       -1.374164        0.359403
N           1.840131        0.007043       -0.500732
H           1.855304        0.905131       -0.979967
H           1.434796       -0.653966       -1.161052
```

---

### Compound_6_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.588838 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.434743 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      54.9552 cm-1
2.      95.6260 cm-1
3.      99.4098 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.468311       -0.097447       -0.093003
C          -0.293212        0.457014        0.408602
C           0.774026       -0.338970        1.011565
H           0.451646       -1.248601        1.509627
H           1.402842        0.231319        1.693960
C          -0.107226        1.953209        0.305698
H           0.045911        2.304657       -0.722265
H          -0.984460        2.490508        0.676080
H           0.755552        2.285526        0.886753
O          -2.388883        0.594351       -0.634345
C          -1.729591       -1.600740       -0.035683
H          -2.739170       -1.764319        0.345055
H          -1.700433       -2.009791       -1.048544
H          -1.035895       -2.175411        0.575665
C           2.521258        0.157302       -0.822232
H           3.059281        0.803939       -0.135723
H           1.766579        0.725573       -1.354033
H           3.211270       -0.302295       -1.523024
N           1.835453       -0.898429       -0.037028
H           2.520952       -1.475828        0.450031
H           1.327155       -1.513298       -0.669305
```

---

### Compound_6_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.614183 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.460257 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      76.7380 cm-1
2.     113.8862 cm-1
3.     135.9701 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.167381       -0.537111        0.049570
C          -0.574046        0.668591        0.064946
C           0.916496        0.794538        0.300427
H           1.132703        0.725013        1.372953
H           1.254848        1.789988       -0.013592
C          -1.297218        1.978350       -0.072237
```

```
H          -2.372666        1.865261       -0.177159
H          -1.118483        2.614070        0.801102
H          -0.934415        2.537951       -0.939882
O          -0.453239       -1.699367        0.200675
C          -2.623802       -0.829901       -0.114924
H          -3.228488        0.065587       -0.211911
H          -2.782512       -1.454089       -0.997338
H          -2.984935       -1.397267        0.746293
C           3.115095       -0.235772       -0.005441
H           3.582829        0.738054       -0.196155
H           3.647648       -0.994191       -0.576855
H           3.228529       -0.463647        1.054635
N           1.698345       -0.262976       -0.357802
H           1.595345       -0.165776       -1.361695
H           0.502234       -1.457355        0.064771
```

---

### Compound_6_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.614183 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.460258 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      76.7560 cm-1
2.     114.0075 cm-1
3.     135.8346 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.167613       -0.536946        0.049505
C           0.573888        0.668555        0.064964
C          -0.916607        0.793879        0.301015
H          -1.132498        0.723534        1.373545
H          -1.255354        1.789439       -0.012188
C           1.296670        1.978515       -0.072372
H           1.119200        2.613771        0.801584
H           2.371960        1.865614       -0.179016
H           0.932516        2.538537       -0.939157
O           0.453792       -1.699401        0.200797
C           2.624100       -0.829370       -0.115098
H           2.783030       -1.453734       -0.997343
H           3.228494        0.066295       -0.212309
```

```
H           2.985429       -1.396328        0.746289
C          -3.115285       -0.235674       -0.005778
H          -3.582500        0.738446       -0.196224
H          -3.648021       -0.993624       -0.577633
H          -3.229074       -0.463922        1.054171
N          -1.698393       -0.263357       -0.357815
H          -1.595268       -0.165406       -1.361642
H          -0.501779       -1.457676        0.064831
```

---

### Compound_6_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.614183 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.460254 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      76.8010 cm-1
  2.     113.8888 cm-1
  3.     135.9693 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.167454       -0.537029       -0.049507
C          -0.573972        0.668538       -0.064867
C           0.916519        0.794315       -0.300572
H           1.132689        0.724695       -1.373102
H           1.255080        1.789731        0.013380
C          -1.296933        1.978425        0.072254
H          -2.372307        1.865511        0.178195
H          -0.933266        2.538297        0.939330
H          -1.118897        2.613795       -0.801499
O          -0.453549       -1.699338       -0.200777
C          -2.623919       -0.829628        0.114998
H          -2.782662       -1.454407        0.996988
H          -3.228372        0.065936        0.212718
H          -2.985324       -1.396282       -0.746572
C           3.115194       -0.235706        0.005598
H           3.647819       -0.994184        0.576869
H           3.582643        0.738175        0.196733
H           3.228851       -0.463154       -1.054563
N           1.698368       -0.263302        0.357675
```

```
H           1.595152       -0.166233        1.361566
H           0.501795       -1.457555       -0.064974
```

---

### Compound_7_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.321038 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.202182 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      76.0117 cm-1
  2.     113.2289 cm-1
  3.     144.9725 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.561703       -0.031445       -0.001173
O           2.720193       -0.092178       -0.489285
C           0.664259       -1.083237        0.172514
C          -0.729554       -0.853913        0.570993
H          -1.304120       -1.773107        0.651626
H          -0.884255       -0.280343        1.488717
H           0.949446       -2.063698       -0.179050
C          -2.864203        0.413286       -0.141841
H          -3.465699       -0.481407       -0.012735
H          -3.274839        1.027335       -0.937661
H          -2.838181        0.977531        0.785465
N          -1.479500        0.012529       -0.490035
H          -0.875797        0.833895       -0.611205
H          -1.455443       -0.496584       -1.370894
N           1.072963        1.280298        0.339082
H           1.834109        1.944775        0.317499
H           0.605765        1.331100        1.236229
```

---

### Compound_7_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.329021 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.210749 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      93.0741 cm-1
2.     137.4544 cm-1
3.     158.1906 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.365695       -0.103285        0.056687
O          -0.812404       -1.239664        0.319383
C          -0.664667        1.084835        0.008691
C           0.782682        1.052906        0.333231
H           1.304872        1.967795        0.062499
H           1.010943        0.828510        1.380955
H          -1.125219        2.009028       -0.304285
C           2.804624       -0.458824       -0.002325
H           2.790745       -0.732573        1.048707
H           3.462042        0.394104       -0.150151
H           3.152132       -1.300423       -0.594652
N           1.431596       -0.103237       -0.416712
H           0.725121       -0.869912       -0.212922
H           1.388534        0.093958       -1.413523
N          -2.734129       -0.139717       -0.269050
H          -3.236929        0.715069       -0.082106
H          -3.196937       -0.941357        0.133039
```

---

### Compound_7_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.320696 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.201749 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      66.5320 cm-1
2.     106.7677 cm-1
3.     148.8317 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.399377       -0.169464        0.025107
O           2.366621       -0.831685       -0.432898
C           0.371374       -0.640632        0.841158
C          -0.808942        0.170144        1.147550
H          -1.523255       -0.344500        1.784970
H          -0.618801        1.155409        1.580236
H           0.352795       -1.695483        1.071044
C          -2.242660       -0.616730       -0.828049
H          -1.472412       -1.366861       -0.977095
H          -2.655324       -0.302764       -1.781894
H          -3.028946       -1.009404       -0.189984
N          -1.617990        0.543872       -0.152005
H          -0.918216        0.976463       -0.763696
H          -2.319832        1.250908        0.059945
N           1.293857        1.197649       -0.407048
H           1.049073        1.851812        0.325949
H           2.155989        1.487353       -0.847506
```

---

## Compound_7_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -343.323183 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.205095 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      65.8012 cm-1
2.     101.3239 cm-1
3.     113.7354 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.321240       -0.051348        0.096778
O          -1.187446       -1.057319        0.846285
C          -0.381333        0.971937       -0.084242
C           0.879408        0.967854        0.631806
H           1.275520        1.956982        0.855867
H           0.856333        0.359434        1.533768
H          -0.605978        1.800457       -0.742801
C           1.894062       -1.129856       -0.468700
H           1.935038       -1.666053        0.473884
H           2.675925       -1.478410       -1.136833
H           0.915293       -1.254748       -0.919086
N           2.082343        0.315251       -0.192883
H           2.960034        0.468566        0.302900
H           2.144072        0.825797       -1.071377
N          -2.514181        0.028426       -0.657963
H          -2.783462        0.958123       -0.943804
H          -3.275719       -0.468867       -0.220731
```

---

### Compound_8_HEI_Conformation_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.744227 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.499437 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      54.7998 cm-1
2.     100.0325 cm-1
3.     129.7604 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.307832       -0.232404       -0.045067
C          -1.216268       -1.441818       -0.109984
C          -2.664142       -1.139325        0.268570
C          -3.147486        0.124500       -0.430451
C          -2.299031        1.312186        0.010417
C          -0.830045        1.003789        0.050968
H          -3.298211       -1.991615        0.017613
H          -1.189512       -1.885368       -1.111622
H          -0.833533       -2.216435        0.559921
H          -3.059639       -0.006831       -1.512828
```

```
H          -4.200419        0.315318       -0.217236
H          -2.446885        2.166799       -0.654450
H          -2.608492        1.649469        1.006129
H          -2.733753       -0.996790        1.351271
O          -0.084329        2.138130        0.208599
C           1.199806       -0.503805        0.044146
C           1.571461       -0.679207        1.524115
H           2.610626       -0.983814        1.651341
H           1.407909        0.248458        2.072357
H           0.942962       -1.451408        1.965299
C           1.594695       -1.764670       -0.741727
H           2.674473       -1.904278       -0.709858
H           1.139267       -2.661629       -0.327339
H           1.289225       -1.679246       -1.785554
N           1.927634        0.676742       -0.511090
H           1.751029        0.698222       -1.509350
H           0.858275        1.845789        0.031288
C           3.369757        0.755954       -0.280428
H           3.916637       -0.149239       -0.561926
H           3.763667        1.583939       -0.867415
H           3.572076        0.965230        0.767848
```

---

### Compound_8_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.746118 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.501232 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      57.5607 cm-1
2.      94.4836 cm-1
3.     132.8220 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.171118       -0.259002       -0.055876
C          -1.001020       -1.488129        0.238043
C          -2.419799       -1.169826        0.707207
C          -3.051571       -0.089287       -0.160634
C          -2.232633        1.193377       -0.062670
C          -0.757111        0.945014       -0.177612
H          -3.023368       -2.079236        0.699305
```

```
H          -1.049011       -2.125718       -0.654523
H          -0.510029       -2.094819        1.000420
H          -3.074536       -0.428785       -1.200254
H          -4.084388        0.099637        0.136153
H          -2.515863        1.898210       -0.848274
H          -2.434359        1.702807        0.886195
H          -2.386485       -0.818755        1.743068
O          -0.068085        2.097409       -0.432452
C           1.324645       -0.443287       -0.345840
C           1.531927       -0.464992       -1.869205
H           2.587527       -0.602275       -2.116988
H           0.971831       -1.288476       -2.310070
H           1.186923        0.465796       -2.317230
C           1.894342       -1.743022        0.239255
H           1.735613       -1.817372        1.313616
H           1.440010       -2.615749       -0.226803
H           2.968064       -1.782253        0.049110
N           2.075439        0.742643        0.160795
H           3.003026        0.737817       -0.245991
H           0.897000        1.856467       -0.320331
C           2.172553        0.874791        1.614535
H           2.664726        1.817373        1.849936
H           1.169043        0.897284        2.037792
H           2.729586        0.066450        2.095686
```

---

### Compound_8_HEI_Conformation_2_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.746118 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.501233 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      57.5419 cm-1
2.      94.4525 cm-1
3.     132.8158 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.171249        0.258849        0.055846
C          -1.001147        1.488031       -0.237790
C          -2.420037        1.169899       -0.706738
C          -3.051699        0.089211        0.160990
```

```
C          -2.232824       -1.193461        0.062665
C          -0.757291       -0.945146        0.177427
H          -3.023563        2.079343       -0.698503
H          -1.048916        2.125545        0.654853
H          -0.510214        2.094719       -1.000208
H          -3.074505        0.428512        1.200684
H          -4.084569       -0.099633       -0.135688
H          -2.515950       -1.898415        0.848207
H          -2.434717       -1.702728       -0.886258
H          -2.386956        0.819060       -1.742691
O          -0.068252       -2.097628        0.432016
C           1.324696        0.443262        0.345595
C           1.531856        0.465349        1.868982
H           2.587396        0.603014        2.116842
H           0.971451        1.288736        2.309648
H           1.187112       -0.465480        2.317150
C           1.894160        1.743000       -0.239752
H           1.735253        1.817195       -1.314103
H           1.439792        2.615733        0.226271
H           2.967916        1.782392       -0.049790
N           2.075540       -0.742627       -0.160651
H           3.002645       -0.738669        0.247183
H           0.896926       -1.856556        0.319830
C           2.173675       -0.874552       -1.614276
H           2.665365       -1.817407       -1.849653
H           1.170404       -0.896173       -2.038189
H           2.731536       -0.066427       -2.094856
```

---

### Compound_8_HEI_Conformation_3_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.744227 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.499437 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      54.7995 cm-1
2.     100.0322 cm-1
3.     129.7599 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.307832       -0.232404       -0.045067
C          -1.216268       -1.441818       -0.109985
C          -2.664142       -1.139325        0.268569
C          -3.147486        0.124500       -0.430451
C          -2.299031        1.312186        0.010417
C          -0.830045        1.003789        0.050968
H          -3.298212       -1.991615        0.017611
H          -1.189512       -1.885368       -1.111623
H          -0.833533       -2.216435        0.559920
H          -3.059640       -0.006830       -1.512828
H          -4.200420        0.315319       -0.217236
H          -2.446885        2.166799       -0.654449
H          -2.608492        1.649470        1.006130
H          -2.733753       -0.996791        1.351270
O          -0.084329        2.138130        0.208599
C           1.199806       -0.503805        0.044146
C           1.571461       -0.679205        1.524116
H           2.610626       -0.983813        1.651342
H           1.407909        0.248460        2.072356
H           0.942962       -1.451406        1.965300
C           1.594695       -1.764671       -0.741726
H           1.289224       -1.679248       -1.785552
H           2.674474       -1.904278       -0.709857
H           1.139269       -2.661629       -0.327335
N           1.927634        0.676741       -0.511091
H           1.751028        0.698221       -1.509351
H           0.858275        1.845788        0.031286
C           3.369757        0.755954       -0.280429
H           3.572076        0.965230        0.767846
H           3.916637       -0.149239       -0.561927
H           3.763666        1.583939       -0.867417
```

---

### Compound_8_HEI_Conformation_4_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.746118 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.501233 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      57.5406 cm-1
2.      94.4522 cm-1
3.     132.8125 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.171256        0.258844        0.055852
C          -1.001117        1.488056       -0.237766
C          -2.419948        1.169971       -0.706922
C          -3.051719        0.089196        0.160619
C          -2.232832       -1.193466        0.062268
C          -0.757314       -0.945163        0.177240
H          -3.023475        2.079414       -0.698672
H          -1.048996        2.125481        0.654934
H          -0.510089        2.094819       -1.000064
H          -3.074655        0.428393        1.200344
H          -4.084552       -0.099618       -0.136206
H          -2.516057       -1.898500        0.847703
H          -2.434605       -1.702637       -0.886732
H          -2.386738        0.819235       -1.742906
O          -0.068308       -2.097670        0.431801
C           1.324653        0.443226        0.345805
C           1.531628        0.465159        1.869220
H           2.587138        0.602797        2.117222
H           0.971171        1.288502        2.309900
H           1.186827       -0.465715        2.317251
C           1.894192        1.743022       -0.239341
H           2.967924        1.782394       -0.049238
H           1.735421        1.817324       -1.313705
H           1.439765        2.615710        0.226711
N           2.075558       -0.742612       -0.160469
H           3.002612       -0.738697        0.247480
H           0.896885       -1.856588        0.319756
C           2.173872       -0.874389       -1.614096
H           2.665587       -1.817222       -1.849509
H           1.170653       -0.895963       -2.038134
H           2.731795       -0.066218       -2.094525
```

### Compound_8_HEI_Conformation_5_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.744227 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.499437 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      54.8221 cm-1
2.     100.0577 cm-1
3.     129.7679 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.307807       -0.232304       -0.044977
C          -1.216181       -1.441802       -0.109848
C          -2.664069       -1.139400        0.268705
C          -3.147545        0.124277       -0.430474
C          -2.299206        1.312085        0.010249
C          -0.830180        1.003824        0.051025
H          -3.298076       -1.991788        0.017919
H          -1.189392       -1.885449       -1.111435
H          -0.833406       -2.216341        0.560132
H          -3.059655       -0.007172       -1.512834
H          -4.200509        0.315012       -0.217329
H          -2.446987        2.166509       -0.654886
H          -2.608826        1.649646        1.005817
H          -2.733629       -0.996703        1.351390
O          -0.084664        2.138298        0.208789
C           1.199895       -0.503780        0.044115
C           1.571710       -0.679743        1.523972
H           2.610913       -0.984332        1.650944
H           1.408198        0.247720        2.072573
H           0.943330       -1.452154        1.964962
C           1.594698       -1.764353       -0.742279
H           2.674406       -1.904382       -0.709971
H           1.138759       -2.661368       -0.328585
H           1.289727       -1.678265       -1.786200
N           1.927686        0.676900       -0.510650
H           1.750751        0.699102       -1.508833
H           0.857975        1.846052        0.031480
C           3.369881        0.756038       -0.280366
H           3.763577        1.584152       -0.867317
H           3.916681       -0.149090       -0.562230
H           3.572503        0.965108        0.767897
```

---

### Compound_8_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.746394 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.501541 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      56.8811 cm-1
2.      96.5333 cm-1
3.     137.9139 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.176844        0.267134       -0.050687
C           1.028380        1.460843        0.322078
C           2.517529        1.253905        0.054909
C           2.969815       -0.109241        0.562337
C           2.214746       -1.210001       -0.175205
C           0.748067       -0.921551       -0.310941
H           2.704274        1.312991       -1.021658
H           0.689606        2.335975       -0.238864
H           0.881353        1.717459        1.377380
H           4.045350       -0.240524        0.433965
H           2.764994       -0.180406        1.634467
H           2.635842       -1.352610       -1.176782
H           2.325139       -2.169609        0.336007
H           3.092435        2.055245        0.522564
O           0.055649       -2.021981       -0.733311
C          -1.324590        0.510815       -0.238619
C          -1.585703        0.875860       -1.707938
H          -2.643576        1.094977       -1.873633
H          -1.011674        1.759381       -1.983746
H          -1.292211        0.055826       -2.362564
C          -1.847182        1.647535        0.655245
H          -1.427341        2.607343        0.362036
H          -2.931787        1.714219        0.557014
H          -1.607644        1.485176        1.704728
N          -2.077598       -0.750271        0.018203
H          -3.006074       -0.658886       -0.375305
H          -0.909698       -1.775171       -0.638860
C          -2.172617       -1.177533        1.414679
H          -2.664569       -2.148477        1.452011
H          -1.169120       -1.286863        1.823849
H          -2.729036       -0.484897        2.051310
```

---

### Compound_8_HEI_Conformation_6_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.746394 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.501541 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      56.8808 cm-1
2.      96.5331 cm-1
3.     137.9134 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.176844       -0.267134        0.050687
C           1.028380       -1.460843       -0.322078
C           2.517529       -1.253905       -0.054909
C           2.969815        0.109241       -0.562337
C           2.214746        1.210001        0.175205
C           0.748067        0.921551        0.310941
H           2.704274       -1.312991        1.021658
H           0.689606       -2.335975        0.238864
H           0.881353       -1.717459       -1.377380
H           4.045350        0.240524       -0.433965
H           2.764994        0.180406       -1.634467
H           2.635842        1.352610        1.176782
H           2.325139        2.169609       -0.336007
H           3.092435       -2.055245       -0.522564
O           0.055649        2.021981        0.733311
C          -1.324590       -0.510815        0.238619
C          -1.585703       -0.875860        1.707938
H          -2.643576       -1.094977        1.873633
H          -1.011674       -1.759381        1.983746
H          -1.292211       -0.055826        2.362564
C          -1.847182       -1.647535       -0.655245
H          -1.427341       -2.607343       -0.362036
H          -2.931787       -1.714219       -0.557014
H          -1.607644       -1.485176       -1.704728
N          -2.077598        0.750271       -0.018203
H          -3.006074        0.658886        0.375305
H          -0.909698        1.775171        0.638860
C          -2.172617        1.177533       -1.414679
H          -2.664569        2.148477       -1.452011
H          -1.169120        1.286863       -1.823849
H          -2.729036        0.484897       -2.051310
```

---

### Compound_9_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.723749 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.481249 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      63.2323 cm-1
  2.      68.6187 cm-1
  3.     110.7531 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.985189       -0.417156       -0.513631
C           0.074944       -1.163526        0.310759
C           1.482817       -0.553492        0.243935
C           1.364123        0.925111        0.634742
C           0.333836        1.709641       -0.175714
C          -0.736431        1.009549       -0.708200
H          -0.211012       -1.165008        1.362498
H           0.104771       -2.209561       -0.000812
H           1.101080        0.997383        1.695998
H           2.326421        1.427003        0.516577
H          -1.423872        1.544055       -1.357003
O           0.543978        2.952209       -0.333118
C           2.378917       -1.289772        1.245163
H           2.466472       -2.347952        0.989346
H           3.382754       -0.861235        1.248226
H           1.978258       -1.217957        2.258002
C           2.096158       -0.690938       -1.155778
H           3.118321       -0.308305       -1.156694
H           2.129751       -1.737988       -1.463114
H           1.528421       -0.133316       -1.898468
C          -1.352858       -1.158031       -1.798123
H          -2.106493       -0.609500       -2.364609
H          -0.463897       -1.240889       -2.419318
H          -1.720316       -2.168446       -1.605150
C          -2.453249        0.172684        1.630744
H          -1.829915       -0.309630        2.375362
H          -3.481494        0.201276        1.978790
H          -2.086992        1.175938        1.431729
N          -2.385379       -0.583833        0.361004
H          -2.562655       -1.573666        0.522839
H          -3.122178       -0.257459       -0.259659
```

---

### Compound_9_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.724548 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.480868 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      90.7295 cm-1
  2.      97.6214 cm-1
  3.     110.0950 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.959023        0.522289        0.415626
C           0.210986       -0.724374        0.881177
C          -1.083371       -1.060137        0.123153
C          -1.980757        0.182119        0.139422
C          -1.294366        1.500971       -0.216807
C           0.078183        1.600607       -0.056265
H           0.875514       -1.590656        0.895658
H          -0.054164       -0.540372        1.924095
H          -2.823222        0.047749       -0.542585
H          -2.410889        0.306479        1.139046
H           0.539266        2.570054       -0.221599
O          -2.052864        2.451587       -0.585331
C          -0.829380       -1.491455       -1.330497
H          -1.740319       -1.913914       -1.756258
H          -0.561006       -0.647794       -1.969147
H          -0.053498       -2.256658       -1.397414
C          -1.772771       -2.220400        0.850129
H          -2.732105       -2.450497        0.383495
H          -1.158667       -3.123159        0.819371
H          -1.956406       -1.971548        1.896581
C           1.973935        0.979182        1.460969
H           2.577072        1.808341        1.088153
H           1.426221        1.332095        2.332029
H           2.638510        0.177362        1.783548
C           2.991677       -0.870635       -0.724255
H           2.615748       -1.793334       -0.296771
H           3.754322       -0.446947       -0.081474
H           3.411043       -1.069835       -1.706749
N           1.873757        0.098632       -0.867042
H           2.227243        0.981921       -1.228661
H           1.212995       -0.231406       -1.565289
```

### Compound_9_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -522.71851 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -522.474347 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      64.8670 cm-1
2.     107.0804 cm-1
3.     129.9535 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.122764        0.054672       -0.594791
C           0.012417       -0.961208       -0.825755
C           1.355690       -0.724693       -0.106194
C           1.708816        0.761973       -0.208955
C           0.599211        1.720883        0.214866
C          -0.710988        1.320480        0.028389
H          -0.341347       -1.975749       -0.624218
H           0.222160       -0.937349       -1.895920
H           2.590788        0.979387        0.396469
H           1.973890        1.003308       -1.244372
H          -1.492483        2.058012        0.190511
O           0.959951        2.860086        0.652593
C           1.343963       -1.139795        1.370191
H           2.356624       -1.085147        1.773026
H           0.717600       -0.485467        1.970538
H           0.995194       -2.166975        1.492031
C           2.419698       -1.566051       -0.823930
H           3.400602       -1.410037       -0.371822
H           2.186747       -2.631458       -0.759815
H           2.486716       -1.297525       -1.879469
C          -1.921729        0.248703       -1.892549
H          -2.756882        0.934055       -1.739296
H          -1.262316        0.688791       -2.637000
H          -2.307094       -0.693225       -2.292785
C          -1.934507       -0.893980        1.762506
H          -1.472049        0.001874        2.164342
H          -1.255278       -1.734022        1.830257
H          -2.855264       -1.118715        2.292623
N          -2.251795       -0.634833        0.340387
H          -2.559225       -1.494861       -0.110098
H          -3.044264        0.002347        0.298875
```

### Compound_10_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.974211 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.80985 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
  1.      89.8071 cm-1
  2.      94.2828 cm-1
  3.     109.5301 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.729012        0.209347        0.491283
C           0.243258       -0.985830        1.324214
C          -1.194740       -1.273734        0.861349
C          -1.599467       -0.057649        0.023283
C          -0.481192        0.742623       -0.119514
H           0.257780       -0.689258        2.371943
H           0.908401       -1.845884        1.238262
H          -1.266544       -2.176686        0.249727
H          -1.878033       -1.404693        1.701685
O          -2.773184        0.101130       -0.417859
O          -0.400823        1.877055       -0.940852
H          -0.628773        2.662444       -0.433774
C           1.630346        1.188225        1.229003
H           1.928664        2.015521        0.584100
H           1.077593        1.601796        2.070646
H           2.529258        0.706839        1.618891
C           1.141064       -1.359436       -1.601411
H           0.181426       -0.984497       -1.943222
H           1.807961       -1.516738       -2.443676
H           1.004611       -2.290082       -1.061653
N           1.727078       -0.350315       -0.691328
H           2.579951       -0.706977       -0.265498
H           1.990529        0.473663       -1.227687
```

### Compound_10_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.974894 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.81017 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
1.      57.5986 cm-1
2.      97.2742 cm-1
3.     133.4639 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.546521        0.483582        0.376684
C           0.266395        1.766326        0.118743
C           1.606674        1.313322       -0.490172
C           1.676102       -0.173642       -0.158791
C           0.456097       -0.560864        0.337708
H           0.430180        2.253357        1.078993
H          -0.275135        2.479201       -0.505517
H           1.649872        1.469104       -1.572327
H           2.452890        1.852634       -0.060538
O           2.702454       -0.909558       -0.318849
O           0.181915       -1.869812        0.742422
H           1.012050       -2.344056        0.592609
C          -1.490480        0.533041        1.564519
H          -2.006006       -0.413958        1.712457
H          -0.902818        0.732316        2.458981
H          -2.233094        1.326116        1.463078
C          -2.270071       -0.939191       -1.077809
H          -2.802459       -0.958995       -2.024809
H          -1.537184       -1.737284       -1.037930
H          -2.975997       -1.044907       -0.261296
N          -1.556887        0.353185       -0.939711
H          -0.954926        0.489955       -1.747754
H          -2.223298        1.123742       -0.931848
```

---

### Compound_10_HEI_Conformation_2_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -479.974895 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -479.810222 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 63)

```
  1.      57.4628 cm-1
  2.      97.1204 cm-1
  3.     133.1112 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.545838        0.483480        0.377695
C           0.266617        1.766289        0.119455
C           1.606718        1.313400       -0.489894
C           1.676186       -0.173724       -0.159196
C           0.456377       -0.560881        0.338403
H           0.430605        2.253488        1.079601
H          -0.275262        2.478990       -0.504696
H           1.649694        1.469608       -1.571989
H           2.453135        1.852349       -0.060209
O           2.702266       -0.909496       -0.320250
O           0.182185       -1.869726        0.743461
H           1.011623       -2.344658        0.592385
C          -1.490805        0.532451        1.564609
H          -2.006663       -0.414556        1.711396
H          -0.904007        0.731029        2.459810
H          -2.233155        1.325742        1.462937
C          -2.270243       -0.938836       -1.078684
H          -2.801718       -0.959300       -2.026197
H          -1.537390       -1.736924       -1.037700
H          -2.977025       -1.044323       -0.262874
N          -1.557278        0.353503       -0.940326
H          -0.954995        0.490629       -1.748040
H          -2.223579        1.124115       -0.932164
```

---

### Compound_11_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1374.808368 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1374.728631 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      34.2850 cm-1
2.      47.5659 cm-1
3.      99.9266 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.173864        0.573188        0.230891
C          -1.190261        1.588994       -0.179418
C          -2.150891       -0.481730       -0.316337
C          -0.715826       -0.641521        0.149265
O          -2.955642       -1.352482       -0.501955
O          -1.012883        2.781185       -0.224451
Cl         -0.065657       -2.167680        0.466809
Cl          3.076332       -0.208916       -1.202981
N          -2.334385        0.881914       -0.484797
H          -3.196648        1.300769       -0.798918
N           1.135600        1.000758        0.587868
H           1.169716        2.014623        0.456415
H           1.882059        0.562350       -0.123563
C           1.573578        0.657793        1.980328
H           2.571977        1.060348        2.112393
H           0.883014        1.096774        2.692293
H           1.591685       -0.421381        2.077691
```

---

### Compound_12_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -826.23292 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -826.088311 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      58.8327 cm-1
2.     158.2966 cm-1
3.     178.3054 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.393193        1.743074        0.092485
H          -1.194445        2.446390       -0.161038
C          -0.669932        0.415663       -0.005279
C           0.326539       -0.657658        0.377103
C           0.380124       -0.831987        1.899955
H           1.122931       -1.577859        2.190932
H           0.613117        0.113858        2.386770
H          -0.594388       -1.166858        2.249600
C           0.113235       -2.004557       -0.301889
H          -0.004199       -1.908162       -1.378763
H           0.953126       -2.667332       -0.092387
H          -0.787926       -2.467540        0.091585
O           0.761514        2.230597        0.439968
C           2.025777       -0.096505       -1.463238
H           1.203357        0.352091       -2.012140
H           2.926028        0.494301       -1.606240
H           2.195869       -1.111415       -1.806809
N           1.687073       -0.080628       -0.022773
H           1.575530        0.966749        0.281211
H           2.418237       -0.536675        0.515832
Cl         -2.295539       -0.095654       -0.447865
```

---

### Compound_12_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -826.222721 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -826.07774 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      48.0452 cm-1
2.     104.8301 cm-1
3.     125.4258 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.776235        1.077097       -0.236600
H           1.392947        2.112116       -0.240294
C           0.805543        0.146994        0.063651
C          -0.636327        0.373379        0.338132
C          -1.031510        1.847515        0.331309
H          -2.098538        1.955304        0.514800
```

```
H          -0.506543        2.362629        1.131581
H          -0.787523        2.335093       -0.610478
C          -1.144871       -0.303594        1.612053
H          -0.985414       -1.379280        1.589827
H          -0.584184        0.102979        2.451186
H          -2.201157       -0.103961        1.783856
O           2.999514        0.894007       -0.481546
C          -2.883827       -0.381864       -0.873403
H          -3.298229        0.617033       -0.802237
H          -3.201133       -0.845399       -1.802874
H          -3.207089       -0.986252       -0.034353
N          -1.397985       -0.301527       -0.876040
H          -1.075907        0.190800       -1.707965
H          -1.004336       -1.241328       -0.946151
Cl          1.296202       -1.571663        0.073346
```

---

### Compound_12_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -826.220688 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -826.076395 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      18.9245 cm-1
  2.      82.6532 cm-1
  3.     138.3976 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.542642        1.073182        0.450369
H          -1.107332        2.050510        0.724314
C          -0.627119        0.213793       -0.125911
C           0.812706        0.479540       -0.340049
C           1.153006        1.966820       -0.485396
H           2.228451        2.097081       -0.609871
H           0.659066        2.358425       -1.370855
H           0.835859        2.556534        0.371262
C           1.447759       -0.291839       -1.493532
H           1.315312       -1.364960       -1.400822
H           0.970689        0.021051       -2.420075
H           2.512253       -0.067347       -1.565702
O          -2.765015        0.886093        0.685677
```

```
C           1.453440       -1.336588        1.464894
H           1.782203       -2.035627        0.704842
H           0.400613       -1.479988        1.676464
H           2.042659       -1.467198        2.367592
N           1.645460        0.050806        0.970281
H           2.636704        0.218823        0.800300
H           1.364074        0.699385        1.703046
Cl         -1.248327       -1.391795       -0.592949
```

---

### Compound_13_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1666.836532 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1666.771809 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      31.7392 cm-1
  2.      49.8953 cm-1
  3.      90.7357 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.600500        1.781782        0.206980
H           2.609460        2.078339        0.520336
C           1.395007        0.318743        0.119482
C           0.245641       -0.247373       -0.290621
O           0.745581        2.609655       -0.039101
C          -1.434827        0.375396       -2.012477
H          -0.660692        0.612041       -2.734996
H          -2.273914        1.055360       -2.113708
H          -1.771336       -0.648030       -2.129594
N          -0.894963        0.556122       -0.628846
H          -1.720985        0.348102        0.090016
H          -0.613508        1.541880       -0.485224
Cl          2.753051       -0.630603        0.585089
Cl         -3.110552        0.019457        1.188972
Cl         -0.001727       -1.925859       -0.395961
```

---

### Compound_13_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1666.820959 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1666.752659 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      46.4722 cm-1
2.     126.6712 cm-1
3.     151.9804 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.385312        1.683611       -0.190275
H          -2.433050        1.949885       -0.193449
C          -1.033344        0.385184       -0.150691
C           0.373246       -0.102113       -0.049935
O          -0.576977        2.747526       -0.205808
C           2.721208        0.643742       -0.383079
H           2.980495        0.769858        0.663094
H           3.236517        1.401720       -0.966231
H           3.038358       -0.345295       -0.718109
N           1.281349        0.849941       -0.568282
H           1.069890        0.978784       -1.552493
H           0.348486        2.414763       -0.197166
Cl         -2.314314       -0.785187        0.018588
Cl          0.772378       -0.451837        1.697489
Cl          0.562577       -1.748979       -0.937685
```

---

### Compound_14_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.855386 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.740812 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      62.9271 cm-1
2.      91.8377 cm-1
```

```
   3.     124.4306 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.128122        1.414407        0.087694
O          -1.340594        1.890234        0.200704
C           0.076114        0.064057        0.146242
C          -1.063336       -0.874454        0.381358
H          -0.838356       -1.898532        0.096932
H          -1.399736       -0.874201        1.421954
C          -3.547830       -0.957730       -0.020382
H          -3.753233       -0.669535        1.006619
H          -3.522655       -2.041802       -0.099517
H          -4.319057       -0.557947       -0.672294
N          -2.242718       -0.391564       -0.417226
H          -2.153870        0.685630       -0.234065
H          -2.063767       -0.555145       -1.404572
C           0.966112        2.425260       -0.122987
H           0.748855        3.008402       -1.019938
H           0.973703        3.120084        0.719292
H           1.952753        1.981382       -0.219785
Br          1.799472       -0.771672       -0.031749
```

---

## Compound_14_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.8651 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.749736 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
   1.      57.1507 cm-1
   2.     102.1934 cm-1
   3.     103.9724 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.315119        1.337885        0.103657
O           1.575845        1.784959        0.356188
C           0.012270        0.037968        0.245996
```

```
C           0.954320       -1.041002        0.722783
H           0.651599       -2.002618        0.295154
H           0.883108       -1.140745        1.809064
C           2.701188       -1.041536       -0.996657
H           3.753645       -0.820246       -1.162405
H           2.110565       -0.420577       -1.669497
H           2.514068       -2.091537       -1.246797
N           2.349998       -0.725379        0.388379
H           2.142410        0.970928        0.491983
H           2.965656       -1.212459        1.025400
C          -0.591684        2.440447       -0.324843
H          -0.643680        3.195480        0.462212
H          -0.181608        2.924924       -1.212900
H          -1.594764        2.090587       -0.541900
Br         -1.771572       -0.602809       -0.066403
```

---

### Compound_14_HEI_Conformation_2_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.8651 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.749735 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      56.9215 cm-1
2.     102.1237 cm-1
3.     104.8938 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.314715        1.337905       -0.103291
O          -1.575189        1.785673       -0.355501
C          -0.012091        0.037946       -0.245731
C          -0.954226       -1.041475       -0.721221
H          -0.652239       -2.002652       -0.292025
H          -0.881928       -1.142740       -1.807309
C          -2.704171       -1.040922        0.995283
H          -3.756536       -0.817700        1.159179
H          -2.113584       -0.421496        1.669582
H          -2.519726       -2.091472        1.245084
N          -2.349848       -0.724576       -0.389011
H          -2.141984        0.972216       -0.492060
H          -2.965280       -1.209960       -1.027534
```

```
C           0.592942        2.440216        0.324197
H           0.644869        3.194779       -0.463324
H           0.183403        2.925446        1.212130
H           1.595957        2.090068        0.541301
Br          1.771745       -0.603196        0.066475
```

---

### Compound_14_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.855386 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.74082 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      62.9011 cm-1
2.      91.9712 cm-1
3.     124.4778 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.128191        1.414318        0.087657
O          -1.340770        1.890044        0.200582
C           0.076154        0.064001        0.146179
C          -1.063260       -0.874639        0.381199
H          -0.838250       -1.898604        0.096373
H          -1.399440       -0.874792        1.421874
C          -3.547779       -0.957902       -0.020397
H          -3.522638       -2.041928       -0.100320
H          -4.319084       -0.557656       -0.671944
H          -3.753090       -0.670433        1.006831
N          -2.242736       -0.391434       -0.416987
H          -2.063862       -0.554565       -1.404421
H          -2.153558        0.685933       -0.233412
C           0.965833        2.425377       -0.122871
H           0.973375        3.120064        0.719545
H           1.952537        1.981633       -0.219691
H           0.748440        3.008642       -1.019690
Br          1.799553       -0.771587       -0.031757
```

---

### Compound_14_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.849125 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.733935 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      42.4877 cm-1
2.      58.1680 cm-1
3.      83.3363 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.029484        1.441973       -0.040461
O           2.226447        1.361038       -0.423801
C           0.205870        0.366162        0.267278
C          -1.190949        0.343707        0.681668
H          -1.418697       -0.403945        1.439939
H          -1.540902        1.310323        1.028925
C          -3.581582       -0.138290       -0.120909
H          -3.911814        0.821510        0.263912
H          -3.684939       -0.902268        0.643073
H          -4.157805       -0.408098       -1.000171
N          -2.145487       -0.030366       -0.490358
H          -1.809288       -0.914654       -0.872613
H          -2.013710        0.661405       -1.226737
C           0.463137        2.853516        0.108826
H           1.076915        3.395135        0.830339
H           0.561803        3.362573       -0.850912
H          -0.575376        2.917749        0.423324
Br          0.946425       -1.420511        0.021869
```

---

### Compound_14_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.849846 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.733613 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      60.3046 cm-1
2.      72.2656 cm-1
3.     106.2987 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.395066        1.575015        0.003313
O           0.392132        2.347037       -0.605018
C          -0.096334        0.283022        0.417528
C          -0.930444       -0.708927        1.079363
H          -0.420973       -1.269410        1.862083
H          -1.840614       -0.282515        1.487621
C          -2.276735       -1.352317       -1.002577
H          -3.202011       -0.970921       -0.582467
H          -2.480368       -2.175794       -1.679203
H          -1.744036       -0.558970       -1.516254
N          -1.417100       -1.835649        0.107890
H          -1.902625       -2.552951        0.644509
H          -0.577644       -2.272564       -0.273111
C          -1.783274        2.133836        0.312457
H          -2.434504        1.490299        0.897818
H          -1.658388        3.076349        0.846788
H          -2.282278        2.356850       -0.632140
Br          1.663349       -0.410026       -0.052321
```

---

### Compound_14_HEI_Conformation_5_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2900.849846 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2900.733613 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      60.3053 cm-1
2.      72.2656 cm-1
3.     106.2978 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.395067        1.575015        0.003313
O           0.392131        2.347037       -0.605018
C          -0.096334        0.283022        0.417528
C          -0.930444       -0.708927        1.079363
H          -0.420973       -1.269410        1.862083
H          -1.840614       -0.282516        1.487621
C          -2.276735       -1.352318       -1.002577
H          -3.202011       -0.970922       -0.582467
H          -2.480367       -2.175795       -1.679203
H          -1.744036       -0.558971       -1.516254
N          -1.417099       -1.835649        0.107890
H          -1.902624       -2.552952        0.644509
H          -0.577643       -2.272564       -0.273111
C          -1.783275        2.133835        0.312457
H          -2.434505        1.490298        0.897818
H          -1.658389        3.076348        0.846788
H          -2.282279        2.356849       -0.632140
Br          1.663349       -0.410025       -0.052321
```

---

### Compound_15_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.682691 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.589002 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      30.8052 cm-1
  2.      85.9019 cm-1
  3.     105.5329 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.798013       -0.062739        0.011925
C           0.366966       -0.799081       -0.643005
C           1.399828        0.231535       -1.080239
C           0.820747        1.511888       -0.687465
C          -0.408128        1.427398       -0.042487
H           1.670142        0.096357       -2.129887
H           1.283185        2.458201       -0.927056
Cl         -1.009916       -0.639488        1.707877
Cl         -2.309192       -0.380509       -0.910472
```

```
O           0.484489       -1.987843       -0.774690
O          -1.158720        2.312154        0.402065
C           2.752821       -0.021909        1.117040
H           2.439049        0.981920        1.380995
H           3.753660       -0.221629        1.484876
H           2.054202       -0.746740        1.522300
N           2.760778       -0.134795       -0.365770
H           3.474139        0.480841       -0.753075
H           3.013536       -1.082505       -0.647271
```

---

### Compound_15_HEI_Conformation_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.682691 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.589002 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      30.8307 cm-1
2.      85.8048 cm-1
3.     105.5814 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.797908       -0.062714        0.011872
C           0.366834       -0.799188       -0.643351
C           1.399869        0.231296       -1.080497
C           0.820723        1.511753       -0.688141
C          -0.408122        1.427416       -0.043068
H           1.670437        0.095875       -2.130041
H           1.283186        2.458003       -0.927932
Cl         -1.008863       -0.638992        1.708189
Cl         -2.309561       -0.380854       -0.909551
O           0.484000       -1.987942       -0.775398
O          -1.158732        2.312280        0.401234
C           2.752104       -0.021805        1.117228
H           2.437758        0.981914        1.380923
H           3.752895       -0.220990        1.485468
H           2.053679       -0.746910        1.522318
N           2.760634       -0.134864       -0.365562
H           3.474024        0.480845       -0.752696
H           3.013639       -1.082558       -0.646896
```

### Compound_15_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1358.682744 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1358.588805 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      57.4075 cm-1
2.      92.9265 cm-1
3.     104.6989 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.829156       -0.123646        0.008239
C           0.401570       -0.554154       -0.782880
C           1.348138        0.638566       -0.806644
C           0.433924        1.766566       -0.627326
C          -0.809545        1.420803       -0.101575
H           1.972500        0.631365       -1.698576
H           0.713593        2.784471       -0.854862
Cl         -0.552317       -0.644061        1.743580
Cl         -2.325877       -0.853513       -0.592095
O           0.565006       -1.601488       -1.349637
O          -1.787356        2.112622        0.217099
C           3.380309       -0.612409        0.208976
H           4.081593       -0.579313        1.036533
H           3.904652       -0.490583       -0.733183
H           2.836400       -1.550444        0.214527
N           2.407402        0.505508        0.356077
H           1.896400        0.423908        1.236375
H           2.899700        1.397372        0.398980
```

### Compound_16_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.314534 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.231689 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      32.5910 cm-1
2.      67.5348 cm-1
3.      84.0287 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.150193       -0.103122        0.001061
C          -0.078814       -1.143584        0.366375
C           1.109741       -0.681117       -0.187481
C           1.048361        0.575282       -0.923369
C          -0.405887        0.996454       -0.747274
H           1.338387        0.550497       -1.977168
Cl         -1.949690        0.573603        1.465607
Cl         -2.405204       -0.816841       -1.079055
O          -0.334876       -2.174498        1.000617
O          -0.849708        2.052174       -1.109105
Cl          2.590854       -1.578733       -0.111473
C           1.867274        1.919008        1.116815
H           2.146492        0.993153        1.606290
H           2.549050        2.717098        1.390153
H           0.850067        2.188995        1.380674
N           1.948378        1.718892       -0.356616
H           1.688988        2.577340       -0.845079
H           2.910839        1.515245       -0.623772
```

---

### Compound_16_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.312725 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.229758 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      26.0458 cm-1
2.      64.6804 cm-1
```

```
   3.     121.7061 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.284406       -0.059332        0.000347
C          -0.400274        1.176756        0.246498
C           0.909088        0.765792        0.022707
C           1.086514       -0.620853       -0.420848
C          -0.303608       -1.204940       -0.170130
H           1.414008       -0.774072       -1.453873
Cl         -2.201418        0.128880       -1.555364
Cl         -2.438497       -0.364675        1.328919
O          -0.869944        2.284893        0.534777
O          -0.521463       -2.380384       -0.050470
Cl          2.231175        1.892008        0.000447
C           3.483330       -1.456594       -0.098177
H           4.083611       -2.082033        0.554338
H           3.488739       -1.852401       -1.108336
H           3.846292       -0.435714       -0.087774
N           2.077260       -1.468515        0.401701
H           1.716745       -2.426896        0.398892
H           2.045781       -1.145945        1.369969
```

---

### Compound_16_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1818.313188 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1818.23024 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
   1.      51.6365 cm-1
   2.      69.1152 cm-1
   3.     111.2774 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.145506       -0.057760       -0.008413
C          -0.261259       -1.305692        0.200482
C           1.014903       -0.923342       -0.208284
```

```
C           1.175169        0.471911       -0.606145
C          -0.275626        0.883519       -0.831745
H           1.786375        0.668501       -1.485789
Cl         -1.447711        0.775367        1.598414
Cl         -2.694721       -0.422265       -0.782419
O          -0.698529       -2.377994        0.628465
O          -0.649793        1.752850       -1.570922
Cl          2.383661       -1.986329       -0.148298
C           2.089783        2.775809        0.117921
H           2.557599        3.285301        0.953805
H           2.747379        2.786727       -0.744997
H           1.142167        3.242716       -0.126277
N           1.840890        1.357597        0.503285
H           2.722260        0.904042        0.744688
H           1.258886        1.308887        1.341485
```

---

### Compound_17_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2333.393077 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2333.309024 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      23.9989 cm-1
2.      42.0725 cm-1
3.      57.5987 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.565377        0.955494       -0.328877
C           1.611475       -0.256571       -0.121064
C           0.291906        0.381778        0.184428
C           0.477900        1.853538        0.154869
N           1.802954        2.086368       -0.141236
H           2.184684        3.019624       -0.220136
O          -0.359059        2.712001        0.349507
O           3.730412        0.907033       -0.597680
C          -0.880699       -0.200793        0.451067
Cl         -1.116522       -1.883005        0.493988
Cl         -3.995260        0.095089       -1.433643
C          -2.775241        0.346970        1.965275
H          -2.100959        0.544394        2.792316
```

```
H          -3.128413       -0.677142        1.991466
H          -3.617790        1.029520        1.986819
N          -2.060756        0.583955        0.672786
H          -1.775866        1.575415        0.603393
H          -2.790573        0.396668       -0.162779
Cl          2.244465       -1.230246        1.241713
Cl          1.591929       -1.218043       -1.629159
```

---

### Compound_17_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2333.363375 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2333.276611 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
  1.      43.2894 cm-1
  2.      57.7104 cm-1
  3.      92.9030 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.351191        0.977011        0.041974
C          -1.348184       -0.218758       -0.037240
C          -0.046358        0.419746       -0.203823
C          -0.218960        1.825399       -0.184274
N          -1.591664        2.101268       -0.062110
H          -1.969116        3.036435       -0.058929
O           0.634070        2.723665       -0.252071
O          -3.547041        0.901876        0.166218
C           1.266202       -0.150527       -0.088217
Cl          1.414940       -1.839730       -0.618617
Cl          1.951538       -0.101779        1.701497
C           3.701985        0.484273       -0.722127
H           4.188836        1.073592       -1.492491
H           3.923894       -0.568480       -0.857700
H           4.007454        0.817740        0.260288
N           2.235736        0.698388       -0.877135
H           1.943006        1.685394       -0.647630
H           1.979852        0.560074       -1.856006
Cl         -1.897245       -1.269892       -1.436671
Cl         -1.545681       -1.213866        1.475923
```

### Compound_18_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.513266 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.422927 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      61.5054 cm-1
2.      84.4023 cm-1
3.     136.0259 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.242436        1.833993        0.218460
O           1.228217        2.380078       -0.331620
C          -0.011436        0.501460        0.467627
C          -1.204705       -0.023585        1.115627
H          -1.015800       -0.778743        1.877707
H          -1.798476        0.781471        1.544496
C          -2.739201        0.128941       -0.923196
H          -3.369691        0.868743       -0.440123
H          -3.322450       -0.473622       -1.611755
H          -1.920369        0.617077       -1.440693
N          -2.161001       -0.753067        0.123112
H          -2.905177       -1.208148        0.649923
H          -1.619277       -1.497415       -0.317158
Br          1.260399       -0.834187       -0.123996
H          -0.584019        2.473175        0.597514
```

### Compound_18_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.515028 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.425247 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      52.6393 cm-1
  2.     129.8063 cm-1
  3.     183.8288 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.174821        1.609459        0.008599
O           1.386198        2.060172        0.094338
C          -0.140259        0.289976        0.126632
C           0.906530       -0.738516        0.395761
H           0.604076       -1.744880        0.119543
H           1.229917       -0.752464        1.440029
C           3.382889       -1.033394        0.022105
H           3.261024       -2.111580       -0.041401
H           3.601820       -0.746153        1.046358
H           4.189850       -0.712185       -0.629745
N           2.132042       -0.364874       -0.398437
H           2.153806        0.703416       -0.261755
H           1.948272       -0.536142       -1.384084
Br         -1.951728       -0.317510       -0.039472
H          -0.636060        2.320441       -0.191654
```

---

### Compound_18_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.515727 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.425633 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      59.4999 cm-1
  2.     139.2444 cm-1
  3.     179.9155 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.431497        1.530151       -0.191722
O           1.656270        1.925711       -0.026498
C          -0.031505        0.323790        0.232631
```

```
C           0.837065       -0.649505        0.959461
H           0.501454       -1.678716        0.857156
H           0.926617       -0.425060        2.025316
C           2.423322       -1.222430       -0.901776
H           3.423476       -1.009516       -1.266985
H           1.685685       -0.838770       -1.599745
H           2.292764       -2.293216       -0.772732
N           2.231347       -0.536947        0.396734
H           2.318553        0.535018        0.259545
H           2.912052       -0.863523        1.076182
Br         -1.846595       -0.204514       -0.086059
H          -0.261638        2.192656       -0.723380
```

---

### Compound_18_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.512809 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.423098 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      62.6689 cm-1
  2.      81.4501 cm-1
  3.     100.4272 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.859808        1.811152        0.040637
O           2.041479        2.013806       -0.326829
C           0.192099        0.627040        0.274268
C          -1.201258        0.516505        0.687904
H          -1.391231       -0.214590        1.473013
H          -1.591532        1.484987        0.996020
C          -3.552908       -0.120794       -0.098244
H          -3.938270        0.830982        0.253635
H          -3.613262       -0.862941        0.691396
H          -4.110002       -0.453349       -0.968171
N          -2.123964        0.056736       -0.471041
H          -1.741764       -0.818320       -0.830405
H          -2.029877        0.735206       -1.225789
Br          1.113297       -1.054210       -0.004028
H           0.200011        2.684366        0.235795
```

### Compound_18_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.510627 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.420472 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
1.      35.9793 cm-1
2.      99.0414 cm-1
3.     137.0783 cm-1
```

**B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates**

```
C           0.367870        1.771798       -0.150272
O           1.466812        2.370159        0.007102
C           0.056140        0.510006        0.319076
C           0.953258       -0.344715        1.088552
H           0.482093       -0.868226        1.918795
H           1.797808        0.239759        1.447474
C           2.452942       -0.992595       -0.862570
H           3.320941       -0.517381       -0.417670
H           1.889995       -0.271828       -1.445600
H           2.753730       -1.834976       -1.476781
N           1.572450       -1.479665        0.233028
H           0.798735       -2.014396       -0.161732
H           2.086754       -2.118606        0.837940
Br         -1.668767       -0.261797       -0.115929
H          -0.446111        2.277953       -0.701654
```

### Compound_18_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2861.510892 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2861.420337 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 39)

```
  1.      61.3525 cm-1
  2.     111.0217 cm-1
  3.     135.7969 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.819690        1.794036       -0.077902
O           1.943503        1.901292       -0.620822
C           0.116141        0.666933        0.302256
C          -1.187651        0.705523        0.954127
H          -1.350079       -0.083898        1.684470
H          -1.354443        1.671485        1.428020
C          -2.489017       -0.714223       -0.760846
H          -2.547105       -1.523853       -0.040480
H          -1.597970       -0.819327       -1.368132
H          -3.375796       -0.701527       -1.386551
N          -2.404071        0.573262       -0.020233
H          -2.338444        1.341326       -0.686582
H          -3.261912        0.719798        0.512239
Br          0.951413       -1.064562        0.065563
H           0.251788        2.718889        0.164714
```

---

### Compound_19_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.267455 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.138832 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
  1.      84.0370 cm-1
  2.     145.9365 cm-1
  3.     193.8796 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.014417        0.216998       -0.044038
O           1.906591       -1.073137        0.100851
C           0.981953        1.102344        0.024186
```

```
C          -0.406552        0.627703        0.330405
H          -0.519623        0.368832        1.388953
H           1.146776        2.157150       -0.138554
H           3.014402        0.615043       -0.264692
C          -1.498677        1.604809       -0.066210
H          -2.493327        1.231592        0.173908
H          -1.353485        2.539059        0.474939
H          -1.450888        1.824654       -1.133996
N          -0.579352       -0.708615       -0.373750
H          -0.676746       -0.538837       -1.372437
H           0.407021       -1.151659       -0.214210
C          -1.670708       -1.573599        0.118013
H          -1.493582       -1.791517        1.167467
H          -2.630795       -1.078789        0.003805
H          -1.669619       -2.499656       -0.449876
```

---

### Compound_19_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.267455 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.138834 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      84.0642 cm-1
2.     146.2592 cm-1
3.     193.9990 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.014415       -0.216998        0.044070
O           1.906441        1.073140       -0.101049
C           0.981949       -1.102343       -0.023873
C          -0.406459       -0.627715       -0.330363
H          -0.519255       -0.368957       -1.388957
H           1.146784       -2.157151        0.138854
H           3.014445       -0.614905        0.264680
C          -1.498711       -1.604747        0.066056
H          -2.493276       -1.231461       -0.174344
H          -1.353429       -2.539037       -0.475001
H          -1.451208       -1.824523        1.133872
N          -0.579258        0.708621        0.373670
H           0.407254        1.151808        0.214000
```

```
H          -0.676454        0.538971        1.372406
C          -1.670738        1.573505       -0.117875
H          -1.668565        2.500244        0.448901
H          -1.494808        1.790041       -1.167837
H          -2.630942        1.079300       -0.001953
```

---

### Compound_19_HEI_Conformation_4_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -327.267455 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.138835 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      84.0570 cm-1
2.     146.0055 cm-1
3.     193.8591 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.014415        0.216981       -0.043991
O           1.906544       -1.073152        0.101020
C           0.981957        1.102341        0.024060
C          -0.406546        0.627752        0.330342
H          -0.519577        0.368985        1.388918
H           1.146816        2.157138       -0.138694
H           3.014431        0.614972       -0.264571
C          -1.498657        1.604856       -0.066313
H          -2.493302        1.231813        0.174083
H          -1.353264        2.539213        0.474595
H          -1.451040        1.824457       -1.134155
N          -0.579322       -0.708666       -0.373666
H           0.407111       -1.151730       -0.213964
H          -0.676572       -0.538996       -1.372387
C          -1.670753       -1.573598        0.117981
H          -1.669268       -2.499886       -0.449530
H          -1.494057       -1.791068        1.167599
H          -2.630877       -1.079008        0.003138
```

---

### Compound_20_HEI_Conformation_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.58772 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.433289 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      24.3144 cm-1
2.      71.0716 cm-1
3.      91.1318 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.333825       -1.334539       -0.122049
O          -2.554384       -1.350485       -0.456803
C          -0.595556       -0.283441        0.397057
H          -0.756973       -2.280360       -0.232334
C           0.817332       -0.507198        0.704276
H           1.177250        0.014961        1.591922
H           1.074514       -1.562896        0.774144
C           3.232565       -0.182436       -0.153958
H           3.414118       -1.245349       -0.027756
H           3.492173        0.348703        0.756477
H           3.814005        0.199763       -0.987219
N           1.785340        0.020717       -0.422136
H           1.506631       -0.444638       -1.284587
H           1.588723        1.009277       -0.564524
C          -1.224809        1.057043        0.673809
H          -2.290441        0.898969        0.854979
H          -0.809674        1.479225        1.596263
C          -1.084071        2.103266       -0.444041
H          -0.042621        2.394657       -0.603259
H          -1.465230        1.713489       -1.388782
H          -1.634586        3.016880       -0.206511
```

---

### Compound_20_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.587877 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.433113 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      44.7672 cm-1
2.      67.4673 cm-1
3.      86.6607 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.190999       -1.399357       -0.225009
O           2.351385       -1.719020        0.171643
C           0.522505       -0.199436       -0.061390
H           0.610859       -2.164115       -0.789077
C          -0.818564       -0.051835       -0.630773
H          -1.025087        0.922478       -1.076542
H          -1.064994       -0.832227       -1.348329
C          -3.325900        0.046821       -0.037850
H          -3.388362        1.051822       -0.443184
H          -4.028321       -0.069998        0.781513
H          -3.534562       -0.680205       -0.816505
N          -1.942598       -0.176879        0.457059
H          -1.850212       -1.103533        0.870067
H          -1.724535        0.482063        1.202364
C           1.155139        0.977145        0.636368
H           0.439785        1.475737        1.302350
H           1.953977        0.604243        1.279595
C           1.734525        2.029470       -0.319806
H           2.514933        1.589348       -0.942494
H           0.964059        2.424795       -0.985103
H           2.167340        2.873056        0.223544
```

---

### Compound_20_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.587877 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.433113 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      44.7579 cm-1
2.      67.4677 cm-1
3.      86.6648 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.190987       -1.399360       -0.225006
O           2.351371       -1.719026        0.171647
C           0.522498       -0.199434       -0.061393
H           0.610842       -2.164118       -0.789070
C          -0.818569       -0.051827       -0.630776
H          -1.025088        0.922487       -1.076545
H          -1.065004       -0.832218       -1.348332
C          -3.325905        0.046831       -0.037850
H          -3.534568       -0.680203       -0.816497
H          -3.388366        1.051828       -0.443195
H          -4.028325       -0.069978        0.781515
N          -1.942602       -0.176865        0.457058
H          -1.850214       -1.103516        0.870073
H          -1.724537        0.482082        1.202358
C           1.155137        0.977144        0.636367
H           0.439772        1.475756        1.302321
H           1.953951        0.604238        1.279621
C           1.734568        2.029446       -0.319805
H           2.514979        1.589300       -0.942473
H           0.964125        2.424782       -0.985122
H           2.167392        2.873027        0.223546
```

---

### Compound_20_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.586442 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.430767 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      43.9895 cm-1
  2.      70.8069 cm-1
  3.     119.3837 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.073082       -1.402511        0.107985
O          -2.122604       -1.682383       -0.542607
```

```
C          -0.376758       -0.206339        0.154944
H          -0.630536       -2.207282        0.738457
C           0.803583       -0.124091        1.019811
H           0.990619        0.866364        1.434199
H           0.793335       -0.853022        1.828712
C           2.495851        0.430995       -0.851013
H           2.564515        1.449357       -0.481147
H           1.704962        0.350892       -1.588068
H           3.443586        0.123819       -1.282271
N           2.160373       -0.462961        0.285763
H           2.918862       -0.457334        0.967899
H           2.073435       -1.419804       -0.052811
C          -0.889393        1.024721       -0.550679
H          -0.070227        1.614889       -0.971008
H          -1.503252        0.707151       -1.395999
C          -1.727567        1.943595        0.350481
H          -2.077518        2.827384       -0.189171
H          -2.599506        1.411625        0.733975
H          -1.145859        2.287521        1.208575
```

---

### Compound_20_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.586441 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.43076 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      44.5779 cm-1
2.      71.0670 cm-1
3.     119.5042 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.074088       -1.402233        0.107955
O          -2.123880       -1.681610       -0.542403
C          -0.377016       -0.206468        0.154625
H          -0.631918       -2.207145        0.738513
C           0.803251       -0.124732        1.019582
H           0.990548        0.865570        1.434240
H           0.792680       -0.853853        1.828318
C           2.496119        0.430331       -0.850745
H           2.564614        1.448621       -0.480639
```

```
H           1.705575        0.350415       -1.588205
H           3.444054        0.123235       -1.281636
N           2.160057       -0.463876        0.285653
H           2.918432       -0.458859        0.967918
H           2.072776       -1.420558       -0.053299
C          -0.889065        1.024875       -0.550944
H          -0.069786        1.614151       -0.972329
H          -1.504095        0.707607       -1.395523
C          -1.725409        1.944846        0.350785
H          -2.597541        1.413863        0.735238
H          -1.142510        2.288353        1.208248
H          -2.074942        2.828889       -0.188733
```

---

### Compound_20_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.608864 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.453603 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      64.1224 cm-1
  2.      94.1800 cm-1
  3.     121.1954 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.502313        1.594612       -0.016683
O           0.713810        2.177702       -0.214377
C          -0.704555        0.314582        0.312703
H          -1.326313        2.285015       -0.154078
C           0.455113       -0.623147        0.548871
H           0.125213       -1.665948        0.467707
H           0.821872       -0.500805        1.574273
C           2.782870       -1.122728       -0.014625
H           3.155245       -0.812848        0.962012
H           3.559258       -0.930167       -0.753156
H           2.593748       -2.202776        0.020103
N           1.589816       -0.348270       -0.346167
H           1.306782       -0.554752       -1.297695
H           1.359136        1.423956       -0.267159
C          -2.094524       -0.230494        0.496887
H          -2.156014       -0.751444        1.458688
```

```
H          -2.802626        0.598777        0.552140
C          -2.529213       -1.192943       -0.614861
H          -3.522164       -1.599162       -0.415228
H          -2.557685       -0.679106       -1.576736
H          -1.839915       -2.033761       -0.706436
```

---

### Compound_20_HEI_Conformation_7_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -366.608976 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.453662 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      80.3435 cm-1
  2.      90.4485 cm-1
  3.     118.4601 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.457075        1.586706        0.019548
O          -0.731208        2.140886       -0.351859
C           0.688736        0.281478        0.197465
H           1.235411        2.326215        0.166754
C          -0.386764       -0.751796       -0.039327
H          -0.153222       -1.668602        0.518553
H          -0.406543       -1.038745       -1.096075
C          -2.798021       -1.158085       -0.117508
H          -2.672284       -2.171738        0.282657
H          -2.820468       -1.223885       -1.205429
H          -3.756454       -0.768151        0.221154
N          -1.729373       -0.250124        0.291218
H          -1.780177       -0.100273        1.292732
H          -1.396328        1.406385       -0.275599
C           2.054910       -0.215707        0.582072
H           2.700407        0.636826        0.802419
H           1.983945       -0.799719        1.506431
C           2.713439       -1.085175       -0.496055
H           3.695317       -1.432506       -0.171084
H           2.109372       -1.965368       -0.721690
H           2.840049       -0.521184       -1.421645
```

### Compound_21_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -2277.972607 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -2277.910708 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.       9.4403 cm-1
2.      15.1559 cm-1
3.      33.8476 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.530280       -0.265122       -0.088563
C          -0.383692       -0.902280        0.713640
C           0.690903        0.123925        0.826262
C           0.265628        1.276082        0.206214
C          -1.051780        1.172618       -0.370648
Cl         -3.031954       -0.258506        0.869777
Cl         -1.752741       -1.154535       -1.621902
O          -0.375822       -2.018791        1.154551
O          -1.687331        2.013102       -0.963929
C           2.253908       -1.220085        2.234821
H           1.707229       -1.201347        3.176704
H           3.317342       -1.140896        2.435551
H           2.052370       -2.154924        1.723919
N           1.883782       -0.082284        1.387525
H           2.461640        0.741973        1.480558
H           2.760707       -0.670795       -0.533364
Cl          1.198127        2.702777        0.106719
Cl          2.971940       -1.058169       -1.745851
```

---

### 23_carboxin_mmff_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.754425 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.497667 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      18.9243 cm-1
  2.      30.5008 cm-1
  3.      54.4453 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.187154       -0.537785       -0.164337
N           1.259378        0.305785        0.157714
O           0.409580       -1.647166       -0.692613
C          -1.099640       -0.033007        0.170779
C           2.626257        0.090421        0.072249
C          -2.371127       -0.588218       -0.320117
S          -1.339057        1.525522        0.960608
C           3.467561        1.153538        0.447769
C           3.221750       -1.107500       -0.353268
C          -2.363496       -1.853661       -1.150960
O          -3.187654        0.388406       -1.010832
C          -2.073892        2.490709       -0.435498
C           4.845934        1.025654        0.401811
C           4.607081       -1.218881       -0.393919
C          -2.471555        1.510716       -1.527708
C           5.433189       -0.164549       -0.020947
H           0.984463        1.198768        0.537560
H           3.023540        2.084777        0.777827
H           2.590869       -1.927756       -0.646831
H          -1.811547       -1.662320       -2.066262
H          -1.876907       -2.679037       -0.644102
H          -3.390871       -2.116244       -1.406448
H          -1.364256        3.221498       -0.822912
H          -2.942246        3.013786       -0.038896
H           5.464836        1.862563        0.698145
H           5.043894       -2.152499       -0.725228
H          -3.143263        1.986176       -2.240575
H          -1.587268        1.168011       -2.066620
H           6.509000       -0.265303       -0.058440
N          -3.313583       -0.829212        0.918359
H          -4.268418       -0.941614        0.583117
H          -3.265803        0.068648        1.411873
C          -2.920286       -1.930270        1.825795
H          -3.482312       -1.843820        2.750348
H          -3.131952       -2.882237        1.352152
H          -1.856393       -1.830672        2.020724
```

### Compound_22_HEI_Conformation_2_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.754425 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.497666 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      18.9369 cm-1
  2.      30.5567 cm-1
  3.      54.4494 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.187148       -0.537741       -0.164504
N           1.259386        0.305871        0.157397
O           0.409550       -1.647161       -0.692712
C          -1.099624       -0.032953        0.170670
C           2.626260        0.090462        0.072085
C          -2.371170       -0.588214       -0.320012
S          -1.338966        1.525595        0.960510
C           3.467546        1.153498        0.447892
C           3.221786       -1.107394       -0.353574
C          -2.363615       -1.853598       -1.150940
O          -3.187889        0.388413       -1.010489
C          -2.074022        2.490733       -0.435504
C           4.845920        1.025598        0.402072
C           4.607121       -1.218794       -0.394070
C          -2.471906        1.510692       -1.527587
C           5.433206       -0.164545       -0.020817
H           0.984477        1.198827        0.537308
H           3.023503        2.084688        0.778064
H           2.590928       -1.927591       -0.647356
H          -1.811896       -1.662138       -2.066359
H          -1.876822       -2.678956       -0.644241
H          -3.391023       -2.116267       -1.406214
H          -1.364431        3.221479       -0.823085
H          -2.942287        3.013858       -0.038768
H           5.464801        1.862447        0.698624
H           5.043956       -2.152365       -0.725489
H          -3.143757        1.986111       -2.240349
H          -1.587723        1.167957       -2.066653
H           6.509020       -0.265313       -0.058197
N          -3.313388       -0.829356        0.918637
```

```
H          -4.268304       -0.941689        0.583595
H          -3.265468        0.068439        1.412259
C          -2.919894       -1.930564        1.825797
H          -3.481565       -1.844164        2.750573
H          -3.131848       -2.882446        1.352115
H          -1.855916       -1.831108        2.020343
```

---

### Compound_22_HEI_Conformation_3_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.753269 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.496276 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      22.3163 cm-1
  2.      31.7204 cm-1
  3.      63.9586 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.247149        0.277114        0.183997
N           1.375527       -0.546376        0.171982
O           0.377422        1.531823        0.415389
C          -0.986450       -0.307125       -0.069783
C           2.720059       -0.220639        0.089070
C          -2.231688        0.507040        0.145524
S          -1.217901       -1.939330       -0.686102
C           3.651168       -1.268098        0.201146
C           3.204323        1.080012       -0.121690
C          -2.497656        0.861623        1.607015
O          -3.359441       -0.074510       -0.470177
C          -2.661088       -2.331647        0.347218
C           5.011942       -1.025988        0.105195
C           4.572415        1.305768       -0.212253
C          -3.795956       -1.340921        0.045312
C           5.489621        0.265814       -0.101488
H           1.163945       -1.532577        0.155543
H           3.292672       -2.276851        0.365126
H           2.503901        1.893167       -0.203348
H          -2.592049       -0.057878        2.177973
H          -1.657571        1.422102        2.010198
H          -3.415072        1.436302        1.724625
```

```
H          -2.357652       -2.291829        1.391631
H          -2.986756       -3.344956        0.119061
H           5.703393       -1.853774        0.194108
H           4.923251        2.316909       -0.375364
H          -4.437798       -1.733604       -0.739370
H          -4.401100       -1.184763        0.941869
H           6.551461        0.455802       -0.173440
N          -2.023842        1.803470       -0.639712
H          -1.961722        1.520478       -1.615795
H          -1.046033        2.061328       -0.323658
C          -3.006139        2.902774       -0.485583
H          -2.781770        3.666102       -1.224697
H          -4.006854        2.514366       -0.644964
H          -2.919683        3.326436        0.508473
```

---

### Compound_22_HEI_Conformation_4_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1164.754425 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1164.497666 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 102)

```
  1.      18.9297 cm-1
  2.      30.5482 cm-1
  3.      54.4457 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.187142       -0.537758       -0.164465
N          -1.259382        0.305854        0.157429
O          -0.409540       -1.647179       -0.692672
C           1.099626       -0.032965        0.170703
C          -2.626255        0.090447        0.072105
C           2.371163       -0.588209       -0.320022
S           1.338970        1.525590        0.960522
C          -3.221782       -1.107409       -0.353550
C          -3.467540        1.153490        0.447894
C           2.363597       -1.853598       -1.150942
O           3.187845        0.388424       -1.010536
C           2.073969        2.490735       -0.435518
C          -4.607117       -1.218802       -0.394066
C          -4.845915        1.025598        0.402055
```

```
C           2.471840        1.510700       -1.527612
C          -5.433202       -0.164545       -0.020833
H          -0.984476        1.198809        0.537345
H          -2.590924       -1.927611       -0.647315
H          -3.023496        2.084679        0.778063
H           1.876871       -2.678972       -0.644211
H           1.811804       -1.662165       -2.066321
H           3.390997       -2.116223       -1.406288
H           2.942234        3.013879       -0.038809
H           1.364353        3.221465       -0.823079
H          -5.043951       -2.152372       -0.725483
H          -5.464794        1.862452        0.698592
H           1.587652        1.167961       -2.066664
H           3.143674        1.986129       -2.240382
H          -6.509015       -0.265307       -0.058229
N           3.313429       -0.829326        0.918594
H           3.265522        0.068474        1.412208
H           4.268332       -0.941659        0.583519
C           2.919978       -1.930525        1.825783
H           3.481668       -1.844096        2.750544
H           1.856003       -1.831083        2.020353
H           3.131940       -2.882409        1.352112
```

---

### Compound_23_HEI_Conformation_10_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.58664 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.351611 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      37.6696 cm-1
2.      54.7800 cm-1
3.      77.2883 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.243444       -0.257110        0.755838
C          -1.009081       -0.257686        0.128531
C          -0.013394        0.723172        0.583923
C           1.425011        0.288679        0.907817
C           2.354668       -0.091702       -0.247048
C           3.721890       -0.538429        0.265161
```

```
C          -0.743475       -1.227496       -0.996008
C          -0.230711       -2.604741       -0.548940
O          -3.241681       -1.004412        0.529195
H          -2.344713        0.501991        1.563190
H          -0.410364        1.234556        1.460605
H           1.336252       -0.557376        1.590929
H           1.906006        1.089098        1.479294
H           2.496649        0.758426       -0.919839
H           1.917977       -0.888256       -0.845837
H           4.198237        0.249488        0.851674
H           3.627400       -1.417958        0.904792
H           4.388583       -0.793062       -0.559082
H          -1.680127       -1.379439       -1.538607
H          -0.042782       -0.808773       -1.725192
H          -0.068515       -3.268394       -1.402232
H           0.710224       -2.526015       -0.002993
H          -0.956274       -3.076635        0.113988
N           0.125000        1.928136       -0.457668
H           0.898336        2.531498       -0.181461
H           0.379215        1.526377       -1.357186
C          -1.110242        2.733561       -0.607627
H          -1.924519        2.054536       -0.837439
H          -1.306588        3.242025        0.331310
H          -0.973892        3.456760       -1.405687
```

---

### Compound_23_HEI_Conformation_15_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.583061 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.347606 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      61.1399 cm-1
2.      71.1025 cm-1
3.     101.6996 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.388224        0.113504       -0.735471
C           1.124464       -0.068238       -0.190033
C           0.022825        0.661869       -0.820159
C          -1.350242        0.013480       -1.027316
```

```
C          -2.255076       -0.244030        0.178843
C          -3.522522       -0.991061       -0.229432
C           0.955116       -1.009457        0.977604
C           0.617657       -2.456546        0.589341
O           3.484555       -0.401134       -0.370862
H           2.411868        0.802498       -1.609929
H           0.359118        1.021059       -1.791667
H          -1.154586       -0.932754       -1.535230
H          -1.910874        0.623530       -1.742327
H          -2.543352        0.702294        0.642817
H          -1.729765       -0.816121        0.941301
H          -4.177442       -1.153997        0.626871
H          -4.084069       -0.431200       -0.979833
H          -3.278470       -1.965846       -0.655852
H           1.897665       -1.018987        1.530139
H           0.199778       -0.649724        1.678863
H           0.553883       -3.100473        1.470275
H          -0.335517       -2.519595        0.063062
H           1.385515       -2.861408       -0.071133
N          -0.251414        2.110608       -0.094130
H           0.437320        2.739415       -0.499018
H          -1.163590        2.466242       -0.375627
C          -0.109508        2.154142        1.381245
H           0.858122        1.732235        1.631740
H          -0.169174        3.185900        1.715203
H          -0.898599        1.569773        1.838425
```

---

### Compound_23_HEI_Conformation_16_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.614504 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.379512 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      44.6192 cm-1
2.      66.1372 cm-1
3.      82.3519 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.608697       -0.466293       -1.401901
C          -1.070151        0.377753       -0.516141
```

```
C           0.135457       -0.001436        0.321203
C           1.433306        0.348499       -0.419759
C           2.701682        0.248117        0.426512
C           3.945288        0.693840       -0.338229
C          -1.622854        1.766028       -0.342076
C          -2.410264        1.952963        0.960568
O          -1.211926       -1.752223       -1.617214
H          -2.442141       -0.173996       -2.030493
H           0.114498        0.590562        1.247194
H           1.339159        1.371602       -0.789693
H           1.516752       -0.294001       -1.300886
H           2.851861       -0.777658        0.774117
H           2.580634        0.861386        1.323897
H           4.098952        0.078295       -1.226803
H           3.850252        1.730856       -0.666267
H           4.841097        0.618469        0.279259
H          -0.803226        2.492289       -0.365885
H          -2.268550        2.006942       -1.189009
H          -1.798389        1.720775        1.833267
H          -2.758285        2.982151        1.063567
H          -3.279889        1.294706        0.979574
N           0.113834       -1.438465        0.660521
H          -0.577888       -1.950420       -0.875192
H           1.037389       -1.728985        0.951535
C          -0.849995       -1.774709        1.707491
H          -1.859384       -1.573390        1.350561
H          -0.773889       -2.834714        1.943673
H          -0.693010       -1.196390        2.625646
```

---

### Compound_23_HEI_Conformation_17_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.596017 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.360579 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      42.8883 cm-1
2.      60.4265 cm-1
3.      84.2955 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.135742        0.945417       -0.483863
C           0.857156        0.803027       -0.027847
C           0.181031       -0.500729       -0.386194
C          -1.191971       -0.810030        0.212929
C          -2.331296       -0.537968       -0.771891
C          -3.706427       -0.669195       -0.127533
C           0.240510        1.844013        0.867414
C          -0.905468        2.672920        0.271731
O           2.808981        0.049031       -1.151499
H           2.659862        1.878972       -0.231598
H           0.102506       -0.580202       -1.475387
H          -1.347480       -0.244966        1.131603
H          -1.238512       -1.864128        0.496729
H          -2.243988       -1.237185       -1.607599
H          -2.218867        0.459630       -1.199993
H          -3.846398       -1.664486        0.299304
H          -3.830105        0.056751        0.678703
H          -4.502689       -0.501691       -0.853518
H          -0.108007        1.396988        1.805462
H           1.039547        2.531530        1.156780
H          -1.781920        2.063296        0.057809
H          -1.214967        3.460345        0.962758
H          -0.592518        3.143648       -0.661966
N           1.189618       -1.612879       -0.087187
H           0.899614       -2.475449       -0.539382
H           2.050809       -1.197413       -0.598674
C           1.495328       -1.850201        1.338372
H           0.618075       -2.229549        1.854644
H           2.302553       -2.573628        1.408773
H           1.805680       -0.908085        1.779140
```

---

### Compound_23_HEI_Conformation_18_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.589951 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.355238 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      49.8854 cm-1
2.      77.2971 cm-1
3.      84.8336 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.091354        0.235395       -1.063292
C           1.129365       -0.097620       -0.128943
C          -0.226911        0.448603       -0.283086
C          -1.396568       -0.521619       -0.113413
C          -2.780160        0.040658       -0.442085
C          -3.863538       -1.033339       -0.387964
C           1.468455       -0.986490        1.041701
C           1.379001       -2.493149        0.756282
O           3.305111       -0.131183       -1.108124
H           1.726623        0.905842       -1.873207
H          -0.316743        0.971664       -1.235875
H          -1.393746       -0.937247        0.898027
H          -1.191682       -1.357413       -0.783323
H          -2.756511        0.491750       -1.437515
H          -3.055760        0.841262        0.251536
H          -4.843947       -0.619961       -0.625594
H          -3.653343       -1.832401       -1.101112
H          -3.919990       -1.481057        0.605940
H           2.488970       -0.760861        1.361748
H           0.828956       -0.761285        1.903594
H           1.685003       -3.083201        1.624036
H           0.363077       -2.788019        0.492166
H           2.029281       -2.755571       -0.078569
N          -0.471154        1.615644        0.774540
H          -0.258746        1.227046        1.691524
H          -1.456685        1.870866        0.789644
C           0.354584        2.823899        0.540635
H           0.221278        3.516412        1.365948
H           1.390597        2.510418        0.465432
H           0.037060        3.283687       -0.390196
```

---

### Compound_23_HEI_Conformation_19_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.596837 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.36188 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
  1.      24.4311 cm-1
  2.      61.9629 cm-1
  3.      84.7728 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.957284        0.537083        1.045967
C           1.058105       -0.319433        0.481806
C          -0.244679        0.300549        0.034101
C          -1.228577       -0.591538       -0.714620
C          -2.096881       -1.438768        0.224858
C          -3.174547       -0.634324        0.949128
C           1.415664       -1.760103        0.227201
C           2.011340       -2.041926       -1.161335
O           1.800458        1.828494        1.155795
H           2.906808        0.112228        1.404349
H          -0.752377        0.736646        0.899370
H          -0.689041       -1.235689       -1.407178
H          -1.894543        0.023627       -1.322099
H          -1.464884       -1.945538        0.956521
H          -2.573017       -2.225125       -0.363932
H          -2.746492        0.144472        1.581772
H          -3.843179       -0.149713        0.234926
H          -3.777911       -1.279124        1.588985
H           2.151012       -2.063655        0.977494
H           0.555524       -2.416265        0.378483
H           2.931972       -1.472723       -1.299583
H           2.242716       -3.102679       -1.287375
H           1.326582       -1.754068       -1.960530
N           0.125681        1.551745       -0.759423
H           0.875922        1.955874       -0.084006
H           0.576512        1.280512       -1.629355
C          -0.946926        2.538814       -0.996268
H          -0.516392        3.420041       -1.464024
H          -1.716771        2.126689       -1.641193
H          -1.380577        2.812203       -0.038058
```

---

### Compound_23_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.590402 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.355541 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      53.4810 cm-1
2.      60.2149 cm-1
3.      66.2884 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.882480       -0.520221       -1.290769
C          -0.987372       -0.361221       -0.245193
C           0.169596        0.525293       -0.458054
C           1.503350        0.081162        0.131081
C           2.019680       -1.190333       -0.539805
C           3.355668       -1.648809        0.036345
C          -1.180869       -1.094857        1.055735
C          -1.510928       -0.222960        2.276898
O          -2.937156       -1.220664       -1.336760
H          -1.605673        0.046500       -2.208238
H           0.285384        0.744940       -1.520320
H           1.395904       -0.089816        1.204950
H           2.254046        0.864087        0.012005
H           2.122168       -1.008147       -1.613037
H           1.276514       -1.981681       -0.433144
H           3.707807       -2.555404       -0.456939
H           4.122837       -0.881735       -0.086708
H           3.267893       -1.861913        1.103607
H          -2.001001       -1.797116        0.901296
H          -0.301973       -1.702386        1.301753
H          -0.672973        0.420019        2.559841
H          -2.373339        0.416521        2.079924
H          -1.737493       -0.836618        3.151671
N          -0.152357        1.977344        0.126288
H          -1.111444        2.154214       -0.166110
H          -0.182092        1.913246        1.142381
C           0.730321        3.096776       -0.294694
H           0.798750        3.090073       -1.378404
H           0.302952        4.035490        0.045157
H           1.713679        2.964650        0.141114
```

---

### Compound_23_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.589844 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.354889 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      36.2229 cm-1
2.      65.3546 cm-1
3.      70.6841 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.028421        0.008405       -1.316115
C          -1.077975       -0.373024       -0.383520
C           0.220838        0.315533       -0.393401
C           1.461253       -0.554863       -0.199626
C           2.800181        0.140770       -0.444537
C           3.976129       -0.828707       -0.361143
C          -1.348667       -1.503644        0.575630
C          -1.397674       -1.125180        2.064137
O          -3.191246       -0.458777       -1.505699
H          -1.693675        0.829798       -1.987813
H           0.326322        0.915717       -1.297716
H           1.361984       -1.383078       -0.903393
H           1.454739       -1.005243        0.796277
H           2.964418        0.943570        0.281044
H           2.782348        0.616354       -1.428539
H           4.923122       -0.318999       -0.539907
H           4.027573       -1.296581        0.623719
H           3.876795       -1.623797       -1.102268
H          -2.313186       -1.928710        0.295663
H          -0.613758       -2.308490        0.455582
H          -0.418428       -0.819696        2.444065
H          -2.099607       -0.307450        2.238434
H          -1.710379       -1.972575        2.677921
N           0.289763        1.439283        0.748187
H           0.059749        0.982959        1.628262
H           1.245379        1.780535        0.834317
C          -0.628375        2.580177        0.524132
H          -0.307653        3.112216       -0.366173
H          -1.627408        2.182460        0.379255
H          -0.600442        3.239451        1.386219
```

---

### Compound_23_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.589345 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.354241 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      39.8453 cm-1
2.      63.7353 cm-1
3.      74.3853 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.513533        0.569074        1.382571
C          -0.903661        0.428545        0.149414
C           0.567329        0.383762        0.100776
C           1.210716       -0.697442       -0.766031
C           1.041938       -2.098699       -0.173151
C           1.813347       -2.313301        1.127402
C          -1.728492        0.366391       -1.113550
C          -2.280382       -1.021835       -1.470979
O          -2.752056        0.643262        1.643784
H          -0.803452        0.612583        2.238880
H           0.966118        0.349151        1.113761
H           2.278779       -0.507127       -0.891651
H           0.766713       -0.664762       -1.763046
H           1.379768       -2.823651       -0.916527
H          -0.018248       -2.291936       -0.006106
H           2.875231       -2.095879        0.994133
H           1.440996       -1.674865        1.929432
H           1.723758       -3.346171        1.465536
H          -2.576965        1.046244       -0.999368
H          -1.159207        0.741425       -1.971125
H          -2.856393       -1.424871       -0.637561
H          -2.934806       -0.974928       -2.345134
H          -1.478702       -1.726324       -1.692865
N           1.119959        1.783056       -0.414849
H           0.951636        1.846697       -1.417692
H           0.506476        2.472121        0.016823
C           2.540212        2.100744       -0.112035
H           3.185447        1.410080       -0.642145
H           2.754308        3.117708       -0.426935
H           2.690433        2.003575        0.958768
```

---

### Compound_23_HEI_Conformation_5_DFT_reopt

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.588389 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.353143 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
  1.      58.2109 cm-1
  2.      69.7271 cm-1
  3.      78.4270 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.214637        0.402447       -1.073598
C           1.201277        0.047100       -0.199705
C          -0.176184        0.410124       -0.566228
C          -1.288064       -0.555961       -0.176158
C          -2.704205       -0.135060       -0.568248
C          -3.721963       -1.245852       -0.323277
C           1.525803       -0.721735        1.058845
C           1.691963       -2.233896        0.846460
O           3.459657        0.200218       -0.957884
H           1.862943        0.928078       -1.990850
H          -0.238233        0.619973       -1.634805
H          -1.250284       -0.773284        0.892597
H          -1.048265       -1.494859       -0.678020
H          -2.719092        0.151158       -1.623530
H          -3.015004        0.747862       -0.001525
H          -4.728167       -0.928986       -0.598275
H          -3.476613       -2.133666       -0.908687
H          -3.737373       -1.534994        0.729192
H           2.460690       -0.332707        1.471902
H           0.765939       -0.562737        1.827235
H           1.969892       -2.740427        1.774514
H           0.767291       -2.684388        0.482903
H           2.470348       -2.427422        0.108077
N          -0.559961        1.862964        0.013942
H           0.140354        2.487646       -0.378956
H          -1.461168        2.157801       -0.360652
C          -0.554643        1.997691        1.490825
H           0.427827        1.716188        1.852615
H          -0.768990        3.028537        1.756208
H          -1.311333        1.344579        1.912036
```

### Compound_23_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.587682 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.35235 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      46.3708 cm-1
2.      57.9927 cm-1
3.      64.6021 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.554088        0.448610       -1.393146
C          -0.821598        0.239989       -0.235084
C           0.642044        0.161207       -0.358308
C           1.391247       -0.897285        0.449869
C           1.277454       -2.306463       -0.147171
C          -0.059974       -3.009223        0.074443
C          -1.511708        0.080755        1.093422
C          -1.263084        1.200560        2.115140
O          -2.809644        0.542095       -1.533669
H          -0.930503        0.522922       -2.311906
H           0.921564        0.085106       -1.409676
H           1.034515       -0.899942        1.482092
H           2.451228       -0.641293        0.490135
H           2.071957       -2.917021        0.287040
H           1.490137       -2.250155       -1.218623
H          -0.266674       -3.123243        1.140154
H          -0.881817       -2.448907       -0.368156
H          -0.046297       -4.005820       -0.369243
H          -2.581501        0.030806        0.886912
H          -1.248928       -0.871862        1.564754
H          -1.490240        2.179003        1.687706
H          -1.882312        1.068261        3.005131
H          -0.225519        1.217956        2.458798
N           1.294942        1.578419        0.031223
H           0.598986        2.263715       -0.257532
H           1.351536        1.644240        1.045873
C           2.611946        1.892081       -0.579196
H           2.505970        1.851922       -1.658893
H           2.924292        2.886100       -0.272297
H           3.342724        1.161130       -0.251287
```

### Compound_23_HEI_Conformation_8_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -484.5863 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -484.350839 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 84)

```
1.      47.6461 cm-1
2.      59.7247 cm-1
3.      80.2426 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.198523       -0.242078       -1.009415
C          -0.951209       -0.391786       -0.421279
C           0.054421        0.642557       -0.695181
C           1.499402        0.225208       -1.010726
C           2.412500       -0.182155        0.150885
C           3.758620       -0.696199       -0.353711
C          -0.670857       -1.601494        0.431455
C          -0.667563       -1.356746        1.948349
O          -3.209153       -1.000768       -0.925239
H          -2.293134        0.663817       -1.648049
H          -0.306610        1.277081       -1.503949
H           1.987240        1.039778       -1.553605
H           1.425608       -0.606602       -1.713153
H           1.940460       -0.950258        0.761358
H           2.595362        0.670359        0.810755
H           3.626651       -1.583382       -0.975625
H           4.265765        0.060039       -0.955856
H           4.415578       -0.961144        0.475017
H          -1.453014       -2.329445        0.209737
H           0.273796       -2.075714        0.148109
H          -1.602603       -0.891573        2.264026
H          -0.548930       -2.290591        2.502801
H           0.149416       -0.701774        2.261361
N           0.164065        1.720157        0.498220
H           0.446717        1.226564        1.341193
H           0.910923        2.378609        0.281862
C          -1.093085        2.460422        0.755722
H          -1.329718        3.055364       -0.121029
H          -1.880044        1.735060        0.931572
H          -0.960935        3.102486        1.621253
```

### Compound_24_HEI_Conformation_10_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862305 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.625016 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      26.9396 cm-1
2.      41.6451 cm-1
3.      63.9210 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.197341        0.252070       -0.751443
C          -0.979649        1.153108       -0.074269
C          -0.490240        2.440649        0.522989
C          -2.427714        0.810103        0.031722
O          -0.599450       -0.876610       -1.208194
O           1.128704        0.612215       -0.950277
C           2.091333       -0.429645       -1.134135
C           2.805991       -0.792296        0.167716
C           3.541171        0.410188        0.760109
C           1.852905       -1.416198        1.188621
H          -0.870017        2.582998        1.540845
H           0.597191        2.451981        0.573052
H          -0.794100        3.330087       -0.045174
H          -2.979246        0.855344       -0.913554
H          -2.949818        1.433041        0.755867
H           1.603561       -1.303672       -1.561560
H           2.813621       -0.042239       -1.854768
H           3.551965       -1.546194       -0.108969
H           4.243426        0.838291        0.042145
H           2.833697        1.190428        1.044002
H           4.101870        0.123633        1.651186
H           2.392705       -1.710788        2.090068
H           1.078413       -0.704374        1.478738
H           1.358929       -2.299437        0.782564
N          -2.572219       -0.635536        0.468572
H          -2.222306       -0.723939        1.419389
H          -1.863908       -1.097238       -0.175489
C          -3.925102       -1.217604        0.344882
```

```
H          -4.625928       -0.645272        0.947009
H          -4.223797       -1.181743       -0.698726
H          -3.902863       -2.249254        0.683986
```

---

### Compound_24_HEI_Conformation_11_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862294 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.626176 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      24.3335 cm-1
  2.      30.6628 cm-1
  3.      73.8467 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.439524       -0.026598       -0.371896
C          -1.346513        0.998263       -0.253955
C          -0.992254        2.453086       -0.139745
C          -2.784807        0.608667       -0.323920
O          -0.735369       -1.273822       -0.429974
O           0.896787        0.329915       -0.417002
C           1.853352       -0.703726       -0.189829
C           3.242674       -0.083325       -0.170754
C           3.395703        0.926996        0.965541
C           4.295813       -1.187584       -0.075678
H           0.061702        2.576039        0.104026
H          -1.174832        3.020837       -1.062335
H          -1.572890        2.950092        0.645313
H          -3.117849        0.263314       -1.309113
H          -3.448334        1.411980       -0.008355
H           1.647904       -1.199489        0.764460
H           1.783101       -1.458601       -0.975030
H           3.378248        0.441436       -1.121862
H           2.654358        1.721316        0.890623
H           3.267512        0.434991        1.933401
H           4.387457        1.381690        0.951067
H           5.301438       -0.765891       -0.091000
H           4.185833       -1.749603        0.855049
H           4.212674       -1.891950       -0.904975
N          -3.030946       -0.583064        0.580793
```

```
H          -2.201418       -1.193398        0.317388
H          -2.899346       -0.289761        1.545691
C          -4.328106       -1.270228        0.408065
H          -4.389813       -2.098790        1.107607
H          -5.139051       -0.570048        0.590848
H          -4.389450       -1.644770       -0.609522
```

---

### Compound_24_HEI_Conformation_12_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.859634 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.622905 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.3803 cm-1
2.      43.7638 cm-1
3.      53.5816 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.283838        1.199324       -0.278991
C          -1.503180        1.050463        0.356567
C          -2.365502        2.243441        0.670264
C          -1.984182       -0.299104        0.709062
O           0.333766        2.230040       -0.611395
O           0.279674       -0.069414       -0.632751
C           1.673952       -0.100040       -0.923122
C           2.537110       -0.142542        0.335803
C           2.213615       -1.360667        1.198342
C           4.014484       -0.110144       -0.053869
H          -1.951704        3.137170        0.204093
H          -3.390622        2.127064        0.299565
H          -2.448102        2.451084        1.745057
H          -1.276071       -0.913830        1.266539
H          -2.927103       -0.274699        1.251538
H           1.831244       -1.005360       -1.513699
H           1.938415        0.765096       -1.530364
H           2.311569        0.760593        0.910191
H           1.159389       -1.380309        1.472998
H           2.438015       -2.284830        0.658844
H           2.803944       -1.357726        2.115994
H           4.651756       -0.110141        0.831363
```

```
H           4.277367       -0.986733       -0.651632
H           4.252423        0.778967       -0.640383
N          -2.250659       -1.156109       -0.551937
H          -1.354796       -1.121769       -1.049966
H          -2.930505       -0.666890       -1.130268
C          -2.673030       -2.555221       -0.299887
H          -1.906925       -3.044051        0.294240
H          -3.612846       -2.545728        0.243984
H          -2.794928       -3.073210       -1.246382
```

---

### Compound_24_HEI_Conformation_13_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.857091 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.621083 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      24.8943 cm-1
2.      36.6243 cm-1
3.      69.1618 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.449861       -0.181329        0.481530
C           1.453778        0.770050        0.285368
C           1.225096        2.058001       -0.466545
C           2.781149        0.470743        0.786751
O           0.529143       -1.282153        1.068612
O          -0.776956        0.204264       -0.059085
C          -1.879986       -0.669365        0.159121
C          -3.123218       -0.053299       -0.466620
C          -4.287527       -1.039803       -0.373105
C          -3.478459        1.284093        0.182010
H           0.247563        2.490399       -0.248432
H           1.979262        2.800221       -0.187436
H           1.279181        1.958053       -1.559325
H           2.789716       -0.309722        1.542458
H           3.341837        1.341730        1.127376
H          -1.674578       -1.647176       -0.282843
H          -2.033550       -0.821697        1.231729
H          -2.904352        0.122200       -1.524772
H          -4.051979       -1.984247       -0.866506
```

```
H          -4.529056       -1.256988        0.670338
H          -5.182597       -0.628824       -0.841537
H          -4.355789        1.726502       -0.292593
H          -3.706370        1.145266        1.242266
H          -2.654259        1.991798        0.104635
N           3.773898       -0.117956       -0.334739
H           4.713571       -0.195781        0.051529
H           3.821334        0.573123       -1.080077
C           3.330771       -1.419823       -0.886769
H           3.389908       -2.164789       -0.099901
H           2.300404       -1.307709       -1.208549
H           3.966184       -1.699163       -1.721865
```

---

### Compound_24_HEI_Conformation_14_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.85657 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.620582 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      24.2202 cm-1
  2.      39.6498 cm-1
  3.      69.9429 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.396765       -0.262632       -0.618456
C           1.303651        0.768782       -0.359144
C           0.916885        2.034862        0.364693
C           2.683721        0.575979       -0.756679
O           0.609368       -1.358676       -1.180914
O          -0.893788        0.028895       -0.181903
C          -1.903673       -0.939028       -0.449646
C          -3.230660       -0.430913        0.101045
C          -3.187689       -0.256668        1.619917
C          -3.682239        0.853339       -0.596311
H           1.610526        2.843832        0.114890
H          -0.085173        2.369327        0.093655
H           0.925396        1.947938        1.460026
H           2.812969       -0.208286       -1.496990
H           3.197379        1.486567       -1.067019
H          -1.981134       -1.109627       -1.526315
```

```
H          -1.638968       -1.891404        0.015973
H          -3.959117       -1.215604       -0.129401
H          -2.884765       -1.181456        2.114646
H          -2.477878        0.522479        1.899638
H          -4.168210        0.026510        2.005736
H          -4.669000        1.159194       -0.245228
H          -2.985472        1.667847       -0.395406
H          -3.736727        0.716299       -1.677972
N           3.639629        0.080453        0.444436
H           3.604174        0.796101        1.166944
H           4.603107        0.046012        0.114930
C           3.239558       -1.227180        1.014400
H           2.186045       -1.166912        1.268306
H           3.390784       -1.992228        0.259865
H           3.836108       -1.440752        1.896286
```

---

### Compound_24_HEI_Conformation_15_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.857517 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.620837 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      31.4565 cm-1
  2.      40.9919 cm-1
  3.      57.5280 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.349453        0.483591       -0.761307
C          -1.539530        0.900982       -0.164044
C          -1.588707        1.943801        0.925716
C          -2.767291        0.239977       -0.565004
O          -0.188388       -0.393682       -1.636593
O           0.766776        1.188013       -0.293765
C           2.047940        0.694168       -0.673579
C           2.516692       -0.468091        0.200318
C           3.874684       -0.965797       -0.292938
C           2.567964       -0.076757        1.675851
H          -0.900176        2.768633        0.737074
H          -2.593810        2.370071        0.998182
H          -1.341665        1.560542        1.925071
```

```
H          -2.690579       -0.267222       -1.522382
H          -3.653372        0.874474       -0.537303
H           2.035928        0.391774       -1.720144
H           2.729646        1.540359       -0.559847
H           1.787482       -1.273253        0.078495
H           3.828841       -1.280378       -1.337088
H           4.629256       -0.178908       -0.212620
H           4.218101       -1.814921        0.299539
H           2.861749       -0.926133        2.294875
H           3.296509        0.722469        1.837531
H           1.597891        0.278079        2.022593
N          -3.204064       -0.949786        0.425497
H          -4.109535       -1.315035        0.134005
H          -3.338594       -0.537743        1.346163
C          -2.205395       -2.042315        0.507882
H          -2.154801       -2.535337       -0.457269
H          -1.245123       -1.593337        0.740099
H          -2.497829       -2.747631        1.280046
```

---

### Compound_24_HEI_Conformation_16_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.856812 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.62006 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      32.6864 cm-1
2.      50.0628 cm-1
3.      63.1199 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.504768       -1.195746       -0.112765
C          -1.781204       -0.647675       -0.247697
C          -2.952155       -1.338510        0.403657
C          -2.016411        0.591415       -0.963676
O          -0.202446       -2.259062        0.463147
O           0.506809       -0.434694       -0.724289
C           1.827447       -0.970276       -0.768627
C           2.820438       -0.072720       -0.033078
C           2.893990        1.322931       -0.653032
C           2.517139       -0.004688        1.463424
```

```
H          -3.153963       -1.008810        1.432700
H          -3.872618       -1.162944       -0.162555
H          -2.794124       -2.416487        0.453005
H          -1.196970        0.894349       -1.606094
H          -2.959344        0.617289       -1.512324
H           1.823149       -1.967426       -0.333406
H           2.111224       -1.046233       -1.822561
H           3.797541       -0.551723       -0.161631
H           3.142069        1.270801       -1.714874
H           1.937846        1.838268       -0.558308
H           3.652862        1.931050       -0.158171
H           3.253343        0.611449        1.981972
H           1.533350        0.432305        1.637531
H           2.526081       -0.997635        1.914566
N          -2.198975        1.868317        0.003581
H          -2.999009        1.675849        0.602014
H          -2.444725        2.680818       -0.559535
C          -1.008561        2.154334        0.836422
H          -0.733695        1.234591        1.342815
H          -0.199362        2.467959        0.185713
H          -1.241223        2.933957        1.555442
```

---

### Compound_24_HEI_Conformation_16_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.856812 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.620062 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      32.6745 cm-1
2.      49.9631 cm-1
3.      63.2538 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.504980       -1.195551       -0.112908
C          -1.781442       -0.647477       -0.247733
C          -2.952248       -1.338322        0.403859
C          -2.016605        0.591582       -0.963635
O          -0.202627       -2.258849        0.462987
O           0.506543       -0.434508       -0.724487
C           1.827148       -0.970169       -0.769077
```

```
C           2.820227       -0.072922       -0.033273
C           2.893557        1.323003       -0.652623
C           2.517157       -0.005583        1.463304
H          -3.152987       -1.009636        1.433435
H          -3.873039       -1.161520       -0.161410
H          -2.794856       -2.416460        0.451899
H          -1.197406        0.894219       -1.606488
H          -2.959874        0.617848       -1.511662
H           1.822820       -1.967488       -0.334251
H           2.110827       -1.045684       -1.823066
H           3.797338       -0.551804       -0.162192
H           3.141712        1.271367       -1.714471
H           1.937300        1.838092       -0.557751
H           3.652284        1.931049       -0.157453
H           3.253325        0.610477        1.981994
H           1.533309        0.431128        1.637772
H           2.526383       -0.998720        1.914019
N          -2.198127        1.868854        0.003704
H          -2.998430        1.677146        0.602007
H          -2.443007        2.681587       -0.559455
C          -1.007617        2.153693        0.836752
H          -0.733493        1.233607        1.342934
H          -0.198105        2.466858        0.186223
H          -1.239716        2.933290        1.555980
```

---

### Compound_24_HEI_Conformation_19_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.856528 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.619473 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      33.2834 cm-1
2.      36.5334 cm-1
3.      68.2795 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.255338       -0.369623        0.005078
C           1.131594        0.681048        0.280675
C           0.902132        2.090393       -0.205430
C           2.334330        0.381439        1.035731
```

```
O           0.352062       -1.565656        0.352170
O          -0.842091        0.035153       -0.764840
C          -1.949867       -0.854503       -0.888308
C          -3.138056       -0.391922       -0.044901
C          -2.812861       -0.417781        1.448846
C          -3.632704        0.987919       -0.479612
H          -0.155298        2.356852       -0.189704
H           1.430431        2.804727        0.433810
H           1.250787        2.276946       -1.230501
H           2.274831       -0.555007        1.583080
H           2.667114        1.188093        1.689778
H          -2.228205       -0.860653       -1.944842
H          -1.641304       -1.857554       -0.599798
H          -3.936920       -1.117511       -0.235437
H          -2.507201       -1.413516        1.771579
H          -1.998395        0.272081        1.676541
H          -3.680277       -0.118715        2.039479
H          -4.513779        1.285182        0.091395
H          -2.857997        1.739348       -0.320046
H          -3.897468        0.997645       -1.538791
N           3.634302        0.167539        0.116029
H           4.455412        0.060911        0.710019
H           3.768698        1.024715       -0.415727
C           3.513649       -0.982626       -0.811524
H           3.482353       -1.895440       -0.225558
H           2.584363       -0.866649       -1.359823
H           4.361641       -0.996267       -1.489625
```

---

### Compound_24_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.858942 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.622285 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      32.5347 cm-1
2.      38.9051 cm-1
3.      63.1988 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.928132       -1.284809       -0.097246
C          -1.975165       -0.441414        0.237359
C          -3.405769       -0.894211        0.126402
C          -1.685553        0.939872        0.661870
O          -0.933487       -2.484359       -0.438903
O           0.322205       -0.601653       -0.061629
C           1.500522       -1.392379       -0.182829
C           2.722636       -0.507792        0.033807
C           2.856504        0.569802       -1.043081
C           2.745480        0.101702        1.436198
H          -3.928439       -0.916448        1.091101
H          -4.003981       -0.253090       -0.532818
H          -3.445998       -1.903431       -0.281814
H          -0.941157        1.036877        1.453275
H          -2.581479        1.483520        0.954402
H           1.480448       -2.194649        0.558075
H           1.539188       -1.855728       -1.171499
H           3.581691       -1.180498       -0.058689
H           2.811118        0.139412       -2.044762
H           2.062221        1.312891       -0.959127
H           3.805401        1.098738       -0.944416
H           3.667893        0.660416        1.600999
H           1.908264        0.787066        1.573232
H           2.676570       -0.671061        2.203864
N          -1.055520        1.766429       -0.490398
H          -1.709019        1.772480       -1.270412
H          -0.255028        1.193157       -0.775063
C          -0.630689        3.143374       -0.139676
H          -1.500703        3.708691        0.180378
H           0.090372        3.085112        0.670026
H          -0.177468        3.614765       -1.006536
```

---

### Compound_24_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.858993 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.622542 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.0769 cm-1
2.      52.2023 cm-1
3.      61.6385 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.772900       -1.325032        0.060889
C           2.006366       -0.736763       -0.164067
C           3.283433       -1.471337        0.143085
C           2.074776        0.642751       -0.680059
O           0.485525       -2.476958        0.442602
O          -0.295049       -0.403200       -0.157478
C          -1.616701       -0.932745       -0.173173
C          -2.611712        0.214632       -0.279105
C          -4.015967       -0.346071       -0.507692
C          -2.578739        1.112580        0.957177
H           3.871504       -1.715794       -0.751063
H           3.948406       -0.899976        0.801683
H           3.061317       -2.412470        0.645140
H           1.480775        0.836734       -1.574530
H           3.096911        0.968297       -0.862134
H          -1.728148       -1.609746       -1.024997
H          -1.799963       -1.512129        0.734455
H          -2.333233        0.813213       -1.152093
H          -4.325566       -0.971494        0.333165
H          -4.743570        0.460149       -0.606776
H          -4.060189       -0.953935       -1.412627
H          -3.282845        1.939549        0.855837
H          -2.853240        0.544815        1.849631
H          -1.590422        1.538853        1.126539
N           1.489435        1.657330        0.334464
H           2.011733        1.573824        1.203994
H           0.550344        1.288166        0.514350
C           1.433396        3.067080       -0.122986
H           0.979597        3.680744        0.649250
H           2.443220        3.409987       -0.327380
H           0.837011        3.110602       -1.029103
```

---

### Compound_24_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862294 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.626179 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      24.2891 cm-1
  2.      30.6131 cm-1
```

```
    3.      73.8436 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.439563       -0.026626       -0.371665
C          -1.346477        0.998289       -0.253718
C          -0.992129        2.453136       -0.139984
C          -2.784803        0.608753       -0.323840
O          -0.735512       -1.273842       -0.429776
O           0.896754        0.329836       -0.416755
C           1.853369       -0.703809       -0.189889
C           3.242650       -0.083295       -0.170759
C           3.395586        0.926842        0.965701
C           4.295929       -1.187437       -0.075956
H           0.061982        2.576222        0.103075
H          -1.175339        3.020618       -1.062611
H          -1.572241        2.950343        0.645334
H          -3.117843        0.263598       -1.309118
H          -3.448255        1.412088       -0.008170
H           1.647982       -1.199814        0.764277
H           1.783105       -1.458474       -0.975299
H           3.378123        0.441667       -1.121764
H           2.653936        1.720906        0.891052
H           3.267753        0.434610        1.933491
H           4.387183        1.381872        0.951116
H           5.301494       -0.765596       -0.091097
H           4.185986       -1.749764        0.854590
H           4.212938       -1.891557       -0.905477
N          -3.030949       -0.583048        0.580703
H          -2.899278       -0.289893        1.545649
H          -2.201391       -1.193336        0.317164
C          -4.328093       -1.270240        0.407897
H          -4.389360       -1.644850       -0.609673
H          -4.389781       -2.098808        1.107426
H          -5.139104       -0.570128        0.590634
```

---

### Compound_24_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.859634 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.622905 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.3804 cm-1
2.      43.7640 cm-1
3.      53.5821 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.283836        1.199323       -0.278993
C          -1.503177        1.050464        0.356567
C          -2.365497        2.243443        0.670267
C          -1.984180       -0.299102        0.709063
O           0.333767        2.230038       -0.611399
O           0.279674       -0.069416       -0.632754
C           1.673952       -0.100044       -0.923123
C           2.537108       -0.142543        0.335803
C           2.213610       -1.360663        1.198347
C           4.014484       -0.110149       -0.053869
H          -3.390618        2.127066        0.299573
H          -2.448091        2.451087        1.745060
H          -1.951700        3.137171        0.204092
H          -1.276070       -0.913830        1.266539
H          -2.927101       -0.274696        1.251539
H           1.831243       -1.005366       -1.513698
H           1.938417        0.765090       -1.530368
H           2.311570        0.760596        0.910187
H           1.159384       -1.380302        1.473003
H           2.438009       -2.284829        0.658852
H           2.803940       -1.357720        2.115998
H           4.651754       -0.110144        0.831364
H           4.277365       -0.986742       -0.651627
H           4.252424        0.778959       -0.640386
N          -2.250659       -1.156108       -0.551937
H          -1.354796       -1.121771       -1.049966
H          -2.930503       -0.666886       -1.130268
C          -2.673035       -2.555218       -0.299887
H          -2.794936       -3.073206       -1.246382
H          -3.612851       -2.545721        0.243984
H          -1.906932       -3.044051        0.294240
```

---

### Compound_24_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862261 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.625669 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      32.3980 cm-1
2.      39.7165 cm-1
3.      77.7887 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.433401        0.040007        0.170935
C           1.365557        1.028592       -0.033411
C           1.054110        2.430350       -0.473211
C           2.778060        0.665838        0.278790
O           0.700000       -1.168554        0.507620
O          -0.892419        0.388407       -0.021865
C          -1.839644       -0.674895       -0.103466
C          -3.224568       -0.079558       -0.310946
C          -4.235276       -1.204271       -0.537172
C          -3.638878        0.808004        0.862047
H           1.125994        3.169259        0.336519
H           1.739349        2.768922       -1.258195
H           0.042604        2.495168       -0.870941
H           2.986691        0.509728        1.343112
H           3.488019        1.399858       -0.098506
H          -1.581724       -1.336628       -0.934865
H          -1.817567       -1.271334        0.811843
H          -3.185635        0.536270       -1.215036
H          -3.961975       -1.821400       -1.394669
H          -4.294832       -1.854079        0.339380
H          -5.231528       -0.798947       -0.717477
H          -4.623391        1.245564        0.689488
H          -3.689767        0.222950        1.784166
H          -2.927436        1.618167        1.015918
N           3.108121       -0.672441       -0.355266
H           2.247598       -1.228654       -0.077083
H           3.087381       -0.564813       -1.366426
C           4.368461       -1.307043        0.084856
H           4.312229       -1.485219        1.154717
H           4.494793       -2.250902       -0.437709
H           5.204365       -0.647791       -0.133952
```

---

### Compound_24_HEI_Conformation_5_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862261 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.625666 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.4099 cm-1
  2.      39.7430 cm-1
  3.      77.7911 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.433396        0.039963        0.171149
C           1.365540        1.028565       -0.033274
C           1.053942        2.430275       -0.473169
C           2.778054        0.665841        0.278880
O           0.700013       -1.168554        0.507890
O          -0.892421        0.388372       -0.021703
C          -1.839650       -0.674923       -0.103315
C          -3.224551       -0.079621       -0.311030
C          -4.235225       -1.204381       -0.537186
C          -3.638993        0.808134        0.861771
H           1.124898        3.169145        0.336695
H           1.739704        2.769152       -1.257558
H           0.042733        2.494789       -0.871712
H           2.986726        0.509590        1.343173
H           3.487966        1.399941       -0.098369
H          -1.581625       -1.336749       -0.934607
H          -1.817713       -1.271262        0.812067
H          -3.185521        0.536063       -1.215217
H          -3.961796       -1.821673       -1.394525
H          -4.294899       -1.854022        0.339482
H          -5.231453       -0.799098       -0.717712
H          -4.623516        1.245613        0.689057
H          -3.689925        0.223246        1.783994
H          -2.927607        1.618364        1.015545
N           3.108174       -0.672354       -0.355370
H           2.247847       -1.228721       -0.077172
H           3.087269       -0.564604       -1.366516
C           4.368644       -1.306912        0.084471
H           4.312574       -1.485319        1.154299
H           4.495000       -2.250648       -0.438306
H           5.204444       -0.647528       -0.134314
```

---

### Compound_24_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.858544 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.621051 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      39.5523 cm-1
  2.      54.2422 cm-1
  3.      65.1777 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.598988       -1.290564       -0.257664
C          -1.848741       -0.724150       -0.078740
C          -2.985321       -1.526432        0.495275
C          -2.078447        0.685513       -0.448871
O          -0.214204       -2.459670       -0.068237
O           0.357899       -0.314476       -0.698600
C           1.682794       -0.751469       -0.997734
C           2.713310       -0.149604       -0.043877
C           2.786902        1.373791       -0.154026
C           2.475184       -0.592697        1.399474
H          -3.774405       -1.752415       -0.234112
H          -2.617226       -2.480674        0.870791
H          -3.476169       -1.013819        1.330713
H          -1.774301        0.958596       -1.460816
H          -3.113169        0.988692       -0.302964
H           1.710920       -1.837692       -0.944219
H           1.901737       -0.440061       -2.022584
H           3.677943       -0.553156       -0.370884
H           2.937130        1.691332       -1.187177
H           1.872355        1.844887        0.210174
H           3.609913        1.766726        0.444607
H           3.241970       -0.187266        2.061202
H           1.505480       -0.241767        1.757315
H           2.487222       -1.679351        1.486704
N          -1.232298        1.641034        0.423980
H          -0.281611        1.276268        0.299558
H          -1.483284        1.488939        1.398381
C          -1.308027        3.078692        0.068127
H          -0.988519        3.194812       -0.962937
H          -2.334596        3.414953        0.177124
H          -0.656850        3.648446        0.724169
```

### Compound_24_HEI_Conformation_6_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.858545 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.621036 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      38.7702 cm-1
2.      54.5312 cm-1
3.      68.5807 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.598872       -1.290102       -0.258151
C          -1.848280       -0.723661       -0.076813
C          -2.984392       -1.527851        0.495469
C          -2.079211        0.685742       -0.447177
O          -0.214412       -2.459520       -0.070191
O           0.357815       -0.314046       -0.699603
C           1.682882       -0.750979       -0.998181
C           2.712983       -0.149929       -0.043352
C           2.787205        1.373499       -0.152652
C           2.473815       -0.593697        1.399615
H          -3.764310       -1.770178       -0.238683
H          -2.613045       -2.474163        0.887707
H          -3.487505       -1.007584        1.318596
H          -1.777351        0.958670       -1.459900
H          -3.113731        0.988627       -0.299144
H           1.710809       -1.837257       -0.945405
H           1.902418       -0.438887       -2.022696
H           3.677695       -0.553632       -0.369985
H           2.937833        1.691546       -1.185598
H           1.872778        1.844813        0.211591
H           3.610244        1.765752        0.446406
H           3.240196       -0.188669        2.062073
H           1.503891       -0.242809        1.756938
H           2.485659       -1.680400        1.486318
N          -1.231547        1.641794        0.423625
H          -0.281050        1.276862        0.297931
H          -1.480994        1.490323        1.398529
C          -1.307824        3.079197        0.066929
H          -0.989574        3.194722       -0.964604
H          -2.334296        3.415479        0.176963
H          -0.655901        3.649442        0.721826
```

---

### Compound_24_HEI_Conformation_8_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.859257 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.621742 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      40.9648 cm-1
2.      54.9395 cm-1
3.      64.2794 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.497581       -1.257201       -0.265321
C           1.819925       -0.894921       -0.080335
C           2.809428       -1.864241        0.508024
C           2.280435        0.450352       -0.478465
O          -0.076241       -2.339928       -0.043284
O          -0.278694       -0.158573       -0.767882
C          -1.684579       -0.331754       -0.924185
C          -2.466339        0.506043        0.084511
C          -3.959664        0.436995       -0.234358
C          -2.184761        0.069262        1.521171
H           3.524982       -2.261998       -0.224261
H           3.406772       -1.410733        1.306902
H           2.287114       -2.718761        0.937353
H           2.050666        0.741330       -1.505313
H           3.346701        0.587304       -0.310823
H          -1.935484       -0.018295       -1.940352
H          -1.928666       -1.387760       -0.812710
H          -2.140074        1.545490       -0.030927
H          -4.167579        0.778849       -1.249734
H          -4.327159       -0.588050       -0.143171
H          -4.533935        1.057958        0.454204
H          -2.691753        0.723730        2.231824
H          -2.538906       -0.950074        1.688575
H          -1.118071        0.090172        1.744491
N           1.579726        1.551084        0.347988
H           1.763846        1.372017        1.332967
H           0.584886        1.356310        0.189524
C           1.920067        2.948123       -0.014678
H           1.673673        3.103002       -1.060653
```

```
H          1.348400        3.631531        0.605860
H          2.983426        3.102453        0.141473
```

---

### Compound_24_HEI_Conformation_9_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.859274 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.6219 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      29.3242 cm-1
  2.      45.8826 cm-1
  3.      63.1129 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -0.297543        1.263996       -0.412352
C         -1.449402        0.986572        0.300806
C         -2.435597        2.073087        0.635149
C         -1.717799       -0.393624        0.750569
O          0.159319        2.350200       -0.817106
O          0.402199        0.060513       -0.756266
C          1.780258        0.154621       -1.110963
C          2.690025       -0.292256        0.032853
C          2.550716        0.621589        1.250800
C          2.447664       -1.754722        0.406781
H         -2.440590        2.348016        1.698287
H         -2.201798        2.978112        0.074929
H         -3.464639        1.790923        0.385141
H         -0.903107       -0.869215        1.299292
H         -2.626475       -0.465566        1.344790
H          1.926320       -0.494080       -1.977310
H          1.998953        1.180784       -1.402152
H          3.712813       -0.202604       -0.350056
H          2.765016        1.659766        0.994358
H          1.535442        0.578774        1.648777
H          3.235147        0.317734        2.044290
H          3.143671       -2.080509        1.181281
H          1.434913       -1.890738        0.789150
H          2.571718       -2.410562       -0.457098
N         -1.922096       -1.350658       -0.446149
H         -1.062506       -1.222321       -0.991917
```

```
H          -2.688398       -0.990823       -1.011337
C          -2.137271       -2.777500       -0.104014
H          -1.283168       -3.129057        0.466632
H          -3.040735       -2.863466        0.492196
H          -2.236354       -3.356845       -1.017005
```

---

### Compound_25_HEI_Conformation_11_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.375857 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.118482 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      43.7477 cm-1
2.      54.4635 cm-1
3.      61.8443 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.535449       -0.909061        0.485496
C           1.360358       -0.317319        1.423651
C           2.812727       -0.245536        1.129493
O           0.965849       -1.286251       -0.673137
N          -0.818357       -1.130394        0.799134
C          -1.887530       -0.860287       -0.185867
C          -1.670546        0.492796       -0.892324
C          -1.484099        1.722282       -0.031097
C          -0.939712        2.931880       -0.751046
O          -1.749080        1.763504        1.155028
H           0.975559        0.118209        2.332443
H           3.319917       -1.216180        1.096160
H           3.359335        0.399554        1.813524
H          -1.044579       -0.693934        1.681126
H          -2.515552        0.706291       -1.555708
H          -0.800396        0.417973       -1.547281
H          -1.009498        3.814454       -0.120383
H           0.107100        2.751183       -1.005016
H          -1.470087        3.096026       -1.689888
C          -1.928787       -1.960660       -1.252632
H          -2.759525       -1.785668       -1.938732
H          -0.998807       -1.989090       -1.812173
H          -2.076000       -2.930085       -0.775139
```

```
C          -3.215491       -0.884630        0.577872
H          -4.044152       -0.698682       -0.105740
H          -3.361743       -1.865699        1.031380
H          -3.238651       -0.128482        1.358902
N           2.996935        0.290910       -0.283775
H           2.683047        1.257794       -0.305994
H           2.263365       -0.298851       -0.788540
C           4.350129        0.155421       -0.859169
H           5.066237        0.692597       -0.242357
H           4.354361        0.560309       -1.867188
H           4.610886       -0.898673       -0.888301
```

---

### Compound_25_HEI_Conformation_13_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.373473 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.11663 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      31.6080 cm-1
  2.      38.4848 cm-1
  3.      44.3296 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.086120       -0.606787       -0.099138
C           2.126146       -1.130948       -0.846142
C           3.348146       -0.307379       -1.014950
O           1.149098        0.555760        0.455839
N          -0.055077       -1.397337        0.128603
C          -1.391575       -0.838697        0.370832
C          -1.731428        0.201917       -0.747428
C          -3.036577        0.934109       -0.548695
C          -2.959202        2.336238       -0.003092
O          -4.106605        0.425333       -0.834512
H           2.098732       -2.134138       -1.243337
H           3.215436        0.584711       -1.636900
H           4.193529       -0.868565       -1.406672
H          -0.089935       -2.183947       -0.502695
H          -1.785788       -0.335496       -1.694860
H          -0.911445        0.914982       -0.787756
H          -3.947389        2.704244        0.261100
```

```
H          -2.291448        2.383534        0.856635
H          -2.525190        2.982051       -0.771239
C          -2.366206       -2.016188        0.304825
H          -2.324167       -2.504197       -0.670734
H          -2.112932       -2.750354        1.070098
H          -3.387914       -1.680942        0.466666
C          -1.467195       -0.207592        1.764485
H          -0.804639        0.648952        1.839852
H          -2.489169        0.101339        1.989768
H          -1.165260       -0.943360        2.509963
N           3.747338        0.270805        0.336520
H           4.027658       -0.493667        0.945791
H           2.799551        0.615310        0.669366
C           4.770235        1.336406        0.312896
H           5.686985        0.951949       -0.126672
H           4.396761        2.163463       -0.283947
H           4.960059        1.674637        1.327547
```

---

### Compound_25_HEI_Conformation_14_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.367617 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.11043 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      31.4933 cm-1
2.      42.9261 cm-1
3.      58.0390 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.608133       -0.925906        1.054081
C           1.728747       -1.669303        0.682384
C           2.607340       -1.260477       -0.426642
O          -0.100365       -1.105376        2.078834
N           0.320706        0.184002        0.168700
C          -0.833677        1.074705        0.376831
C          -2.172219        0.310890        0.412740
C          -2.533313       -0.524094       -0.790300
C          -3.967673       -0.986427       -0.852080
O          -1.738356       -0.830513       -1.661427
H           2.055538       -2.463008        1.337669
```

```
H           2.142070       -1.183326       -1.414219
H           3.483940       -1.895900       -0.523888
H           0.298709       -0.145354       -0.788799
H          -2.996496        1.002183        0.606288
H          -2.146094       -0.379591        1.260445
H          -4.601911       -0.131298       -1.098445
H          -4.089483       -1.753320       -1.612843
H          -4.299144       -1.358504        0.117789
C          -0.664264        1.845432        1.689289
H          -0.670740        1.166957        2.537268
H           0.284069        2.384616        1.678575
H          -1.469515        2.572257        1.804775
C          -0.827621        2.079096       -0.781746
H          -1.670917        2.764347       -0.689947
H           0.093036        2.662896       -0.765488
H          -0.899154        1.576492       -1.745116
N           3.135580        0.178866       -0.194918
H           3.694915        0.172915        0.654548
H           2.265402        0.699121        0.015757
C           3.872048        0.794923       -1.322239
H           4.168126        1.804390       -1.052281
H           4.750695        0.195772       -1.543185
H           3.217717        0.822349       -2.188532
```

---

### Compound_25_HEI_Conformation_15_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.373931 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.116793 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      32.5097 cm-1
2.      48.8306 cm-1
3.      57.0477 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           -0.981679       -0.072450       -0.137583
C           -1.650638       -1.283418       -0.185976
C           -3.060007       -1.324347        0.276164
O           -1.546653        1.010074        0.283499
N            0.327744        0.001826       -0.641348
```

```
C           1.326559        0.942635       -0.106935
C           2.701451        0.505972       -0.678703
C           3.182911       -0.839974       -0.179013
C           4.397183       -0.853917        0.704492
O           2.602046       -1.868244       -0.483314
H          -1.199133       -2.170777       -0.602724
H          -3.191244       -1.190254        1.355837
H          -3.582079       -2.233264       -0.015225
H           0.728141       -0.917584       -0.765942
H           3.433207        1.274789       -0.438378
H           2.613478        0.445151       -1.765158
H           4.627653       -1.863536        1.033852
H           5.246321       -0.436165        0.158551
H           4.233050       -0.204027        1.566260
C           1.054267        2.363219       -0.612312
H           1.822011        3.049265       -0.250885
H           1.057423        2.381662       -1.702771
H           0.082009        2.697209       -0.262232
C           1.369605        0.931560        1.429926
H           2.168080        1.575937        1.800760
H           0.422099        1.289545        1.825108
H           1.535890       -0.077136        1.810906
N          -3.808004       -0.135728       -0.311306
H          -3.868788       -0.255809       -1.319202
H          -3.092903        0.631351       -0.118909
C          -5.133091        0.152857        0.273450
H          -5.786285       -0.706078        0.141577
H          -5.561619        1.021670       -0.218172
H          -5.007997        0.357893        1.332784
```

---

### Compound_25_HEI_Conformation_16_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.364656 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.107534 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      23.5333 cm-1
2.      41.9603 cm-1
3.      51.0343 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.999008        1.428690       -0.004446
C          -2.387130        1.611882       -0.015166
C          -3.325759        0.521728        0.263242
O          -0.144629        2.249490       -0.426492
N          -0.564965        0.144984        0.470756
C           0.846522       -0.212927        0.681282
C           1.518273       -0.280323       -0.718739
C           3.011981       -0.511106       -0.677321
C           3.893692        0.687154       -0.909477
O           3.484280       -1.618126       -0.489833
H          -2.766794        2.514375       -0.471290
H          -3.210055        0.004122        1.219953
H          -4.365716        0.825062        0.174702
H          -1.126134       -0.179806        1.246203
H           1.299153        0.652743       -1.229703
H           1.062304       -1.106171       -1.265627
H           4.935500        0.447283       -0.712822
H           3.782480        1.002104       -1.950468
H           3.572234        1.528012       -0.295144
C           1.563800        0.770767        1.617586
H           2.578600        0.433697        1.835823
H           1.599765        1.763465        1.178967
H           1.024124        0.829930        2.563827
C           0.840532       -1.601981        1.324715
H           1.855489       -1.964122        1.471542
H           0.348062       -1.563407        2.298532
H           0.307291       -2.315282        0.695771
N          -3.144994       -0.648009       -0.764303
H          -2.136617       -0.839779       -0.736287
H          -3.345117       -0.273161       -1.688750
C          -3.930637       -1.877232       -0.502240
H          -3.699884       -2.624002       -1.256067
H          -4.988052       -1.631991       -0.532529
H          -3.667730       -2.252719        0.482177
```

---

### Compound_25_HEI_Conformation_18_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.370487 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.113397 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      33.4875 cm-1
2.      40.8274 cm-1
```

```
   3.      57.5412 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.733207       -0.721138        0.065960
C           1.864099       -1.115127       -0.671006
C           3.187001       -1.076233       -0.086548
O           0.745719       -0.325497        1.263549
N          -0.492298       -0.740745       -0.625935
C          -1.797761       -0.929120        0.026494
C          -2.205065        0.343597        0.819389
C          -2.025721        1.614312        0.018025
C          -0.822329        2.455426        0.337756
O          -2.833129        1.951857       -0.830408
H           1.750937       -1.477315       -1.684435
H           3.173676       -1.083761        1.001264
H           3.873306       -1.833469       -0.461813
H          -0.433316       -1.222642       -1.509356
H          -1.599601        0.392006        1.719960
H          -3.257259        0.253749        1.092509
H           0.045522        1.820284        0.505399
H          -0.643762        3.190723       -0.443241
H          -1.015350        2.976649        1.280749
C          -2.804642       -1.195400       -1.095214
H          -2.835510       -0.369077       -1.802460
H          -2.532989       -2.106787       -1.631511
H          -3.803803       -1.331372       -0.682930
C          -1.793713       -2.123328        0.991250
H          -2.777418       -2.253327        1.445364
H          -1.544514       -3.037484        0.449885
H          -1.059594       -1.971384        1.778804
N           3.998566        0.273939       -0.406862
H           4.955848        0.186208       -0.067464
H           4.048271        0.349056       -1.420747
C           3.363222        1.491045        0.150869
H           2.332103        1.506495       -0.185271
H           3.395342        1.431131        1.233787
H           3.893731        2.372868       -0.195902
```

---

### Compound_25_HEI_Conformation_19_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.37555 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.11851 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      28.5539 cm-1
2.      44.1679 cm-1
3.      56.8810 cm-1
```

## B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.711457       -0.276334        0.430404
C          -1.591926        0.289132        1.340833
C          -2.894934        0.773686        0.832245
O          -1.017475       -0.447825       -0.809291
N           0.540456       -0.706590        0.876823
C           1.674485       -1.059143        0.020093
C           2.015015        0.052584       -1.023043
C           2.331942        1.398985       -0.414496
C           1.204371        2.383765       -0.275354
O           3.463682        1.677292       -0.055435
H          -1.372578        0.341582        2.396107
H          -2.831515        1.628040        0.148527
H          -3.599263        1.024006        1.622299
H           0.803294       -0.325382        1.770774
H           1.163465        0.139463       -1.693536
H           2.890652       -0.271810       -1.585447
H           1.554809        3.303112        0.187163
H           0.788400        2.599208       -1.261989
H           0.392997        1.949388        0.313195
C           2.864136       -1.299064        0.952175
H           3.106152       -0.409070        1.532856
H           2.634597       -2.111510        1.642167
H           3.747040       -1.573472        0.376754
C           1.382215       -2.352350       -0.752015
H           0.526438       -2.217918       -1.407003
H           2.249124       -2.642112       -1.347475
H           1.161965       -3.156348       -0.048819
N          -3.525305       -0.309565       -0.039457
H          -3.742808       -1.110976        0.547846
H          -2.686774       -0.566932       -0.633240
C          -4.695993        0.100585       -0.842183
H          -5.489441        0.440177       -0.181531
H          -4.397466        0.910063       -1.502103
H          -5.041922       -0.743236       -1.432248
```

---

## Compound_25_HEI_Conformation_20_DFT

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.366842 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.109266 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      29.8453 cm-1
2.      31.1076 cm-1
3.      44.3991 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.099983       -1.521026       -0.493663
C          -2.283176       -0.975702       -1.016978
C          -2.614031        0.442840       -0.883778
O          -0.826693       -2.746987       -0.425047
N          -0.195498       -0.564403        0.060745
C           1.183751       -0.886908        0.454236
C           1.840257        0.448387        0.894203
C           1.993349        1.470876       -0.213306
C           3.387826        1.899618       -0.565181
O           1.020571        1.925259       -0.793499
H          -3.062263       -1.663736       -1.311283
H          -1.868294        1.155270       -1.246627
H          -3.570510        0.703307       -1.329281
H          -0.206604        0.313883       -0.441604
H           2.812534        0.228523        1.331029
H           1.214696        0.897660        1.668727
H           3.381082        2.625440       -1.373819
H           3.871455        2.325092        0.317040
H           3.976622        1.024555       -0.848850
C           1.186094       -1.818975        1.668610
H           0.645361       -1.359842        2.497243
H           0.702348       -2.757068        1.413185
H           2.209220       -2.017483        1.990736
C           1.992479       -1.507666       -0.696194
H           1.980028       -0.861261       -1.575315
H           3.031060       -1.662166       -0.398974
H           1.557161       -2.463761       -0.972485
N          -2.740714        0.860834        0.630321
H          -3.526233        0.349612        1.025645
H          -1.890767        0.477139        1.058496
C          -2.855535        2.314585        0.893791
H          -2.917163        2.488496        1.963997
H          -3.747594        2.692300        0.402956
H          -1.975867        2.806677        0.489640
```

---

### Compound_25_HEI_Conformation_21_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.367091 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.110177 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      22.1078 cm-1
2.      35.6987 cm-1
3.      54.5552 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.749729       -0.560464        1.001502
C           1.808237       -1.425499        0.719404
C           2.492372       -1.431596       -0.581982
O           0.232669       -0.363573        2.132031
N           0.289841        0.201778       -0.138469
C          -0.843341        1.138506       -0.049982
C          -2.131556        0.462288        0.459254
C          -2.659247       -0.715301       -0.321768
C          -4.067344       -1.138369        0.015021
O          -2.010488       -1.311241       -1.163516
H           2.268973       -1.941608        1.548537
H           1.876654       -1.674842       -1.452699
H           3.360158       -2.086296       -0.595142
H           0.126965       -0.422215       -0.919301
H          -2.934849        1.198086        0.549037
H          -1.941749        0.091394        1.470378
H          -4.762574       -0.399385       -0.390934
H          -4.287476       -2.111572       -0.416436
H          -4.220481       -1.158687        1.094415
C          -0.486432        2.298563        0.884206
H          -0.333824        1.943107        1.898890
H           0.430506        2.778497        0.539245
H          -1.284255        3.042599        0.880596
C          -1.060784        1.700041       -1.460102
H          -1.898680        2.397926       -1.461806
H          -0.169356        2.233089       -1.791731
H          -1.274433        0.907911       -2.176076
N           3.021667       -0.008857       -0.951029
```

```
H           2.176057        0.574658       -0.836490
H           3.299158        0.025878       -1.929788
C           4.114967        0.482651       -0.083494
H           3.795134        0.370507        0.947626
H           5.004916       -0.113034       -0.266461
H           4.311546        1.527138       -0.305844
```

---

### Compound_25_HEI_Conformation_22_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.364966 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.108028 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      22.2133 cm-1
2.      33.7502 cm-1
3.      49.6841 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.057165        1.102231       -0.263213
C          -2.348891        1.232424       -0.787596
C          -3.165883        0.079039       -1.166815
O          -0.384261        2.019854        0.271565
N          -0.521728       -0.229393       -0.299947
C           0.841774       -0.572745        0.120452
C           1.880113        0.226178       -0.734158
C           3.314052        0.060097       -0.291645
C           3.906838        1.172107        0.534214
O           3.973680       -0.916478       -0.602710
H          -2.833911        2.189829       -0.666694
H          -2.738842       -0.601990       -1.907656
H          -4.160188        0.358806       -1.505345
H          -0.762014       -0.708589       -1.157092
H           1.593677        1.272961       -0.686207
H           1.801921       -0.124682       -1.764149
H           3.226229        1.470955        1.330764
H           4.869885        0.879577        0.945012
H           4.037688        2.046839       -0.108598
C           1.007380       -0.302521        1.618091
H           0.924513        0.758003        1.834493
H           0.227439       -0.830536        2.167273
```

```
H           1.972642       -0.670025        1.968526
C           1.002071       -2.073287       -0.135403
H           0.276474       -2.631612        0.456578
H           0.842111       -2.308393       -1.189512
H           2.002821       -2.405445        0.131622
N          -3.406170       -0.894652        0.052251
H          -2.457583       -1.100223        0.385050
H          -3.818322       -1.769587       -0.267012
C          -4.215470       -0.306507        1.143461
H          -4.212307       -0.974704        1.999118
H          -3.770691        0.647962        1.406769
H          -5.230516       -0.159948        0.785750
```

---

### Compound_25_HEI_Conformation_23_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.36755 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.110617 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      33.6544 cm-1
  2.      41.9100 cm-1
  3.      56.7584 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.163657       -0.385886        0.222238
C          -2.411932       -1.035502        0.199551
C          -3.590105       -0.410352        0.758009
O          -0.946047        0.749575        0.726347
N          -0.103709       -1.070758       -0.401618
C           1.311987       -0.876842       -0.066916
C           1.758624        0.490867       -0.664785
C           3.160585        0.909349       -0.287177
C           3.294806        1.953765        0.789869
O           4.141073        0.444860       -0.842077
H          -2.499457       -2.025554       -0.228707
H          -3.361591        0.360128        1.491349
H          -4.327971       -1.104616        1.156217
H          -0.325077       -2.030996       -0.612801
H           1.040234        1.233727       -0.330309
H           1.709636        0.406885       -1.750783
```

```
H           4.332304        2.068132        1.093621
H           2.923774        2.904384        0.397478
H           2.669955        1.707527        1.648094
C           1.550716       -0.935189        1.448928
H           1.021803       -0.130439        1.953059
H           1.185099       -1.886255        1.837878
H           2.614201       -0.865526        1.683178
C           2.078667       -2.016038       -0.741455
H           1.888795       -2.024240       -1.815371
H           3.149225       -1.906599       -0.584758
H           1.767240       -2.976694       -0.326670
N          -4.468560        0.401820       -0.320584
H          -5.340142        0.710044        0.109415
H          -4.715181       -0.262251       -1.051378
C          -3.750408        1.553726       -0.915277
H          -3.573549        2.287681       -0.135805
H          -2.802492        1.189231       -1.296575
H          -4.346832        1.985141       -1.713790
```

---

### Compound_25_HEI_Conformation_24_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.368035 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.111662 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      26.9973 cm-1
2.      37.8889 cm-1
3.      45.8259 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.113631        0.158108       -0.196790
C          -2.216896        0.577423       -0.962583
C          -3.329084       -0.311677       -1.218585
O          -0.974390       -0.988386        0.308405
N          -0.115844        1.128943        0.022187
C           1.283003        0.817742        0.327721
C           1.842437       -0.171687       -0.748258
C           3.236501       -0.678247       -0.470047
C           3.358783       -2.063224        0.110618
O           4.224130       -0.009203       -0.720954
```

```
H          -2.237820        1.574656       -1.382378
H          -3.069905       -1.363619       -1.117723
H          -3.841955       -0.136949       -2.162685
H          -0.210539        1.926110       -0.587917
H           1.856801        0.353218       -1.704056
H           1.149685       -1.007495       -0.807511
H           4.377482       -2.258936        0.435848
H           2.660654       -2.203354        0.935257
H           3.079791       -2.786151       -0.660772
C           2.046395        2.142227        0.264629
H           1.960855        2.595115       -0.724991
H           1.643325        2.839138        1.000100
H           3.102973        1.988587        0.471678
C           1.406406        0.238545        1.740773
H           0.885820       -0.711144        1.815815
H           2.454752        0.102580        2.011418
H           0.961277        0.932930        2.453624
N          -4.535527       -0.157767       -0.166884
H          -5.334699       -0.709365       -0.477615
H          -4.818909        0.819458       -0.194278
C          -4.159239       -0.528953        1.218199
H          -3.952593       -1.593911        1.243971
H          -3.262115        0.024224        1.474845
H          -4.971243       -0.284156        1.896577
```

---

### Compound_25_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.367617 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.110431 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      31.4295 cm-1
2.      42.9627 cm-1
3.      58.0894 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.608223       -0.925489        1.054497
C          -1.728876       -1.668969        0.683078
C          -2.607350       -1.260580       -0.426183
O           0.100303       -1.104692        2.079271
```

```
N          -0.320757        0.184165        0.168816
C           0.833747        1.074780        0.376661
C           2.172199        0.310796        0.412616
C           2.533087       -0.524512       -0.790261
C           3.967510       -0.986606       -0.852275
O           1.737944       -0.831329       -1.661075
H          -2.055628       -2.462474        1.338625
H          -2.141919       -1.183732       -1.413705
H          -3.483908       -1.896059       -0.523365
H          -0.298860       -0.145427       -0.788605
H           2.146035       -0.379526        1.260438
H           2.996594        1.002004        0.605966
H           4.089177       -1.754078       -1.612472
H           4.601397       -0.131501       -1.099628
H           4.299537       -1.357760        0.117752
C           0.827719        2.078908       -0.782143
H           0.899076        1.576080       -1.745405
H          -0.092849        2.662846       -0.765919
H           1.671121        2.764054       -0.690591
C           0.664553        1.845836        1.688952
H           0.671027        1.167570        2.537090
H           1.469895        2.572597        1.804181
H          -0.283718        2.385123        1.678199
N          -3.135695        0.178854       -0.195054
H          -2.265599        0.699061        0.016030
H          -3.695523        0.173119        0.654087
C          -3.871446        0.794727       -1.322950
H          -4.167729        1.804220       -1.053335
H          -3.216542        0.822047       -2.188813
H          -4.749924        0.195513       -1.544388
```

---

### Compound_25_HEI_Conformation_4_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.368017 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.110868 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      27.5684 cm-1
2.      54.9045 cm-1
3.      69.3516 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.892836       -1.800329       -0.261272
C          -2.262217       -1.536696       -0.111881
C          -2.777616       -0.301322        0.485753
O          -0.393212       -2.769910       -0.891771
N          -0.040027       -0.826276        0.319633
C           1.418201       -0.822301        0.279281
C           1.862419        0.534378        0.896140
C           1.476730        1.743126        0.069951
C           2.592100        2.508516       -0.581634
O           0.314286        2.089409       -0.062509
H          -2.959659       -2.205883       -0.593842
H          -2.416269       -0.051040        1.488843
H          -3.864497       -0.282850        0.517789
H          -0.397898       -0.437707        1.178029
H           2.941546        0.513880        1.037336
H           1.399870        0.638229        1.880571
H           2.202859        3.317932       -1.193203
H           3.251831        2.910062        0.191275
H           3.200049        1.834433       -1.187672
C           2.020937       -1.951537        1.128454
H           3.111561       -1.932919        1.093761
H           1.708456       -1.853546        2.169377
H           1.671475       -2.909531        0.749339
C           1.927669       -0.921228       -1.162954
H           1.681701       -1.893436       -1.576218
H           1.465359       -0.160427       -1.793009
H           3.009076       -0.781671       -1.185814
N          -2.374388        0.972540       -0.326126
H          -1.345579        1.016017       -0.315880
H          -2.655504        0.812336       -1.290783
C          -2.920046        2.250777        0.186341
H          -2.552466        3.070947       -0.422685
H          -4.004976        2.214269        0.151819
H          -2.586672        2.380755        1.211587
```

---

### Compound_25_HEI_Conformation_5_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.372723 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.114935 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      25.4115 cm-1
2.      51.9418 cm-1
3.      67.7160 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.352603       -1.776362       -0.428526
C          -1.756244       -1.779669       -0.431517
C          -2.603472       -0.933151        0.399985
O           0.359629       -2.362256       -1.290510
N           0.304663       -1.110196        0.631344
C           1.635769       -0.518054        0.507280
C           1.745822        0.405763       -0.752564
C           0.993183        1.700849       -0.628554
C           1.799260        2.967426       -0.630543
O          -0.224793        1.742690       -0.517273
H          -2.230499       -2.343727       -1.223148
H          -2.249326       -0.749322        1.415402
H          -3.630971       -1.285662        0.469204
H          -0.302060       -0.548192        1.203194
H           1.347874       -0.159987       -1.595461
H           2.796223        0.616104       -0.946581
H           1.161203        3.836357       -0.494771
H           2.552290        2.924878        0.158813
H           2.344474        3.047695       -1.573720
C           1.884854        0.288058        1.785504
H           2.859283        0.773884        1.747016
H           1.124526        1.056826        1.933995
H           1.867284       -0.373546        2.651467
C           2.715387       -1.601559        0.396078
H           3.707147       -1.147064        0.408425
H           2.635542       -2.280128        1.246108
H           2.586853       -2.175139       -0.515921
N          -2.748709        0.523773       -0.185461
H          -1.792766        0.866967       -0.367888
H          -3.195092        0.430467       -1.094823
C          -3.488779        1.484925        0.665686
H          -2.961419        1.584892        1.610125
H          -3.538392        2.449646        0.169159
H          -4.491609        1.107184        0.843510
```

---

### Compound_25_HEI_Conformation_7_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.366842 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.109262 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      29.9317 cm-1
2.      31.1794 cm-1
3.      44.4481 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.100114       -1.520909       -0.493701
C           2.283244       -0.975482       -1.017115
C           2.614027        0.443064       -0.883834
O           0.826926       -2.746889       -0.425084
N           0.195605       -0.564368        0.060773
C          -1.183618       -0.886955        0.454304
C          -1.840202        0.448323        0.894193
C          -1.993523        1.470664       -0.213425
C          -3.388068        1.899398       -0.565039
O          -1.020865        1.924933       -0.793912
H           3.062364       -1.663467       -1.311453
H           1.868227        1.155491       -1.246561
H           3.570476        0.703627       -1.329349
H           0.206649        0.313947       -0.441524
H          -1.214591        0.897758        1.668586
H          -2.812403        0.228420        1.331172
H          -3.381489        2.625163       -1.373730
H          -3.976928        1.024317       -0.848524
H          -3.871515        2.324931        0.317253
C          -1.992304       -1.507812       -0.696101
H          -1.979937       -0.861413       -1.575229
H          -1.556888       -2.463864       -0.972391
H          -3.030862       -1.662423       -0.398862
C          -1.185866       -1.818966        1.668719
H          -0.645245       -1.359711        2.497359
H          -2.208973       -2.017630        1.990812
H          -0.701951       -2.756990        1.413352
N           2.740775        0.860973        0.630353
H           3.526528        0.349994        1.025523
H           1.891019        0.476926        1.058583
C           2.855099        2.314737        0.893970
H           1.975244        2.806566        0.489905
H           2.916717        2.488566        1.964191
H           3.746999        2.692830        0.403140
```

### Compound_25_HEI_Conformation_9_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -653.376707 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -653.119205 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      37.7910 cm-1
2.      48.3548 cm-1
3.      53.0452 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.732906       -0.170196        0.518673
C           1.764211       -0.509167        1.374862
C           3.100505        0.081073        1.119349
O           0.916423        0.537850       -0.545258
N          -0.576382       -0.579366        0.816406
C          -1.515244       -1.043098       -0.225842
C          -2.087984        0.162943       -1.018520
C          -2.597132        1.270500       -0.121515
C          -1.720834        2.481195        0.030184
O          -3.679779        1.191730        0.432843
H           1.629436       -1.200363        2.192285
H           3.153158        1.167406        1.251351
H           3.892057       -0.372092        1.711560
H          -0.599720       -1.179558        1.627269
H          -2.918852       -0.193784       -1.628627
H          -1.304511        0.548113       -1.664976
H          -2.066503        3.109324        0.847846
H          -0.683304        2.177541        0.161487
H          -1.763925        3.051476       -0.902981
C          -0.842892       -2.002890       -1.216190
H          -1.559946       -2.348047       -1.962323
H          -0.018745       -1.509654       -1.727178
H          -0.454975       -2.874421       -0.686689
C          -2.639118       -1.780739        0.504764
H          -3.388750       -2.127858       -0.205316
H          -2.236573       -2.651947        1.025126
H          -3.128985       -1.134819        1.230507
N           3.441392       -0.105457       -0.354104
H           3.545991       -1.100510       -0.536762
H           2.520085        0.203211       -0.787552
```

```
C          4.603580       0.654769       -0.856830
H          5.495896       0.362610       -0.309077
H          4.415729       1.714613       -0.711070
H          4.736236       0.449558       -1.915285
```

---

### Compound_26_HEI_Conformation_10_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526851 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314963 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.0756 cm-1
  2.      51.2521 cm-1
  3.      67.1941 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -1.435611      -1.428595       0.102556
C         -2.402807      -0.507541       0.482941
C         -2.065920       0.900597       0.733634
O         -1.529164      -2.649214      -0.110643
O         -0.179399      -0.800374      -0.084226
C          0.949412      -1.635671      -0.338415
C          2.148920      -0.742821      -0.592419
C          2.536713       0.134305       0.596342
C          3.755980       1.006299       0.311429
H         -3.431512      -0.827459       0.536371
H         -1.243463       1.063343       1.432682
H         -2.922218       1.486943       1.057220
H          1.124944      -2.285165       0.523945
H          0.749912      -2.275620      -1.198481
H          1.945077      -0.112896      -1.463832
H          2.992365      -1.384709      -0.863417
H          2.734776      -0.505664       1.461479
H          1.689420       0.766074       0.869338
H          3.569528       1.674750      -0.531909
H          4.016127       1.622653       1.173055
H          4.626756       0.396026       0.062286
N         -1.542528       1.597415      -0.551917
H         -2.273486       1.541814      -1.258226
H         -0.781959       0.984262      -0.861383
```

```
C          -1.065969        2.990969       -0.380828
H          -1.891059        3.604684       -0.031993
H          -0.696707        3.367002       -1.330195
H          -0.266611        2.993502        0.353992
```

---

### Compound_26_HEI_Conformation_11_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.528104 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.316733 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.8447 cm-1
  2.      35.0462 cm-1
  3.      73.4943 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.657256       -0.527599        0.191372
C           1.674368       -1.315714       -0.302548
C           3.065231       -0.879441       -0.038404
O           0.819526        0.576221        0.800299
O          -0.626770       -0.988952       -0.029315
C          -1.700600       -0.103160        0.298306
C          -2.994494       -0.765539       -0.136317
C          -4.240323        0.043585        0.232751
C          -4.346848        1.390459       -0.481828
H           1.478650       -2.188927       -0.902619
H           3.359425       -0.894260        1.016116
H           3.804516       -1.438374       -0.606817
H          -1.712110        0.090282        1.373960
H          -1.551963        0.853228       -0.204369
H          -3.051420       -1.751978        0.330052
H          -2.967903       -0.927747       -1.217678
H          -4.260149        0.201042        1.315162
H          -5.122364       -0.555774       -0.003112
H          -5.287611        1.887277       -0.241123
H          -3.538168        2.065350       -0.199551
H          -4.306159        1.259834       -1.565475
N           3.208340        0.594418       -0.414550
H           3.070138        0.682607       -1.418640
H           2.362713        1.000799        0.051672
```

```
C           4.459553        1.258361        0.012054
H           5.307706        0.754762       -0.443319
H           4.533148        1.197673        1.093812
H           4.436269        2.299427       -0.296398
```

---

### Compound_26_HEI_Conformation_12_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.5264 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314719 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      19.1891 cm-1
2.      47.4081 cm-1
3.      56.3876 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.747768       -1.615163       -0.235181
C          -2.013728       -1.160758       -0.576807
C          -2.598318        0.041365        0.034002
O          -0.129717       -2.620380       -0.622465
O          -0.116047       -0.734401        0.687540
C           1.205600       -1.068542        1.119691
C           2.281651       -0.510871        0.200746
C           2.292676        1.012540        0.101142
C           3.421654        1.537359       -0.781393
H          -2.560290       -1.685759       -1.344234
H          -2.601430        0.055346        1.125740
H          -3.605638        0.244387       -0.320936
H           1.299632       -0.637236        2.117903
H           1.295799       -2.150518        1.193965
H           2.160307       -0.948106       -0.792810
H           3.250331       -0.853843        0.578582
H           2.379087        1.439707        1.104558
H           1.337582        1.360856       -0.299337
H           3.338346        1.143751       -1.796541
H           3.407618        2.626299       -0.843405
H           4.395667        1.236988       -0.389668
N          -1.767838        1.305906       -0.307517
H          -1.739534        1.396163       -1.321092
H          -0.821198        1.053293       -0.006199
```

```
C          -2.213719        2.567403        0.331921
H          -3.224804        2.789006        0.004023
H          -1.543649        3.373108        0.047481
H          -2.195146        2.433466        1.409259
```

---

### Compound_26_HEI_Conformation_13_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526584 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314661 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.4684 cm-1
  2.      42.1983 cm-1
  3.      67.0520 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.462340        1.556329       -0.252159
C          -1.502987        1.121726       -1.059917
C          -1.974095       -0.269902       -1.029592
O           0.091285        2.666494       -0.186913
O          -0.047856        0.530834        0.643531
C           1.210563        0.698884        1.299664
C           2.374980        0.271413        0.419493
C           2.322968       -1.194918       -0.001677
C           3.494286       -1.595364       -0.893906
H          -2.008755        1.840596       -1.685451
H          -1.194599       -1.024106       -1.152903
H          -2.765206       -0.461440       -1.750398
H           1.322490        1.737262        1.607212
H           1.155392        0.072082        2.190985
H           3.302018        0.463866        0.969035
H           2.399318        0.910768       -0.466805
H           1.382545       -1.383479       -0.523795
H           2.309475       -1.824677        0.893240
H           4.447748       -1.441406       -0.383963
H           3.436476       -2.645858       -1.182613
H           3.509659       -0.998779       -1.808553
N          -2.570665       -0.639821        0.354168
H          -3.339381       -0.000235        0.545402
H          -1.818666       -0.403602        1.008888
```

```
C          -2.997203       -2.051082        0.512574
H          -3.779353       -2.263788       -0.210005
H          -2.140732       -2.692763        0.329715
H          -3.368230       -2.206832        1.521014
```

---

### Compound_26_HEI_Conformation_14_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.528212 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.316025 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.3480 cm-1
  2.      38.0882 cm-1
  3.      56.0146 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.582841        0.820684        0.247386
C          -1.624423        1.344338       -0.484386
C          -2.974380        0.776202       -0.258025
O          -0.675030       -0.160987        1.049734
O           0.648042        1.432060        0.067141
C           1.807339        0.692876        0.466233
C           2.189259       -0.361104       -0.563327
C           3.410862       -1.189408       -0.158297
C           4.711305       -0.389601       -0.084120
H          -1.469487        2.108014       -1.228351
H          -3.387194        0.956121        0.739879
H          -3.705053        1.103240       -0.993693
H           2.590297        1.441804        0.573064
H           1.636358        0.228444        1.437344
H           2.376947        0.129649       -1.522747
H           1.333206       -1.023645       -0.704320
H           3.533222       -2.002526       -0.877394
H           3.217792       -1.664935        0.807999
H           5.558393       -1.038962        0.140819
H           4.915645        0.108135       -1.034651
H           4.673146        0.378132        0.689488
N          -2.892910       -0.746852       -0.329054
H          -2.062651       -0.930175        0.284091
H          -2.629661       -1.008823       -1.276357
```

```
C          -4.096749       -1.484635        0.112498
H          -3.910956       -2.552093        0.038721
H          -4.938402       -1.210084       -0.517357
H          -4.307569       -1.219029        1.144078
```

---

### Compound_26_HEI_Conformation_15_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.527811 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.315947 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.3829 cm-1
  2.      38.7411 cm-1
  3.      42.6103 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.574675        0.529656       -0.036898
C          -1.640884        1.362813        0.223850
C          -2.928163        0.729034        0.591237
O          -0.625403       -0.739644       -0.031993
O           0.614081        1.160418       -0.366425
C           1.757852        0.333999       -0.602131
C           2.491576        0.000194        0.689175
C           3.703360       -0.910877        0.479417
C           4.829670       -0.277326       -0.337081
H          -1.569532        2.431991        0.110886
H          -2.918729        0.189435        1.543831
H          -3.761497        1.427333        0.602663
H           1.455611       -0.581138       -1.110785
H           2.389522        0.914115       -1.273484
H           1.784349       -0.485425        1.363591
H           2.807523        0.930770        1.169829
H           3.376816       -1.836302       -0.004479
H           4.092567       -1.201378        1.457881
H           5.693437       -0.941083       -0.393715
H           4.517863       -0.058525       -1.358967
H           5.158531        0.660240        0.116620
N          -3.256935       -0.368328       -0.420415
H          -3.406350        0.066849       -1.327894
H          -2.342936       -0.876056       -0.466626
```

```
C          -4.379739       -1.265024       -0.067474
H          -5.288760       -0.679027        0.035952
H          -4.148933       -1.755793        0.873414
H          -4.504343       -2.008721       -0.849045
```

---

### Compound_26_HEI_Conformation_16_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52504 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313919 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      28.5007 cm-1
2.      46.7392 cm-1
3.      77.4022 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.799138       -0.264641       -0.423210
C           1.805544       -1.079148        0.095583
C           3.182971       -0.934154       -0.341293
O           0.905682        0.664630       -1.246571
O          -0.462954       -0.587528        0.075971
C          -1.558642        0.195001       -0.395187
C          -2.818325       -0.289388        0.295622
C          -4.056688        0.487772       -0.145647
C          -5.330254        0.011949        0.547642
H           1.549342       -1.857588        0.798876
H           3.280171       -0.453216       -1.312811
H           3.755739       -1.859938       -0.326970
H          -1.382975        1.252041       -0.180901
H          -1.651111        0.095588       -1.479767
H          -2.692208       -0.196392        1.378029
H          -2.957502       -1.353469        0.084804
H          -4.174211        0.395712       -1.229185
H          -3.906571        1.552188        0.056529
H          -6.200592        0.579961        0.216488
H          -5.519638       -1.042603        0.337022
H          -5.250833        0.123646        1.630941
N           4.052607        0.006698        0.602767
H           5.033584       -0.047000        0.330114
H           3.983755       -0.379307        1.542399
```

```
C           3.601591        1.420061        0.612212
H           4.163169        1.974870        1.357762
H           3.765930        1.839371       -0.375038
H           2.541860        1.427716        0.842805
```

---

### Compound_26_HEI_Conformation_17_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529531 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317287 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      32.4994 cm-1
  2.      36.8404 cm-1
  3.      86.1476 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.556082       -1.133878       -0.028190
C           1.508095       -0.845632       -0.977832
C           2.818831       -0.332609       -0.513517
O           0.689018       -0.942296        1.221542
O          -0.631186       -1.663212       -0.511255
C          -1.796126       -1.584043        0.319437
C          -2.682814       -0.413673       -0.077716
C          -2.050805        0.956579        0.157146
C          -2.963257        2.105335       -0.262350
H           1.287376       -0.902080       -2.030735
H           3.430175       -1.061470        0.027639
H           3.419669        0.084952       -1.318142
H          -2.328753       -2.525295        0.178871
H          -1.491714       -1.507527        1.361781
H          -3.615210       -0.489940        0.491575
H          -2.953869       -0.515602       -1.133037
H          -1.111053        1.017001       -0.395500
H          -1.791135        1.056410        1.214155
H          -3.902501        2.085027        0.294698
H          -2.492330        3.073680       -0.086831
H          -3.208725        2.042042       -1.324709
N           2.602470        0.771773        0.526385
H           3.452415        0.930402        1.061278
H           1.886503        0.316672        1.145229
```

```
C           2.086263        2.047591       -0.017903
H           1.818928        2.705297        0.803785
H           2.852451        2.510469       -0.633573
H           1.210215        1.823595       -0.617927
```

---

### Compound_26_HEI_Conformation_18_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.528473 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.316748 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      22.6766 cm-1
  2.      29.7997 cm-1
  3.      76.9522 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.483216        0.171462        0.209551
C          -1.360901       -0.386284        1.111714
C          -2.455976       -1.232192        0.582346
O          -0.560442        0.049148       -1.052758
O           0.518719        0.953604        0.762230
C           1.507114        1.523961       -0.101875
C           2.854127        0.846301        0.093671
C           2.879294       -0.619166       -0.333295
C           4.234795       -1.278315       -0.094176
H          -1.315213       -0.149618        2.161828
H          -2.130822       -2.184183        0.150699
H          -3.226877       -1.439690        1.320940
H           1.175118        1.440254       -1.134807
H           1.575298        2.581444        0.160549
H           3.143543        0.926647        1.145985
H           3.600136        1.408544       -0.477460
H           2.616255       -0.688694       -1.392106
H           2.105356       -1.164932        0.211026
H           4.503456       -1.247429        0.964003
H           4.231753       -2.323667       -0.406345
H           5.024039       -0.766710       -0.649422
N          -3.128294       -0.534104       -0.605141
H          -2.288164       -0.242793       -1.160030
H          -3.670684       -1.199611       -1.149715
```

```
C          -3.954230        0.641630       -0.250432
H          -3.347686        1.303486        0.359517
H          -4.265251        1.148226       -1.159148
H          -4.824460        0.311051        0.309684
```

---

### Compound_26_HEI_Conformation_19_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525136 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313573 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.2894 cm-1
  2.      45.1707 cm-1
  3.      70.7301 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.726560       -0.912497        0.195378
C          -1.924502       -0.994811       -0.511867
C          -3.166151       -0.510327        0.066116
O          -0.529553       -0.418069        1.321582
O           0.342492       -1.494684       -0.495306
C           1.646456       -1.310957        0.055785
C           2.260853        0.020381       -0.348687
C           3.672776        0.200730        0.203519
C           4.302263        1.530803       -0.201575
H          -1.936966       -1.463162       -1.484778
H          -3.141740       -0.451140        1.152420
H          -4.052112       -1.054933       -0.255882
H           1.605553       -1.394066        1.141714
H           2.243670       -2.137192       -0.333265
H           1.617881        0.827128        0.010712
H           2.279570        0.087502       -1.440341
H           4.305087       -0.622758       -0.141687
H           3.644696        0.127502        1.294608
H           5.308449        1.637551        0.206173
H           4.371300        1.615945       -1.288010
H           3.704967        2.371041        0.158404
N          -3.520438        0.980461       -0.358166
H          -4.459134        1.214963       -0.035682
H          -3.543699        0.996916       -1.375840
```

```
C          -2.543747        1.984737        0.131420
H          -2.784045        2.957629       -0.286534
H          -2.596407        2.014014        1.214865
H          -1.555851        1.663511       -0.180450
```

---

### Compound_26_HEI_Conformation_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529024 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317952 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.2659 cm-1
  2.      38.1699 cm-1
  3.      68.7763 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.739012        0.346614       -0.233084
C          -1.681558        1.316054        0.034039
C          -3.103462        0.964955       -0.186216
O          -0.998186       -0.846085       -0.586894
O           0.580187        0.726996       -0.073035
C           1.568142       -0.303496       -0.145779
C           2.925523        0.333247        0.076256
C           4.060904       -0.686408        0.019935
C           5.432002       -0.053568        0.240619
H          -1.410615        2.280420        0.430802
H          -3.372460        0.770830       -1.229690
H          -3.793537        1.704728        0.211983
H           1.367963       -1.063817        0.613791
H           1.525270       -0.795165       -1.119684
H           2.931314        0.837300        1.046683
H           3.086414        1.105401       -0.681290
H           4.044061       -1.193570       -0.948948
H           3.890008       -1.460237        0.773778
H           5.484903        0.434743        1.215832
H           6.226881       -0.799205        0.197113
H           5.640728        0.702172       -0.519349
N          -3.405155       -0.367702        0.497934
H          -2.596829       -0.946725        0.169138
H          -3.298679       -0.245135        1.502483
```

```
C          -4.709365       -0.984944        0.171352
H          -5.510110       -0.316948        0.476594
H          -4.756089       -1.149473       -0.900993
H          -4.798197       -1.933425        0.692915
```

---

### Compound_26_HEI_Conformation_20_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52619 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313572 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.2825 cm-1
  2.      40.3901 cm-1
  3.      61.9426 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.330346        1.675351        0.046980
C           1.485842        1.394870        0.761121
C           1.976751        0.018333        0.921707
O          -0.259426        2.753197       -0.136084
O          -0.174735        0.504558       -0.584829
C          -1.527394        0.530340       -1.042878
C          -2.518532        0.278062        0.085862
C          -2.245820       -0.990450        0.897585
C          -2.276551       -2.277252        0.075902
H           2.056888        2.214115        1.169253
H           1.239032       -0.692836        1.298320
H           2.868115       -0.040008        1.541382
H          -1.732977        1.487332       -1.520024
H          -1.586982       -0.252559       -1.797942
H          -3.518612        0.226279       -0.356478
H          -2.514019        1.142320        0.753157
H          -2.987424       -1.054466        1.697427
H          -1.274329       -0.896361        1.387478
H          -1.479165       -2.297519       -0.668059
H          -2.150717       -3.152670        0.714446
H          -3.226466       -2.383845       -0.452988
N           2.369437       -0.610098       -0.440254
H           3.099545       -0.034388       -0.854864
H           1.528188       -0.480817       -1.011484
```

```
C           2.771044       -2.036907       -0.396639
H           2.990681       -2.382109       -1.402432
H           3.650594       -2.135581        0.232478
H           1.950765       -2.612332        0.021577
```

---

### Compound_26_HEI_Conformation_21_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524965 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313837 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      21.5789 cm-1
  2.      34.4818 cm-1
  3.      54.4833 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.618523       -0.130594        0.173945
C          -1.683757       -1.003332        0.387829
C          -2.788061       -1.077586       -0.552905
O          -0.460171        0.676399       -0.761671
O           0.356220       -0.223302        1.173921
C           1.568940        0.501067        0.968873
C           2.569664       -0.277495        0.128829
C           3.888752        0.470596       -0.047815
C           4.904174       -0.307825       -0.880046
H          -1.667019       -1.662833        1.242696
H          -2.530665       -0.718427       -1.547477
H          -3.250323       -2.060875       -0.620861
H           1.352017        1.462553        0.503866
H           1.971843        0.680238        1.967140
H           2.125762       -0.479513       -0.848707
H           2.754965       -1.245807        0.602789
H           4.314912        0.691048        0.935506
H           3.694116        1.437854       -0.520224
H           4.514038       -0.514714       -1.878712
H           5.836787        0.246492       -0.994185
H           5.140111       -1.266042       -0.412581
N          -4.022896       -0.157617       -0.156942
H          -4.298489       -0.427713        0.785387
H          -4.812882       -0.363092       -0.768047
```

```
C          -3.715533        1.293587       -0.187604
H          -3.506351        1.578011       -1.213737
H          -4.564261        1.852323        0.195119
H          -2.836613        1.458525        0.425987
```

---

### Compound_26_HEI_Conformation_22_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525137 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313304 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      34.0038 cm-1
  2.      39.4896 cm-1
  3.      54.8343 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.719243       -1.535970        0.047035
C           2.093442       -1.397442       -0.084646
C           2.796976       -0.181471        0.347782
O          -0.018000       -2.490456       -0.249596
O           0.131595       -0.360703        0.596156
C          -1.294695       -0.315260        0.674423
C          -1.912107        0.193799       -0.620277
C          -3.441359        0.243854       -0.585671
C          -4.011398        1.257591        0.406202
H           2.646992       -2.187472       -0.567122
H           2.608885        0.126322        1.378340
H           3.871329       -0.242005        0.192343
H          -1.678397       -1.307504        0.909741
H          -1.515396        0.352199        1.506403
H          -1.586998       -0.462529       -1.429315
H          -1.516692        1.191227       -0.836226
H          -3.827746       -0.753048       -0.353453
H          -3.803666        0.483565       -1.587883
H          -3.755644        1.007212        1.436346
H          -3.625057        2.258860        0.203114
H          -5.099343        1.300708        0.340412
N           2.323850        1.057170       -0.456421
H           2.493039        0.871295       -1.442891
H           1.307531        1.050354       -0.324799
```

```
C           2.909441        2.356342       -0.046162
H           2.489341        3.151062       -0.655231
H           2.672528        2.526382        0.999728
H           3.986322        2.313798       -0.179152
```

---

### Compound_26_HEI_Conformation_23_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525071 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313438 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.8456 cm-1
  2.      37.0949 cm-1
  3.      47.3826 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.625606        1.434410       -0.147720
C          -1.916719        1.429660        0.360570
C          -2.573181        0.188038        0.792012
O           0.079280        2.383312       -0.529053
O          -0.112312        0.111493       -0.259623
C           1.273864       -0.032750       -0.573989
C           2.145194        0.046714        0.671177
C           3.640737       -0.087353        0.374700
C           4.051265       -1.458884       -0.160895
H          -2.469275        2.356044        0.374859
H          -2.002571       -0.416578        1.499275
H          -3.567881        0.357143        1.196978
H           1.358126       -1.007262       -1.052971
H           1.566552        0.735253       -1.289769
H           1.835726       -0.734098        1.372149
H           1.955637        1.005885        1.156578
H           4.196393        0.117324        1.292597
H           3.936428        0.687827       -0.338566
H           5.132759       -1.522010       -0.288288
H           3.749818       -2.250884        0.528245
H           3.595117       -1.671298       -1.128471
N          -2.765677       -0.792466       -0.396373
H          -3.323776       -0.319175       -1.104018
H          -1.820845       -0.888212       -0.780887
```

```
C          -3.342590       -2.115330       -0.055971
H          -3.402544       -2.725806       -0.951842
H          -2.699688       -2.594071        0.676414
H          -4.333771       -1.968291        0.362434
```

---

### Compound_26_HEI_Conformation_24_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525266 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313747 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      22.7812 cm-1
2.      33.0978 cm-1
3.      70.3384 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.576211       -1.071078        0.020477
C           1.567274       -0.743224       -0.902655
C           2.913652       -0.416993       -0.464377
O           0.663667       -1.105833        1.262737
O          -0.634050       -1.412443       -0.591926
C          -1.776774       -1.535479        0.257569
C          -2.389333       -0.187599        0.611130
C          -2.859919        0.614372       -0.599583
C          -3.457853        1.965141       -0.216564
H           1.339810       -0.762292       -1.958106
H           3.152757       -0.810658        0.521602
H           3.695115       -0.688530       -1.172206
H          -2.487905       -2.136252       -0.311972
H          -1.508253       -2.078229        1.162836
H          -1.657700        0.392428        1.178534
H          -3.235097       -0.368000        1.282864
H          -3.599834        0.028333       -1.153519
H          -2.017385        0.764963       -1.277582
H          -2.725784        2.580154        0.311393
H          -3.787537        2.521075       -1.095548
H          -4.320021        1.841048        0.442392
N           3.154672        1.144022       -0.286687
H           4.142767        1.319425       -0.106794
H           2.934480        1.578322       -1.181030
```

```
C           2.322956        1.755902        0.779217
H           2.629593        1.341064        1.733886
H           1.288834        1.495890        0.580692
H           2.459229        2.833061        0.771589
```

---

### Compound_26_HEI_Conformation_25_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525874 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.31335 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.2680 cm-1
  2.      31.2800 cm-1
  3.      65.2918 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.898775        1.474293       -0.281901
C           2.140992        0.922464        0.001243
C           2.300508       -0.195316        0.937149
O           0.598378        2.416390       -1.034406
O          -0.142485        0.792370        0.398612
C          -1.470436        1.278345        0.198993
C          -2.443475        0.341463        0.891164
C          -2.411121       -1.110683        0.404727
C          -2.603880       -1.274839       -1.100792
H           2.992869        1.270286       -0.561330
H           1.873664       -0.034780        1.928751
H           3.336577       -0.505967        1.046817
H          -1.559383        2.286049        0.610172
H          -1.676837        1.345536       -0.869051
H          -3.446242        0.750147        0.735515
H          -2.260475        0.365253        1.968254
H          -3.191581       -1.663833        0.932232
H          -1.470559       -1.578658        0.705032
H          -3.528980       -0.798238       -1.432023
H          -1.782181       -0.829261       -1.662671
H          -2.655030       -2.329348       -1.374018
N           1.529019       -1.472771        0.469738
H           1.534741       -2.172645        1.209508
H           0.566683       -1.138399        0.366404
```

```
C           2.011198       -2.060438       -0.801368
H           1.332346       -2.847518       -1.114799
H           2.041383       -1.267425       -1.541778
H           3.007362       -2.463615       -0.644120
```

---

### Compound_26_HEI_Conformation_26_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524988 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313265 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.6009 cm-1
  2.      42.4675 cm-1
  3.      73.0476 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.486394       -0.164695       -0.041149
C          -1.322564        0.840139       -0.525670
C          -2.458485        1.306743        0.250092
O          -0.578210       -0.792346        1.031019
O           0.561409       -0.455079       -0.920434
C           1.566599       -1.360974       -0.461866
C           2.639989       -0.671880        0.368403
C           3.394933        0.422184       -0.382365
C           4.463237        1.096357        0.473976
H          -1.098592        1.306204       -1.473739
H          -2.366329        1.103354        1.315147
H          -2.705491        2.355178        0.092331
H           1.104044       -2.165006        0.108886
H           2.004431       -1.781617       -1.369079
H           3.346178       -1.437301        0.707031
H           2.176944       -0.254432        1.265734
H           2.682322        1.169884       -0.736670
H           3.857936       -0.009112       -1.275360
H           5.205773        0.372865        0.817799
H           4.988764        1.875196       -0.080625
H           4.019931        1.558734        1.358604
N          -3.824131        0.584576       -0.128033
H          -4.601594        1.056722        0.332891
H          -3.952138        0.710838       -1.130219
```

```
C          -3.839527       -0.863543        0.194980
H          -3.795849       -0.975096        1.273482
H          -2.961987       -1.312361       -0.257539
H          -4.747739       -1.312671       -0.195523
```

---

### Compound_26_HEI_Conformation_27_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524942 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313498 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.4172 cm-1
  2.      35.5294 cm-1
  3.      68.3281 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.921093        1.401108        0.074740
C          -2.248544        1.108036       -0.209648
C          -2.634092       -0.108669       -0.932047
O          -0.426390        2.381836        0.656013
O          -0.058156        0.366561       -0.365032
C           1.343520        0.564148       -0.181319
C           2.052020       -0.708085       -0.607949
C           3.577236       -0.607458       -0.527357
C           4.119095       -0.438946        0.891749
H          -3.012978        1.751511        0.196158
H          -2.124075       -0.261751       -1.884366
H          -3.707075       -0.180572       -1.091862
H           1.680132        1.411947       -0.784568
H           1.543470        0.805290        0.862139
H           1.757093       -0.942278       -1.633594
H           1.705459       -1.535939        0.017940
H           3.916720        0.225162       -1.150437
H           4.005493       -1.510516       -0.967704
H           3.774203       -1.249152        1.537984
H           5.209781       -0.449386        0.897416
H           3.797853        0.501499        1.340493
N          -2.243478       -1.409509       -0.153831
H          -1.237342       -1.299238        0.000652
H          -2.374930       -2.225044       -0.749303
```

```
C          -2.952926       -1.590521        1.133734
H          -4.004726       -1.769693        0.930520
H          -2.525503       -2.433163        1.668278
H          -2.834160       -0.676964        1.707803
```

---

### Compound_26_HEI_Conformation_28_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525329 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.31264 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      37.4576 cm-1
  2.      60.8253 cm-1
  3.      79.2983 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.701307        1.730092        0.176872
C          -1.916708        1.190358        0.577139
C          -2.112051       -0.259123        0.719856
O          -0.365648        2.917151        0.025020
O           0.243935        0.714856       -0.115512
C           1.548577        1.136791       -0.515990
C           2.393984       -0.078813       -0.855893
C           2.875474       -0.915751        0.333033
C           1.792399       -1.724846        1.044396
H          -2.753960        1.855181        0.720043
H          -1.389464       -0.767550        1.360631
H          -3.114512       -0.515865        1.053338
H           1.463665        1.794475       -1.382358
H           2.011531        1.714119        0.288615
H           3.270078        0.291132       -1.395178
H           1.843851       -0.710240       -1.560510
H           3.368117       -0.253641        1.051618
H           3.647867       -1.601367       -0.024904
H           1.039017       -1.078354        1.490081
H           1.284559       -2.391361        0.343569
H           2.224219       -2.341746        1.834131
N          -1.919451       -0.991783       -0.634945
H          -2.585890       -0.600950       -1.297753
H          -0.988780       -0.688332       -0.938628
```

```
C          -2.014205       -2.470643       -0.588473
H          -1.824727       -2.877304       -1.577200
H          -1.273033       -2.841865        0.112462
H          -3.009653       -2.748295       -0.255048
```

---

### Compound_26_HEI_Conformation_29_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526584 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314661 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.4685 cm-1
  2.      42.1988 cm-1
  3.      67.0527 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.462344        1.556329       -0.252158
C          -1.502993        1.121728       -1.059915
C          -1.974100       -0.269901       -1.029592
O           0.091281        2.666494       -0.186910
O          -0.047857        0.530832        0.643529
C           1.210561        0.698883        1.299663
C           2.374979        0.271415        0.419492
C           2.322970       -1.194915       -0.001680
C           3.494291       -1.595359       -0.893906
H          -2.008761        1.840598       -1.685446
H          -1.194604       -1.024104       -1.152911
H          -2.765215       -0.461436       -1.750394
H           1.322485        1.737260        1.607213
H           1.155390        0.072079        2.190983
H           3.302016        0.463869        0.969036
H           2.399316        0.910771       -0.466805
H           1.382548       -1.383476       -0.523801
H           2.309475       -1.824676        0.893237
H           4.447751       -1.441401       -0.383960
H           3.436482       -2.645853       -1.182615
H           3.509666       -0.998772       -1.808552
N          -2.570661       -0.639825        0.354169
H          -3.339377       -0.000242        0.545410
H          -1.818658       -0.403607        1.008885
```

```
C          -2.997195       -2.051087        0.512573
H          -3.779348       -2.263793       -0.210002
H          -2.140722       -2.692767        0.329708
H          -3.368216       -2.206842        1.521015
```

---

### Compound_26_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529146 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.31762 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.1525 cm-1
  2.      43.9015 cm-1
  3.      65.3695 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.604298        0.125996       -0.480716
C           1.341759       -1.010856       -0.732978
C           2.816600       -0.899396       -0.652303
O           1.088360        1.243595       -0.116601
O          -0.764041        0.001991       -0.620624
C          -1.567480        1.099463       -0.177435
C          -3.024578        0.696889       -0.294149
C          -3.430226       -0.443041        0.637619
C          -4.905368       -0.812214        0.510283
H           0.874219       -1.959513       -0.938404
H           3.270275       -0.250207       -1.408358
H           3.321255       -1.861901       -0.682250
H          -1.316102        1.346396        0.856998
H          -1.358815        1.980922       -0.786595
H          -3.238054        0.421588       -1.331276
H          -3.632226        1.580021       -0.075404
H          -3.211449       -0.152696        1.669725
H          -2.811882       -1.317429        0.426187
H          -5.141820       -1.133053       -0.506525
H          -5.173655       -1.625153        1.186445
H          -5.545622        0.041253        0.743914
N           3.197966       -0.215774        0.659933
H           2.924705       -0.823004        1.429179
H           2.539002        0.598753        0.657431
```

```
C          4.610424        0.205361        0.787918
H          5.254701       -0.665962        0.710153
H          4.837809        0.903606       -0.012050
H          4.754768        0.688889        1.749659
```

---

### Compound_26_HEI_Conformation_30_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524092 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.312783 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.7280 cm-1
  2.      36.3746 cm-1
  3.      78.4375 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -0.711749       -0.441347       -0.352666
C         -1.812533       -1.071708        0.227621
C         -3.153849       -0.842627       -0.279397
O         -0.699243        0.375803       -1.293396
O          0.495786       -0.822314        0.232528
C          1.681022       -0.229209       -0.296683
C          2.852020       -0.696385        0.548139
C          4.204441       -0.189010        0.041746
C          4.378623        1.326756        0.132580
H         -1.660391       -1.771255        1.036086
H         -3.171501       -0.489333       -1.308622
H         -3.825352       -1.691946       -0.166135
H          1.818771       -0.530921       -1.339230
H          1.586073        0.856946       -0.283762
H          2.856161       -1.788981        0.560107
H          2.700279       -0.369776        1.581068
H          4.345955       -0.512215       -0.993840
H          4.993465       -0.673331        0.621319
H          3.673148        1.856072       -0.508673
H          4.221522        1.675052        1.155842
H          5.383676        1.623844       -0.169895
N         -3.940012        0.304526        0.495176
H         -4.909942        0.325854        0.181282
H         -3.951636        0.038930        1.478009
```

```
C          -3.325427        1.647250        0.351669
H          -3.848666        2.355603        0.986906
H          -2.283336        1.566280        0.640972
H          -3.395790        1.947272       -0.688771
```

---

### Compound_26_HEI_Conformation_31_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52767 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.315418 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.0851 cm-1
  2.      44.2642 cm-1
  3.      57.7661 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.255476       -0.729369        0.523093
C          -1.035955        0.042945        1.353815
C          -2.469587        0.186829        1.008513
O          -0.656397       -1.277821       -0.552083
O           1.060950       -0.894210        0.915406
C           1.985416       -1.360413       -0.074131
C           2.421810       -0.290535       -1.067409
C           3.271872        0.846090       -0.492465
C           2.508305        1.845588        0.375744
H          -0.618354        0.574408        2.192651
H          -3.053624       -0.736798        1.075338
H          -2.975123        0.953051        1.591031
H           2.844960       -1.714785        0.496710
H           1.550833       -2.205166       -0.606620
H           1.536806        0.116500       -1.562530
H           2.999073       -0.804660       -1.841882
H           3.731349        1.384608       -1.325528
H           4.098658        0.416552        0.082150
H           3.158896        2.662597        0.692741
H           1.673871        2.280040       -0.179423
H           2.096116        1.369437        1.263177
N          -2.592685        0.566295       -0.465802
H          -2.178800        1.486719       -0.596287
H          -1.942641       -0.130077       -0.903865
```

```
C          -3.954056        0.507269       -1.041466
H          -3.910198        0.773306       -2.093536
H          -4.333095       -0.504600       -0.933939
H          -4.600334        1.200633       -0.510312
```

---

### Compound_26_HEI_Conformation_32_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52707 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.315217 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.8246 cm-1
  2.      39.3140 cm-1
  3.      67.4145 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.530068       -0.698196        0.324501
C           1.338212       -0.001508        1.195243
C           2.804921       -0.106457        1.015174
O           0.939899       -1.378519       -0.670008
O          -0.826764       -0.608186        0.560195
C          -1.702749       -1.136098       -0.440264
C          -3.127833       -0.716076       -0.123675
C          -3.475818        0.740194       -0.446682
C          -2.772268        1.787792        0.414672
H           0.926354        0.661633        1.937711
H           3.225030       -1.090979        1.245593
H           3.356599        0.639484        1.582550
H          -1.402777       -0.773151       -1.425811
H          -1.622050       -2.225360       -0.454348
H          -3.334176       -0.927469        0.929656
H          -3.788029       -1.366141       -0.703988
H          -4.556888        0.863223       -0.340647
H          -3.252475        0.927027       -1.501669
H          -2.968262        1.614826        1.475089
H          -1.693029        1.762071        0.274642
H          -3.126025        2.790609        0.168895
N           3.162125        0.076458       -0.463999
H           4.096006       -0.279212       -0.650874
H           2.456777       -0.559431       -0.912316
```

```
C           3.021077        1.458054       -0.975144
H           2.027800        1.809926       -0.714410
H           3.774557        2.089744       -0.512730
H           3.146959        1.455407       -2.053788
```

---

### Compound_26_HEI_Conformation_33_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52711 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314958 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.1905 cm-1
  2.      38.1134 cm-1
  3.      51.8021 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.283509       -0.075695        0.384163
C           1.055800        1.027252        0.677532
C           2.365427        1.144664       -0.004391
O           0.630111       -1.019817       -0.392793
O          -0.933903       -0.146490        1.037019
C          -1.811330       -1.220251        0.682989
C          -2.627059       -0.959250       -0.577233
C          -3.665944        0.161337       -0.477489
C          -3.086574        1.575220       -0.437638
H           0.755465        1.752789        1.415250
H           2.306308        1.285213       -1.088592
H           2.994749        1.929696        0.407667
H          -1.233966       -2.136595        0.567331
H          -2.475437       -1.331881        1.541749
H          -3.141538       -1.895673       -0.813881
H          -1.943347       -0.763667       -1.406519
H          -4.286871       -0.006116        0.408358
H          -4.337865        0.081474       -1.336153
H          -3.882214        2.322303       -0.446722
H          -2.478250        1.731477        0.450978
H          -2.449751        1.755982       -1.306661
N           3.123802       -0.174855        0.128922
H           2.379473       -0.859334       -0.141841
H           3.330429       -0.328094        1.113327
```

```
C           4.341441       -0.311758       -0.700243
H           5.049549        0.466831       -0.430242
H           4.782640       -1.289622       -0.531599
H           4.062722       -0.209462       -1.744865
```

---

### Compound_26_HEI_Conformation_34_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525303 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314026 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.9072 cm-1
  2.      37.5103 cm-1
  3.      65.0408 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.795485        1.599873       -0.053315
C           2.129895        1.411541        0.282281
C           2.638569        0.103915        0.716603
O           0.197345        2.628781       -0.410737
O           0.070150        0.383698        0.017391
C          -1.330999        0.443728       -0.247838
C          -1.901334       -0.948080       -0.046874
C          -3.395585       -1.041850       -0.365209
C          -4.287643       -0.233924        0.576791
H           2.814789        2.235938        0.160931
H           2.085148       -0.362792        1.533627
H           3.693627        0.128282        0.977351
H          -1.795877        1.169099        0.420099
H          -1.502199        0.784745       -1.272052
H          -1.724516       -1.261097        0.986084
H          -1.351021       -1.643091       -0.686096
H          -3.691284       -2.092354       -0.322457
H          -3.565418       -0.719752       -1.396767
H          -4.097271        0.836885        0.498190
H          -5.342421       -0.396841        0.351760
H          -4.119293       -0.524877        1.616001
N           2.510555       -0.957032       -0.411319
H           1.519963       -0.913250       -0.668604
H           3.038312       -0.623045       -1.215186
```

```
C           2.905996       -2.338558       -0.045026
H           2.295215       -2.660614        0.792928
H           2.748007       -2.997868       -0.893109
H           3.954083       -2.339842        0.238829
```

---

### Compound_26_HEI_Conformation_35_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526205 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314044 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      37.8552 cm-1
  2.      57.5974 cm-1
  3.      66.6725 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.284773        1.375782       -0.137356
C          -2.367426        0.595147        0.247511
C          -2.198807       -0.625632        1.041612
O          -1.256965        2.439254       -0.779725
O          -0.057481        0.796335        0.270044
C           1.130833        1.556288        0.043900
C           2.325875        0.717403        0.453951
C           2.560938       -0.510856       -0.422686
C           3.797794       -1.302324       -0.007764
H          -3.344097        0.854465       -0.129436
H          -1.622057       -0.503280        1.959807
H          -3.144220       -1.106310        1.280619
H           1.195927        1.834486       -1.009583
H           1.088837        2.478852        0.627105
H           2.210896        0.412299        1.498114
H           3.210220        1.360034        0.413389
H           2.658238       -0.191840       -1.464391
H           1.687485       -1.165741       -0.385708
H           3.708830       -1.654861        1.021905
H           3.947244       -2.173485       -0.646801
H           4.696074       -0.684455       -0.068954
N          -1.360140       -1.712049        0.288283
H          -0.491382       -1.220592        0.061836
H          -1.126330       -2.474033        0.922095
```

```
C          -1.996165       -2.238430       -0.941266
H          -2.277597       -1.389883       -1.556874
H          -2.878848       -2.806167       -0.661670
H          -1.292288       -2.874117       -1.469396
```

---

### Compound_26_HEI_Conformation_36_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526229 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314402 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.6598 cm-1
  2.      49.9850 cm-1
  3.      57.9158 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.174774        1.402436        0.187551
C           2.164148        0.609998        0.755066
C           1.913555       -0.785090        1.133521
O           1.205042        2.596106       -0.157301
O          -0.011323        0.661291       -0.034726
C          -1.156875        1.373707       -0.501515
C          -2.275700        0.375964       -0.731212
C          -2.732547       -0.350928        0.531881
C          -3.879776       -1.322145        0.269313
H           3.161212        1.013164        0.835881
H           1.050468       -0.938239        1.783280
H           2.781808       -1.260671        1.583027
H          -1.451095        2.120173        0.241477
H          -0.911787        1.903473       -1.422735
H          -1.955234       -0.353619       -1.481358
H          -3.120836        0.917566       -1.166380
H          -3.039460        0.389255        1.277012
H          -1.886605       -0.889100        0.963744
H          -3.586580       -2.087326       -0.452744
H          -4.190987       -1.829333        1.183565
H          -4.750040       -0.802006       -0.136740
N           1.541343       -1.678669       -0.095763
H           1.224069       -2.592615        0.221886
H           0.735426       -1.194931       -0.502473
```

```
C           2.620659       -1.826521       -1.099024
H           3.432088       -2.397717       -0.657313
H           2.233642       -2.339465       -1.974074
H           2.965330       -0.831630       -1.362980
```

---

### Compound_26_HEI_Conformation_37_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524032 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.312249 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.6232 cm-1
  2.      36.2368 cm-1
  3.      47.3891 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.554177       -0.330080       -0.002273
C           1.715347       -1.090852        0.124224
C           2.845132       -0.607723        0.899166
O           0.320093        0.800563        0.465125
O          -0.427228       -0.976412       -0.761560
C          -1.701521       -0.339001       -0.858200
C          -2.625178       -0.743568        0.282396
C          -4.037550       -0.168532        0.151451
C          -4.106812        1.351709        0.296104
H           1.761583       -2.069365       -0.330140
H           2.573242        0.144973        1.636829
H           3.431051       -1.394945        1.370528
H          -1.566075        0.740059       -0.887861
H          -2.120606       -0.665884       -1.811892
H          -2.180726       -0.419927        1.226788
H          -2.676581       -1.834901        0.310395
H          -4.672900       -0.627657        0.912283
H          -4.459382       -0.463768       -0.814296
H          -3.556901        1.860485       -0.496255
H          -5.138941        1.702762        0.257211
H          -3.681540        1.670031        1.250330
N           3.940417        0.141215        0.022701
H           4.770270        0.318603        0.588166
H           4.216216       -0.504620       -0.714496
```

```
C           3.453063        1.405617       -0.581455
H           3.248572        2.110494        0.217955
H           4.209252        1.802197       -1.252190
H           2.537678        1.184322       -1.119263
```

---

### Compound_26_HEI_Conformation_38_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.524094 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.312187 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.6909 cm-1
  2.      37.4849 cm-1
  3.      52.3902 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.658386       -0.795841        0.261600
C           1.823316       -1.092918       -0.443076
C           3.128277       -0.745706        0.093364
O           0.547207       -0.201637        1.350786
O          -0.490648       -1.271164       -0.381016
C          -1.748751       -0.841385        0.140444
C          -2.139645        0.533694       -0.384775
C          -3.470006        1.042648        0.174843
C          -4.685180        0.222416       -0.257761
H           1.756690       -1.620972       -1.382683
H           3.129497       -0.614135        1.173615
H           3.927778       -1.424708       -0.198655
H          -2.461965       -1.600250       -0.179079
H          -1.716302       -0.831732        1.230162
H          -2.188531        0.496743       -1.477124
H          -1.344023        1.233648       -0.123198
H          -3.608106        2.078523       -0.143516
H          -3.414402        1.065645        1.267373
H          -4.751055        0.170913       -1.346848
H          -4.640818       -0.799958        0.119258
H          -5.610216        0.667524        0.111195
N           3.672906        0.652499       -0.430352
H           3.686559        0.599613       -1.447061
H           4.637964        0.778224       -0.126653
```

```
C           2.847446        1.809750       -0.004576
H           1.821629        1.608278       -0.293455
H           2.914918        1.899503        1.074766
H           3.214512        2.712107       -0.484175
```

---

### Compound_26_HEI_Conformation_39_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.525111 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313569 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.1521 cm-1
  2.      31.6456 cm-1
  3.      51.8536 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.409794        1.301237       -0.064354
C           1.687402        1.501314        0.439167
C           2.563675        0.377906        0.794475
O          -0.462426        2.127935       -0.378538
O           0.145054       -0.082651       -0.261583
C          -1.200154       -0.454493       -0.567429
C          -2.030408       -0.641472        0.693902
C          -3.462755       -1.102696        0.413880
C          -4.326182       -0.055796       -0.289828
H           2.061600        2.510506        0.511315
H           2.118083       -0.366486        1.456669
H           3.511105        0.702032        1.217736
H          -1.638304        0.297377       -1.219982
H          -1.127757       -1.395171       -1.115591
H          -2.048697        0.302430        1.244404
H          -1.526920       -1.373247        1.330421
H          -3.933055       -1.372759        1.362041
H          -3.437404       -2.019075       -0.183824
H          -3.942990        0.187145       -1.281388
H          -5.350734       -0.409985       -0.411412
H          -4.359332        0.870509        0.287670
N           2.933552       -0.473837       -0.451535
H           2.024048       -0.729224       -0.847359
H           3.384794        0.140101       -1.127012
```

```
C           3.759552       -1.676481       -0.184861
H           3.230200       -2.308053        0.522021
H           3.925009       -2.216155       -1.112392
H           4.708918       -1.362481        0.238681
```

---

### Compound_26_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529098 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317554 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      24.2528 cm-1
2.      40.4091 cm-1
3.      69.4164 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.587289        0.086376        0.059932
C           1.349809        1.197845       -0.228592
C           2.780487        1.162193        0.152764
O           1.030979       -0.991485        0.566877
O          -0.753463        0.176261       -0.259480
C          -1.531586       -1.019753       -0.161490
C          -2.967344       -0.679451       -0.510101
C          -3.634525        0.276788        0.476264
C          -5.084015        0.583485        0.110923
H           0.943536        2.046586       -0.753344
H           2.968071        1.122888        1.230824
H           3.355335        1.985778       -0.263527
H          -1.134516       -1.773407       -0.845861
H          -1.464999       -1.424854        0.850093
H          -3.531385       -1.616196       -0.547457
H          -3.001367       -0.254888       -1.517802
H          -3.061407        1.204801        0.520408
H          -3.592098       -0.160224        1.478546
H          -5.148805        1.047102       -0.875793
H          -5.684622       -0.328423        0.086804
H          -5.541516        1.265096        0.829342
N           3.402784       -0.139706       -0.349998
H           2.687989       -0.836363       -0.032073
H           3.385218       -0.132653       -1.367324
```

```
C           4.756601       -0.451728        0.158171
H           5.080804       -1.405857       -0.246882
H           5.444378        0.333088       -0.144284
H           4.715472       -0.507271        1.241916
```

---

### Compound_26_HEI_Conformation_40_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52619 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313572 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      28.2680 cm-1
2.      40.3874 cm-1
3.      61.9389 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.330400        1.675352        0.046968
C           1.485894        1.394849        0.761103
C           1.976767        0.018300        0.921701
O          -0.259350        2.753211       -0.136096
O          -0.174712        0.504569       -0.584833
C          -1.527379        0.530379       -1.042857
C          -2.518497        0.278124        0.085906
C          -2.245824       -0.990426        0.897584
C          -2.276696       -2.277204        0.075868
H           2.056962        2.214082        1.169228
H           1.239036       -0.692844        1.298339
H           2.868140       -0.040053        1.541361
H          -1.732951        1.487375       -1.519998
H          -1.586998       -0.252521       -1.797919
H          -3.518594        0.226407       -0.356401
H          -2.513913        1.142364        0.753223
H          -2.987385       -1.054412        1.697468
H          -1.274298       -0.896415        1.387422
H          -1.479371       -2.297496       -0.668158
H          -2.150863       -3.152647        0.714378
H          -3.226660       -2.383725       -0.452950
N           2.369411       -0.610163       -0.440256
H           1.528151       -0.480879       -1.011470
H           3.099519       -0.034474       -0.854894
```

```
C           2.770996       -2.036977       -0.396621
H           1.950719       -2.612381        0.021627
H           2.990603       -2.382205       -1.402411
H           3.650559       -2.135651        0.232477
```

---

### Compound_26_HEI_Conformation_41_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.5261 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.313512 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      35.1526 cm-1
2.      53.3067 cm-1
3.      59.2257 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.145103        1.538063        0.017373
C           1.455377        1.616361       -0.433008
C           2.479382        0.648606       -0.015286
O          -0.822666        2.278753       -0.218806
O          -0.040635        0.397024        0.849721
C          -1.344109        0.130005        1.372587
C          -1.838232       -1.223494        0.884210
C          -2.053961       -1.311692       -0.628349
C          -3.178681       -0.417013       -1.145094
H           1.707823        2.379914       -1.151770
H           2.580416        0.513199        1.063206
H           3.458787        0.867551       -0.433205
H          -1.266244        0.129934        2.462009
H          -2.011846        0.934270        1.073843
H          -2.777293       -1.445355        1.400957
H          -1.123509       -1.989635        1.197473
H          -2.268075       -2.351077       -0.888116
H          -1.123965       -1.056099       -1.142889
H          -2.955047        0.635753       -0.973652
H          -3.327024       -0.555021       -2.217133
H          -4.122028       -0.649155       -0.645496
N           2.127113       -0.785291       -0.492891
H           1.180341       -0.926210       -0.127635
H           2.052622       -0.768763       -1.508051
```

```
C           3.040805       -1.861424       -0.039319
H           3.065131       -1.858170        1.046094
H           4.034232       -1.667280       -0.432221
H           2.678197       -2.819518       -0.399177
```

---

### Compound_26_HEI_Conformation_42_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52486 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.312543 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.8636 cm-1
  2.      49.2491 cm-1
  3.      57.7067 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.139271        1.598489       -0.194232
C          -1.310029        1.372378       -0.904480
C          -1.969679        0.059501       -0.915048
O           0.552624        2.626624       -0.105103
O           0.241180        0.449771        0.552339
C           1.545224        0.455123        1.139332
C           2.642948        0.043838        0.165007
C           2.716927       -1.449777       -0.161218
C           1.504022       -2.013587       -0.899544
H          -1.782305        2.206932       -1.398905
H          -1.328499       -0.778558       -1.190406
H          -2.858207        0.041611       -1.541139
H           1.749441        1.448951        1.534056
H           1.489820       -0.247753        1.972288
H           3.596990        0.351732        0.602908
H           2.524421        0.624061       -0.753500
H           2.866686       -2.007709        0.768453
H           3.611847       -1.623201       -0.764752
H           1.297249       -1.440918       -1.806181
H           1.673633       -3.051896       -1.189337
H           0.609918       -1.977714       -0.279853
N          -2.449978       -0.346121        0.504750
H          -3.090749        0.372412        0.835461
H          -1.601538       -0.269184        1.074158
```

```
C          -3.052826       -1.696195        0.619512
H          -3.933819       -1.741687       -0.013720
H          -2.323194       -2.429614        0.289991
H          -3.326173       -1.884400        1.653367
```

---

### Compound_26_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.529259 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.31741 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.9845 cm-1
  2.      42.5057 cm-1
  3.      69.7151 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.643374       -0.962992        0.137334
C          -1.677357       -1.204112       -0.738211
C          -2.971040       -0.529654       -0.475291
O          -0.686664       -0.147697        1.112164
O           0.521964       -1.677390       -0.094279
C           1.723434       -1.175098        0.499016
C           2.327094       -0.034858       -0.305516
C           3.630416        0.477720        0.302615
C           4.252798        1.614235       -0.503895
H          -1.551844       -1.827509       -1.607859
H          -3.478606       -0.851185        0.440023
H          -3.672789       -0.613715       -1.301549
H           1.526477       -0.857829        1.522461
H           2.405395       -2.025669        0.524560
H           1.602503        0.781202       -0.363159
H           2.505530       -0.376055       -1.329177
H           4.343608       -0.348276        0.380145
H           3.442028        0.816057        1.325591
H           3.570753        2.464288       -0.571394
H           5.180135        1.965443       -0.049313
H           4.480812        1.291805       -1.521898
N          -2.718701        0.955298       -0.228049
H          -1.916571        0.910868        0.446415
H          -2.366769        1.369071       -1.088563
```

```
C          -3.861251        1.728101        0.306312
H          -4.687831        1.682434       -0.397388
H          -4.161185        1.292551        1.254713
H          -3.557459        2.760078        0.455472
```

---

### Compound_26_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.528897 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317329 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.2622 cm-1
  2.      35.0466 cm-1
  3.      66.9676 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.607136        0.605609       -0.002700
C          -1.685886        1.264349        0.546484
C          -2.889162        0.459771        0.859100
O          -0.585773       -0.626910       -0.308380
O           0.505642        1.389130       -0.261756
C           1.650341        0.746597       -0.828982
C           2.566335        0.158226        0.232283
C           3.822097       -0.468094       -0.369641
C           4.757800       -1.049717        0.686575
H          -1.687312        2.331758        0.693338
H          -2.748630       -0.290627        1.643813
H          -3.754395        1.065388        1.117120
H           1.332072       -0.026692       -1.527230
H           2.170383        1.527304       -1.386230
H           2.012856       -0.593932        0.798803
H           2.848167        0.946869        0.935884
H           4.356901        0.284633       -0.956511
H           3.531600       -1.254065       -1.072818
H           4.256354       -1.826385        1.267608
H           5.645707       -1.492618        0.233317
H           5.088525       -0.277110        1.383718
N          -3.262685       -0.385199       -0.358696
H          -2.333613       -0.796320       -0.608511
H          -3.527334        0.242110       -1.114916
```

```
C          -4.295606       -1.421336       -0.137896
H          -5.216557       -0.945950        0.187895
H          -4.464781       -1.963559       -1.063537
H          -3.942804       -2.104591        0.628879
```

---

### Compound_26_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526271 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314963 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      38.0638 cm-1
2.      48.9322 cm-1
3.      62.9676 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.178030       -1.585694       -0.013375
C           2.450081       -1.078677        0.217314
C           2.663719        0.317834        0.620305
O           0.818718       -2.731754       -0.331971
O           0.188667       -0.578804        0.125533
C          -1.172468       -0.974518       -0.038365
C          -2.043335        0.258259        0.102749
C          -3.528774       -0.060433       -0.052558
C          -4.413823        1.175191        0.084316
H           3.301266       -1.715853        0.035948
H           2.086604        0.645976        1.487031
H           3.712261        0.550316        0.789437
H          -1.309305       -1.436818       -1.017967
H          -1.433422       -1.721341        0.715327
H          -1.745743        0.995254       -0.648873
H          -1.864547        0.714630        1.080284
H          -3.819074       -0.803021        0.696047
H          -3.698563       -0.525720       -1.027663
H          -4.285320        1.641813        1.063079
H          -4.164043        1.920945       -0.673134
H          -5.469059        0.923992       -0.029791
N           2.188088        1.304770       -0.480550
H           2.704573        1.094850       -1.332271
H           1.216311        1.026226       -0.647327
```

```
C          2.280648       2.744775      -0.139222
H          1.894625       3.338006      -0.962591
H          1.692375       2.926099       0.755190
H          3.320904       2.995300       0.045651
```

---

### Compound_26_HEI_Conformation_7_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.526671 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.314997 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.2669 cm-1
2.      55.2547 cm-1
3.      60.3441 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -1.449873      -1.419683      -0.111353
C         -2.496876      -0.516749       0.023132
C         -2.282105       0.843390       0.532076
O         -1.459097      -2.601531      -0.495102
O         -0.208605      -0.827203       0.231128
C          0.940547      -1.675412       0.226300
C          2.158095      -0.840944       0.574274
C          2.518930       0.211707      -0.471604
C          3.780066       0.991529      -0.111462
H         -3.477404      -0.808696      -0.318767
H         -1.742214       0.906101       1.478776
H         -3.204229       1.413069       0.615607
H          0.802750      -2.479214       0.952316
H          1.054309      -2.136100      -0.757162
H          3.002471      -1.525188       0.699062
H          2.000254      -0.361162       1.544549
H          1.689150       0.911173      -0.594388
H          2.650996      -0.278371      -1.440498
H          3.658694       1.512434       0.840531
H          4.638687       0.323711      -0.015670
H          4.019224       1.736610      -0.871242
N         -1.367613       1.666291      -0.418458
H         -0.534841       1.078277      -0.515275
H         -1.813428       1.695589      -1.333158
```

```
C          -1.010497        3.027494        0.049129
H          -0.514495        2.942073        1.011170
H          -0.345095        3.495432       -0.669984
H          -1.919635        3.612100        0.152180
```

---

### Compound_26_HEI_Conformation_8_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52945 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317199 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.8707 cm-1
  2.      47.4942 cm-1
  3.      74.7006 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.441038       -0.975668        0.147155
C           1.211312       -0.633484        1.235050
C           2.600901       -0.185626        0.978121
O           0.803025       -0.867088       -1.067133
O          -0.821315       -1.470491        0.432992
C          -1.799501       -1.395553       -0.611420
C          -2.358628        0.008806       -0.782423
C          -3.054120        0.552734        0.463000
C          -3.590174        1.968121        0.268292
H           0.816233       -0.645522        2.237244
H           3.262394       -0.955252        0.567323
H           3.081011        0.244806        1.853440
H          -1.369396       -1.752059       -1.545997
H          -2.587032       -2.084646       -0.303982
H          -3.064147       -0.009822       -1.619363
H          -1.546207        0.678522       -1.075753
H          -2.352540        0.537293        1.299458
H          -3.874787       -0.117287        0.737019
H          -2.782175        2.660940        0.023305
H          -4.314928        2.005376       -0.547946
H          -4.083171        2.336955        1.168926
N           2.587105        0.878999       -0.115214
H           1.962065        0.425758       -0.825474
H           2.096810        1.697267        0.238938
```

```
C           3.904133        1.248217       -0.678272
H           3.766334        1.998153       -1.451606
H           4.536688        1.642124        0.112450
H           4.359660        0.359759       -1.105368
```

---

### Compound_26_HEI_Conformation_9_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -520.52891 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.317028 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.0396 cm-1
  2.      45.3353 cm-1
  3.      75.2908 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.447440       -0.223293        0.399145
C          -1.277332        0.570194        1.160946
C          -2.536259        1.039668        0.538018
O          -0.704074       -0.624785       -0.778641
O           0.725472       -0.627185        1.014898
C           1.644339       -1.408401        0.244216
C           2.575410       -0.549797       -0.598667
C           3.445445        0.402804        0.217617
C           4.366864        1.252706       -0.652749
H          -1.055689        0.803363        2.189305
H          -2.403378        1.726586       -0.304174
H          -3.219518        1.499084        1.248039
H           2.216852       -1.975167        0.980353
H           1.095048       -2.106106       -0.385455
H           1.979043        0.015885       -1.318386
H           3.214859       -1.221767       -1.180572
H           4.042566       -0.176777        0.928396
H           2.802202        1.052414        0.814795
H           5.040295        0.625762       -1.241274
H           3.790588        1.863248       -1.351284
H           4.979073        1.925023       -0.049882
N          -3.258322       -0.146913       -0.098723
H          -2.473810       -0.598011       -0.624743
H          -3.533739       -0.789130        0.640785
```

```
C          -4.404922        0.183578       -0.973316
H          -4.821446       -0.732628       -1.381396
H          -5.159252        0.708772       -0.393983
H          -4.053261        0.818839       -1.780773
```

---

### Compound_27_HEI_Conformation_10_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195783 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.93209 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      34.2899 cm-1
  2.      40.0692 cm-1
  3.      64.2024 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.641324       -1.263847       -0.380247
C          -1.822986       -0.965491        0.273103
C          -2.855580       -2.028442        0.535078
C          -2.088791        0.418568        0.712207
O          -0.187814       -2.356201       -0.771556
O           0.103767       -0.072743       -0.671332
C           1.483112       -0.197272       -0.997176
C           2.396842        0.232193        0.159320
C           3.846022        0.081905       -0.316459
H          -2.582217       -2.950182        0.022540
H          -2.967414       -2.274624        1.599091
H          -3.851778       -1.740189        0.179455
H          -1.297174        0.876308        1.307621
H          -3.027966        0.506758        1.254631
H           1.686948       -1.228978       -1.280738
H           1.664381        0.445479       -1.862109
H           4.067253       -0.953556       -0.582605
H           4.040177        0.705224       -1.191816
H           4.541022        0.382758        0.469198
C           2.153983       -0.663504        1.378789
H           1.120083       -0.590244        1.716800
H           2.358287       -1.708996        1.143029
H           2.802962       -0.367890        2.205171
C           2.123607        1.694213        0.528367
```

```
H           1.093657        1.825850        0.859338
H           2.782663        2.017240        1.336303
H           2.291613        2.351373       -0.327588
N          -2.207384        1.382737       -0.490181
H          -2.946164        1.038340       -1.099720
H          -1.320479        1.240882       -0.986763
C          -2.417301        2.812011       -0.154972
H          -3.353334        2.912267        0.386284
H          -1.593010        3.146083        0.467642
H          -2.450954        3.396480       -1.069452
```

---

### Compound_27_HEI_Conformation_11_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.193333 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.930252 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      32.8376 cm-1
2.      40.6102 cm-1
3.      50.1357 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.600337       -0.410868        0.870927
C          -1.690739       -0.948663        0.187315
C          -1.546990       -2.021964       -0.863971
C          -3.005584       -0.403464        0.470904
O          -0.595646        0.504914        1.719873
O           0.605660       -1.039530        0.530916
C           1.823168       -0.435142        0.951193
C           2.571260        0.228424       -0.214665
C           3.862222        0.831939        0.349373
H          -0.853704       -2.808435       -0.560503
H          -2.513440       -2.497666       -1.054125
H          -1.185420       -1.652880       -1.832752
H          -3.057778        0.121154        1.420731
H          -3.820791       -1.122389        0.385374
H           1.614211        0.297729        1.728659
H           2.443549       -1.229659        1.373812
H           3.644957        1.589514        1.104936
H           4.487355        0.064174        0.810151
```

```
H           4.443659        1.305040       -0.443739
C           1.707592        1.334091       -0.831309
H           0.780580        0.924048       -1.232436
H           1.448784        2.090496       -0.089107
H           2.240723        1.824599       -1.647814
C           2.912746       -0.815981       -1.283006
H           2.007769       -1.274852       -1.680660
H           3.454714       -0.356354       -2.111781
H           3.540475       -1.607404       -0.867701
N          -3.470729        0.722755       -0.576455
H          -4.435868        0.986145       -0.382788
H          -3.464755        0.291351       -1.498012
C          -2.598757        1.921725       -0.581256
H          -2.703861        2.427656        0.372947
H          -1.575222        1.584201       -0.704802
H          -2.888439        2.580598       -1.394532
```

---

### Compound_27_HEI_Conformation_12_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.193037 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.929443 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      34.2708 cm-1
2.      38.1104 cm-1
3.      56.8370 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.567501       -0.303865        0.036844
C           1.528306        0.685484        0.248405
C           1.408147        2.081329       -0.310324
C           2.713636        0.328627        1.006563
O           0.571394       -1.483901        0.446125
O          -0.504870        0.147389       -0.744263
C          -1.680822       -0.651986       -0.804271
C          -2.829603       -0.062070        0.027290
C          -4.044791       -0.979748       -0.147042
H           0.375392        2.431345       -0.305668
H           1.995749        2.783909        0.288961
H           1.763799        2.185404       -1.344706
```

```
H           2.588180       -0.575311        1.595645
H           3.114184        1.135317        1.621512
H          -1.979674       -0.691462       -1.854888
H          -1.450811       -1.661195       -0.466275
H          -4.341201       -1.046661       -1.195937
H          -3.829673       -1.989305        0.208791
H          -4.897416       -0.599079        0.417831
C          -3.169549        1.346098       -0.472710
H          -2.311243        2.010251       -0.373273
H          -3.463427        1.326379       -1.524481
H          -3.996851        1.769023        0.100445
C          -2.432894       -0.003076        1.506351
H          -1.552021        0.623029        1.649532
H          -3.246266        0.414669        2.102752
H          -2.205027       -0.998300        1.890375
N           3.982537       -0.022519        0.087334
H           4.797909       -0.172939        0.679646
H           4.180342        0.801736       -0.475727
C           3.763326       -1.191265       -0.797459
H           3.662170       -2.076877       -0.178624
H           2.843140       -1.019930       -1.346661
H           4.603251       -1.297451       -1.477369
```

---

### Compound_27_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195129 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.932213 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      20.4084 cm-1
  2.      43.4105 cm-1
  3.      67.0053 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.021097       -1.355392       -0.071553
C          -2.204264       -0.697565        0.222419
C          -3.532479       -1.390062        0.076906
C          -2.167066        0.712226        0.649134
O          -0.818808       -2.541714       -0.398695
O           0.098431       -0.474873       -0.010797
```

```
C           1.388538       -1.066851       -0.103687
C           2.468458        0.006797        0.049812
C           3.826284       -0.701775       -0.035586
H          -4.024196       -1.602296        1.035504
H          -4.246263       -0.801708       -0.511207
H          -3.403325       -2.345143       -0.431682
H          -1.474196        0.936359        1.461313
H          -3.150944        1.094605        0.912741
H           1.502949       -1.820736        0.679401
H           1.499122       -1.571722       -1.066051
H           3.947012       -1.207750       -0.995352
H           4.639178        0.018184        0.069125
H           3.932026       -1.446135        0.755712
C           2.337283        0.704027        1.408644
H           1.377108        1.210707        1.498632
H           2.417001       -0.017007        2.224650
H           3.127577        1.445890        1.535740
C           2.366014        1.038383       -1.079498
H           3.183727        1.758004       -1.014363
H           2.416940        0.555770       -2.057202
H           1.433114        1.598811       -1.027357
N          -1.654860        1.634420       -0.488424
H          -2.260741        1.505227       -1.295804
H          -0.748186        1.222935       -0.730624
C          -1.520831        3.070910       -0.145030
H          -2.500092        3.462534        0.113229
H          -0.850861        3.160616        0.704599
H          -1.114946        3.610434       -0.995454
```

---

### Compound_27_HEI_Conformation_1_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195129 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.932189 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      20.6290 cm-1
2.      43.4411 cm-1
3.      68.7833 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.020918       -1.355266       -0.071596
C          -2.204217       -0.697666        0.222440
C          -3.532130       -1.390775        0.077019
C          -2.167325        0.712113        0.649088
O          -0.818607       -2.541610       -0.398618
O           0.098508       -0.474644       -0.011108
C           1.388620       -1.066596       -0.104278
C           2.468588        0.006901        0.049855
C           3.826370       -0.701676       -0.036167
H          -4.022142       -1.606458        1.035737
H          -4.247232       -0.801007       -0.508039
H          -3.403214       -2.344190       -0.434852
H          -1.474435        0.936460        1.461230
H          -3.151277        1.094285        0.912811
H           1.502969       -1.820985        0.678355
H           1.499288       -1.570919       -1.066940
H           3.947046       -1.206871       -0.996365
H           4.639311        0.018167        0.069107
H           3.932109       -1.446699        0.754527
C           2.337608        0.703258        1.409145
H           1.377523        1.210076        1.499510
H           2.417263       -0.018320        2.224692
H           3.128050        1.444912        1.536671
C           2.366042        1.039219       -1.078776
H           3.184020        1.758550       -1.013525
H           2.416428        0.557195       -2.056812
H           1.433329        1.599910       -1.025890
N          -1.655426        1.634478       -0.488501
H          -2.261463        1.505367       -1.295779
H          -0.748800        1.223036       -0.730962
C          -1.521382        3.070922       -0.144906
H          -2.500647        3.462496        0.113514
H          -0.851312        3.160496        0.704695
H          -1.115576        3.610588       -0.995312
```

---

### Compound_27_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.198026 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.935257 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      22.1510 cm-1
2.      30.6646 cm-1
```

```
   3.      74.6709 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.699826       -0.030892       -0.287937
C          -1.587317        1.004986       -0.125219
C          -1.203543        2.433059        0.135639
C          -3.028741        0.665592       -0.303705
O          -1.021639       -1.259227       -0.473725
O           0.643819        0.292049       -0.230593
C           1.564766       -0.780709       -0.053792
C           2.981386       -0.217974        0.077104
C           3.930426       -1.408210        0.262193
H          -1.326307        3.084923       -0.740090
H          -1.809411        2.875839        0.934033
H          -0.159978        2.502948        0.437868
H          -3.317308        0.420663       -1.332111
H          -3.688161        1.456474        0.049763
H           1.305013       -1.347088        0.845117
H           1.512007       -1.464456       -0.903641
H           3.680102       -1.976373        1.160224
H           3.883838       -2.086404       -0.592050
H           4.960463       -1.062162        0.360256
C           3.074032        0.706990        1.296141
H           2.404705        1.559945        1.191249
H           2.804121        0.173862        2.210185
H           4.091794        1.083237        1.413937
C           3.364606        0.550729       -1.192795
H           2.703286        1.402033       -1.349514
H           4.388168        0.922582       -1.119796
H           3.302360       -0.094346       -2.071735
N          -3.352193       -0.595633        0.473775
H          -3.265359       -0.395414        1.467140
H          -2.524777       -1.203556        0.198302
C          -4.654828       -1.225204        0.171435
H          -5.457077       -0.522883        0.382172
H          -4.672725       -1.497557       -0.879769
H          -4.772603       -2.115612        0.782181
```

---

### Compound_27_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.194858 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.931645 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      33.5813 cm-1
2.      42.7942 cm-1
3.      53.3580 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.761165       -1.303439       -0.248347
C           2.069473       -0.883128       -0.088349
C           3.116135       -1.817175        0.457288
C           2.462134        0.483260       -0.485135
O           0.249157       -2.420508       -0.048743
O          -0.086068       -0.227087       -0.684238
C          -1.458759       -0.511729       -0.934042
C          -2.401168        0.140059        0.088035
C          -2.084891       -0.364779        1.499381
H           3.806769       -2.200629       -0.306112
H           3.737425       -1.336387        1.220795
H           2.644281       -2.683784        0.919927
H           2.189723        0.773096       -1.501854
H           3.526255        0.662884       -0.347179
H          -1.688648       -0.129603       -1.932288
H          -1.598587       -1.590906       -0.927134
H          -1.062194       -0.117303        1.785265
H          -2.758967        0.090909        2.226948
H          -2.194721       -1.447766        1.560313
C          -3.831041       -0.258575       -0.296985
H          -4.077694        0.082409       -1.304592
H          -3.957907       -1.342256       -0.265927
H          -4.551454        0.184812        0.392096
C          -2.273455        1.666770        0.041908
H          -2.994815        2.132213        0.715783
H          -1.282129        1.998048        0.351650
H          -2.456167        2.046738       -0.964963
N           1.741719        1.547267        0.371367
H           1.959493        1.367173        1.349296
H           0.751771        1.312216        0.239077
C           2.017086        2.959671        0.012968
H           1.433839        3.615140        0.652670
H           3.077040        3.154553        0.145673
H           1.739865        3.112725       -1.025487
```

---

### Compound_27_HEI_Conformation_3_DFT_reopt

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.194858 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.931644 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      33.5829 cm-1
  2.      42.7928 cm-1
  3.      53.3543 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.761165       -1.303439       -0.248347
C           2.069473       -0.883128       -0.088349
C           3.116135       -1.817175        0.457288
C           2.462134        0.483260       -0.485135
O           0.249157       -2.420508       -0.048743
O          -0.086068       -0.227087       -0.684238
C          -1.458759       -0.511729       -0.934042
C          -2.401168        0.140059        0.088035
C          -2.084891       -0.364779        1.499381
H           3.806769       -2.200629       -0.306112
H           3.737425       -1.336387        1.220795
H           2.644281       -2.683784        0.919927
H           2.189723        0.773096       -1.501854
H           3.526255        0.662884       -0.347179
H          -1.688648       -0.129603       -1.932288
H          -1.598587       -1.590906       -0.927134
H          -1.062194       -0.117303        1.785265
H          -2.758967        0.090909        2.226948
H          -2.194721       -1.447766        1.560313
C          -3.831041       -0.258575       -0.296985
H          -4.077694        0.082409       -1.304592
H          -3.957907       -1.342256       -0.265927
H          -4.551454        0.184812        0.392096
C          -2.273455        1.666770        0.041908
H          -2.994815        2.132213        0.715783
H          -1.282129        1.998048        0.351650
H          -2.456167        2.046738       -0.964963
N           1.741719        1.547267        0.371367
H           1.959493        1.367173        1.349296
H           0.751771        1.312216        0.239077
C           2.017086        2.959671        0.012968
H           1.433839        3.615140        0.652670
H           3.077040        3.154553        0.145673
H           1.739865        3.112725       -1.025487
```

---

### Compound_27_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195782 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.932091 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      34.2838 cm-1
2.      40.0986 cm-1
3.      64.1377 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.641119       -1.263805       -0.380379
C          -1.822764       -0.965637        0.273100
C          -2.855234       -2.028663        0.535260
C          -2.088741        0.418383        0.712231
O          -0.187444       -2.356058       -0.771776
O           0.103752       -0.072570       -0.671517
C           1.483131       -0.196889       -0.997299
C           2.396782        0.232318        0.159359
C           3.845991        0.082288       -0.316408
H          -2.581515       -2.950616        0.023301
H          -2.967374       -2.274297        1.599365
H          -3.851383       -1.740815        0.179151
H          -1.297148        0.876263        1.307567
H          -3.027886        0.506418        1.254728
H           1.687074       -1.228496       -1.281150
H           1.664379        0.446129       -1.862037
H           4.067320       -0.953081       -0.582833
H           4.040127        0.705867       -1.191583
H           4.540936        0.382979        0.469361
C           2.153958       -0.663740        1.378572
H           1.120035       -0.590679        1.716555
H           2.358382       -1.709146        1.142537
H           2.802871       -0.368280        2.205062
C           2.123410        1.694207        0.528818
H           1.093438        1.825649        0.859800
H           2.782412        2.017059        1.336868
H           2.291380        2.351631       -0.326941
N          -2.207621        1.382556       -0.490175
```

```
H          -2.946410        1.038028       -1.099629
H          -1.320750        1.240861       -0.986854
C          -2.417768        2.811791       -0.154956
H          -3.353707        2.911849        0.386500
H          -1.593415        3.146069        0.467464
H          -2.451759        3.396228       -1.069445
```

---

### Compound_27_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.195782 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.93209 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      34.2890 cm-1
2.      40.1008 cm-1
3.      64.1550 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.641139       -1.263817       -0.380373
C          -1.822763       -0.965617        0.273120
C          -2.855263       -2.028613        0.535264
C          -2.088707        0.418413        0.712236
O          -0.187497       -2.356086       -0.771768
O           0.103761       -0.072605       -0.671532
C           1.483144       -0.196957       -0.997288
C           2.396781        0.232311        0.159357
C           3.845997        0.082237       -0.316376
H          -2.967550       -2.274103        1.599387
H          -3.851370       -1.740835        0.178970
H          -2.581445       -2.950626        0.023466
H          -1.297088        0.876274        1.307556
H          -3.027837        0.506468        1.254761
H           1.687080       -1.228583       -1.281075
H           1.664414        0.446008       -1.862062
H           4.040157        0.705769       -1.191581
H           4.540931        0.382962        0.469390
H           4.067319       -0.953150       -0.582744
C           2.153928       -0.663668        1.378621
H           1.119992       -0.590592        1.716568
H           2.358367       -1.709088        1.142661
```

```
H           2.802814       -0.368149        2.205112
C           2.123422        1.694226        0.528721
H           2.782413        2.017118        1.336765
H           2.291419        2.351596       -0.327076
H           1.093444        1.825701        0.859674
N          -2.207592        1.382553       -0.490167
H          -2.946380        1.038016       -1.099617
H          -1.320719        1.240855       -0.986845
C          -2.417749        2.811795       -0.154977
H          -3.353703        2.911858        0.386453
H          -1.593415        3.146090        0.467458
H          -2.451719        3.396213       -1.069479
```

---

### Compound_27_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.198756 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.934999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
  1.      29.1739 cm-1
  2.      40.3098 cm-1
  3.      56.0616 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.539242        0.313633       -0.739605
C          -1.440349        1.136677       -0.112793
C          -1.127356        2.497459        0.439006
C          -2.837258        0.621400       -0.017512
O          -0.790376       -0.872137       -1.157280
O           0.738029        0.825644       -0.927489
C           1.818843       -0.093512       -1.081951
C           2.584296       -0.339318        0.226677
C           3.749575       -1.282219       -0.094748
H          -1.531998        3.318822       -0.167440
H          -1.539046        2.628693        1.445899
H          -0.051285        2.649382        0.501794
H          -3.369066        0.561227       -0.973155
H          -3.447724        1.202664        0.671286
H           1.443731       -1.033860       -1.482296
H           2.492184        0.356205       -1.814455
```

```
H           4.418957       -0.843616       -0.837653
H           4.334548       -1.487671        0.803257
H           3.388170       -2.235465       -0.485688
C           1.665438       -0.990223        1.267067
H           0.817702       -0.345674        1.499761
H           1.274861       -1.941487        0.903366
H           2.213270       -1.177753        2.192550
C           3.126962        0.985380        0.773289
H           3.792865        1.462456        0.050937
H           2.313998        1.677136        0.992500
H           3.691010        0.819194        1.692996
N          -2.811985       -0.812944        0.476238
H          -2.473675       -0.819611        1.435320
H          -2.038499       -1.207619       -0.136718
C          -4.079742       -1.563452        0.355122
H          -4.361095       -1.601527       -0.693213
H          -3.936021       -2.571741        0.732409
H          -4.857214       -1.062149        0.925717
```

---

### Compound_27_HEI_Conformation_6_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.198756 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.934999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      29.1749 cm-1
2.      40.3100 cm-1
3.      56.0622 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.539242        0.313633       -0.739605
C          -1.440349        1.136677       -0.112793
C          -1.127356        2.497459        0.439006
C          -2.837258        0.621400       -0.017512
O          -0.790376       -0.872137       -1.157280
O           0.738029        0.825644       -0.927489
C           1.818843       -0.093512       -1.081951
C           2.584296       -0.339318        0.226677
C           3.749575       -1.282219       -0.094748
H          -1.531998        3.318822       -0.167440
```

```
H          -1.539046        2.628693        1.445899
H          -0.051285        2.649382        0.501794
H          -3.369066        0.561227       -0.973155
H          -3.447724        1.202664        0.671286
H           1.443731       -1.033860       -1.482296
H           2.492184        0.356205       -1.814455
H           4.418957       -0.843616       -0.837653
H           4.334548       -1.487671        0.803257
H           3.388170       -2.235465       -0.485688
C           1.665438       -0.990223        1.267067
H           0.817702       -0.345674        1.499761
H           1.274861       -1.941487        0.903366
H           2.213270       -1.177753        2.192550
C           3.126962        0.985380        0.773289
H           3.792865        1.462456        0.050937
H           2.313998        1.677136        0.992500
H           3.691010        0.819194        1.692996
N          -2.811985       -0.812944        0.476238
H          -2.473675       -0.819611        1.435320
H          -2.038499       -1.207619       -0.136718
C          -4.079742       -1.563452        0.355122
H          -4.361095       -1.601527       -0.693213
H          -3.936021       -2.571741        0.732409
H          -4.857214       -1.062149        0.925717
```

---

### Compound_27_HEI_Conformation_7_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.197716 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.934401 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      24.8380 cm-1
2.      41.9281 cm-1
3.      54.1400 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.554646        0.091866       -0.299343
C           1.482189        1.040598        0.052879
C           1.268954        2.526135       -0.001306
C           2.781689        0.523998        0.573793
```

```
O           0.749333       -1.174215       -0.264562
O          -0.661248        0.568440       -0.774695
C          -1.728677       -0.354220       -0.973416
C          -2.791928       -0.266532        0.131332
C          -2.176258       -0.625144        1.487957
H           1.255809        2.992809        0.992545
H           2.057377        3.035964       -0.567729
H           0.319712        2.763404       -0.477113
H           2.722818        0.057687        1.563520
H           3.549275        1.295249        0.612186
H          -2.183966       -0.096560       -1.932761
H          -1.330576       -1.365200       -1.033546
H          -1.761959       -1.633950        1.474825
H          -1.373014        0.064826        1.747587
H          -2.932291       -0.575533        2.273846
C          -3.898899       -1.268193       -0.216284
H          -4.346807       -1.040273       -1.185770
H          -3.509582       -2.287509       -0.254546
H          -4.691292       -1.239167        0.533428
C          -3.375116        1.149635        0.186043
H          -3.829775        1.421704       -0.769015
H          -4.144408        1.219231        0.957408
H          -2.599138        1.880605        0.412208
N           3.284793       -0.589157       -0.323129
H           3.514030       -0.194922       -1.232227
H           2.394549       -1.155209       -0.438768
C           4.409562       -1.388613        0.206616
H           5.262230       -0.740269        0.390480
H           4.095997       -1.855303        1.135849
H           4.675819       -2.154457       -0.516070
```

---

### Compound_27_HEI_Conformation_7_DFT_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.197716 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.934393 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      24.8952 cm-1
2.      42.1113 cm-1
3.      54.1770 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.554538        0.092020       -0.299529
C           1.482098        1.040696        0.052786
C           1.269021        2.526248       -0.001538
C           2.781519        0.524035        0.573852
O           0.749119       -1.174081       -0.264623
O          -0.661245        0.568633       -0.775133
C          -1.728743       -0.353974       -0.973736
C          -2.791694       -0.266570        0.131327
C          -2.175619       -0.625338        1.487728
H           1.256417        2.993046        0.992260
H           2.057214        3.035933       -0.568417
H           0.319566        2.763543       -0.476906
H           2.722530        0.057878        1.563645
H           3.549177        1.295220        0.612203
H          -2.184290       -0.096064       -1.932888
H          -1.330670       -1.364945       -1.034230
H          -1.760955       -1.633989        1.474220
H          -1.372559        0.064835        1.747387
H          -2.931512       -0.576201        2.273781
C          -3.898656       -1.268291       -0.216145
H          -4.346810       -1.040305       -1.185503
H          -3.509256       -2.287568       -0.254609
H          -4.690879       -1.239419        0.533753
C          -3.375010        1.149528        0.186420
H          -3.830041        1.421666       -0.768442
H          -4.144031        1.218955        0.958071
H          -2.599023        1.880551        0.412393
N           3.284578       -0.589282       -0.322871
H           3.514047       -0.195180       -1.231968
H           2.394227       -1.155189       -0.438605
C           4.409102       -1.388893        0.207155
H           5.261825       -0.740674        0.391210
H           4.095241       -1.855518        1.136322
H           4.675415       -2.154791       -0.515453
```

---

### Compound_27_HEI_Conformation_8_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.192823 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.930577 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      26.4242 cm-1
2.      32.8017 cm-1
3.      56.7006 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.707276       -0.222849       -0.614461
C          -1.703088        0.735206       -0.407848
C          -1.438623        2.065053        0.253093
C          -3.059030        0.399933       -0.795612
O          -0.818220       -1.356297       -1.130252
O           0.548933        0.197473       -0.180358
C           1.645859       -0.669887       -0.439033
C           2.920838       -0.073830        0.161908
C           4.071802       -1.034195       -0.161224
H          -0.454198        2.457106       -0.003414
H          -2.179637        2.804837       -0.066340
H          -1.482291        2.039264        1.350959
H          -3.113262       -0.437087       -1.485749
H          -3.646455        1.241997       -1.163780
H           1.454659       -1.654922       -0.007179
H           1.770768       -0.801852       -1.517608
H           4.198954       -1.148147       -1.239568
H           5.009888       -0.657483        0.249343
H           3.891601       -2.023066        0.265001
C           2.775555        0.059127        1.682282
H           1.957838        0.731334        1.939525
H           2.573821       -0.911832        2.139642
H           3.693449        0.453931        2.121610
C           3.208595        1.298651       -0.457600
H           3.311885        1.221811       -1.542089
H           2.403555        2.000381       -0.242976
H           4.137603        1.710913       -0.059494
N          -3.974583       -0.096399        0.433558
H          -4.932598       -0.223361        0.110542
H          -3.994074        0.661575        1.112138
C          -3.476235       -1.332888        1.080489
H          -3.577994       -2.154173        0.378472
H          -2.428112       -1.180108        1.317800
H          -4.049400       -1.531663        1.981186
```

---

### Compound_27_HEI_Conformation_9_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -599.193206 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -598.930476 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 96)

```
1.      26.0451 cm-1
2.      42.1267 cm-1
3.      63.5103 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.756169       -1.194360       -0.092006
C           2.062639       -0.733019       -0.258358
C           3.200047       -1.493210        0.374446
C           2.364951        0.482756       -0.989788
O           0.394934       -2.231176        0.498003
O          -0.215650       -0.370367       -0.688656
C          -1.566343       -0.817271       -0.706435
C          -2.504467        0.157610        0.017035
C          -3.929442       -0.392662       -0.111588
H           4.110142       -1.409194       -0.228627
H           3.465191       -1.148678        1.384156
H           2.959188       -2.552615        0.465640
H           1.552888        0.837459       -1.614743
H           3.293586        0.439745       -1.561473
H          -1.870596       -0.898946       -1.754785
H          -1.625058       -1.802251       -0.247286
H          -4.224731       -0.481129       -1.159117
H          -4.013256       -1.379350        0.348160
H          -4.642212        0.269833        0.382268
C          -2.428866        1.542999       -0.633712
H          -1.417895        1.944312       -0.578234
H          -2.714872        1.494568       -1.686572
H          -3.101220        2.242140       -0.133028
C          -2.120964        0.254131        1.497113
H          -1.096005        0.604233        1.612036
H          -2.778140        0.952295        2.018756
H          -2.201998       -0.717986        1.986019
N           2.660396        1.747989       -0.037495
H           2.943106        2.539163       -0.613452
H           3.463442        1.506023        0.538710
C           1.517543        2.117918        0.827872
H           0.710667        2.478388        0.198970
H           1.199796        1.222250        1.351937
H           1.823338        2.886811        1.530889
```

### Compound_28_HEI_Conformation_1_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.866482 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.628906 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      21.0112 cm-1
2.      34.1885 cm-1
3.      80.9604 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.778711        0.220836       -0.273836
C          -1.644720        1.258641       -0.004039
C          -3.090707        1.014003       -0.212345
O          -1.128658       -0.949724       -0.624932
O           0.564076        0.500915       -0.118584
C           1.470484       -0.597999       -0.192449
C           2.892725       -0.105619        0.080671
C           3.822141       -1.321573       -0.017648
H          -3.382655        0.840764       -1.253287
H          -3.720503        1.802779        0.191737
H           1.190322       -1.357563        0.541855
H           1.417752       -1.057794       -1.181884
H           3.776910       -1.773491       -1.010383
H           4.855599       -1.026707        0.170162
H           3.552166       -2.084619        0.714983
C           2.984254        0.497154        1.487298
H           2.326821        1.359992        1.587317
H           2.699067       -0.236738        2.243984
H           4.005236        0.819585        1.698937
C           3.302064        0.938598       -0.964555
H           4.329656        1.265212       -0.795582
H           3.241863        0.523843       -1.972943
H           2.654568        1.813466       -0.918637
N          -3.482894       -0.292893        0.475763
H          -2.718093       -0.927520        0.144132
H          -3.363670       -0.175764        1.479408
C          -4.827536       -0.820705        0.156343
H          -4.981173       -1.755739        0.687050
H          -5.579728       -0.096224        0.455933
```

```
H          -4.887430       -0.991829       -0.914349
H          -1.299756        2.199064        0.392713
```

---

### Compound_28_HEI_Conformation_2_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.864222 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.62619 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      28.5176 cm-1
  2.      53.9326 cm-1
  3.      76.5918 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.962118        1.740170       -0.043616
C           2.265821        1.346117        0.228314
C           2.584360       -0.026731        0.639604
O           0.512348        2.854861       -0.358004
O           0.065871        0.644663        0.039678
C          -1.325241        0.932818       -0.061560
C          -2.134038       -0.362324        0.038283
C          -1.795721       -1.298387       -1.127815
H           1.992664       -0.409401        1.473165
H           3.638931       -0.166849        0.863361
H          -1.615666        1.614611        0.741890
H          -1.532641        1.431140       -1.010588
H          -2.425270       -2.189062       -1.096397
H          -1.956812       -0.803636       -2.087283
H          -0.758502       -1.630542       -1.089188
C          -3.616479        0.024720       -0.038377
H          -3.892014        0.690256        0.781687
H          -3.843423        0.532159       -0.977912
H          -4.245712       -0.864185        0.023948
C          -1.855575       -1.066057        1.371493
H          -2.089074       -0.411043        2.213212
H          -2.467954       -1.964671        1.463586
H          -0.809225       -1.358788        1.451351
N           2.256135       -1.046563       -0.486591
H           2.813089       -0.803442       -1.303226
H           1.281638       -0.835709       -0.719710
```

```
C           2.422141       -2.475965       -0.128946
H           2.126790       -3.097381       -0.968874
H           3.463371       -2.656134        0.120907
H           1.793524       -2.690606        0.729887
H           3.063269        2.056871        0.078653
```

---

### Compound_28_HEI_Conformation_3_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.866952 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.628385 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      30.3416 cm-1
2.      48.0268 cm-1
3.      64.8019 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.610915       -0.773532       -0.446302
C          -1.520216       -1.364969        0.401621
C          -2.928811       -0.914443        0.314681
O          -0.877519        0.164350       -1.259454
O           0.683551       -1.264519       -0.369343
C           1.741852       -0.479410       -0.920445
C           2.516804        0.305621        0.147655
C           3.651196        1.050523       -0.565522
H          -3.429124       -1.146985       -0.630718
H          -3.547088       -1.284131        1.128950
H           2.415751       -1.183737       -1.412388
H           1.337557        0.200316       -1.668067
H           4.242450        1.623186        0.150865
H           4.322181        0.354820       -1.073552
H           3.258442        1.746401       -1.309536
C           3.103433       -0.657845        1.184898
H           3.772797       -1.379985        0.712488
H           3.674744       -0.110703        1.937062
H           2.313314       -1.210209        1.692906
C           1.593594        1.313689        0.841620
H           1.175301        2.020109        0.123609
H           0.765590        0.809254        1.340116
H           2.146969        1.878996        1.593875
```

```
N          -2.967168        0.612388        0.358692
H          -2.226834        0.849560       -0.343012
H          -2.626644        0.914569        1.268578
C          -4.266860        1.242807        0.038939
H          -4.161168        2.322900        0.079898
H          -4.561680        0.939863       -0.961399
H          -5.012844        0.915176        0.757637
H          -1.218247       -2.079408        1.149360
```

---

### Compound_28_HEI_Conformation_4_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.866329 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.627934 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      29.4820 cm-1
  2.      44.1770 cm-1
  3.      58.8810 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.648079        0.322803       -0.233227
C          -1.567155        1.311635        0.040944
C          -2.895658        0.892256        0.545460
O          -0.871204       -0.923284       -0.136058
O           0.584941        0.767284       -0.684636
C           1.608419       -0.192445       -0.944943
C           2.725685       -0.154214        0.106995
C           3.368064        1.236923        0.140790
H          -2.883973        0.426741        1.536406
H          -3.622890        1.700490        0.557565
H           1.169274       -1.186815       -0.990401
H           2.024831        0.055979       -1.924251
H           2.635524        1.997712        0.409611
H           4.176657        1.268867        0.873380
H           3.785944        1.497489       -0.834021
C           3.773478       -1.196537       -0.300202
H           3.342379       -2.199297       -0.324944
H           4.182432       -0.979321       -1.289131
H           4.601820       -1.204314        0.410036
C           2.162677       -0.498800        1.489835
```

```
H           2.956936       -0.482610        2.238439
H           1.399562        0.219013        1.791326
H           1.710771       -1.491407        1.492370
N          -3.448200       -0.216422       -0.347956
H          -2.614265       -0.845256       -0.423266
H          -3.618919        0.170617       -1.273396
C          -4.641479       -0.927801        0.160926
H          -4.393922       -1.380352        1.116531
H          -5.455595       -0.219857        0.288808
H          -4.928286       -1.699315       -0.547543
H          -1.356494        2.351666       -0.145737
```

---

### Compound_28_HEI_Conformation_5_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.863946 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.626182 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      22.2912 cm-1
  2.      32.8674 cm-1
  3.      51.7519 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.670028        1.673621       -0.046361
C          -2.043050        1.534061        0.095467
C          -2.757539        0.334440       -0.360963
O           0.064206        2.630676        0.244043
O          -0.086166        0.490147       -0.589477
C           1.311635        0.493093       -0.871709
C           2.099499       -0.470142        0.026419
C           1.933160       -0.078539        1.498095
H          -2.563857        0.042182       -1.394703
H          -3.832241        0.404607       -0.212134
H           1.427856        0.192855       -1.916315
H           1.690617        1.505846       -0.750324
H           2.500133       -0.756008        2.138988
H           2.288969        0.937095        1.674022
H           0.887096       -0.123685        1.802178
C           3.575347       -0.358073       -0.375093
H           3.946814        0.657347       -0.225687
```

```
H           4.187638       -1.032470        0.225455
H           3.719327       -0.620509       -1.425149
C           1.626915       -1.912570       -0.186519
H           0.586207       -2.044132        0.109823
H           1.716784       -2.204246       -1.234591
H           2.225012       -2.603716        0.409792
N          -2.305710       -0.923592        0.425821
H          -2.477667       -0.752241        1.414501
H          -1.289373       -0.926266        0.299660
C          -2.903991       -2.208771       -0.009462
H          -2.498254       -3.018185        0.589944
H          -3.981131       -2.154518        0.116307
H          -2.660855       -2.365093       -1.056019
H          -2.589112        2.316975        0.597732
```

---

### Compound_28_HEI_Conformation_6_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.862437 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.625492 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      24.3845 cm-1
  2.      33.0826 cm-1
  3.      61.3083 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.826915       -0.224717       -0.497059
C           1.774013       -1.037735        0.126236
C           3.163976       -1.016217       -0.292554
O           1.004531        0.603528       -1.411133
O          -0.458138       -0.417429        0.005630
C          -1.499051        0.364716       -0.569623
C          -2.818024        0.073314        0.149451
C          -3.184801       -1.408455        0.008263
H           3.302650       -0.638435       -1.303673
H           3.682154       -1.966537       -0.175518
H          -1.256894        1.426899       -0.486061
H          -1.595815        0.131604       -1.633491
H          -4.143453       -1.612468        0.488614
H          -3.268466       -1.689776       -1.043607
```

```
H          -2.430158       -2.044058        0.469941
C          -3.899806        0.934226       -0.514202
H          -4.002254        0.691014       -1.573568
H          -4.866349        0.767011       -0.036463
H          -3.663701        1.996950       -0.431747
C          -2.705170        0.445492        1.632382
H          -1.937086       -0.147755        2.127274
H          -2.447844        1.500279        1.749804
H          -3.653614        0.271402        2.143727
N           4.072994       -0.036832        0.573612
H           3.976904       -0.330555        1.543558
H           5.052371       -0.164612        0.320733
C           3.693817        1.391814        0.446514
H           3.887110        1.707595       -0.573610
H           2.633927        1.472574        0.662018
H           4.276522        1.985803        1.144113
H           1.460681       -1.722516        0.900236
```

---

### Compound_28_HEI_Conformation_8_DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -559.863004 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.624923 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      32.2093 cm-1
2.      41.1536 cm-1
3.      60.4886 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.696226       -0.907417       -0.345629
C           1.741562       -1.078175        0.559036
C           3.118540       -0.828106        0.166442
O           0.757048       -0.514502       -1.525311
O          -0.542219       -1.262399        0.205671
C          -1.722941       -0.914063       -0.510421
C          -2.455545        0.283404        0.113295
C          -2.856539       -0.040010        1.556656
H           3.280192       -0.892393       -0.907798
H           3.850892       -1.441281        0.689013
H          -1.467273       -0.699219       -1.546577
```

```
H          -2.375321       -1.790359       -0.483744
H          -3.388488        0.800767        2.005979
H          -3.512882       -0.912204        1.593015
H          -1.977917       -0.251717        2.165711
C          -3.711816        0.542642       -0.725822
H          -4.365630       -0.331936       -0.737425
H          -4.280210        1.379773       -0.317094
H          -3.452285        0.784681       -1.758348
C          -1.554891        1.523261        0.092886
H          -0.647741        1.356122        0.673945
H          -1.260841        1.777667       -0.926026
H          -2.077220        2.380391        0.522018
N           3.609478        0.642746        0.508529
H           3.453069        0.778207        1.505431
H           4.614451        0.714055        0.352326
C           2.897324        1.698283       -0.253741
H           3.145490        1.587402       -1.304289
H           1.832893        1.549846       -0.110224
H           3.204049        2.675353        0.107203
H           1.528278       -1.428079        1.558086
```

---

### Methylamine DFT

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp Energy | -95.912855 |
| B3LYP-D3(BJ)/def2tzvpp Free Energy (Quasiharmonic) | -95.869911 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 15)

```
1.     295.4482 cm-1
2.     865.4259 cm-1
3.     977.0619 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp Molecular Geometry in Cartesian Coordinates

```
C          -0.708078        0.000002        0.016983
H          -1.120014        0.878928       -0.479475
H          -1.064335        0.000412        1.053581
H          -1.119919       -0.879383       -0.478737
N           0.752282        0.000002       -0.126346
H           1.143375        0.807994        0.343572
H           1.143391       -0.807976        0.343582
```

### Methylamine AM1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -95.910176 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -95.867368 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 15)

```
1.     246.9909 cm-1
2.     924.0309 cm-1
3.    1011.6568 cm-1
```

### AM1 Molecular Geometry in Cartesian Coordinates

```
C          -0.691612        0.000000        0.015054
H          -1.104625        0.910488       -0.494793
H          -1.061575        0.000001        1.078525
H          -1.104625       -0.910489       -0.494792
N           0.734981        0.000000       -0.112863
H           1.137814        0.814476        0.305388
H           1.137814       -0.814476        0.305388
```

### Methylamine

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -95.871051 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -95.827609 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 15)

```
1.     312.5625 cm-1
2.     891.8549 cm-1
3.     982.9709 cm-1
```

#### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.710922        0.000002        0.017190
H          -1.120657        0.883959       -0.482478
H          -1.065460        0.000489        1.059700
H          -1.120544       -0.884501       -0.481600
N           0.754152        0.000003       -0.127394
H           1.146557        0.812325        0.346495
H           1.146572       -0.812307        0.346503
```

### Compound_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -730.183772 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -730.106871 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      56.6008 cm-1
2.     129.4268 cm-1
3.     137.8776 cm-1
```

#### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.346843       -1.645979        0.000034
H           0.414306       -2.447267        0.000151
C           0.201863       -0.281993        0.000007
C          -0.508190        0.874215        0.000009
C          -2.017416        0.865513        0.000045
H          -2.411237        0.340503        0.876299
H          -2.396501        1.890811        0.000269
H          -2.411249        0.340906       -0.876451
C           0.121587        2.233585       -0.000032
H          -0.226389        2.792567        0.878818
H           1.210809        2.213756       -0.000118
H          -0.226527        2.792571       -0.878825
O          -1.540324       -1.924198       -0.000068
Cl          1.980199       -0.282489        0.000001
```

---

### Compound_12_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -730.187311 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -730.109926 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      74.1939 cm-1
  2.     107.7305 cm-1
  3.     160.7270 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.083232        1.275611        0.000020
H          -0.580407        2.253950       -0.000012
C          -0.189598        0.118141        0.000007
C           1.167827        0.168069       -0.000050
C           1.958122        1.447810       -0.000136
H           2.614172        1.459233        0.879495
H           2.614132        1.459135       -0.879799
H           1.365783        2.361358       -0.000177
C           1.994628       -1.088738       -0.000044
H           1.767994       -1.702334        0.879922
H           1.768057       -1.702287       -0.880061
H           3.062033       -0.856581       -0.000004
```

```
O          -2.308081        1.220459        0.000068
Cl         -1.013741       -1.444794        0.000077
```

---

### Compound_12_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -826.064133 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -825.917702 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      52.8728 cm-1
  2.     152.3641 cm-1
  3.     174.2292 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.423326        1.754909        0.084481
H          -1.244579        2.438655       -0.179132
C          -0.668977        0.411470       -0.000136
C           0.342163       -0.647037        0.395943
C           0.434489       -0.779213        1.926313
H           1.192263       -1.515332        2.224005
H           0.668365        0.185194        2.387057
H          -0.534490       -1.114531        2.306417
C           0.130516       -2.019086       -0.244415
H          -0.022554       -1.952334       -1.324268
H           0.990637       -2.666978       -0.043402
H          -0.753963       -2.489092        0.191228
O           0.722334        2.279419        0.424509
C           1.993109       -0.109840       -1.513855
H           1.142409        0.322825       -2.040618
H           2.886848        0.489786       -1.691869
H           2.162417       -1.135289       -1.840575
N           1.699480       -0.077198       -0.055746
H           1.630032        0.951070        0.245680
H           2.452893       -0.534191        0.463482
Cl         -2.299597       -0.137763       -0.446697
```

---

### Compound_12_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -826.056104 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -825.910062 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      44.5751 cm-1
2.      99.1030 cm-1
3.     114.1605 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.757274        1.104646       -0.228392
H           1.361946        2.136579       -0.217753
C           0.805463        0.148412        0.070181
C          -0.644508        0.347321        0.353727
C          -1.052101        1.823286        0.421166
H          -2.121953        1.915471        0.624818
H          -0.518010        2.305909        1.242636
H          -0.825400        2.361569       -0.503208
C          -1.153524       -0.397544        1.595147
H          -1.009896       -1.477844        1.514393
H          -0.579708       -0.044265        2.456119
H          -2.210825       -0.192819        1.786073
O           2.993033        0.946899       -0.489730
C          -2.896764       -0.346009       -0.906571
H          -3.308349        0.655451       -0.795494
H          -3.207653       -0.770805       -1.861939
H          -3.226129       -0.987990       -0.091965
N          -1.404061       -0.270740       -0.897012
H          -1.077192        0.256961       -1.711808
H          -1.019743       -1.214065       -1.017886
Cl          1.337179       -1.570873        0.055375
```

---

### Compound_12_HEI_3_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -826.056104 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -825.910065 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      44.4599 cm-1
  2.      99.1666 cm-1
  3.     114.0973 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.756835        1.105052       -0.228255
H           1.361112        2.136820       -0.217359
C           0.805412        0.148320        0.070019
C          -0.644569        0.346771        0.353858
C          -1.052265        1.822680        0.422637
H          -2.122025        1.914637        0.626914
H          -0.517742        2.304748        1.244157
H          -0.826099        2.361586       -0.501510
C          -1.153346       -0.399217        1.594706
H          -1.010562       -1.479517        1.512559
H          -0.578737       -0.047410        2.455753
H          -2.210381       -0.193955        1.786537
O           2.992727        0.947919       -0.489548
C          -2.897115       -0.345165       -0.906640
H          -3.308423        0.656326       -0.794781
H          -3.208305       -0.769210       -1.862250
H          -3.226480       -0.987620       -0.092405
N          -1.404354       -0.270246       -0.897317
H          -1.077557        0.258020       -1.711805
H          -1.020288       -1.213596       -1.018975
Cl          1.337908       -1.570771        0.054872
```

---

### Compound_12_HEI_4_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -826.054389 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -825.908305 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      30.4263 cm-1
  2.     105.9285 cm-1
  3.     142.4314 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.528021        1.092511        0.447399
H          -1.085977        2.067163        0.726365
C          -0.622153        0.218568       -0.130519
C           0.828593        0.465278       -0.345515
C           1.181847        1.952170       -0.523896
H           2.263532        2.074497       -0.646852
H           0.692332        2.326482       -1.425795
H           0.863333        2.569926        0.319139
C           1.460833       -0.336962       -1.487836
H           1.342798       -1.414193       -1.365374
H           0.969455       -0.053665       -2.422513
H           2.527287       -0.103650       -1.577434
O          -2.765727        0.921599        0.683769
C           1.413028       -1.317640        1.518408
H           1.708011       -2.053662        0.772737
H           0.354078       -1.413981        1.749448
H           2.013688       -1.437651        2.420844
N           1.648203        0.051746        0.974942
H           2.650366        0.180866        0.800844
H           1.396313        0.731838        1.697416
Cl         -1.265387       -1.391325       -0.600696
```

---

### Compound_19_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -231.267756 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -231.20477 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.     129.8537 cm-1
  2.     200.5661 cm-1
  3.     212.9987 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.392002        0.332949        0.000003
O           2.475807       -0.248610       -0.000025
```

```
C           0.094301       -0.330204       -0.000013
C          -1.043640        0.392818        0.000021
H           0.083708       -1.418834       -0.000054
H           1.361605        1.440886        0.000044
C          -2.426351       -0.167311        0.000009
H          -2.980230        0.188565        0.878941
H          -2.980243        0.188632       -0.878887
H          -2.426857       -1.261115       -0.000033
H          -0.962303        1.481236        0.000061
```

---

### Compound_19_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -231.263535 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -231.200889 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.     138.3491 cm-1
2.     200.2738 cm-1
3.     204.2758 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.511636        0.421527       -0.000004
O          -2.039707       -0.688916       -0.000004
C          -0.066214        0.679690       -0.000001
C           0.848508       -0.309764        0.000002
H           0.487690       -1.338482        0.000002
H           0.239495        1.724519       -0.000001
H          -2.151785        1.324528       -0.000005
C           2.327423       -0.115274        0.000005
H           2.774652       -0.599687        0.878545
H           2.774655       -0.599685       -0.878535
H           2.604466        0.943062        0.000006
```

---

### Compound_19_HEI_3

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -327.142055 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -327.011837 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      81.8989 cm-1
2.     138.0733 cm-1
3.     194.2173 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.042497        0.196461       -0.063740
O           1.946274       -1.087328        0.163587
C           0.999505        1.086122       -0.032252
C          -0.383221        0.626579        0.331101
H          -0.458650        0.352720        1.393797
H           1.155557        2.133117       -0.273321
H           3.041044        0.586248       -0.325975
C          -1.484995        1.618277       -0.019228
H          -2.476155        1.262079        0.277190
H          -1.295648        2.557565        0.510209
H          -1.490209        1.833368       -1.094352
N          -0.604198       -0.712314       -0.377615
H          -0.670504       -0.541079       -1.384868
H           0.333136       -1.199603       -0.209465
C          -1.745932       -1.539343        0.089330
H          -1.626824       -1.720400        1.158491
H          -2.685637       -1.019822       -0.098955
H          -1.734042       -2.487952       -0.449407
```

---

### Compound_19_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -327.142055 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -327.011837 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      81.8989 cm-1
2.     138.0729 cm-1
3.     194.2172 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.042498        0.196461       -0.063741
O           1.946274       -1.087327        0.163588
C           0.999505        1.086122       -0.032252
C          -0.383221        0.626579        0.331100
H          -0.458649        0.352719        1.393797
H           1.155557        2.133116       -0.273323
H           3.041044        0.586248       -0.325976
C          -1.484995        1.618277       -0.019227
H          -2.476155        1.262079        0.277191
H          -1.295647        2.557565        0.510210
H          -1.490209        1.833368       -1.094351
N          -0.604198       -0.712315       -0.377616
H           0.333135       -1.199603       -0.209466
H          -0.670505       -0.541079       -1.384869
C          -1.745932       -1.539343        0.089330
H          -1.734041       -2.487953       -0.449405
H          -1.626826       -1.720397        1.158492
H          -2.685637       -1.019823       -0.098958
```

---

### Compound_19_HEI_4_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -327.142055 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -327.011837 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      81.8988 cm-1
2.     138.0730 cm-1
3.     194.2172 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.042497        0.196461       -0.063740
O           1.946274       -1.087328        0.163588
C           0.999505        1.086122       -0.032252
C          -0.383221        0.626579        0.331100
H          -0.458650        0.352720        1.393797
H           1.155557        2.133116       -0.273322
H           3.041044        0.586248       -0.325975
C          -1.484995        1.618277       -0.019228
H          -2.476155        1.262079        0.277190
H          -1.295647        2.557565        0.510209
H          -1.490209        1.833368       -1.094351
N          -0.604198       -0.712314       -0.377615
H           0.333136       -1.199603       -0.209465
H          -0.670505       -0.541079       -1.384868
C          -1.745932       -1.539343        0.089330
H          -1.734042       -2.487952       -0.449406
H          -1.626825       -1.720399        1.158491
H          -2.685637       -1.019823       -0.098956
```

---

### Compound_26_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.465363 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.318854 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      40.4830 cm-1
2.      57.9629 cm-1
3.      71.9282 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.801905       -0.425651       -0.093557
C          -2.699041        0.753242       -0.075806
C          -2.302367        2.002942        0.193210
O          -2.193148       -1.555774       -0.363230
O          -0.528338       -0.137147        0.210803
C           0.422344       -1.235791        0.205802
C           1.789363       -0.669219        0.544235
C           2.332217        0.313917       -0.499242
C           3.726269        0.836726       -0.140192
```

```
H          -3.734608        0.522475       -0.308575
H          -1.267399        2.235740        0.424205
H          -3.011016        2.826083        0.186958
H           0.407697       -1.698198       -0.786411
H           0.094185       -1.976905        0.940384
H           1.745237       -0.186732        1.530138
H           2.476738       -1.520858        0.641919
H           1.637091        1.156680       -0.601050
H           2.364992       -0.184525       -1.478530
H           3.712945        1.362820        0.822877
H           4.447975        0.013750       -0.060378
H           4.096763        1.536036       -0.898824
```

---

### Compound_26_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.465317 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.318509 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      39.1597 cm-1
  2.      59.2487 cm-1
  3.      77.5532 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.430580       -0.266783        0.042118
C          -2.425088        0.681804       -0.515651
C          -3.495441        1.067117        0.187883
O          -1.485297       -0.782795        1.149926
O          -0.443857       -0.496772       -0.844516
C           0.636049       -1.384626       -0.441057
C           1.705801       -0.645792        0.352558
C           2.371077        0.500459       -0.417330
C           3.462225        1.197153        0.401216
H          -2.236746        1.047323       -1.520769
H          -3.670072        0.694281        1.193546
H          -4.220047        1.762618       -0.224292
H           1.031898       -1.760524       -1.387237
H           0.210547       -2.211914        0.130896
H           1.269579       -0.269968        1.286559
H           2.464024       -1.389266        0.636956
```

```
H           1.608529        1.232873       -0.711221
H           2.801968        0.107218       -1.349071
H           4.254238        0.492112        0.684242
H           3.925612        2.012893       -0.166002
H           3.049443        1.622897        1.324692
```

---

### Compound_26_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.465764 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.319313 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      36.9083 cm-1
  2.      61.4744 cm-1
  3.      69.6670 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.630222        0.241482        0.021456
C          -2.443771       -0.979917       -0.192924
C          -3.760667       -0.994312        0.040713
O          -2.052690        1.318120        0.421573
O          -0.340599        0.017578       -0.284586
C           0.582044        1.129008       -0.125170
C           1.973857        0.636990       -0.479137
C           2.516727       -0.435917        0.471779
C           3.935707       -0.879392        0.103589
H          -1.914374       -1.858777       -0.549031
H          -4.277744       -0.107223        0.396475
H          -4.350991       -1.891507       -0.118184
H           0.524265        1.476767        0.911242
H           0.255709        1.939968       -0.782854
H           1.971477        0.260827       -1.511240
H           2.638342        1.511927       -0.465563
H           2.506833       -0.043038        1.498449
H           1.845354       -1.303696        0.463120
H           3.965716       -1.300910       -0.909259
H           4.633810       -0.033058        0.133159
H           4.305861       -1.644516        0.795962
```

### Compound_26_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.464602 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.317493 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      32.5865 cm-1
2.      57.5115 cm-1
3.      64.2977 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.375497        0.243728       -0.151652
C           2.328041       -0.892648       -0.188955
C           3.543230       -0.805206        0.363023
O           1.591845        1.334967        0.357170
O           0.222933       -0.082348       -0.765642
C          -0.839913        0.910626       -0.788211
C          -1.660550        0.886210        0.496659
C          -2.265436       -0.481140        0.848921
C          -3.239730       -1.026041       -0.201485
H           1.985975       -1.796595       -0.684158
H           3.871036        0.105668        0.856686
H           4.236640       -1.640072        0.334305
H          -1.436623        0.632984       -1.658255
H          -0.395882        1.894342       -0.955100
H          -1.034651        1.237753        1.325059
H          -2.464618        1.625541        0.371961
H          -2.787197       -0.382772        1.809646
H          -1.456233       -1.204807        1.011169
H          -2.737253       -1.240091       -1.152066
H          -3.701791       -1.958929        0.141904
H          -4.044456       -0.307142       -0.403177
```

---

### Compound_26_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.46532 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.318466 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      51.9272 cm-1
2.      58.4751 cm-1
3.      74.0540 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.576830        0.035751        0.190959
C          -2.857878        0.199461       -0.538066
C          -3.873754       -0.653821       -0.367627
O          -1.325897       -0.850091        0.996211
O          -0.708802        1.008565       -0.148216
C           0.610324        0.979890        0.461017
C           1.560708        0.079743       -0.316987
C           2.974419        0.101755        0.277605
C           3.948710       -0.789680       -0.498709
H          -2.925930        1.044707       -1.216516
H          -3.791171       -1.496382        0.313628
H          -4.809400       -0.529921       -0.904176
H           0.509943        0.656846        1.500021
H           0.938045        2.021290        0.435116
H           1.172959       -0.946360       -0.312792
H           1.591497        0.412844       -1.362804
H           2.933290       -0.225017        1.325879
H           3.349778        1.134531        0.287618
H           4.031793       -0.464688       -1.543407
H           4.951400       -0.760543       -0.056646
H           3.611192       -1.833696       -0.499036
```

---

### Compound_26_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.46567 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.319438 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      38.5933 cm-1
2.      62.2757 cm-1
3.      85.2550 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.775531        0.200762       -0.000001
C           2.861600       -0.809010        0.000001
C           4.150150       -0.450255       -0.000000
O           1.930942        1.414419       -0.000003
O           0.568183       -0.392714        0.000001
C          -0.595333        0.475907       -0.000000
C          -1.832342       -0.403919        0.000001
C          -3.120466        0.428781        0.000000
C          -4.379558       -0.443551        0.000002
H           2.555791       -1.851087        0.000002
H           4.441509        0.596660       -0.000002
H           4.941638       -1.193373        0.000001
H          -0.549376        1.114524        0.887751
H          -0.549377        1.114521       -0.887754
H          -1.811634       -1.055794        0.883324
H          -1.811634       -1.055797       -0.883319
H          -3.129585        1.086463       -0.880178
H          -3.129584        1.086466        0.880176
H          -5.287341        0.170816        0.000001
H          -4.410449       -1.089669       -0.886274
H          -4.410449       -1.089666        0.886280
```

---

### Compound_26_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.465096 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.318257 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      33.7832 cm-1
2.      46.1998 cm-1
3.      79.8544 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.451772        0.272348        0.076534
C           2.389660       -0.773215       -0.399503
C           3.658620       -0.818670        0.020799
O           1.721722        1.163069        0.871116
O           0.239434        0.119565       -0.483708
C          -0.790714        1.072344       -0.107130
C          -2.081434        0.662201       -0.795915
C          -2.606503       -0.729353       -0.409782
C          -2.937213       -0.881933        1.079263
H           1.992010       -1.497021       -1.104776
H           4.042409       -0.087098        0.726780
H           4.341324       -1.586319       -0.330330
H          -0.466841        2.069010       -0.421370
H          -0.878887        1.068959        0.982462
H          -2.832638        1.423258       -0.542955
H          -1.934428        0.713887       -1.882374
H          -1.870896       -1.488784       -0.703452
H          -3.508882       -0.927435       -1.002485
H          -2.042935       -0.794318        1.707419
H          -3.651303       -0.114731        1.405614
H          -3.383308       -1.862805        1.280605
```

---

### Compound_26_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.465136 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.318185 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      46.2951 cm-1
  2.      53.4541 cm-1
  3.      89.2964 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           -1.354195        0.233142        0.175618
C           -2.437371       -0.291710       -0.691533
C           -3.420473       -1.053180       -0.198845
```

```
O          -1.255349        0.039511        1.379015
O          -0.483969        0.962615       -0.549123
C           0.675550        1.540571        0.113312
C           1.937872        0.784059       -0.276142
C           1.984611       -0.665333        0.219956
C           3.287700       -1.370995       -0.167721
H          -2.387700       -0.027994       -1.743813
H          -3.456277       -1.310088        0.856389
H          -4.210244       -1.436341       -0.837697
H           0.507729        1.524536        1.191774
H           0.709844        2.574742       -0.236664
H           2.048759        0.809600       -1.368781
H           2.787876        1.343902        0.139090
H           1.133434       -1.222706       -0.192219
H           1.865923       -0.677743        1.311787
H           3.413691       -1.393573       -1.257691
H           4.157485       -0.854553        0.257828
H           3.301862       -2.406114        0.192985
```

---

### Compound_26_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.464843 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.31807 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      38.8337 cm-1
2.      47.6526 cm-1
3.      74.1240 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.503324       -0.471404       -0.250961
C           2.569953        0.541446       -0.428651
C           2.665376        1.674415        0.277512
O           1.418528       -1.473282       -0.951532
O           0.652855       -0.183723        0.747702
C          -0.465947       -1.087084        0.968002
C          -1.638314       -0.762071        0.052067
C          -2.192966        0.655395        0.232905
C          -3.389168        0.935232       -0.681816
H           3.286083        0.294415       -1.207089
```

```
H           1.947815        1.925807        1.052408
H           3.469472        2.380698        0.091984
H          -0.725464       -0.928207        2.017145
H          -0.118684       -2.113158        0.829932
H          -1.337638       -0.919267       -0.991480
H          -2.426561       -1.497962        0.265815
H          -1.398421        1.385341        0.032649
H          -2.488923        0.796004        1.282293
H          -3.110262        0.827176       -1.737749
H          -4.211460        0.236603       -0.481200
H          -3.770572        1.953016       -0.538426
```

---

### Compound_26_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -424.464371 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -424.317247 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      41.9716 cm-1
  2.      57.5535 cm-1
  3.      64.5755 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.472852        0.085069       -0.161561
C          -2.847449       -0.419136        0.074383
C          -3.856554        0.410503        0.361692
O          -1.132339        1.259549       -0.131914
O          -0.630740       -0.933221       -0.423107
C           0.767547       -0.610820       -0.655187
C           1.535591       -0.542393        0.659610
C           3.047322       -0.356619        0.453675
C           3.432418        0.982131       -0.188374
H          -2.989600       -1.493460        0.004040
H          -3.698712        1.483438        0.430380
H          -4.861263        0.037107        0.534239
H           0.817354        0.324978       -1.214134
H           1.130229       -1.428609       -1.282163
H           1.140244        0.281726        1.266547
H           1.352749       -1.471942        1.213234
H           3.435961       -1.184629       -0.155909
```

```
H           3.536596       -0.440046        1.432320
H           4.521969        1.095252       -0.230200
H           3.053834        1.069793       -1.213348
H           3.029135        1.823358        0.389728
```

---

### Compound_26_HEI_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329857 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116391 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      35.3066 cm-1
  2.      53.7661 cm-1
  3.      67.4743 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.444711       -1.426464        0.102470
C          -2.408998       -0.498744        0.489767
C          -2.059931        0.912763        0.742721
O          -1.552352       -2.657318       -0.119879
O          -0.182894       -0.807719       -0.083303
C           0.948944       -1.649487       -0.333766
C           2.152306       -0.753478       -0.591495
C           2.537650        0.135099        0.596751
C           3.768889        1.000017        0.310596
H          -3.446124       -0.810930        0.534402
H          -1.231302        1.070440        1.442734
H          -2.915571        1.509092        1.065955
H           1.120874       -2.295684        0.537353
H           0.745818       -2.293179       -1.195852
H           1.949478       -0.127465       -1.472474
H           3.000164       -1.401503       -0.855766
H           2.728322       -0.501105        1.473254
H           1.688645        0.778232        0.858962
H           3.591900        1.664271       -0.545193
H           4.026497        1.626779        1.172696
H           4.642369        0.378784        0.074027
N          -1.533108        1.603120       -0.548688
H          -2.263946        1.538118       -1.262572
H          -0.764953        0.990236       -0.857237
```

```
C          -1.062221        3.006791       -0.392032
H          -1.896513        3.620149       -0.049420
H          -0.693549        3.372867       -1.351135
H          -0.259947        3.020376        0.346464
```

---

### Compound_26_HEI_11_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330049 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.11707 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.8251 cm-1
  2.      38.5111 cm-1
  3.      73.8736 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.650940       -0.527737        0.209026
C           1.676667       -1.308770       -0.296671
C           3.068632       -0.878099       -0.011969
O           0.808683        0.568926        0.846797
O          -0.635548       -0.989431       -0.033291
C          -1.717335       -0.101092        0.283295
C          -3.009201       -0.766693       -0.171449
C          -4.266407        0.030056        0.210097
C          -4.361554        1.410605       -0.451909
H           1.484390       -2.165026       -0.931391
H           3.343800       -0.872850        1.052016
H           3.818580       -1.450349       -0.561728
H          -1.739687        0.088815        1.363688
H          -1.559364        0.858287       -0.220606
H          -3.062801       -1.766675        0.278879
H          -2.977631       -0.908588       -1.260860
H          -4.306084        0.143689        1.302897
H          -5.147262       -0.562654       -0.068784
H          -5.317847        1.892577       -0.216553
H          -3.563069        2.081545       -0.114805
H          -4.287843        1.326876       -1.544073
N           3.235771        0.595126       -0.413958
H           3.076820        0.670979       -1.421873
H           2.413015        1.037804        0.054257
```

```
C           4.514350        1.245813       -0.025462
H           5.341514        0.714738       -0.499029
H           4.612389        1.197889        1.059732
H           4.499047        2.286607       -0.351860
```

---

### Compound_26_HEI_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32922 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115782 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      33.0243 cm-1
2.      48.6155 cm-1
3.      65.0307 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.777337       -1.618820       -0.231981
C          -2.043994       -1.143799       -0.561278
C          -2.601184        0.075334        0.055931
O          -0.174886       -2.642076       -0.636084
O          -0.121483       -0.752648        0.689194
C           1.207456       -1.102611        1.105276
C           2.278745       -0.532576        0.179685
C           2.312246        0.998453        0.125185
C           3.426507        1.533333       -0.779556
H          -2.606201       -1.656506       -1.333281
H          -2.585814        0.095674        1.151918
H          -3.613478        0.297939       -0.287623
H           1.309058       -0.683566        2.112579
H           1.289751       -2.190733        1.163086
H           2.131817       -0.940523       -0.828625
H           3.253247       -0.902631        0.531762
H           2.439018        1.394936        1.142793
H           1.346596        1.376546       -0.235442
H           3.302826        1.173193       -1.808866
H           3.430041        2.629479       -0.805458
H           4.411671        1.201948       -0.427212
N          -1.749677        1.323950       -0.308901
H          -1.730192        1.404699       -1.329152
H          -0.797197        1.061107       -0.018672
```

```
C          -2.164315        2.607723        0.321733
H          -3.180254        2.842058        0.001583
H          -1.479153        3.398189        0.013043
H          -2.131780        2.486104        1.405017
```

---

### Compound_26_HEI_13

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329448 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116175 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      20.3377 cm-1
  2.      43.6098 cm-1
  3.      66.6064 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.472814        1.582968       -0.260939
C          -1.490585        1.102598       -1.078605
C          -1.923318       -0.307799       -1.027082
O           0.053591        2.721206       -0.213842
O          -0.050137        0.593748        0.672524
C           1.235792        0.765106        1.286093
C           2.366313        0.279983        0.382880
C           2.274551       -1.206497        0.023154
C           3.419175       -1.668167       -0.883850
H          -2.014076        1.798282       -1.724851
H          -1.117124       -1.044452       -1.120998
H          -2.701661       -0.537879       -1.757709
H           1.372062        1.816920        1.551646
H           1.192229        0.169741        2.204297
H           3.318357        0.478013        0.897312
H           2.372896        0.885023       -0.534123
H           1.313182       -1.398494       -0.469929
H           2.273584       -1.801647        0.948111
H           4.392938       -1.511964       -0.401844
H           3.332636       -2.733990       -1.127173
H           3.422185       -1.108175       -1.827913
N          -2.533681       -0.662936        0.357637
H          -3.318936       -0.029010        0.529740
H          -1.795266       -0.401600        1.026106
```

```
C          -2.945010       -2.082295        0.540453
H          -3.715296       -2.319620       -0.194352
H          -2.072002       -2.716984        0.385233
H          -3.332208       -2.218619        1.550911
```

---

### Compound_26_HEI_14

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330202 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.11637 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.4641 cm-1
  2.      40.5375 cm-1
  3.      58.0008 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.574140       -0.840949        0.251563
C           1.616319       -1.325787       -0.517330
C           2.971398       -0.771305       -0.266595
O           0.670266        0.101516        1.110068
O          -0.660907       -1.449896        0.046417
C          -1.827138       -0.712541        0.449318
C          -2.184401        0.377934       -0.558564
C          -3.408169        1.209957       -0.145197
C          -4.718742        0.414269       -0.092787
H           1.453835       -2.041885       -1.313329
H           3.374667       -0.969455        0.736273
H           3.709775       -1.086798       -1.006525
H          -2.615837       -1.466082        0.517219
H          -1.666930       -0.280939        1.442238
H          -2.364917       -0.085584       -1.538730
H          -1.316911        1.040082       -0.670386
H          -3.520990        2.038955       -0.856142
H          -3.218243        1.670350        0.835122
H          -5.568050        1.071058        0.129776
H          -4.916809       -0.075724       -1.055032
H          -4.694332       -0.364399        0.678326
N           2.905202        0.761621       -0.312288
H           2.097131        0.958784        0.321703
H           2.615888        1.041444       -1.253223
```

```
C          4.133699        1.487090        0.104410
H          3.950059        2.561093        0.052490
H          4.952238        1.212788       -0.562946
H          4.375499        1.199994        1.128391
```

---

### Compound_26_HEI_15

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32971 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116196 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      30.4851 cm-1
2.      38.7921 cm-1
3.      51.0730 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -0.565653        0.503665       -0.042284
C         -1.630503        1.344646        0.232865
C         -2.917530        0.715357        0.621838
O         -0.616011       -0.772798       -0.024205
O          0.618601        1.136556       -0.408638
C          1.776034        0.312984       -0.617185
C          2.514672        0.033834        0.690355
C          3.734769       -0.883434        0.515444
C          4.851554       -0.285813       -0.350243
H         -1.561811        2.417075        0.097392
H         -2.888592        0.143905        1.560100
H         -3.746251        1.424595        0.672549
H          1.480633       -0.624603       -1.097902
H          2.399770        0.883786       -1.310436
H          1.808328       -0.429383        1.389722
H          2.829600        0.988980        1.134158
H          3.408522       -1.840781        0.083973
H          4.138517       -1.117350        1.509281
H          5.726991       -0.945673       -0.371693
H          4.528965       -0.133993       -1.386801
H          5.174034        0.686623        0.044265
N         -3.296409       -0.353776       -0.414259
H         -3.429532        0.108447       -1.317479
H         -2.411973       -0.904652       -0.485230
```

```
C          -4.461827       -1.213775       -0.078972
H          -5.346851       -0.585025        0.030793
H          -4.252844       -1.730837        0.858272
H          -4.612453       -1.939532       -0.879314
```

---

### Compound_26_HEI_16

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32749 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114841 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.2081 cm-1
  2.      44.5611 cm-1
  3.      76.9054 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.802711       -0.267384        0.427006
C          -1.812862       -1.079933       -0.097526
C          -3.197989       -0.937672        0.338446
O          -0.907754        0.659883        1.269654
O           0.462401       -0.581158       -0.083524
C           1.566389        0.187103        0.407841
C           2.825493       -0.284387       -0.305150
C           4.072368        0.479848        0.155463
C           5.345938        0.017356       -0.559310
H          -1.556699       -1.853094       -0.814891
H          -3.303440       -0.461732        1.316848
H          -3.773103       -1.867494        0.313368
H           1.390377        1.253632        0.221436
H           1.660194        0.052239        1.492889
H           2.694793       -0.158605       -1.388997
H           2.963170       -1.359376       -0.123631
H           4.195703        0.355409        1.240604
H           3.925216        1.555276       -0.017896
H           6.223322        0.576461       -0.213213
H           5.533704       -1.048577       -0.377923
H           5.262248        0.161174       -1.644068
N          -4.061974        0.008962       -0.606453
H          -5.049701       -0.041168       -0.335973
H          -3.997204       -0.376616       -1.552538
```

```
C          -3.609298        1.427929       -0.618653
H          -4.182698        1.983224       -1.361997
H          -3.765420        1.845806        0.375761
H          -2.547783        1.433742       -0.862355
```

---

### Compound_26_HEI_17

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.331221 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.117342 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      36.6134 cm-1
  2.      37.8686 cm-1
  3.      88.1403 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.549854       -1.156019       -0.028557
C           1.503959       -0.841799       -0.977699
C           2.818551       -0.345159       -0.499384
O           0.688342       -0.999891        1.232577
O          -0.644060       -1.672805       -0.526264
C          -1.817273       -1.588984        0.301227
C          -2.689550       -0.397877       -0.087218
C          -2.036480        0.966497        0.160674
C          -2.944184        2.135023       -0.235116
H           1.272073       -0.846999       -2.035457
H           3.408121       -1.076535        0.070344
H           3.443518        0.054825       -1.300751
H          -2.360094       -2.526335        0.141113
H          -1.514030       -1.531035        1.349897
H          -3.626057       -0.467247        0.486675
H          -2.964742       -0.486878       -1.148078
H          -1.097619        1.025444       -0.403768
H          -1.765342        1.050343        1.221946
H          -3.881852        2.117852        0.335395
H          -2.457105        3.100179       -0.050827
H          -3.203010        2.088593       -1.300896
N           2.612424        0.787857        0.526704
H           3.474273        0.961036        1.050135
H           1.913856        0.355881        1.174878
```

```
C           2.087178        2.059164       -0.036378
H           1.841298        2.737325        0.781809
H           2.848590        2.502386       -0.680240
H           1.194566        1.822665       -0.614900
```

---

### Compound_26_HEI_18

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330171 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116617 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      24.9375 cm-1
  2.      43.0810 cm-1
  3.      78.5166 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.476106        0.172867        0.184248
C          -1.348580       -0.406435        1.087812
C          -2.439745       -1.256876        0.550258
O          -0.552292        0.057330       -1.086120
O           0.513969        0.974529        0.745641
C           1.519859        1.536860       -0.111617
C           2.864899        0.848367        0.102122
C           2.886518       -0.625180       -0.317630
C           4.246355       -1.286845       -0.072908
H          -1.313964       -0.162663        2.142483
H          -2.104595       -2.182945        0.062593
H          -3.192141       -1.513674        1.299174
H           1.194916        1.451746       -1.151538
H           1.589161        2.598017        0.153654
H           3.146773        0.934440        1.161491
H           3.621852        1.405785       -0.469839
H           2.625010       -0.700636       -1.382093
H           2.108111       -1.170199        0.231811
H           4.515600       -1.250980        0.990701
H           4.241293       -2.339196       -0.381481
H           5.040366       -0.776763       -0.633660
N          -3.168695       -0.526428       -0.596018
H          -2.365442       -0.223811       -1.192624
H          -3.740554       -1.182354       -1.133839
```

```
C          -3.981847        0.646720       -0.181728
H          -3.344269        1.299759        0.414067
H          -4.335509        1.167844       -1.072316
H          -4.827274        0.298889        0.414033
```

---

### Compound_26_HEI_19

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327521 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114637 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      22.4523 cm-1
  2.      41.9221 cm-1
  3.      69.7012 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.731550       -0.928996        0.195300
C          -1.927080       -0.990199       -0.525251
C          -3.177333       -0.502053        0.048659
O          -0.538406       -0.450590        1.341146
O           0.342947       -1.513794       -0.494531
C           1.652639       -1.322676        0.055373
C           2.257318        0.019384       -0.348706
C           3.675755        0.207551        0.201099
C           4.295783        1.548748       -0.203820
H          -1.933555       -1.441250       -1.512334
H          -3.170281       -0.459469        1.140760
H          -4.067547       -1.034796       -0.297051
H           1.612711       -1.413601        1.145149
H           2.251372       -2.148081       -0.344479
H           1.607770        0.825104        0.016962
H           2.272339        0.089498       -1.445525
H           4.316024       -0.613378       -0.152658
H           3.652990        0.131031        1.297521
H           5.308359        1.660372        0.201986
H           4.359625        1.638649       -1.295751
H           3.691729        2.387669        0.164672
N          -3.510098        0.998589       -0.359770
H          -4.454703        1.242281       -0.043222
H          -3.526863        1.031624       -1.382663
```

```
C          -2.527964        1.996178        0.150223
H          -2.768906        2.979165       -0.256425
H          -2.585346        2.007099        1.238538
H          -1.536773        1.675402       -0.167272
```

---

### Compound_26_HEI_1_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.331049 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.118259 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.8157 cm-1
  2.      38.3336 cm-1
  3.      71.3378 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.735188        0.346264       -0.259507
C          -1.683938        1.306630        0.047913
C          -3.109165        0.961923       -0.184765
O          -0.992794       -0.840095       -0.660355
O           0.588303        0.729859       -0.089210
C           1.578311       -0.307899       -0.127661
C           2.941842        0.337152        0.070534
C           4.078521       -0.691503        0.046683
C           5.456173       -0.052105        0.246888
H          -1.413448        2.254814        0.495889
H          -3.373636        0.766755       -1.233500
H          -3.803078        1.703665        0.215949
H           1.374300       -1.039847        0.665048
H           1.530379       -0.833656       -1.087695
H           2.951412        0.876497        1.027780
H           3.103438        1.084868       -0.718310
H           4.060971       -1.231994       -0.910208
H           3.906480       -1.443075        0.830098
H           5.511270        0.469270        1.210984
H           6.252448       -0.805529        0.226615
H           5.667454        0.681543       -0.541431
N          -3.426577       -0.376244        0.499334
H          -2.645503       -0.980321        0.157119
H          -3.291558       -0.262684        1.507413
```

```
C          -4.757883       -0.967412        0.203822
H          -5.535098       -0.279322        0.540161
H          -4.837028       -1.122104       -0.872880
H          -4.848871       -1.921578        0.724712
```

---

### Compound_26_HEI_20

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328957 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114922 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.1828 cm-1
  2.      37.0477 cm-1
  3.      66.7146 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.307547       -1.688910        0.045781
C          -1.458999       -1.406273        0.773771
C          -1.953544       -0.023582        0.929858
O           0.286208       -2.779527       -0.135447
O           0.185718       -0.524754       -0.608295
C           1.552804       -0.528557       -1.042540
C           2.519581       -0.244298        0.105929
C           2.205124        1.030247        0.903377
C           2.210770        2.313098        0.064634
H          -2.030605       -2.227976        1.190429
H          -1.210795        0.696169        1.292841
H          -2.843923        0.037992        1.558991
H           1.783765       -1.489598       -1.510659
H           1.604959        0.253047       -1.805533
H           3.530772       -0.174494       -0.321913
H           2.522757       -1.105773        0.785712
H           2.942441        1.122401        1.712036
H           1.227221        0.916714        1.388145
H           1.410453        2.309140       -0.684471
H           2.064670        3.196479        0.697622
H           3.164380        2.434621       -0.465956
N          -2.363337        0.589799       -0.437645
H          -3.091359       -0.002041       -0.847338
H          -1.522893        0.467779       -1.020555
```

```
C          -2.788706        2.016521       -0.407909
H          -3.023708        2.343627       -1.421555
H          -3.667784        2.106623        0.231435
H          -1.969299        2.611458       -0.003189
```

---

### Compound_26_HEI_21_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327431 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114467 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.2689 cm-1
  2.      34.4579 cm-1
  3.      67.6311 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.620394       -0.101095        0.167619
C          -1.680014       -0.959302        0.473870
C          -2.798149       -1.137398       -0.446903
O          -0.463686        0.607235       -0.858506
O           0.353349       -0.070719        1.179103
C           1.574843        0.622333        0.894150
C           2.580749       -0.260377        0.160227
C           3.911683        0.457910       -0.089733
C           4.932895       -0.422144       -0.817688
H          -1.658478       -1.522451        1.401414
H          -2.558635       -0.875202       -1.480391
H          -3.254451       -2.130516       -0.411231
H           1.359867        1.524756        0.313864
H           1.969082        0.918121        1.872473
H           2.144728       -0.577134       -0.796020
H           2.756170       -1.170102        0.751665
H           4.332798        0.789493        0.870324
H           3.728215        1.368583       -0.677567
H           4.549715       -0.741911       -1.795102
H           5.875246        0.113000       -0.985159
H           5.158120       -1.325481       -0.236550
N          -4.037409       -0.193414       -0.123312
H          -4.308050       -0.378088        0.846543
H          -4.837119       -0.460796       -0.706760
```

```
C          -3.749489        1.258681       -0.288502
H          -3.539338        1.447547       -1.341297
H          -4.613332        1.837838        0.040130
H          -2.872727        1.492457        0.313832
```

---

### Compound_26_HEI_22

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327994 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114692 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.6761 cm-1
  2.      36.6003 cm-1
  3.      55.7976 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.723222       -1.546415        0.045825
C           2.099039       -1.397941       -0.101911
C           2.803033       -0.177663        0.340065
O          -0.017299       -2.509758       -0.265840
O           0.133366       -0.387424        0.630088
C          -1.299653       -0.327506        0.681586
C          -1.881871        0.236964       -0.612684
C          -3.417683        0.274374       -0.624106
C          -4.029649        1.216769        0.420383
H           2.653500       -2.178831       -0.609564
H           2.628606        0.116289        1.381876
H           3.879469       -0.225583        0.163033
H          -1.698423       -1.327071        0.877959
H          -1.524266        0.317560        1.535333
H          -1.525287       -0.381812       -1.445171
H          -1.487263        1.251073       -0.771775
H          -3.804828       -0.743440       -0.472434
H          -3.750367        0.582976       -1.623790
H          -3.813019        0.889297        1.443785
H          -3.636199        2.235282        0.305928
H          -5.119876        1.264924        0.314298
N           2.302399        1.067042       -0.443080
H           2.446362        0.889493       -1.440788
H           1.284116        1.056682       -0.289937
```

```
C           2.891556        2.374257       -0.041166
H           2.446923        3.169113       -0.641316
H           2.677741        2.538400        1.015570
H           3.969521        2.336768       -0.203392
```

---

### Compound_26_HEI_23

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327941 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114647 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      32.6072 cm-1
  2.      38.0197 cm-1
  3.      44.0681 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.626216        1.444623       -0.152917
C          -1.907248        1.426276        0.390814
C          -2.548622        0.167660        0.818040
O           0.071396        2.415117       -0.534727
O          -0.114200        0.125399       -0.315700
C           1.285538       -0.017504       -0.595638
C           2.117916        0.003762        0.684451
C           3.629012       -0.105344        0.429268
C           4.065838       -1.440701       -0.186842
H          -2.469691        2.352306        0.429536
H          -1.952095       -0.451993        1.497188
H          -3.537162        0.323454        1.255087
H           1.371754       -0.977273       -1.112055
H           1.602721        0.779416       -1.275165
H           1.791018       -0.818061        1.337189
H           1.905160        0.939676        1.216067
H           4.153784        0.037523        1.382956
H           3.946541        0.721373       -0.222394
H           5.157561       -1.494583       -0.273112
H           3.736456       -2.283787        0.434427
H           3.649264       -1.584187       -1.190574
N          -2.771634       -0.787515       -0.389677
H          -3.347946       -0.296030       -1.078355
H          -1.834301       -0.879094       -0.805777
```

```
C          -3.346904       -2.123153       -0.069411
H          -3.432921       -2.707877       -0.986066
H          -2.682220       -2.625257        0.634423
H          -4.329940       -1.980849        0.381189
```

---

### Compound_26_HEI_24

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327484 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114651 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      19.9272 cm-1
  2.      24.9088 cm-1
  3.      66.4702 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.577549       -1.094732        0.004825
C           1.539542       -0.710980       -0.932440
C           2.903051       -0.384764       -0.523683
O           0.698251       -1.179236        1.253246
O          -0.645679       -1.440648       -0.590982
C          -1.785455       -1.537945        0.274453
C          -2.372978       -0.171095        0.620732
C          -2.851763        0.626039       -0.597161
C          -3.438785        1.989180       -0.217862
H           1.277486       -0.682383       -1.985210
H           3.188645       -0.821574        0.436709
H           3.663952       -0.610596       -1.276068
H          -2.511619       -2.134765       -0.288208
H          -1.512546       -2.080555        1.184018
H          -1.621484        0.408611        1.172804
H          -3.215695       -0.331893        1.309889
H          -3.606247        0.038017       -1.140129
H          -2.011437        0.766862       -1.288499
H          -2.693468        2.607386        0.299224
H          -3.775262        2.541597       -1.103555
H          -4.299600        1.875839        0.453866
N           3.124287        1.169902       -0.283358
H           4.121454        1.359723       -0.139193
H           2.858318        1.646412       -1.149536
```

```
C           2.330958        1.725646        0.848604
H           2.680507        1.261725        1.770819
H           1.286432        1.470125        0.676442
H           2.467275        2.807124        0.887215
```

---

### Compound_26_HEI_25

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32867 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114437 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.3987 cm-1
  2.      36.0455 cm-1
  3.      69.5413 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.902722        1.470904        0.281336
C          -2.150958        0.926178       -0.008850
C          -2.311060       -0.198440       -0.946267
O          -0.600933        2.419171        1.046780
O           0.140617        0.784434       -0.393396
C           1.473172        1.280907       -0.211436
C           2.445111        0.337090       -0.907253
C           2.425036       -1.114625       -0.402548
C           2.639580       -1.260642        1.107618
H          -3.005181        1.270274        0.562730
H          -1.876241       -0.043438       -1.940440
H          -3.351823       -0.509174       -1.059183
H           1.549142        2.288305       -0.638014
H           1.688628        1.358821        0.858515
H           3.452201        0.754398       -0.765115
H           2.249632        0.349016       -1.987823
H           3.205395       -1.672612       -0.936507
H           1.476936       -1.591039       -0.684410
H           3.568229       -0.767832        1.423363
H           1.815597       -0.816737        1.678071
H           2.706622       -2.317165        1.392139
N          -1.544764       -1.478715       -0.467971
H          -1.558977       -2.192085       -1.202859
H          -0.572350       -1.155936       -0.373169
```

```
C          -2.024158       -2.054827        0.816336
H          -1.349924       -2.854642        1.124595
H          -2.033314       -1.253673        1.555231
H          -3.032701       -2.443580        0.667990
```

---

### Compound_26_HEI_26

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327235 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.113975 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.2544 cm-1
  2.      40.6836 cm-1
  3.      73.2648 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.484169       -0.189577       -0.033880
C          -1.305179        0.833322       -0.517457
C          -2.445401        1.317581        0.254154
O          -0.583274       -0.820323        1.048724
O           0.555590       -0.505775       -0.921092
C           1.580493       -1.388747       -0.445077
C           2.644274       -0.664458        0.377421
C           3.380388        0.438570       -0.390368
C           4.453376        1.131452        0.455543
H          -1.072691        1.296793       -1.470953
H          -2.367406        1.116117        1.325496
H          -2.679050        2.373120        0.090340
H           1.128047       -2.196004        0.138035
H           2.024797       -1.813421       -1.352201
H           3.368984       -1.416758        0.723893
H           2.174118       -0.243109        1.275551
H           2.652726        1.180811       -0.742096
H           3.843002        0.005926       -1.289652
H           5.212071        0.414689        0.795779
H           4.965786        1.917915       -0.111657
H           4.011634        1.595240        1.347064
N          -3.816415        0.611246       -0.136979
H          -4.597470        1.092187        0.321611
H          -3.941645        0.743931       -1.144362
```

```
C          -3.858064       -0.844180        0.177970
H          -3.810486       -0.961859        1.260470
H          -2.988349       -1.307435       -0.285875
H          -4.782003       -1.271850       -0.213474
```

---

### Compound_26_HEI_27

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327797 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114899 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.7885 cm-1
  2.      36.2701 cm-1
  3.      70.8356 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.933475        1.401995        0.063190
C          -2.262633        1.106359       -0.229308
C          -2.643247       -0.125980       -0.941434
O          -0.441345        2.396278        0.651032
O          -0.064042        0.365302       -0.364247
C           1.342781        0.561433       -0.174501
C           2.047833       -0.721046       -0.595693
C           3.579658       -0.620076       -0.531686
C           4.136855       -0.405193        0.881264
H          -3.034491        1.747859        0.179840
H          -2.132921       -0.287720       -1.897693
H          -3.721046       -0.209447       -1.096347
H           1.681463        1.409494       -0.784067
H           1.536136        0.805114        0.874087
H           1.741836       -0.967111       -1.621073
H           1.705657       -1.545514        0.046039
H           3.917228        0.194828       -1.187889
H           4.002953       -1.543648       -0.947307
H           3.785458       -1.190074        1.563697
H           5.232968       -0.430265        0.877728
H           3.830983        0.560766        1.299152
N          -2.237808       -1.415453       -0.147576
H          -1.224116       -1.304855       -0.007290
H          -2.374881       -2.246314       -0.730458
```

```
C          -2.928587       -1.584672        1.158614
H          -3.989091       -1.759301        0.971393
H          -2.492691       -2.431259        1.690183
H          -2.792811       -0.663946        1.726087
```

---

### Compound_26_HEI_28

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328196 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.113954 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      40.9107 cm-1
  2.      63.4984 cm-1
  3.      81.2536 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.703174        1.732257        0.178328
C          -1.920955        1.190644        0.583956
C          -2.113118       -0.265777        0.727370
O          -0.371618        2.932796        0.018952
O           0.246307        0.719389       -0.111833
C           1.554217        1.140886       -0.520874
C           2.397902       -0.082834       -0.859829
C           2.879943       -0.921217        0.334888
C           1.790029       -1.724439        1.053910
H          -2.765774        1.856150        0.719487
H          -1.386560       -0.775284        1.370465
H          -3.120538       -0.527699        1.057521
H           1.462080        1.796336       -1.393862
H           2.019936        1.722362        0.285100
H           3.279099        0.286486       -1.402357
H           1.842932       -0.716836       -1.566482
H           3.380655       -0.256578        1.053963
H           3.650654       -1.616127       -0.025694
H           1.035484       -1.068896        1.497520
H           1.277241       -2.397097        0.353895
H           2.222635       -2.340862        1.851499
N          -1.914747       -0.993453       -0.632860
H          -2.576500       -0.592893       -1.303340
H          -0.976423       -0.693823       -0.934385
```

```
C          -2.019597       -2.478151       -0.601162
H          -1.826276       -2.874923       -1.598570
H          -1.280518       -2.860988        0.103081
H          -3.023898       -2.750854       -0.274299
```

---

### Compound_26_HEI_29

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329448 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116175 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      20.3377 cm-1
  2.      43.6098 cm-1
  3.      66.6064 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.472814        1.582968       -0.260939
C          -1.490585        1.102598       -1.078605
C          -1.923318       -0.307799       -1.027082
O           0.053591        2.721206       -0.213842
O          -0.050137        0.593748        0.672524
C           1.235792        0.765106        1.286093
C           2.366313        0.279983        0.382880
C           2.274551       -1.206497        0.023154
C           3.419175       -1.668167       -0.883850
H          -2.014076        1.798282       -1.724851
H          -1.117124       -1.044452       -1.120998
H          -2.701661       -0.537879       -1.757709
H           1.372062        1.816920        1.551646
H           1.192229        0.169741        2.204297
H           3.318357        0.478013        0.897312
H           2.372896        0.885023       -0.534123
H           1.313182       -1.398494       -0.469929
H           2.273584       -1.801647        0.948111
H           4.392938       -1.511964       -0.401844
H           3.332636       -2.733990       -1.127173
H           3.422185       -1.108175       -1.827913
N          -2.533681       -0.662936        0.357637
H          -3.318936       -0.029010        0.529740
H          -1.795266       -0.401600        1.026106
```

```
C          -2.945010       -2.082295        0.540453
H          -3.715296       -2.319620       -0.194352
H          -2.072002       -2.716984        0.385233
H          -3.332208       -2.218619        1.550911
```

---

### Compound_26_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330987 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.118026 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      24.9617 cm-1
  2.      45.4119 cm-1
  3.      64.1104 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.602746        0.151274       -0.481911
C           1.336780       -0.999373       -0.715734
C           2.816674       -0.890243       -0.667460
O           1.097383        1.284977       -0.156911
O          -0.773203        0.022675       -0.598341
C          -1.575747        1.103313       -0.100325
C          -3.039842        0.715232       -0.248292
C          -3.457707       -0.489998        0.601494
C          -4.946525       -0.822129        0.461511
H           0.860477       -1.959577       -0.870660
H           3.257795       -0.230705       -1.427925
H           3.322300       -1.857084       -0.711179
H          -1.326865        1.288699        0.952932
H          -1.356046        2.017465       -0.662676
H          -3.254039        0.516242       -1.308053
H          -3.643614        1.589452        0.034727
H          -3.223889       -0.282810        1.655988
H          -2.856158       -1.361320        0.314789
H          -5.200577       -1.057943       -0.580010
H          -5.223602       -1.686228        1.077186
H          -5.571248        0.025409        0.772021
N           3.233001       -0.217127        0.649085
H           2.939217       -0.818212        1.423389
H           2.609348        0.621739        0.665113
```

```
C           4.666923        0.152955        0.775980
H           5.275507       -0.749363        0.698725
H           4.919467        0.843344       -0.029652
H           4.827657        0.633367        1.742131
```

---

### Compound_26_HEI_30

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.326495 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.113656 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.0292 cm-1
2.      37.4019 cm-1
3.      78.5573 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.714223       -0.435984        0.360425
C           1.819232       -1.077020       -0.208968
C           3.167874       -0.843924        0.296257
O           0.697764        0.394278        1.304513
O          -0.495309       -0.815428       -0.233085
C          -1.687881       -0.216750        0.287756
C          -2.857251       -0.697625       -0.561521
C          -4.220010       -0.202015       -0.053420
C          -4.398874        1.320300       -0.115427
H           1.667896       -1.782696       -1.019552
H           3.193507       -0.478818        1.326188
H           3.840796       -1.698877        0.187254
H          -1.826526       -0.511944        1.336533
H          -1.591950        0.873422        0.260998
H          -2.851704       -1.795609       -0.572957
H          -2.707953       -0.367517       -1.599268
H          -4.370019       -0.547552        0.979508
H          -5.005770       -0.679311       -0.653331
H          -3.706410        1.841277        0.555666
H          -4.221529        1.693525       -1.132561
H          -5.416778        1.607304        0.173983
N           3.951451        0.293724       -0.496543
H           4.927673        0.322259       -0.183879
H           3.967198        0.013879       -1.481138
```

```
C          3.337990        1.645926       -0.377785
H          3.875769        2.344222       -1.020380
H          2.295241        1.562835       -0.680873
H          3.398935        1.959287        0.664282
```

---

### Compound_26_HEI_31

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329364 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115373 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.0627 cm-1
  2.      46.9977 cm-1
  3.      59.9604 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -0.243344       -0.763773        0.509971
C         -1.023170        0.018548        1.342574
C         -2.464478        0.152056        1.010451
O         -0.652214       -1.327746       -0.563257
O          1.080296       -0.922943        0.900380
C          2.013203       -1.356922       -0.102958
C          2.432370       -0.256281       -1.077925
C          3.265611        0.887359       -0.477963
C          2.480768        1.859983        0.410863
H         -0.594543        0.575519        2.166323
H         -3.039340       -0.783500        1.055217
H         -2.978129        0.903999        1.612945
H          2.880373       -1.709025        0.465977
H          1.586702       -2.202284       -0.650410
H          1.537278        0.148213       -1.568857
H          3.022430       -0.748243       -1.864906
H          3.718284        1.452408       -1.304488
H          4.102935        0.459047        0.092849
H          3.121799        2.683432        0.749852
H          1.638463        2.296386       -0.141870
H          2.069740        1.355993        1.289977
N         -2.607347        0.569579       -0.460150
H         -2.174177        1.489371       -0.577565
H         -1.982530       -0.120798       -0.937303
```

```
C          -3.984955        0.554532       -1.017617
H          -3.948058        0.843759       -2.068823
H          -4.386573       -0.454995       -0.923145
H          -4.603911        1.256161       -0.456091
```

---

### Compound_26_HEI_32_reopt_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328572 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115378 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.7080 cm-1
  2.      35.5762 cm-1
  3.      65.8704 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.528430       -0.715979        0.331678
C           1.336971        0.014659        1.184708
C           2.806337       -0.104591        1.017845
O           0.945355       -1.440716       -0.637622
O          -0.834378       -0.609431        0.557717
C          -1.710766       -1.131958       -0.451650
C          -3.141377       -0.713992       -0.130667
C          -3.492253        0.749419       -0.443972
C          -2.774083        1.795092        0.417118
H           0.920657        0.726756        1.886323
H           3.216138       -1.100745        1.236616
H           3.365513        0.634105        1.596051
H          -1.407421       -0.755219       -1.436438
H          -1.625884       -2.224931       -0.473395
H          -3.348761       -0.935061        0.925926
H          -3.803707       -1.363055       -0.719963
H          -4.577311        0.873214       -0.323026
H          -3.279872        0.942652       -1.505803
H          -2.958312        1.616100        1.484352
H          -1.691351        1.767952        0.262642
H          -3.131508        2.804675        0.178902
N           3.190195        0.090304       -0.463889
H           4.142437       -0.242604       -0.633768
H           2.523227       -0.562240       -0.937197
```

```
C           3.027089        1.473224       -0.983186
H           2.013951        1.799248       -0.747591
H           3.755934        2.123008       -0.495891
H           3.184997        1.469941       -2.062525
```

---

### Compound_26_HEI_33_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328753 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114887 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.2432 cm-1
  2.      42.3842 cm-1
  3.      56.5428 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.273310       -0.097127        0.364396
C           1.054687        1.001193        0.681744
C           2.361449        1.135086       -0.009235
O           0.610883       -1.025873       -0.446438
O          -0.940023       -0.181852        1.034196
C          -1.831955       -1.243583        0.662035
C          -2.662830       -0.946019       -0.586304
C          -3.683934        0.194886       -0.453472
C          -3.076012        1.602431       -0.409631
H           0.765654        1.704513        1.452998
H           2.297413        1.263807       -1.098813
H           2.985850        1.932756        0.398458
H          -1.258500       -2.164360        0.520001
H          -2.487981       -1.367152        1.530823
H          -3.200367       -1.874479       -0.828967
H          -1.985846       -0.748573       -1.427405
H          -4.293815        0.028029        0.446913
H          -4.376011        0.136151       -1.304912
H          -3.862407        2.367415       -0.392461
H          -2.442790        1.736994        0.471667
H          -2.452236        1.782911       -1.295096
N           3.149913       -0.176069        0.129983
H           2.440214       -0.882877       -0.166464
H           3.330655       -0.338467        1.124144
```

```
C           4.402932       -0.277210       -0.663109
H           5.085578        0.514356       -0.349642
H           4.856512       -1.254500       -0.492821
H           4.155912       -0.160186       -1.718924
```

---

### Compound_26_HEI_34

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328299 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115808 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      21.1591 cm-1
  2.      35.6732 cm-1
  3.      64.2895 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.805171        1.604788       -0.052908
C           2.144174        1.411741        0.279600
C           2.648629        0.096783        0.718843
O           0.209276        2.646368       -0.421241
O           0.070666        0.393593        0.029106
C          -1.337963        0.455845       -0.226622
C          -1.900700       -0.947678       -0.045231
C          -3.399282       -1.047574       -0.369458
C          -4.300610       -0.233374        0.567425
H           2.838436        2.232537        0.140677
H           2.095969       -0.364923        1.545279
H           3.711267        0.113183        0.969350
H          -1.798900        1.169736        0.463511
H          -1.513330        0.816283       -1.247876
H          -1.723243       -1.275491        0.988616
H          -1.342411       -1.633168       -0.696893
H          -3.692177       -2.104276       -0.319297
H          -3.567928       -0.731133       -1.408697
H          -4.122679        0.843923        0.472375
H          -5.359254       -0.413093        0.345850
H          -4.125624       -0.509129        1.615530
N           2.501060       -0.966254       -0.408986
H           1.502987       -0.922091       -0.658123
H           3.019737       -0.632690       -1.226049
```

```
C           2.899336       -2.356301       -0.053021
H           2.293414       -2.681986        0.793198
H           2.728830       -3.010598       -0.908862
H           3.955421       -2.358381        0.219631
```

---

### Compound_26_HEI_35

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329115 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115364 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      40.2625 cm-1
  2.      59.5779 cm-1
  3.      67.3048 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.293533       -1.371675       -0.134083
C           2.375834       -0.589858        0.263178
C           2.195775        0.638727        1.054558
O           1.275267       -2.443379       -0.788078
O           0.059928       -0.794940        0.261977
C          -1.129924       -1.565909        0.046821
C          -2.329542       -0.724217        0.458309
C          -2.567134        0.506703       -0.423779
C          -3.810897        1.298443       -0.009034
H           3.358736       -0.840642       -0.118769
H           1.608398        0.518843        1.971966
H           3.141147        1.127618        1.299068
H          -1.196714       -1.851811       -1.008967
H          -1.077114       -2.485520        0.642245
H          -2.213729       -0.416208        1.507004
H          -3.216417       -1.372440        0.417762
H          -2.664334        0.185157       -1.470497
H          -1.690785        1.166465       -0.385282
H          -3.723403        1.653760        1.025669
H          -3.960984        2.173273       -0.652610
H          -4.712478        0.675796       -0.072113
N           1.358095        1.719692        0.286801
H           0.479493        1.232604        0.065763
H           1.126109        2.495847        0.913468
```

```
C           1.992497        2.234157       -0.955819
H           2.260337        1.374708       -1.570444
H           2.886923        2.795882       -0.682496
H           1.285746        2.877146       -1.481469
```

---

### Compound_26_HEI_36

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32909 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115699 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      33.1276 cm-1
2.      48.8367 cm-1
3.      59.5638 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.194464        1.395963       -0.189358
C          -2.175320        0.591172       -0.763857
C          -1.904236       -0.807645       -1.139768
O          -1.245735        2.599460        0.165438
O           0.002613        0.670584        0.033697
C           1.151594        1.397395        0.486169
C           2.277068        0.400869        0.725422
C           2.727167       -0.350122       -0.532802
C           3.887903       -1.311796       -0.260899
H          -3.185729        0.977547       -0.831991
H          -1.035511       -0.952764       -1.791741
H          -2.770185       -1.301038       -1.586264
H           1.438230        2.134731       -0.275278
H           0.905406        1.939975        1.404860
H           1.961566       -0.318562        1.494877
H           3.128219        0.955537        1.145645
H           3.024538        0.380568       -1.298985
H           1.877008       -0.905835       -0.947367
H           3.605702       -2.068021        0.483053
H           4.193855       -1.837792       -1.173103
H           4.763317       -0.774929        0.126783
N          -1.517046       -1.689971        0.096590
H          -1.194762       -2.610612       -0.215267
H          -0.705027       -1.200738        0.497780
```

```
C          -2.589099       -1.839204        1.116045
H          -3.407301       -2.413538        0.678909
H          -2.186963       -2.355069        1.988726
H          -2.931741       -0.839807        1.384444
```

---

### Compound_26_HEI_37

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.326404 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.112969 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.5599 cm-1
  2.      37.0737 cm-1
  3.      50.2913 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.554178       -0.293624        0.020986
C          -1.700673       -1.080025       -0.123134
C          -2.837927       -0.621890       -0.915142
O          -0.327326        0.845817       -0.457817
O           0.424025       -0.911950        0.816158
C           1.714131       -0.288688        0.873122
C           2.613459       -0.746622       -0.273628
C           4.050784       -0.213523       -0.170549
C           4.166017        1.309066       -0.319624
H          -1.735303       -2.060942        0.340029
H          -2.578802        0.139525       -1.655418
H          -3.402891       -1.427638       -1.392063
H           1.591913        0.796812        0.873738
H           2.139789       -0.597747        1.834497
H           2.167043       -0.427725       -1.224799
H           2.631046       -1.844824       -0.278889
H           4.657944       -0.695822       -0.947892
H           4.484461       -0.522184        0.791922
H           3.656426        1.839092        0.493211
H           5.215743        1.626110       -0.313149
H           3.720175        1.643185       -1.265423
N          -3.959742        0.099508       -0.047913
H          -4.791366        0.263220       -0.625213
H          -4.237855       -0.557891        0.685911
```

```
C          -3.512816        1.376425        0.575362
H          -3.300821        2.089707       -0.221139
H          -4.300357        1.754338        1.228537
H          -2.605324        1.168569        1.140444
```

---

### Compound_26_HEI_38

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.326455 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.112898 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      32.2244 cm-1
  2.      38.9579 cm-1
  3.      52.7818 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.659124       -0.813944        0.262720
C           1.825115       -1.089517       -0.455839
C           3.138800       -0.740908        0.077514
O           0.547853       -0.232345        1.371246
O          -0.494264       -1.296010       -0.377945
C          -1.757954       -0.852025        0.133816
C          -2.132154        0.529191       -0.402291
C          -3.457817        1.062815        0.161675
C          -4.687732        0.237993       -0.239148
H           1.755967       -1.602841       -1.409567
H           3.154017       -0.627150        1.164477
H           3.943177       -1.411477       -0.237755
H          -2.473055       -1.611312       -0.194506
H          -1.732202       -0.843109        1.228182
H          -2.187283        0.484301       -1.499357
H          -1.322817        1.224889       -0.149007
H          -3.592268        2.096496       -0.183354
H          -3.390368        1.111853        1.258128
H          -4.761578        0.152164       -1.331171
H          -4.651213       -0.777241        0.172613
H          -5.610283        0.707009        0.123139
N           3.665849        0.669928       -0.430607
H           3.674767        0.634989       -1.453691
H           4.638266        0.801200       -0.133556
```

```
C           2.836630        1.823578        0.017694
H           1.807232        1.625233       -0.277402
H           2.906189        1.892498        1.103218
H           3.207720        2.736736       -0.449402
```

---

### Compound_26_HEI_39

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.327911 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.115179 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      22.8505 cm-1
2.      30.5938 cm-1
3.      48.5263 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.424454        1.322691       -0.064501
C           1.699198        1.496421        0.467009
C           2.555481        0.347733        0.817846
O          -0.436166        2.178589       -0.382006
O           0.143412       -0.053421       -0.298427
C          -1.213965       -0.414466       -0.591164
C          -2.018942       -0.643635        0.685783
C          -3.454641       -1.123280        0.421736
C          -4.344536       -0.082040       -0.269434
H           2.093127        2.502589        0.555105
H           2.085633       -0.405203        1.460789
H           3.506597        0.649661        1.261068
H          -1.661557        0.362882       -1.213948
H          -1.147463       -1.340206       -1.172944
H          -2.041458        0.290026        1.263771
H          -1.490098       -1.386910        1.297232
H          -3.910010       -1.402452        1.380884
H          -3.425887       -2.041914       -0.182257
H          -3.983916        0.161333       -1.275388
H          -5.373480       -0.448105       -0.367455
H          -4.373648        0.850872        0.308223
N           2.929521       -0.484669       -0.443542
H           2.018887       -0.723320       -0.860273
H           3.396568        0.139928       -1.106919
```

```
C           3.742995       -1.708036       -0.198684
H           3.195648       -2.353723        0.488820
H           3.911500       -2.224803       -1.144289
H           4.694689       -1.411654        0.244296
```

---

### Compound_26_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330968 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.117915 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.1219 cm-1
2.      38.1619 cm-1
3.      67.9958 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.583466        0.079840        0.086318
C           1.357187        1.187233       -0.218830
C           2.788836        1.151896        0.171735
O           1.021155       -0.998721        0.615781
O          -0.760672        0.176594       -0.241079
C          -1.545083       -1.022127       -0.158749
C          -2.981654       -0.674627       -0.521523
C          -3.658192        0.285886        0.463028
C          -5.113709        0.583913        0.090136
H           0.958579        2.027767       -0.773405
H           2.972858        1.087463        1.253432
H           3.366295        1.987364       -0.229219
H          -1.139101       -1.772995       -0.848460
H          -1.488327       -1.432857        0.855845
H          -3.549233       -1.615382       -0.562831
H          -3.006115       -0.248344       -1.534498
H          -3.088242        1.222263        0.504987
H          -3.617862       -0.149235        1.472250
H          -5.178506        1.044394       -0.904186
H          -5.712569       -0.335858        0.069928
H          -5.578226        1.270796        0.807709
N           3.428715       -0.140479       -0.357927
H           2.745762       -0.862773       -0.035067
H           3.383090       -0.126738       -1.380177
```

```
C           4.808954       -0.431264        0.110656
H           5.140058       -1.378204       -0.317973
H           5.469791        0.377209       -0.206297
H           4.798048       -0.499004        1.199205
```

---

### Compound_26_HEI_40

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328957 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.114922 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.1829 cm-1
  2.      37.0477 cm-1
  3.      66.7146 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.307548       -1.688910        0.045781
C          -1.458999       -1.406273        0.773771
C          -1.953544       -0.023582        0.929858
O           0.286208       -2.779527       -0.135447
O           0.185718       -0.524754       -0.608295
C           1.552804       -0.528557       -1.042540
C           2.519581       -0.244298        0.105929
C           2.205124        1.030247        0.903377
C           2.210771        2.313097        0.064634
H          -2.030605       -2.227975        1.190429
H          -1.210794        0.696169        1.292841
H          -2.843923        0.037992        1.558992
H           1.783765       -1.489599       -1.510659
H           1.604959        0.253047       -1.805533
H           3.530772       -0.174494       -0.321913
H           2.522757       -1.105773        0.785712
H           2.942441        1.122401        1.712037
H           1.227221        0.916714        1.388145
H           1.410454        2.309140       -0.684472
H           2.064670        3.196479        0.697622
H           3.164381        2.434621       -0.465955
N          -2.363337        0.589799       -0.437645
H          -1.522893        0.467779       -1.020555
H          -3.091359       -0.002041       -0.847338
```

```
C          -2.788706        2.016521       -0.407909
H          -1.969299        2.611458       -0.003190
H          -3.023708        2.343627       -1.421555
H          -3.667784        2.106624        0.231435
```

---

### Compound_26_HEI_41

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.328551 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.11452 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.2633 cm-1
  2.      56.7879 cm-1
  3.      59.6441 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.168158        1.553776        0.004462
C           1.487849        1.614812       -0.435587
C           2.497621        0.628477       -0.004671
O          -0.796456        2.312624       -0.250598
O          -0.042330        0.419251        0.840948
C          -1.355772        0.172213        1.364654
C          -1.848557       -1.198173        0.907502
C          -2.063703       -1.324816       -0.608057
C          -3.198409       -0.447255       -1.148504
H           1.756238        2.369514       -1.165882
H           2.589107        0.492796        1.079270
H           3.487329        0.828397       -0.420306
H          -1.280175        0.203313        2.458389
H          -2.019850        0.974266        1.037114
H          -2.792887       -1.408366        1.430937
H          -1.130042       -1.959039        1.243056
H          -2.274237       -2.376680       -0.842647
H          -1.130871       -1.074811       -1.131456
H          -2.982972        0.616693       -1.003099
H          -3.345784       -0.614022       -2.222361
H          -4.145107       -0.674800       -0.640991
N           2.120309       -0.802207       -0.484263
H           1.166590       -0.933097       -0.119086
H           2.041481       -0.783616       -1.504722
```

```
C           3.018516       -1.902355       -0.037199
H           3.041810       -1.906978        1.053015
H           4.018592       -1.719496       -0.432102
H           2.634692       -2.853688       -0.407681
```

---

### Compound_26_HEI_42

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.32754 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.113628 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.2362 cm-1
  2.      53.1800 cm-1
  3.      61.2901 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.136413        1.611668       -0.189866
C          -1.305615        1.379260       -0.909109
C          -1.959170        0.056323       -0.921567
O           0.551674        2.657142       -0.096065
O           0.248404        0.466648        0.561041
C           1.566321        0.461936        1.130701
C           2.647085        0.032258        0.137273
C           2.708879       -1.471523       -0.169870
C           1.470480       -2.043236       -0.869558
H          -1.789019        2.217008       -1.399123
H          -1.308035       -0.781947       -1.189986
H          -2.849446        0.030871       -1.553198
H           1.783612        1.459966        1.520435
H           1.510051       -0.240494        1.969517
H           3.615584        0.342786        0.554904
H           2.512968        0.602340       -0.791807
H           2.881764       -2.019228        0.768337
H           3.591339       -1.656790       -0.797793
H           1.243188       -1.483279       -1.785822
H           1.628233       -3.093195       -1.145362
H           0.588493       -1.990350       -0.224760
N          -2.445916       -0.344950        0.501148
H          -3.088266        0.380251        0.831756
H          -1.598009       -0.268928        1.080440
```

```
C          -3.058035       -1.697053        0.623343
H          -3.938656       -1.740939       -0.018786
H          -2.325032       -2.438226        0.302951
H          -3.339166       -1.873319        1.662369
```

---

### Compound_26_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.331286 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.117812 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.6317 cm-1
  2.      46.9258 cm-1
  3.      68.5280 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.634397       -0.985898        0.137196
C          -1.666847       -1.186054       -0.760474
C          -2.967035       -0.526879       -0.472662
O          -0.684047       -0.213585        1.155271
O           0.535485       -1.695524       -0.120755
C           1.744943       -1.197190        0.473414
C           2.326115       -0.022618       -0.308271
C           3.638635        0.486646        0.298284
C           4.234936        1.661968       -0.482932
H          -1.530183       -1.758666       -1.669433
H          -3.462371       -0.863606        0.448813
H          -3.679654       -0.601317       -1.296677
H           1.554515       -0.914967        1.513010
H           2.434373       -2.047355        0.460281
H           1.589543        0.791450       -0.330363
H           2.493656       -0.332747       -1.349147
H           4.367032       -0.336099        0.334523
H           3.463268        0.790553        1.340027
H           3.538854        2.510060       -0.508368
H           5.171165        2.009357       -0.030014
H           4.449423        1.375816       -1.520484
N          -2.728413        0.965597       -0.208211
H          -1.944980        0.936350        0.484645
H          -2.352385        1.387175       -1.061647
```

```
C          -3.892497        1.738098        0.298948
H          -4.697997        1.691535       -0.435709
H          -4.219723        1.294066        1.239792
H          -3.590269        2.773648        0.461084
```

---

### Compound_26_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.330864 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.117476 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      32.7332 cm-1
  2.      41.2813 cm-1
  3.      67.9630 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.596108       -0.576076       -0.010078
C           1.662762       -1.228923        0.584399
C           2.865541       -0.421001        0.904639
O           0.584819        0.656744       -0.343447
O          -0.511816       -1.370997       -0.288840
C          -1.666867       -0.730285       -0.849749
C          -2.587591       -0.161124        0.225761
C          -3.855576        0.463956       -0.367183
C          -4.794647        1.027531        0.704172
H           1.660281       -2.300032        0.745153
H           2.700988        0.383158        1.635372
H           3.714822       -1.022547        1.234924
H          -1.352006        0.054766       -1.543357
H          -2.179452       -1.516247       -1.414674
H          -2.037138        0.592386        0.803506
H          -2.862321       -0.965249        0.922845
H          -4.390129       -0.290558       -0.962069
H          -3.573740        1.265061       -1.065223
H          -4.295012        1.806470        1.294087
H          -5.692774        1.469475        0.256477
H          -5.117290        0.240246        1.397368
N           3.313793        0.348534       -0.348177
H           2.421620        0.794541       -0.655529
H           3.567788       -0.331417       -1.069461
```

```
C           4.396470        1.348226       -0.153518
H           5.289173        0.837623        0.210916
H           4.605592        1.839495       -1.104828
H           4.061824        2.083293        0.579367
```

---

### Compound_26_HEI_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329345 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116587 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      37.3204 cm-1
2.      49.0073 cm-1
3.      62.8515 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.188746       -1.586895       -0.012216
C           2.462019       -1.073484        0.223413
C           2.667120        0.330351        0.629223
O           0.836491       -2.746054       -0.340780
O           0.191404       -0.586653        0.127830
C          -1.174331       -0.986253       -0.038671
C          -2.045819        0.253214        0.101125
C          -3.537708       -0.066196       -0.050421
C          -4.422837        1.176666        0.085544
H           3.321452       -1.706131        0.033364
H           2.085715        0.656545        1.499565
H           3.718912        0.572606        0.795287
H          -1.305913       -1.449725       -1.023144
H          -1.433119       -1.734366        0.720766
H          -1.747739        0.990520       -0.657531
H          -1.863722        0.713749        1.081946
H          -3.829546       -0.808584        0.705658
H          -3.712288       -0.535264       -1.028940
H          -4.290622        1.647957        1.067735
H          -4.172606        1.923096       -0.679018
H          -5.484006        0.924585       -0.025861
N           2.181185        1.311348       -0.476613
H           2.694636        1.097113       -1.335859
H           1.204314        1.030366       -0.641723
```

```
C           2.270728        2.761120       -0.149241
H           1.879973        3.344032       -0.984176
H           1.679618        2.949758        0.747576
H           3.315976        3.014833        0.031717
```

---

### Compound_26_HEI_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.329725 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.116574 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      24.6407 cm-1
  2.      56.5788 cm-1
  3.      62.8836 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.454517       -1.419962       -0.111931
C          -2.503179       -0.513490        0.030140
C          -2.280634        0.850625        0.543617
O          -1.471168       -2.611125       -0.507789
O          -0.209143       -0.833736        0.229324
C           0.942847       -1.687409        0.230928
C           2.163147       -0.846735        0.578705
C           2.521821        0.209033       -0.473054
C           3.785801        0.995304       -0.112797
H          -3.488339       -0.799318       -0.320467
H          -1.733589        0.910681        1.491634
H          -3.203724        1.427552        0.629476
H           0.799017       -2.488436        0.965735
H           1.055994       -2.152521       -0.755270
H           3.012127       -1.533905        0.702950
H           2.004365       -0.364226        1.553360
H           1.685812        0.909399       -0.596047
H           2.656635       -0.284178       -1.446196
H           3.662848        1.519869        0.843316
H           4.650798        0.326646       -0.017004
H           4.022682        1.743792       -0.878088
N          -1.365753        1.670031       -0.414643
H          -0.525196        1.084425       -0.513034
H          -1.812947        1.691700       -1.335213
```

```
C          -1.009459        3.042671        0.039778
H          -0.506001        2.966291        1.004033
H          -0.346832        3.505411       -0.692500
H          -1.925857        3.625273        0.141214
```

---

### Compound_26_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -520.331319 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -520.117573 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      27.9924 cm-1
2.      48.4166 cm-1
3.      74.8158 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.433756       -1.000444        0.154154
C           1.198410       -0.610103        1.237849
C           2.596632       -0.181516        0.974400
O           0.808721       -0.946851       -1.067808
O          -0.836270       -1.483453        0.453856
C          -1.822567       -1.408631       -0.590168
C          -2.361426        0.006965       -0.780919
C          -3.045101        0.584288        0.462964
C          -3.578539        2.002557        0.238436
H           0.788470       -0.565157        2.239150
H           3.250152       -0.963740        0.563505
H           3.085850        0.256676        1.846713
H          -1.398888       -1.790706       -1.523017
H          -2.620243       -2.083098       -0.262080
H          -3.075827       -0.016282       -1.617353
H          -1.537441        0.663356       -1.091524
H          -2.332931        0.586133        1.297642
H          -3.871485       -0.077734        0.760366
H          -2.765910        2.689504       -0.031391
H          -4.314938        2.023511       -0.575399
H          -4.063761        2.395952        1.139823
N           2.597009        0.881753       -0.131507
H           1.993969        0.431740       -0.858922
H           2.087987        1.701530        0.209388
```

```
C           3.926578        1.266101       -0.672909
H           3.791307        2.014847       -1.454592
H           4.537119        1.671908        0.135293
H           4.401445        0.376410       -1.088268
```

---

### Compound_20_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -270.584312 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -270.494151 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      83.6942 cm-1
2.     176.6403 cm-1
3.     213.8172 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.594585        0.176125       -0.000006
O           2.120437       -0.931326       -0.000026
C           0.136963        0.411601        0.000005
H           2.222681        1.088399        0.000004
C          -0.261853        1.696941        0.000026
H          -1.308069        1.984906        0.000036
H           0.465560        2.505617        0.000035
C          -0.766377       -0.796419       -0.000008
H          -0.509359       -1.413870       -0.871541
H          -0.509347       -1.413898        0.871501
C          -2.264827       -0.493568        0.000007
H          -2.836521       -1.427584       -0.000003
H          -2.559690        0.079466        0.886944
H          -2.559702        0.079493       -0.886908
```

---

### Compound_20_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -270.579184 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -270.48963 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      69.3610 cm-1
2.     108.3553 cm-1
3.     228.9603 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.419393       -0.618359       -0.000010
O           2.528602       -0.099500       -0.000013
C           0.121055        0.108738       -0.000000
H           1.336531       -1.723525       -0.000013
C           0.126046        1.451930        0.000003
H          -0.788735        2.035278        0.000010
H           1.065322        1.997504       -0.000000
C          -1.110686       -0.768663        0.000004
H          -1.060711       -1.435508       -0.873563
H          -1.060703       -1.435511        0.873568
C          -2.446358       -0.026756        0.000013
H          -2.550937        0.609248       -0.886830
H          -3.275360       -0.742067        0.000015
H          -2.550929        0.609243        0.886859
```

---

### Compound_20_HEI_1_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.450545 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.294207 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      60.1970 cm-1
2.      83.1720 cm-1
3.     101.7393 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.342046       -1.335082       -0.121707
O          -2.577515       -1.343187       -0.451937
C          -0.593554       -0.284940        0.396688
H          -0.779891       -2.289996       -0.242657
C           0.826541       -0.523573        0.700611
H           1.192990        0.000412        1.590140
H           1.081141       -1.584780        0.772685
C           3.248027       -0.160774       -0.150734
H           3.454647       -1.218906        0.012923
H           3.489889        0.411462        0.745268
H           3.821813        0.209166       -1.001011
N           1.791004       -0.002463       -0.431401
H           1.533529       -0.493452       -1.292747
H           1.571948        0.982278       -0.602993
C          -1.209210        1.065399        0.685860
H          -2.274116        0.919547        0.908989
H          -0.755810        1.494422        1.593242
C          -1.101617        2.106057       -0.448302
H          -0.059567        2.391450       -0.646848
H          -1.520133        1.710483       -1.381033
H          -1.642188        3.028133       -0.195151
```

---

### Compound_20_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.450661 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.294679 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      43.6456 cm-1
  2.      73.4812 cm-1
  3.      83.3085 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.178242       -1.404825       -0.228950
O           2.346079       -1.742676        0.173387
C           0.521311       -0.194246       -0.059424
```

```
H           0.598852       -2.169264       -0.796881
C          -0.825462       -0.033917       -0.633956
H          -1.027409        0.955069       -1.059756
H          -1.077241       -0.800287       -1.371861
C          -3.340661        0.060005       -0.035367
H          -3.401131        1.081888       -0.410477
H          -4.041136       -0.082549        0.788049
H          -3.551397       -0.647083       -0.838196
N          -1.950449       -0.181357        0.451119
H          -1.864311       -1.121833        0.847652
H          -1.731169        0.459855        1.218867
C           1.160529        0.983451        0.641992
H           0.433339        1.503388        1.287028
H           1.944721        0.611251        1.311954
C           1.774337        2.018967       -0.319886
H           2.562781        1.558436       -0.927149
H           1.016870        2.419167       -1.005948
H           2.211971        2.866259        0.225335
```

---

### Compound_20_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.450661 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.294679 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      43.6450 cm-1
2.      73.4811 cm-1
3.      83.3086 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.178242       -1.404825       -0.228950
O           2.346079       -1.742676        0.173388
C           0.521310       -0.194246       -0.059424
H           0.598851       -2.169264       -0.796881
C          -0.825462       -0.033917       -0.633956
H          -1.027409        0.955069       -1.059756
H          -1.077241       -0.800286       -1.371861
C          -3.340661        0.060006       -0.035367
H          -3.551397       -0.647082       -0.838196
H          -3.401131        1.081888       -0.410476
```

```
H          -4.041136       -0.082549        0.788049
N          -1.950449       -0.181357        0.451119
H          -1.864311       -1.121833        0.847651
H          -1.731169        0.459855        1.218868
C           1.160529        0.983451        0.641992
H           0.433338        1.503388        1.287027
H           1.944720        0.611251        1.311955
C           1.774338        2.018966       -0.319886
H           2.562782        1.558435       -0.927148
H           1.016872        2.419166       -1.005949
H           2.211972        2.866259        0.225335
```

---

### Compound_20_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.449245 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.292225 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      47.3472 cm-1
  2.      64.1506 cm-1
  3.     123.2606 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.056362       -1.411599        0.118825
O          -2.108866       -1.713086       -0.543590
C          -0.374913       -0.201916        0.159452
H          -0.613654       -2.214482        0.754015
C           0.809697       -0.100548        1.030208
H           0.990320        0.902438        1.429161
H           0.807675       -0.818236        1.855749
C           2.488340        0.422246       -0.872654
H           2.543424        1.456760       -0.532374
H           1.693037        0.304326       -1.606865
H           3.444173        0.110585       -1.295157
N           2.167089       -0.442371        0.298571
H           2.934299       -0.404951        0.978508
H           2.100754       -1.416004       -0.012011
C          -0.895554        1.026574       -0.554937
H          -0.072941        1.629412       -0.964813
H          -1.499563        0.706259       -1.412938
```

```
C          -1.755219        1.938303        0.342428
H          -2.113407        2.820996       -0.205126
H          -2.627691        1.393358        0.722188
H          -1.181057        2.292463        1.208452
```

---

### Compound_20_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.449245 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.292225 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      47.3425 cm-1
  2.      64.1468 cm-1
  3.     123.2594 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.056372       -1.411597        0.118823
O          -2.108880       -1.713079       -0.543589
C          -0.374917       -0.201917        0.159450
H          -0.613668       -2.214481        0.754014
C           0.809695       -0.100559        1.030204
H           0.990325        0.902425        1.429161
H           0.807669       -0.818250        1.855743
C           2.488346        0.422246       -0.872646
H           2.543430        1.456756       -0.532351
H           1.693048        0.304338       -1.606864
H           3.444181        0.110587       -1.295146
N           2.167084       -0.442386        0.298565
H           2.934293       -0.404986        0.978504
H           2.100739       -1.416014       -0.012032
C          -0.895550        1.026577       -0.554938
H          -0.072935        1.629406       -0.964820
H          -1.499570        0.706267       -1.412934
C          -1.755198        1.938319        0.342432
H          -2.627673        1.393385        0.722201
H          -1.181025        2.292475        1.208450
H          -2.113380        2.821014       -0.205122
```

---

### Compound_20_HEI_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.466087 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.309848 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      65.7504 cm-1
2.      94.1554 cm-1
3.     124.9893 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.493464        1.600143       -0.015392
O           0.733568        2.175163       -0.215880
C          -0.706083        0.313996        0.316939
H          -1.310069        2.305266       -0.153835
C           0.453242       -0.631978        0.556192
H           0.122236       -1.679491        0.476231
H           0.829977       -0.506023        1.582476
C           2.788973       -1.126011       -0.016709
H           3.163519       -0.804153        0.960614
H           3.562751       -0.930572       -0.764553
H           2.602301       -2.211252        0.024463
N           1.586710       -0.356278       -0.349068
H           1.296930       -0.577626       -1.301569
H           1.378039        1.407114       -0.275154
C          -2.105121       -0.223769        0.499899
H          -2.171391       -0.751691        1.463540
H          -2.812891        0.612838        0.557631
C          -2.546972       -1.181722       -0.620535
H          -3.548850       -1.581640       -0.421608
H          -2.570101       -0.661607       -1.585440
H          -1.861416       -2.032473       -0.714646
```

---

### Compound_20_HEI_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.466252 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.309947 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      81.1758 cm-1
2.      91.9021 cm-1
3.     122.2562 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.447797        1.593109        0.018535
O          -0.752153        2.138465       -0.353484
C           0.691017        0.281957        0.198868
H           1.218465        2.347358        0.160655
C          -0.381872       -0.761279       -0.039758
H          -0.146634       -1.683343        0.517806
H          -0.408125       -1.044006       -1.102332
C          -2.802656       -1.161627       -0.121210
H          -2.676337       -2.184483        0.268666
H          -2.824737       -1.210379       -1.214842
H          -3.762485       -0.769162        0.226519
N          -1.727775       -0.257856        0.299273
H          -1.775561       -0.126313        1.309534
H          -1.418342        1.391528       -0.267292
C           2.066091       -0.207139        0.583960
H           2.712013        0.652530        0.802685
H           2.001214       -0.794225        1.513071
C           2.728952       -1.076441       -0.499331
H           3.719692       -1.416752       -0.174766
H           2.127969       -1.966386       -0.721942
H           2.848542       -0.510569       -1.431190
```

---

### Compound_20_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -366.466087 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -366.309848 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      65.7405 cm-1
2.      94.1464 cm-1
3.     124.9940 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.493472        1.600171       -0.015426
O           0.733557        2.175204       -0.215864
C          -0.706087        0.314015        0.316877
H          -1.310082        2.305279       -0.153904
C           0.453246       -0.631922        0.556203
H           0.122286       -1.679448        0.476248
H           0.829918       -0.505934        1.582508
C           2.788926       -1.126120       -0.016736
H           2.602082       -2.211328        0.024473
H           3.163619       -0.804307        0.960545
H           3.562663       -0.930821       -0.764658
N           1.586754       -0.356210       -0.348999
H           1.296968       -0.577365       -1.301543
H           1.378064        1.407157       -0.275012
C          -2.105123       -0.223750        0.499851
H          -2.171422       -0.751554        1.463554
H          -2.812899        0.612861        0.557458
C          -2.546941       -1.181824       -0.620484
H          -3.548633       -1.582082       -0.421312
H          -2.570483       -0.661698       -1.585372
H          -1.861124       -2.032342       -0.714788
```

---

### Compound_28_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.7893 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.61649 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      37.2268 cm-1
2.      53.1277 cm-1
3.     102.4817 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.717352        0.318180       -0.000057
C          -2.746053       -0.750169        0.000093
C          -4.052677       -0.464491        0.000061
O          -1.939197        1.521739       -0.000220
O          -0.481742       -0.209473        0.000010
C           0.634508        0.715492       -0.000120
C           1.943304       -0.078246        0.000020
C           2.034513       -0.954421       -1.261105
H          -4.402489        0.564332       -0.000077
H          -4.801262       -1.250806        0.000172
H           0.554462        1.349291       -0.889155
H           0.554441        1.349569        0.888714
H           1.969134       -0.343380       -2.170108
H           2.990425       -1.490903       -1.282287
H           1.228305       -1.694987       -1.288911
C           2.034478       -0.954034        1.261416
H           1.969066       -0.342715        2.170229
H           1.228273       -1.694596        1.289423
H           2.990392       -1.490504        1.282793
C           3.088581        0.950606       -0.000121
H           4.056622        0.436644       -0.000031
H           3.048101        1.592750       -0.888587
H           3.048078        1.593016        0.888152
H          -2.381844       -1.773340        0.000231
```

---

### Compound_28_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.788781 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.615303 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      48.2239 cm-1
2.      50.9205 cm-1
3.      69.1586 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.563035       -0.230289       -0.269667
C          -2.696804        0.695152       -0.028350
C          -3.880802        0.252020        0.408513
O          -1.592973       -1.442226       -0.111212
O          -0.482841        0.453604       -0.694803
C           0.751083       -0.265708       -0.950955
C           1.815297        0.056371        0.108389
C           1.341642       -0.397733        1.499180
H          -4.049401       -0.804480        0.598841
H          -4.706866        0.933824        0.585820
H           0.534903       -1.335015       -0.982414
H           1.075467        0.072252       -1.938939
H           1.122522       -1.471760        1.512319
H           2.119343       -0.199339        2.246063
H           0.438053        0.139315        1.809066
C           2.112123        1.565402        0.121611
H           2.456248        1.908203       -0.862251
H           1.220860        2.141991        0.391511
H           2.897472        1.792229        0.852367
C           3.084062       -0.720251       -0.287498
H           3.888220       -0.521134        0.430229
H           2.902085       -1.801892       -0.298858
H           3.439261       -0.422980       -1.281959
H          -2.513035        1.747975       -0.221017
```

---

### Compound_28_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.789028 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.616275 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      30.8710 cm-1
2.      48.2879 cm-1
3.      97.4757 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.800770        0.662647       -0.000109
C          -2.974420       -0.241437        0.000014
C          -2.898109       -1.577743        0.000199
```

```
O          -1.900021        1.884556       -0.000298
O          -0.627447        0.015399        0.000003
C           0.577887        0.819742       -0.000117
C           1.793684       -0.110175        0.000031
C           1.788104       -0.991168        1.261203
H          -1.942873       -2.093726        0.000274
H          -3.796867       -2.187650        0.000280
H           0.565869        1.458234       -0.889294
H           0.565862        1.458509        0.888863
H           0.906023       -1.639560        1.287705
H           2.680024       -1.628375        1.283268
H           1.788436       -0.376830        2.170364
C           3.044020        0.787743       -0.000104
H           3.073661        1.430509       -0.888538
H           3.073657        1.430781        0.888134
H           3.950425        0.171507       -0.000007
C           1.788112       -0.991557       -1.260869
H           2.680032       -1.628772       -1.282731
H           0.906030       -1.639957       -1.287177
H           1.788451       -0.377499       -2.170218
H          -3.930032        0.274869       -0.000062
```

---

## Compound_28_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.788372 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.615 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      35.9941 cm-1
2.      60.7577 cm-1
3.      65.5096 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.608050       -0.644990       -0.127128
C          -2.870381        0.060014        0.197219
C          -3.051549        1.380999        0.080562
O          -1.460416       -1.848337        0.047178
O          -0.662602        0.168706       -0.626183
C           0.649314       -0.371919       -0.927725
C           1.701126        0.136295        0.068631
```

```
C           1.766480        1.672535        0.031687
H          -2.262065        2.035111       -0.276286
H          -4.000709        1.838781        0.343856
H           0.591448       -1.461778       -0.923025
H           0.874060       -0.021448       -1.938747
H           0.811048        2.116119        0.331736
H           2.540891        2.037385        0.716822
H           2.009040        2.032784       -0.975973
C           1.364738       -0.340307        1.491567
H           0.406234        0.066328        1.833284
H           1.309339       -1.434074        1.540585
H           2.137217       -0.006481        2.194319
C           3.052889       -0.454078       -0.371224
H           3.849546       -0.116616        0.301782
H           3.035038       -1.550672       -0.349471
H           3.314651       -0.136750       -1.388226
H          -3.658996       -0.592928        0.559852
```

---

### Compound_28_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.781313 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.608793 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      17.8342 cm-1
2.      55.8025 cm-1
3.      95.3753 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.764777       -0.499562        0.000025
C          -2.392779        0.848798       -0.000021
C          -3.724957        0.981200       -0.000092
O          -2.407745       -1.541332        0.000046
O          -0.421603       -0.590987        0.000046
C           0.446490        0.572649        0.000002
C           1.904315        0.101469        0.000002
C           2.779520        1.368150       -0.000041
H          -4.377523        0.112944       -0.000119
H          -4.189258        1.962627       -0.000125
H           0.240147        1.169073       -0.894532
```

```
H           0.240164        1.169127        0.894503
H           2.591962        1.983613        0.888361
H           3.839979        1.091674       -0.000045
H           2.591943        1.983565       -0.888474
C           2.194263       -0.729010        1.261593
H           1.990156       -0.148834        2.170261
H           1.580573       -1.635248        1.289457
H           3.248147       -1.030098        1.282256
C           2.194241       -0.729082       -1.261547
H           3.248123       -1.030172       -1.282210
H           1.580549       -1.635320       -1.289350
H           1.990120       -0.148956       -2.170244
H          -1.758203        1.726897        0.000003
```

---

### Compound_28_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.779594 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.606434 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      17.9894 cm-1
2.      48.4175 cm-1
3.      74.9106 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.641035       -0.599381       -0.103780
C           1.994774        0.842911       -0.185528
C           3.239421        1.252382        0.088416
O           2.424179       -1.452343        0.293652
O           0.415099       -1.014259       -0.479346
C          -0.647351       -0.170345       -0.994354
C          -1.717489        0.129675        0.066628
C          -2.297459       -1.187525        0.609404
H           4.016422        0.547627        0.369513
H           3.504554        2.303933        0.036213
H          -0.238847        0.744755       -1.426436
H          -1.080885       -0.760431       -1.805914
H          -1.528994       -1.779924        1.117038
H          -3.097919       -0.979933        1.329007
H          -2.718844       -1.795965       -0.200398
```

```
C          -1.136608        0.958365        1.224297
H          -0.327221        0.426785        1.737417
H          -0.749144        1.922424        0.874718
H          -1.917497        1.162797        1.965808
C          -2.824116        0.933820       -0.640085
H          -3.625627        1.173745        0.067718
H          -2.437093        1.877665       -1.043327
H          -3.264603        0.363645       -1.467090
H           1.238223        1.566287       -0.458698
```

---

### Compound_28_HEI_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.654429 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.415109 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      22.3569 cm-1
2.      33.7205 cm-1
3.      74.2529 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.774256        0.206839       -0.290395
C          -1.647716        1.243679       -0.007173
C          -3.094715        1.003885       -0.235131
O          -1.121926       -0.965121       -0.665853
O           0.571083        0.492473       -0.122059
C           1.483732       -0.609378       -0.167787
C           2.909135       -0.101517        0.087249
C           3.846050       -1.321037        0.025071
H          -3.373167        0.806156       -1.279793
H          -3.729784        1.805410        0.147554
H           1.203864       -1.349032        0.593813
H           1.425974       -1.097426       -1.147872
H           3.801240       -1.808080       -0.957202
H           4.884031       -1.014522        0.201294
H           3.581339       -2.065677        0.786379
C           3.004152        0.548308        1.478155
H           2.345649        1.419829        1.552212
H           2.717619       -0.162982        2.263515
H           4.031311        0.877076        1.678819
```

```
C           3.314514        0.913127       -0.995501
H           4.347534        1.247968       -0.840045
H           3.251418        0.465439       -1.995706
H           2.663265        1.793044       -0.975134
N          -3.514032       -0.290490        0.478810
H          -2.778644       -0.959007        0.155237
H          -3.374971       -0.162309        1.484476
C          -4.884014       -0.789564        0.190043
H          -5.052549       -1.712690        0.746372
H          -5.609561       -0.031922        0.490218
H          -4.965477       -0.980453       -0.880658
H          -1.305424        2.177734        0.420979
```

---

### Compound_28_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.653444 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.413204 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      40.3627 cm-1
2.      59.5592 cm-1
3.      86.3856 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.938892        1.748502       -0.046212
C           2.247956        1.368624        0.242059
C           2.578837       -0.005527        0.660836
O           0.482328        2.872191       -0.370165
O           0.050363        0.646243        0.023830
C          -1.351209        0.928227       -0.028226
C          -2.146812       -0.382525        0.038871
C          -1.841159       -1.260192       -1.186792
H           1.972784       -0.400819        1.483892
H           3.635865       -0.132602        0.903728
H          -1.620020        1.575394        0.816782
H          -1.585099        1.466725       -0.953525
H          -2.449184       -2.172685       -1.166937
H          -2.061702       -0.725504       -2.119113
H          -0.789389       -1.564094       -1.213270
C          -3.639915       -0.007556        0.033228
```

```
H          -3.896506        0.614238        0.899917
H          -3.907608        0.547218       -0.874803
H          -4.260611       -0.910595        0.071051
C          -1.814108       -1.147685        1.330938
H          -2.020883       -0.531649        2.215361
H          -2.420258       -2.058916        1.404139
H          -0.758691       -1.436926        1.359679
N           2.289926       -1.027708       -0.478974
H           2.837277       -0.748980       -1.298004
H           1.303717       -0.859146       -0.717521
C           2.520755       -2.460343       -0.143781
H           2.257396       -3.079699       -1.001996
H           3.573183       -2.593297        0.109631
H           1.894877       -2.719142        0.710783
H           3.044418        2.087818        0.088183
```

---

### Compound_28_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.654913 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.414283 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      33.3558 cm-1
2.      49.9575 cm-1
3.      64.4474 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.602450       -0.803459       -0.439610
C          -1.517537       -1.349036        0.442893
C          -2.929799       -0.906527        0.325695
O          -0.869033        0.089614       -1.312742
O           0.696318       -1.291424       -0.328813
C           1.763669       -0.523852       -0.901434
C           2.518841        0.317262        0.144500
C           3.669418        1.031349       -0.586094
H          -3.416954       -1.156548       -0.626830
H          -3.561784       -1.259313        1.143194
H           2.447745       -1.254350       -1.348544
H           1.363281        0.116615       -1.691420
H           4.247073        1.645702        0.115210
```

```
H           4.357262        0.310445       -1.046228
H           3.289434        1.690420       -1.377040
C           3.090664       -0.594670        1.242469
H           3.768198       -1.346246        0.816854
H           3.656467       -0.006909        1.976082
H           2.288974       -1.120777        1.771597
C           1.580314        1.360858        0.773543
H           1.173169        2.035602        0.011481
H           0.738862        0.880220        1.284560
H           2.123030        1.966325        1.510350
N          -2.979558        0.629197        0.340994
H          -2.256913        0.871924       -0.373782
H          -2.621976        0.952589        1.243554
C          -4.294159        1.251180        0.033861
H          -4.189109        2.336785        0.053470
H          -4.607313        0.925082       -0.958769
H          -5.023304        0.930023        0.779337
H          -1.211281       -2.006117        1.247467
```

---

### Compound_28_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.654205 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.414331 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      26.2423 cm-1
2.      36.0271 cm-1
3.      58.1948 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.642770        0.294263       -0.231554
C          -1.562995        1.292975        0.036282
C          -2.890773        0.882931        0.559789
O          -0.864965       -0.957345       -0.108171
O           0.586796        0.734976       -0.711552
C           1.621511       -0.227616       -0.944601
C           2.743370       -0.144640        0.106526
C           3.377560        1.256188        0.093494
H          -2.869832        0.395581        1.544696
H          -3.611513        1.702499        0.594482
```

```
H           1.185253       -1.229242       -0.957885
H           2.030684       -0.002541       -1.937306
H           2.638702        2.023824        0.347459
H           4.196235        1.316060        0.821489
H           3.788211        1.492933       -0.896680
C           3.802972       -1.194793       -0.269659
H           3.379201       -2.207033       -0.262348
H           4.213201       -1.005689       -1.269983
H           4.635789       -1.173274        0.443658
C           2.185229       -0.449354        1.506228
H           2.985450       -0.402880        2.255417
H           1.413617        0.275238        1.789140
H           1.739231       -1.450072        1.543757
N          -3.481862       -0.207126       -0.345827
H          -2.679377       -0.871563       -0.428926
H          -3.633144        0.192784       -1.275645
C          -4.709999       -0.881898        0.150022
H          -4.484544       -1.352285        1.107807
H          -5.498756       -0.138495        0.275900
H          -5.018217       -1.638659       -0.572636
H          -1.356435        2.333313       -0.182966
```

---

### Compound_28_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.652926 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.413179 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      30.9023 cm-1
2.      36.3258 cm-1
3.      47.8193 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.670428        1.677287       -0.045552
C          -2.049239        1.539581        0.087558
C          -2.763698        0.335458       -0.376395
O           0.066896        2.643933        0.258582
O          -0.081098        0.496871       -0.588740
C           1.323211        0.500986       -0.871157
C           2.107281       -0.473980        0.024944
```

```
C           1.943970       -0.086799        1.503362
H          -2.559231        0.038491       -1.411485
H          -3.844227        0.405189       -0.234401
H           1.433764        0.206908       -1.922632
H           1.702530        1.517470       -0.742454
H           2.504415       -0.778079        2.144768
H           2.315256        0.928029        1.686852
H           0.892031       -0.119609        1.808115
C           3.589093       -0.369417       -0.377699
H           3.970222        0.648165       -0.226271
H           4.200137       -1.051515        0.225554
H           3.734188       -0.633177       -1.433061
C           1.625021       -1.917623       -0.195216
H           0.579512       -2.045402        0.105600
H           1.709448       -2.206421       -1.250390
H           2.224549       -2.619051        0.397753
N          -2.317395       -0.921912        0.422144
H          -2.485486       -0.739428        1.415322
H          -1.295982       -0.937411        0.298955
C          -2.927120       -2.214541        0.003612
H          -2.523097       -3.019543        0.618788
H          -4.008280       -2.147952        0.131019
H          -2.683585       -2.386698       -1.045323
H          -2.599331        2.321281        0.598796
```

---

### Compound_28_HEI_6_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.650829 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.412023 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      25.6094 cm-1
2.      31.8616 cm-1
3.      65.8044 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.829558        0.219548       -0.501259
C          -1.779162        1.038747        0.118878
C          -3.176724        1.020711       -0.298118
O          -1.007577       -0.614945       -1.425202
```

```
O           0.457253        0.406452        0.009495
C           1.504692       -0.376159       -0.566627
C           2.827038       -0.070823        0.150623
C           3.188038        1.416408       -0.002805
H          -3.325659        0.642697       -1.312789
H          -3.694169        1.976380       -0.176202
H           1.264371       -1.442693       -0.473954
H           1.594006       -0.145175       -1.636044
H           4.153507        1.628465        0.473098
H           3.265397        1.693810       -1.062029
H           2.430251        2.055815        0.461462
C           3.916171       -0.933813       -0.511109
H           4.017439       -0.697777       -1.577983
H           4.887363       -0.756114       -0.033887
H           3.687072       -2.003103       -0.419830
C           2.720490       -0.433817        1.641553
H           1.950900        0.165423        2.139025
H           2.463140       -1.493194        1.769608
H           3.676052       -0.254809        2.149904
N          -4.082591        0.043715        0.575820
H          -3.986853        0.342120        1.550176
H          -5.068998        0.170487        0.326543
C          -3.708084       -1.393170        0.458782
H          -3.897809       -1.713038       -0.565826
H          -2.645838       -1.476531        0.684379
H          -4.302854       -1.980052        1.159912
H          -1.463986        1.723433        0.899835
```

---

### Compound_28_HEI_8_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.651287 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.411423 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      31.4404 cm-1
2.      43.6461 cm-1
3.      60.8794 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.695723       -0.927464       -0.339072
C           1.740622       -1.070164        0.576880
C           3.126079       -0.822483        0.188121
O           0.759653       -0.562534       -1.539192
O          -0.547214       -1.278223        0.215175
C          -1.732997       -0.926290       -0.502650
C          -2.453298        0.289023        0.111986
C          -2.849180       -0.010966        1.567248
H           3.302635       -0.910473       -0.886872
H           3.859482       -1.421040        0.735689
H          -1.476717       -0.729078       -1.546981
H          -2.390729       -1.803095       -0.458326
H          -3.383997        0.840887        2.005796
H          -3.507424       -0.887756        1.623183
H          -1.964121       -0.210713        2.180827
C          -3.718260        0.546776       -0.724787
H          -4.384567       -0.325412       -0.717529
H          -4.278543        1.399918       -0.323139
H          -3.464934        0.771495       -1.768651
C          -1.542610        1.527195        0.068246
H          -0.627673        1.363592        0.648199
H          -1.252975        1.769047       -0.960918
H          -2.059788        2.397676        0.491032
N           3.604929        0.659451        0.504255
H           3.446046        0.816355        1.503337
H           4.615929        0.736293        0.351993
C           2.891359        1.705711       -0.280520
H           3.137618        1.569507       -1.333508
H           1.822830        1.563704       -0.127263
H           3.207155        2.691797        0.062548
H           1.521118       -1.390838        1.590226
```

---

## Compound_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -247.329462 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -247.277005 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      88.8904 cm-1
2.     254.5227 cm-1
3.     302.9917 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.561131       -0.119970        0.023114
O           1.488438       -0.932515       -0.121488
C          -0.844500       -0.601609        0.154212
C          -1.944964        0.109949       -0.116095
H          -2.931353       -0.336322       -0.027386
H          -1.913023        1.143406       -0.452171
H          -0.916923       -1.646271        0.445458
N           0.776651        1.218774        0.047078
H           0.059886        1.876769        0.318607
H           1.727352        1.560898       -0.009536
```

---

## Compound_7_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -247.331524 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -247.27903 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
  1.      93.0923 cm-1
  2.     254.2696 cm-1
  3.     280.0364 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.481001        0.121306        0.000020
O          -0.530683        1.360337       -0.000088
C           0.801090       -0.643283       -0.000024
C           1.985690       -0.023788       -0.000131
H           2.916325       -0.583007       -0.000161
H           2.046719        1.061195       -0.000190
H           0.739893       -1.729506        0.000034
N          -1.601756       -0.643450        0.000189
H          -2.510834       -0.198848        0.000231
H          -1.569015       -1.653793        0.000278
```

---

## Compound_7_HEI_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -343.187383 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -343.067403 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      81.9786 cm-1
2.     116.3038 cm-1
3.     148.9992 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.558584       -0.032362        0.002548
O           2.724679       -0.083930       -0.501802
C           0.666595       -1.092898        0.174298
C          -0.736864       -0.866514        0.571984
H          -1.315439       -1.790322        0.633294
H          -0.897530       -0.305286        1.501704
H           0.953672       -2.074323       -0.188784
C          -2.866148        0.418841       -0.151606
H          -3.471588       -0.481385       -0.039583
H          -3.262181        1.042554       -0.954020
H          -2.851149        0.977835        0.784653
N          -1.471372        0.017267       -0.484478
H          -0.863423        0.845330       -0.590218
H          -1.437282       -0.478545       -1.379011
N           1.065119        1.281353        0.352331
H           1.827149        1.953472        0.314790
H           0.631112        1.329363        1.273281
```

---

### Compound_7_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -343.193619 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -343.074034 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      97.2201 cm-1
2.     136.5909 cm-1
3.     160.8034 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.383638       -0.102436        0.061290
O          -0.853912       -1.250752        0.349253
C          -0.660078        1.080148        0.017684
C           0.783461        1.029351        0.368524
H           1.318029        1.953226        0.136933
H           0.995113        0.758458        1.412774
H          -1.097057        2.008811       -0.333386
C           2.843108       -0.446570       -0.027705
H           2.845066       -0.740881        1.022652
H           3.482314        0.426522       -0.170836
H           3.194152       -1.274212       -0.645828
N           1.452079       -0.102894       -0.418751
H           0.779729       -0.893265       -0.239342
H           1.394724        0.118399       -1.415975
N          -2.751129       -0.119725       -0.304690
H          -3.244396        0.750271       -0.127751
H          -3.240151       -0.905936        0.112064
```

---

## Compound_7_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -343.186797 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -343.066791 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      76.7016 cm-1
2.     109.9784 cm-1
3.     158.8220 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.389472       -0.164326        0.033442
O           2.365512       -0.824778       -0.444462
C           0.373814       -0.644647        0.862645
C          -0.824825        0.159250        1.162994
H          -1.547735       -0.372607        1.784676
H          -0.649137        1.143918        1.615103
H           0.362978       -1.704354        1.094820
C          -2.209682       -0.618850       -0.858150
H          -1.424104       -1.358123       -1.014098
H          -2.614693       -0.283301       -1.813584
H          -3.002449       -1.034983       -0.234873
N          -1.606160        0.539448       -0.146379
H          -0.895029        0.991599       -0.742541
H          -2.323968        1.241322        0.056654
N           1.264625        1.207131       -0.405313
H           1.071674        1.866994        0.347075
H           2.116431        1.493142       -0.881274
```

---

### Compound_7_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -343.188605 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -343.069539 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      64.3342 cm-1
  2.     100.5025 cm-1
  3.     112.7662 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.325673        0.043370        0.099917
O           1.211167        1.049244        0.872348
C           0.375310       -0.973094       -0.082779
C          -0.892506       -0.968044        0.636938
H          -1.293219       -1.962056        0.854672
H          -0.871024       -0.364683        1.547760
H           0.586817       -1.795987       -0.761497
C          -1.892590        1.138739       -0.479304
H          -1.912354        1.681761        0.465490
H          -2.689342        1.486762       -1.137951
```

```
H          -0.918084        1.251160       -0.952619
N          -2.087486       -0.309009       -0.189536
H          -2.971848       -0.452062        0.309345
H          -2.161749       -0.825494       -1.070090
N           2.513292       -0.025898       -0.678398
H           2.774570       -0.959696       -0.980839
H           3.290938        0.444873       -0.226149
```

---

### Compound_24_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.791059 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.617797 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      35.1631 cm-1
2.      51.0321 cm-1
3.      64.0172 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.992576       -0.302509       -0.355829
C           2.293544        0.291135        0.077346
C           3.421535       -0.689166        0.260686
C           2.415195        1.610032        0.291554
O           0.833060       -1.506184       -0.511271
O           0.027096        0.612204       -0.556998
C          -1.304859        0.164917       -0.918661
C          -2.276005        0.382638        0.240643
C          -3.698468        0.052627       -0.232992
C          -1.891572       -0.442901        1.474172
H           4.332083       -0.172203        0.575735
H           3.168147       -1.443547        1.014445
H           3.629493       -1.228958       -0.670461
H           1.582573        2.290935        0.155128
H           3.361950        2.035920        0.612890
H          -1.584076        0.773170       -1.782891
H          -1.260511       -0.886232       -1.211894
H          -2.237529        1.448342        0.507257
H          -3.985607        0.659750       -1.099905
H          -3.781390       -1.004693       -0.516250
H          -4.422545        0.242309        0.567141
```

```
H          -1.917512       -1.516475        1.248333
H          -0.885632       -0.194625        1.829894
H          -2.592363       -0.252498        2.295214
```

---

### Compound_24_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.79141 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.618022 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      39.1806 cm-1
  2.      56.3206 cm-1
  3.      58.3869 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.999062       -0.563603        0.129404
C          -2.330696        0.086063       -0.084012
C          -2.504770        1.530176        0.308701
C          -3.307470       -0.658231       -0.623126
O          -0.725696       -1.720947       -0.159304
O          -0.119995        0.286357        0.689969
C           1.232012       -0.190005        0.916530
C           2.106742       -0.039639       -0.328280
C           3.506514       -0.589264       -0.021280
C           2.167342        1.417003       -0.803274
H          -3.521977        1.865139        0.086248
H          -2.316064        1.676246        1.378283
H          -1.800008        2.174375       -0.229203
H          -3.139098       -1.695849       -0.893471
H          -4.294829       -0.243211       -0.803907
H           1.601765        0.437739        1.731617
H           1.186037       -1.229850        1.247968
H           1.661255       -0.651981       -1.123199
H           3.467822       -1.640908        0.287006
H           4.148138       -0.519884       -0.906800
H           3.984524       -0.016161        0.784011
H           2.779535        1.501112       -1.708676
H           1.169379        1.806652       -1.030728
H           2.615381        2.058309       -0.032451
```

## Compound_24_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.791578 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.618367 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      35.0092 cm-1
2.      52.4033 cm-1
3.      61.8673 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.989963       -0.433421       -0.177984
C           2.305401        0.245757        0.019649
C           3.401945       -0.619518        0.581473
C           2.464151        1.544030       -0.279634
O           0.786893       -1.597458        0.143523
O           0.056763        0.351165       -0.745176
C          -1.273077       -0.201632       -0.921569
C          -2.124336       -0.062641        0.340530
C          -3.498467       -0.697144        0.085928
C          -2.253943        1.402175        0.774919
H           4.326680       -0.045943        0.688484
H           3.122830       -1.020309        1.562751
H           3.596713       -1.480179       -0.068909
H           1.652409        2.142376       -0.678052
H           3.420570        2.036950       -0.126972
H          -1.696119        0.382633       -1.743139
H          -1.181434       -1.246371       -1.227311
H          -1.626845       -0.625320        1.141338
H          -3.408995       -1.754543       -0.190554
H          -4.122263       -0.634210        0.984578
H          -4.025967       -0.177283       -0.724594
H          -2.847905        1.480304        1.692926
H          -1.273719        1.852071        0.965191
H          -2.755029        1.994535       -0.002392
```

## Compound_24_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.791368 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.618566 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      27.9082 cm-1
2.      58.2202 cm-1
3.      60.4752 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.161851       -0.650625       -0.000014
C          -2.203107        0.425029        0.000002
C          -1.754914        1.863619        0.000030
C          -3.490208        0.048656       -0.000009
O          -1.387427       -1.854140       -0.000034
O           0.077315       -0.137088       -0.000002
C           1.188647       -1.069579       -0.000016
C           2.485734       -0.268423        0.000001
C           2.629549        0.581457       -1.269957
C           2.629542        0.581414        1.269988
H          -2.620599        2.532237        0.000040
H          -1.140969        2.087438        0.879784
H          -1.140963        2.087470       -0.879712
H          -3.769015       -1.000387       -0.000029
H          -4.289949        0.783668        0.000001
H           1.105303       -1.702486        0.889003
H           1.105308       -1.702455       -0.889056
H           3.284325       -1.024629       -0.000009
H           1.853193        1.353899       -1.312820
H           3.604691        1.081350       -1.290014
H           2.545682       -0.035330       -2.173101
H           1.853187        1.353856        1.312872
H           2.545670       -0.035403        2.173111
H           3.604685        1.081306        1.290068
```

---

### Compound_24_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.79172 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.618976 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      30.9213 cm-1
  2.      53.8661 cm-1
  3.      62.4688 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.199302       -0.633133        0.053405
C          -2.393143        0.263414       -0.055085
C          -2.176850        1.724123       -0.354792
C          -3.603566       -0.285840        0.122890
O          -1.234561       -1.830759        0.304953
O          -0.055575        0.037180       -0.159477
C           1.181950       -0.713491       -0.075907
C           2.340519        0.249529       -0.302717
C           2.386280        1.343559        0.771223
C           3.652259       -0.546492       -0.347273
H          -3.135003        2.250031       -0.397031
H          -1.552513        2.197737        0.411271
H          -1.662035        1.860648       -1.312569
H          -3.714500       -1.344081        0.337288
H          -4.507143        0.313365        0.057350
H           1.237717       -1.182040        0.912753
H           1.156978       -1.502542       -0.833771
H           2.189155        0.724076       -1.282584
H           2.539111        0.902640        1.765386
H           3.213593        2.036678        0.579751
H           1.456131        1.920583        0.794528
H           3.836110       -1.052820        0.609273
H           3.635787       -1.307575       -1.136513
H           4.498822        0.121921       -0.539405
```

---

### Compound_24_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.791477 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.618858 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      26.2886 cm-1
2.      53.9753 cm-1
3.      64.3278 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.113833       -0.545885       -0.000071
C          -2.161547        0.518818        0.000028
C          -3.584592        0.027727       -0.000059
C          -1.823679        1.817354        0.000183
O          -1.375816       -1.742828       -0.000198
O           0.139848       -0.070432       -0.000008
C           1.219657       -1.038456       -0.000097
C           2.541743       -0.279115        0.000002
C           2.712720        0.565997       -1.269746
C           2.712689        0.565720        1.269939
H          -4.281249        0.870507        0.000019
H          -3.786533       -0.593650       -0.880260
H          -3.786573       -0.593846        0.879994
H          -0.787918        2.138424        0.000241
H          -2.587308        2.590597        0.000256
H           1.117487       -1.668794        0.888881
H           1.117511       -1.668602       -0.889214
H           3.315830       -1.060394       -0.000074
H           1.961851        1.363345       -1.312049
H           3.703568        1.034006       -1.290065
H           2.608412       -0.047391       -2.173068
H           1.961817        1.363056        1.312399
H           2.608361       -0.047866        2.173125
H           3.703535        1.033726        1.290383
```

---

### Compound_24_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.791838 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.619285 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      29.9179 cm-1
2.      52.6952 cm-1
3.      59.9080 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.166595       -0.511486        0.037050
C           2.356922        0.381873       -0.089583
C           3.690654       -0.282784        0.124843
C           2.213528        1.685920       -0.370970
O           1.249681       -1.700996        0.318006
O          -0.002988        0.108702       -0.183757
C          -1.208633       -0.686950       -0.065474
C          -2.405710        0.223735       -0.308571
C          -3.686321       -0.622574       -0.314720
C          -2.483239        1.347673        0.732129
H           4.502450        0.441611        0.016209
H           3.751342       -0.729990        1.123748
H           3.846616       -1.094096       -0.595662
H           1.237719        2.135382       -0.517976
H           3.081045        2.334475       -0.459158
H          -1.161544       -1.496599       -0.800285
H          -1.238709       -1.127916        0.937020
H          -2.282257        0.673481       -1.303946
H          -3.842058       -1.104720        0.659142
H          -4.559584        0.006706       -0.519138
H          -3.647837       -1.407251       -1.079719
H          -2.607922        0.931860        1.740932
H          -1.576401        1.961151        0.727051
H          -3.339181        2.001819        0.529572
```

---

### Compound_24_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.790599 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.617083 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      34.1740 cm-1
2.      56.1551 cm-1
3.      68.7508 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.965998       -0.545712       -0.306670
C           2.137842        0.281426        0.124065
C           2.016663        1.782862        0.093458
C           3.243280       -0.364253        0.523666
O           0.933226       -1.768671       -0.307176
O          -0.058711        0.231651       -0.699481
C          -1.311401       -0.390168       -1.092995
C          -2.386088       -0.145943       -0.032985
C          -2.044247       -0.829870        1.297342
C          -2.664686        1.350764        0.159800
H           2.943497        2.246497        0.443345
H           1.807366        2.143781       -0.919858
H           1.192788        2.126350        0.729187
H           3.288507       -1.448601        0.532009
H           4.124488        0.180506        0.850132
H          -1.577973        0.088772       -2.038735
H          -1.140095       -1.455379       -1.255820
H          -3.293784       -0.616750       -0.439065
H          -1.872083       -1.903781        1.163307
H          -1.141778       -0.394127        1.743126
H          -2.862621       -0.701453        2.014905
H          -1.783247        1.862860        0.562961
H          -2.932957        1.831839       -0.788725
H          -3.492391        1.501016        0.862396
```

---

### Compound_24_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.790707 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.617423 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      30.1685 cm-1
2.      56.2006 cm-1
3.      60.1027 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.939567       -0.415640       -0.334233
C          -2.093618        0.433930        0.089514
C          -3.347512       -0.313920        0.457189
C          -1.983999        1.770045        0.144194
O          -0.977593       -1.639197       -0.321743
O           0.129728        0.296733       -0.729450
C           1.351904       -0.401419       -1.088177
C           2.419806       -0.203828       -0.011910
C           2.782640        1.276915        0.163199
C           2.014069       -0.844457        1.322081
H          -4.138220        0.382657        0.749051
H          -3.706370       -0.918718       -0.383720
H          -3.164257       -1.004134        1.288731
H          -1.064167        2.279350       -0.120565
H          -2.822596        2.384023        0.461717
H           1.123433       -1.457597       -1.239403
H           1.663405        0.046079       -2.035635
H           3.305478       -0.733772       -0.393195
H           1.925373        1.846355        0.540765
H           3.604407        1.390332        0.879568
H           3.096500        1.725563       -0.787246
H           1.132157       -0.347777        1.744725
H           1.779332       -1.908018        1.201029
H           2.826115       -0.754381        2.052581
```

---

### Compound_24_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -463.790895 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -463.617605 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      31.9148 cm-1
2.      51.1050 cm-1
3.      64.2271 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.014158       -0.462949       -0.325026
C           2.325024        0.140733        0.074661
C           2.434137        1.639843        0.178926
C           3.344008       -0.694677        0.324744
O           0.796787       -1.662575       -0.425985
O           0.092033        0.487517       -0.564226
C          -1.258054        0.091807       -0.920358
C          -2.226603        0.425752        0.213159
C          -3.660845        0.152186       -0.260893
C          -1.901833       -0.354214        1.492586
H           3.444496        1.927316        0.483839
H           2.208904        2.122073       -0.779001
H           1.722734        2.038956        0.910746
H           3.223262       -1.769858        0.238955
H           4.319191       -0.318208        0.619870
H          -1.494728        0.665422       -1.820208
H          -1.266396       -0.974965       -1.154181
H          -2.129597        1.500158        0.423973
H          -3.800861       -0.911919       -0.491268
H          -4.380510        0.422971        0.519621
H          -3.904760        0.729345       -1.160861
H          -1.989997       -1.434848        1.322906
H          -0.885678       -0.147260        1.845817
H          -2.596570       -0.079609        2.294683
```

---

### Compound_24_HEI_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.650205 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.410944 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      30.9969 cm-1
2.      42.5602 cm-1
3.      67.2154 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.191536        0.239027        0.777921
C           0.974839        1.142167        0.090643
C           0.474029        2.415558       -0.540846
```

```
C           2.430711        0.813454        0.013845
O           0.600609       -0.886786        1.253311
O          -1.142335        0.598201        0.965994
C          -2.108850       -0.450444        1.129651
C          -2.820507       -0.790558       -0.185696
C          -3.553163        0.427826       -0.762624
C          -1.861909       -1.401361       -1.217410
H           0.881563        2.551976       -1.554616
H          -0.617051        2.403438       -0.622904
H           0.743728        3.324441        0.024602
H           2.958932        0.821185        0.978322
H           2.973248        1.461868       -0.679003
H          -1.617327       -1.332754        1.547826
H          -2.834570       -0.070495        1.857564
H          -3.573182       -1.551075        0.076122
H          -4.257690        0.850376       -0.034978
H          -2.839402        1.213360       -1.036635
H          -4.118297        0.154677       -1.661971
H          -2.401230       -1.674615       -2.132625
H          -1.075996       -0.687068       -1.489408
H          -1.375976       -2.302780       -0.826374
N           2.602190       -0.622213       -0.474546
H           2.238208       -0.687391       -1.428396
H           1.921387       -1.130906        0.150459
C           3.974615       -1.183563       -0.389451
H           4.650535       -0.574802       -0.992545
H           4.290577       -1.167846        0.654438
H           3.963213       -2.210059       -0.758693
```

---

## Compound_24_HEI_11

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.650374 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.411999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      29.7937 cm-1
2.      33.0713 cm-1
3.      74.5212 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.431860       -0.048476       -0.416948
C          -1.340618        0.981254       -0.276440
C          -0.980816        2.436635       -0.119810
C          -2.781401        0.593210       -0.359214
O          -0.731887       -1.300024       -0.497092
O           0.909422        0.312775       -0.462107
C           1.868856       -0.714559       -0.190445
C           3.259104       -0.083581       -0.158610
C           3.382670        0.962560        0.956129
C           4.318693       -1.183406       -0.007502
H           0.077071        2.549139        0.136443
H          -1.154654        3.033165       -1.032448
H          -1.568312        2.917208        0.677884
H          -3.102239        0.207079       -1.337986
H          -3.452928        1.407931       -0.075791
H           1.642262       -1.186315        0.776339
H           1.814763       -1.490252       -0.962601
H           3.415564        0.417049       -1.125545
H           2.637477        1.755983        0.840400
H           3.232397        0.496056        1.939565
H           4.378471        1.422191        0.951658
H           5.327274       -0.754146       -0.013928
H           4.191390       -1.721413        0.941447
H           4.257771       -1.916086       -0.821523
N          -3.049684       -0.571753        0.588634
H          -2.262900       -1.225861        0.333518
H          -2.874504       -0.256169        1.545998
C          -4.383132       -1.216849        0.478262
H          -4.442677       -2.036367        1.195851
H          -5.158357       -0.477575        0.686865
H          -4.499344       -1.602086       -0.535526
```

---

## Compound_24_HEI_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648834 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.410273 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      31.1717 cm-1
2.      43.6183 cm-1
3.      51.8161 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.284277        1.217105       -0.290113
C          -1.493432        1.050360        0.369587
C          -2.374326        2.229655        0.705845
C          -1.954935       -0.314241        0.718225
O           0.322318        2.268679       -0.624548
O           0.281709       -0.041798       -0.678277
C           1.688894       -0.073641       -0.935813
C           2.520779       -0.154087        0.348034
C           2.176502       -1.403300        1.166704
C           4.013493       -0.109982       -0.003262
H          -1.975773        3.142937        0.252147
H          -3.404374        2.102650        0.335415
H          -2.456924        2.417591        1.789710
H          -1.227271       -0.931046        1.256545
H          -2.892924       -0.306782        1.279111
H           1.849572       -0.969409       -1.547164
H           1.969894        0.808281       -1.519239
H           2.279266        0.734408        0.948483
H           1.111067       -1.431488        1.418058
H           2.414826       -2.314955        0.601387
H           2.748478       -1.429136        2.102157
H           4.629731       -0.137475        0.903082
H           4.294599       -0.972033       -0.623396
H           4.268581        0.801430       -0.557935
N          -2.237729       -1.158594       -0.551347
H          -1.346475       -1.121545       -1.067342
H          -2.927014       -0.660450       -1.120819
C          -2.662654       -2.565876       -0.313579
H          -1.885398       -3.066762        0.264549
H          -3.599101       -2.558810        0.245588
H          -2.799139       -3.068256       -1.272081
```

---

### Compound_24_HEI_13_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645902 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.407873 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      33.9138 cm-1
2.      37.6168 cm-1
```

```
   3.      61.7289 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.450688       -0.210717       -0.495375
C          -1.458409        0.746911       -0.325813
C          -1.232535        2.054444        0.402006
C          -2.794282        0.430306       -0.815366
O          -0.526629       -1.333164       -1.067032
O           0.775728        0.184541        0.049356
C           1.897107       -0.669170       -0.188439
C           3.127235       -0.057327        0.478869
C           4.315205       -1.019595        0.343732
C           3.463130        1.322039       -0.101535
H          -0.246438        2.481234        0.184214
H          -1.985326        2.796671        0.098245
H          -1.298506        1.977450        1.501807
H          -2.811025       -0.384630       -1.540726
H          -3.356255        1.291564       -1.193251
H           1.696679       -1.668544        0.215726
H           2.063384       -0.774543       -1.269583
H           2.897988        0.061207        1.548232
H           4.093258       -1.998321        0.786587
H           4.572165       -1.177492       -0.712325
H           5.202092       -0.615078        0.845143
H           4.336127        1.755212        0.401778
H           3.698136        1.242038       -1.171950
H           2.623089        2.015043        0.009742
N          -3.783984       -0.101014        0.335384
H          -4.724885       -0.222072       -0.052150
H          -3.855432        0.640310        1.036859
C          -3.327990       -1.358882        0.986502
H          -3.362607       -2.159826        0.248022
H          -2.301494       -1.204018        1.318301
H          -3.978497       -1.588176        1.831565
```

---

### Compound_24_HEI_14

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645254 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.407263 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      25.1933 cm-1
  2.      39.7687 cm-1
  3.      72.6499 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.397653       -0.270343       -0.624060
C           1.307427        0.764235       -0.369192
C           0.917144        2.035006        0.354711
C           2.696578        0.570757       -0.762976
O           0.610107       -1.376976       -1.192154
O          -0.894428        0.020887       -0.180204
C          -1.913368       -0.943578       -0.452629
C          -3.241113       -0.426449        0.102236
C          -3.197436       -0.256834        1.627036
C          -3.686583        0.867579       -0.592867
H           1.618786        2.846164        0.110310
H          -0.086806        2.375032        0.074933
H           0.916135        1.946422        1.455552
H           2.836699       -0.220492       -1.501024
H           3.211020        1.484844       -1.079314
H          -1.990049       -1.107813       -1.535012
H          -1.650762       -1.901906        0.012722
H          -3.977892       -1.209834       -0.132167
H          -2.894190       -1.188344        2.121494
H          -2.483682        0.524592        1.911349
H          -4.183071        0.026945        2.015348
H          -4.678258        1.176943       -0.241146
H          -2.983748        1.682555       -0.385690
H          -3.739600        0.735190       -1.680904
N           3.643616        0.090951        0.447683
H           3.603178        0.816302        1.168249
H           4.616266        0.057754        0.126906
C           3.250071       -1.217921        1.035341
H           2.193925       -1.157121        1.297256
H           3.401039       -1.991138        0.282129
H           3.858038       -1.418750        1.918490
```

---

### Compound_24_HEI_15

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.6462 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.407592 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      29.1253 cm-1
2.      40.2821 cm-1
3.      54.3138 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.350133       -0.500026       -0.778389
C           1.535442       -0.904334       -0.155450
C           1.567083       -1.933050        0.955179
C           2.775842       -0.245938       -0.549601
O           0.196556        0.370145       -1.678166
O          -0.773378       -1.206157       -0.318061
C          -2.057745       -0.693539       -0.683163
C          -2.503946        0.473117        0.205403
C          -3.866501        0.990822       -0.272920
C          -2.547353        0.072447        1.684445
H           0.916745       -2.791617        0.747181
H           2.587046       -2.322571        1.084738
H           1.254680       -1.542141        1.938921
H           2.718699        0.251714       -1.518851
H           3.665068       -0.883087       -0.499806
H          -2.051339       -0.388581       -1.733791
H          -2.745509       -1.539267       -0.563389
H          -1.764526        1.275936        0.081914
H          -3.828493        1.312680       -1.321060
H          -4.633698        0.209055       -0.188014
H          -4.194604        1.845240        0.330834
H          -2.832210        0.925412        2.312634
H          -3.284326       -0.726120        1.848417
H          -1.572744       -0.292732        2.025047
N           3.194214        0.951802        0.434855
H           4.112634        1.314082        0.160155
H           3.310542        0.550370        1.368898
C           2.198791        2.057313        0.488805
H           2.162831        2.533798       -0.490599
H           1.229786        1.616892        0.721862
H           2.494020        2.775548        1.254891
```

---

### Compound_24_HEI_16_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645494 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.406881 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      26.9055 cm-1
  2.      46.8732 cm-1
  3.      65.9898 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.524161       -1.197206       -0.107185
C          -1.797727       -0.638264       -0.258395
C          -2.985422       -1.319724        0.383795
C          -2.009415        0.615047       -0.972893
O          -0.237599       -2.272927        0.480061
O           0.505649       -0.444006       -0.703899
C           1.824640       -0.997422       -0.746344
C           2.832648       -0.087057       -0.037850
C           2.912152        1.298563       -0.691990
C           2.541162        0.017822        1.464343
H          -3.134122       -1.059568        1.447100
H          -3.916317       -1.048799       -0.135467
H          -2.892333       -2.412032        0.346366
H          -1.176956        0.912334       -1.609722
H          -2.950787        0.659369       -1.532317
H           1.811805       -1.987766       -0.285034
H           2.096857       -1.101869       -1.805772
H           3.809880       -0.578765       -0.164055
H           3.144578        1.220280       -1.761598
H           1.959299        1.830444       -0.593243
H           3.690137        1.910800       -0.219986
H           3.291892        0.640449        1.965863
H           1.558453        0.470397        1.637798
H           2.544824       -0.970125        1.939961
N          -2.179790        1.884229        0.002934
H          -2.994741        1.703864        0.594623
H          -2.407374        2.712175       -0.555958
C          -0.991877        2.148469        0.857258
H          -0.748357        1.222086        1.376808
H          -0.162856        2.437901        0.212386
H          -1.221748        2.943314        1.567984
```

---

### Compound_24_HEI_16_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645494 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.406866 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.3114 cm-1
2.      46.9531 cm-1
3.      66.1691 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.524060       -1.197092       -0.107276
C          -1.797738       -0.638357       -0.258283
C          -2.985229       -1.320168        0.383930
C          -2.009761        0.614965       -0.972673
O          -0.237277       -2.272866        0.479791
O           0.505578       -0.443619       -0.703941
C           1.824584       -0.996974       -0.746902
C           2.832700       -0.087014       -0.038036
C           2.912085        1.298998       -0.691364
C           2.541462        0.016976        1.464266
H          -3.133348       -1.060870        1.447521
H          -3.916326       -1.048634       -0.134648
H          -2.892392       -2.412475        0.345551
H          -1.177478        0.912427       -1.609658
H          -2.951252        0.659158       -1.531908
H           1.811839       -1.987587       -0.286166
H           2.096627       -1.100784       -1.806437
H           3.809918       -0.578634       -0.164699
H           3.144179        1.221353       -1.761092
H           1.959301        1.830884       -0.591994
H           3.690254        1.910900       -0.219224
H           3.292159        0.639477        1.965996
H           1.558689        0.469259        1.638142
H           2.545407       -0.971230        1.939342
N          -2.180137        1.884063        0.003245
H          -2.994729        1.703379        0.595335
H          -2.408303        2.711932       -0.555528
C          -0.991905        2.148741        0.856998
H          -0.747859        1.222484        1.376528
H          -0.163274        2.438360        0.211712
H          -1.221686        2.943585        1.567758
```

### Compound_24_HEI_16_reopt_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645494 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.406881 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      26.9038 cm-1
2.      46.8730 cm-1
3.      65.9888 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.524161       -1.197207       -0.107184
C          -1.797726       -0.638264       -0.258396
C          -2.985422       -1.319723        0.383794
C          -2.009413        0.615047       -0.972895
O          -0.237599       -2.272927        0.480063
O           0.505651       -0.444008       -0.703899
C           1.824641       -0.997424       -0.746341
C           2.832648       -0.087055       -0.037849
C           2.912151        1.298562       -0.691993
C           2.541161        0.017827        1.464343
H          -3.134124       -1.059564        1.447097
H          -3.916317       -1.048799       -0.135471
H          -2.892332       -2.412031        0.346368
H          -1.176952        0.912334       -1.609722
H          -2.950784        0.659368       -1.532321
H           1.811806       -1.987766       -0.285028
H           2.096860       -1.101874       -1.805769
H           3.809881       -0.578763       -0.164052
H           3.144579        1.220276       -1.761600
H           1.959298        1.830443       -0.593249
H           3.690136        1.910802       -0.219990
H           3.291890        0.640457        1.965862
H           1.558451        0.470402        1.637796
H           2.544823       -0.970118        1.939965
N          -2.179791        1.884228        0.002932
H          -2.994744        1.703864        0.594618
H          -2.407372        2.712175       -0.555960
C          -0.991880        2.148467        0.857260
H          -0.748363        1.222084        1.376810
H          -0.162857        2.437901        0.212392
H          -1.221754        2.943312        1.567987
```

### Compound_24_HEI_18

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645333 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.406627 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      29.3716 cm-1
2.      41.7702 cm-1
3.      61.0947 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.269098       -0.474726        0.844647
C          -1.304347       -0.999131        0.062740
C          -1.058282       -1.921780       -1.112087
C          -2.668085       -0.582648        0.367359
O          -0.354938        0.328581        1.811825
O           0.991819       -0.965512        0.468530
C           2.157695       -0.348043        1.023993
C           2.875380        0.527949       -0.010533
C           3.358978       -0.294105       -1.212494
C           2.001891        1.706215       -0.460542
H          -0.295852       -2.679455       -0.894008
H          -1.981933       -2.456378       -1.376676
H          -0.723670       -1.404151       -2.027792
H          -2.782948       -0.164786        1.368666
H          -3.430209       -1.347234        0.181910
H           1.871361        0.241305        1.898737
H           2.817550       -1.163821        1.344091
H           3.759563        0.932248        0.506923
H           4.006025       -1.121380       -0.894134
H           2.507893       -0.720682       -1.756178
H           3.928018        0.330963       -1.911462
H           2.546563        2.348577       -1.163099
H           1.098877        1.345541       -0.967396
H           1.687262        2.319831        0.391415
N          -3.193837        0.610939       -0.572726
H          -4.178776        0.800509       -0.362832
H          -3.166083        0.271239       -1.537620
C          -2.393530        1.860844       -0.461031
H          -2.520532        2.260301        0.544909
```

```
H          -1.348991        1.598692       -0.625325
H          -2.735923        2.580110       -1.206198
```

---

### Compound_24_HEI_19

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.645179 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.405944 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      36.8857 cm-1
  2.      44.6620 cm-1
  3.      69.9580 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.253401       -0.393079        0.001380
C           1.118455        0.671156        0.277683
C           0.874384        2.077563       -0.224673
C           2.329847        0.390975        1.040924
O           0.355909       -1.595621        0.365518
O          -0.838678       -0.007554       -0.792784
C          -1.965628       -0.886735       -0.877656
C          -3.139149       -0.380845       -0.029605
C          -2.796407       -0.374980        1.465991
C          -3.617575        1.000730       -0.494932
H          -0.189949        2.339437       -0.202873
H           1.406128        2.806548        0.404441
H           1.214580        2.254714       -1.260185
H           2.287798       -0.546643        1.597449
H           2.650862        1.209471        1.694396
H          -2.254143       -0.913219       -1.935536
H          -1.664991       -1.890508       -0.566346
H          -3.956314       -1.100876       -0.193725
H          -2.503344       -1.372958        1.811964
H          -1.964038        0.309179        1.670013
H          -3.656942       -0.045800        2.061124
H          -4.495357        1.325127        0.077151
H          -2.827518        1.748259       -0.357048
H          -3.890970        0.989970       -1.557793
N           3.630575        0.196540        0.121485
H           4.460197        0.105448        0.716290
```

```
H           3.754522        1.058856       -0.415302
C           3.536169       -0.960659       -0.810156
H           3.510354       -1.875810       -0.218659
H           2.608543       -0.855743       -1.372254
H           4.397723       -0.960594       -1.479110
```

---

### Compound_24_HEI_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648109 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.409936 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      24.9213 cm-1
  2.      38.4299 cm-1
  3.      62.6911 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.932187       -1.289754       -0.097881
C          -1.978348       -0.440167        0.241937
C          -3.418530       -0.877663        0.127997
C          -1.675884        0.944641        0.668676
O          -0.946435       -2.500966       -0.444241
O           0.322087       -0.611401       -0.068875
C           1.506033       -1.407646       -0.159174
C           2.727356       -0.510928        0.047659
C           2.868487        0.543847       -1.058260
C           2.734545        0.135676        1.439454
H          -3.944999       -0.892476        1.096960
H          -4.010422       -0.224383       -0.534292
H          -3.474439       -1.890973       -0.282598
H          -0.923052        1.037829        1.458864
H          -2.570508        1.498443        0.964277
H           1.476649       -2.192148        0.607036
H           1.551242       -1.896316       -1.140207
H           3.593426       -1.186378       -0.020412
H           2.835622        0.086125       -2.054493
H           2.065987        1.288623       -1.001528
H           3.819198        1.081421       -0.962258
H           3.659206        0.702746        1.600199
H           1.890580        0.825707        1.551993
```

```
H           2.659206       -0.621713        2.229588
N          -1.045945        1.765508       -0.491896
H          -1.699231        1.759270       -1.279608
H          -0.236330        1.195140       -0.775014
C          -0.629040        3.155551       -0.157865
H          -1.508050        3.718200        0.158760
H           0.098431        3.110853        0.653284
H          -0.180720        3.619078       -1.037607
```

---

### Compound_24_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648281 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.409987 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.1776 cm-1
  2.      51.8584 cm-1
  3.      60.2888 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.771353       -1.331153        0.066542
C           2.007536       -0.743131       -0.171236
C           3.294846       -1.471414        0.131871
C           2.068178        0.640689       -0.694420
O           0.486460       -2.494626        0.456227
O          -0.299044       -0.408011       -0.138884
C          -1.626587       -0.937672       -0.169307
C          -2.618127        0.218865       -0.283521
C          -4.029184       -0.338465       -0.516892
C          -2.586072        1.123256        0.954940
H           3.878404       -1.722134       -0.770235
H           3.966369       -0.885546        0.780196
H           3.085094       -2.413643        0.648735
H           1.457948        0.834853       -1.583457
H           3.091780        0.969770       -0.890374
H          -1.726890       -1.614282       -1.028490
H          -1.817887       -1.519059        0.740493
H          -2.332428        0.816698       -1.161316
H          -4.348503       -0.961592        0.329087
H          -4.755354        0.475526       -0.623941
```

```
H          -4.073267       -0.952811       -1.424287
H          -3.290172        1.956836        0.847621
H          -2.867014        0.557330        1.853282
H          -1.591183        1.547750        1.125888
N           1.496809        1.657056        0.331730
H           2.022974        1.560960        1.204342
H           0.548934        1.300811        0.519612
C           1.456764        3.078090       -0.112266
H           1.009920        3.689073        0.672948
H           2.475986        3.409459       -0.314915
H           0.856058        3.137322       -1.020324
```

---

### Compound_24_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.650374 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.411999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      29.7940 cm-1
  2.      33.0710 cm-1
  3.      74.5212 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.431860       -0.048476       -0.416950
C          -1.340618        0.981254       -0.276441
C          -0.980816        2.436635       -0.119811
C          -2.781400        0.593209       -0.359214
O          -0.731887       -1.300024       -0.497094
O           0.909422        0.312775       -0.462109
C           1.868856       -0.714559       -0.190447
C           3.259104       -0.083580       -0.158609
C           3.382668        0.962559        0.956132
C           4.318693       -1.183405       -0.007501
H           0.077071        2.549139        0.136442
H          -1.154655        3.033166       -1.032448
H          -1.568312        2.917207        0.677885
H          -3.102239        0.207078       -1.337986
H          -3.452928        1.407931       -0.075791
H           1.642261       -1.186316        0.776336
H           1.814765       -1.490251       -0.962604
```

```
H           3.415565        0.417051       -1.125543
H           2.637474        1.755982        0.840404
H           3.232394        0.496053        1.939567
H           4.378469        1.422190        0.951663
H           5.327274       -0.754144       -0.013925
H           4.191389       -1.721414        0.941446
H           4.257773       -1.916083       -0.821524
N          -3.049683       -0.571753        0.588635
H          -2.874501       -0.256170        1.545998
H          -2.262900       -1.225862        0.333518
C          -4.383131       -1.216849        0.478264
H          -4.499346       -1.602085       -0.535524
H          -4.442676       -2.036367        1.195853
H          -5.158356       -0.477575        0.686869
```

---

## Compound_24_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648834 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.410273 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      31.1717 cm-1
  2.      43.6184 cm-1
  3.      51.8161 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.284277        1.217105       -0.290113
C          -1.493432        1.050360        0.369587
C          -2.374326        2.229655        0.705845
C          -1.954935       -0.314241        0.718225
O           0.322318        2.268679       -0.624548
O           0.281709       -0.041798       -0.678277
C           1.688894       -0.073641       -0.935813
C           2.520779       -0.154087        0.348034
C           2.176502       -1.403300        1.166704
C           4.013493       -0.109982       -0.003262
H          -3.404374        2.102650        0.335415
H          -2.456924        2.417591        1.789710
H          -1.975774        3.142937        0.252147
H          -1.227271       -0.931046        1.256545
```

```
H          -2.892924       -0.306782        1.279111
H           1.849572       -0.969409       -1.547164
H           1.969894        0.808281       -1.519239
H           2.279266        0.734408        0.948483
H           1.111067       -1.431488        1.418058
H           2.414826       -2.314955        0.601387
H           2.748478       -1.429136        2.102156
H           4.629731       -0.137475        0.903082
H           4.294599       -0.972033       -0.623396
H           4.268581        0.801430       -0.557935
N          -2.237729       -1.158594       -0.551347
H          -1.346475       -1.121545       -1.067342
H          -2.927014       -0.660450       -1.120819
C          -2.662654       -2.565876       -0.313579
H          -2.799139       -3.068256       -1.272081
H          -3.599101       -2.558810        0.245588
H          -1.885398       -3.066762        0.264549
```

---

### Compound_24_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.65029 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.411933 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.1459 cm-1
  2.      35.6957 cm-1
  3.      74.6486 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.425930        0.030106        0.195530
C           1.365616        1.017846       -0.024998
C           1.057576        2.416414       -0.495759
C           2.776710        0.658328        0.309892
O           0.690125       -1.179346        0.555337
O          -0.902791        0.384936       -0.005778
C          -1.855104       -0.679261       -0.101813
C          -3.240638       -0.075477       -0.320570
C          -4.257007       -1.200819       -0.557459
C          -3.664318        0.813823        0.854902
H           1.117831        3.173788        0.305401
```

```
H           1.756434        2.743703       -1.281117
H           0.046408        2.474015       -0.910404
H           2.967140        0.467732        1.376478
H           3.494307        1.406512       -0.037134
H          -1.587076       -1.337874       -0.938668
H          -1.840682       -1.280314        0.815592
H          -3.193118        0.544783       -1.227680
H          -3.977387       -1.822103       -1.417129
H          -4.328991       -1.854139        0.322355
H          -5.254582       -0.788723       -0.748648
H          -4.653269        1.252524        0.674836
H          -3.721189        0.225913        1.781388
H          -2.951566        1.629197        1.014327
N           3.137246       -0.665954       -0.357389
H           2.312115       -1.261782       -0.082774
H           3.089609       -0.540614       -1.371669
C           4.432227       -1.273820        0.041958
H           4.411813       -1.458016        1.116829
H           4.563838       -2.214984       -0.493940
H           5.243018       -0.585509       -0.202888
```

---

### Compound_24_HEI_5_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.65029 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.411933 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.1459 cm-1
  2.      35.6957 cm-1
  3.      74.6486 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.425930        0.030106        0.195531
C           1.365616        1.017846       -0.024998
C           1.057576        2.416414       -0.495759
C           2.776710        0.658329        0.309892
O           0.690126       -1.179346        0.555337
O          -0.902791        0.384936       -0.005777
C          -1.855104       -0.679261       -0.101813
C          -3.240638       -0.075477       -0.320570
```

```
C          -4.257007       -1.200818       -0.557460
C          -3.664318        0.813823        0.854902
H           1.117833        3.173788        0.305401
H           1.756432        2.743702       -1.281119
H           0.046407        2.474015       -0.910402
H           2.967141        0.467733        1.376477
H           3.494307        1.406512       -0.037136
H          -1.587076       -1.337874       -0.938668
H          -1.840682       -1.280314        0.815592
H          -3.193117        0.544784       -1.227680
H          -3.977387       -1.822102       -1.417130
H          -4.328991       -1.854139        0.322354
H          -5.254582       -0.788723       -0.748649
H          -4.653269        1.252524        0.674835
H          -3.721190        0.225912        1.781388
H          -2.951566        1.629196        1.014328
N           3.137246       -0.665954       -0.357389
H           2.312114       -1.261782       -0.082773
H           3.089608       -0.540615       -1.371669
C           4.432226       -1.273820        0.041958
H           4.411814       -1.458015        1.116829
H           4.563837       -2.214985       -0.493939
H           5.243018       -0.585510       -0.202889
```

---

### Compound_24_HEI_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.647466 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.40843 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      34.0768 cm-1
2.      51.9131 cm-1
3.      65.0406 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.602465       -1.297633       -0.254748
C          -1.855391       -0.724663       -0.081795
C          -3.003763       -1.517757        0.494138
C          -2.076775        0.689340       -0.463743
O          -0.221970       -2.479673       -0.056626
```

```
O           0.362031       -0.327781       -0.694593
C           1.691854       -0.770058       -0.991639
C           2.723783       -0.149471       -0.043787
C           2.792170        1.378000       -0.174988
C           2.487003       -0.575765        1.410492
H          -3.789828       -1.753501       -0.243887
H          -2.644255       -2.472368        0.892270
H          -3.504643       -0.986093        1.318852
H          -1.758549        0.959749       -1.477098
H          -3.115319        1.001109       -0.326739
H           1.719577       -1.860012       -0.923046
H           1.904692       -0.469954       -2.025948
H           3.694530       -0.555684       -0.367720
H           2.938540        1.683983       -1.218152
H           1.872716        1.852952        0.187681
H           3.620734        1.783160        0.417966
H           3.252730       -0.151185        2.070719
H           1.508171       -0.229386        1.764147
H           2.512006       -1.666511        1.513721
N          -1.233527        1.644744        0.419110
H          -0.274599        1.286500        0.300697
H          -1.486808        1.484428        1.397597
C          -1.312842        3.091700        0.076154
H          -0.988866        3.218332       -0.957288
H          -2.346261        3.422047        0.187203
H          -0.661805        3.656698        0.744502
```

---

### Compound_24_HEI_6_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.647466 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.408431 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      34.0633 cm-1
2.      51.8868 cm-1
3.      65.0419 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.602499       -1.297631       -0.254702
C          -1.855416       -0.724637       -0.081779
```

```
C          -3.003835       -1.517723        0.494062
C          -2.076771        0.689374       -0.463724
O          -0.222030       -2.479680       -0.056580
O           0.362027       -0.327795       -0.694518
C           1.691827       -0.770104       -0.991612
C           2.723805       -0.149499       -0.043827
C           2.792182        1.377969       -0.175066
C           2.487095       -0.575760        1.410474
H          -3.789840       -1.753474       -0.244024
H          -2.644354       -2.472328        0.892226
H          -3.504781       -0.986051        1.318731
H          -1.758558        0.959780       -1.477083
H          -3.115308        1.001158       -0.326705
H           1.719536       -1.860055       -0.922984
H           1.904626       -0.470040       -2.025940
H           3.694534       -0.555719       -0.367798
H           2.938500        1.683927       -1.218244
H           1.872744        1.852924        0.187637
H           3.620774        1.783145        0.417837
H           3.252848       -0.151158        2.070655
H           1.508276       -0.229384        1.764164
H           2.512116       -1.666503        1.513727
N          -1.233499        1.644756        0.419120
H          -0.274576        1.286497        0.300697
H          -1.486771        1.484443        1.397610
C          -1.312798        3.091714        0.076169
H          -0.988865        3.218343       -0.957286
H          -2.346206        3.422081        0.187264
H          -0.661723        3.656698        0.744491
```

---

### Compound_24_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648377 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.409167 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      36.9609 cm-1
2.      44.6036 cm-1
3.      59.2617 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.504458       -1.263407       -0.273213
C           1.825931       -0.888746       -0.072354
C           2.825424       -1.851106        0.523032
C           2.279621        0.462962       -0.479662
O          -0.065313       -2.362501       -0.053144
O          -0.277571       -0.173632       -0.788924
C          -1.691325       -0.346093       -0.930845
C          -2.460148        0.499594        0.088688
C          -3.962141        0.444032       -0.219889
C          -2.172156        0.055735        1.527731
H           3.513310       -2.292942       -0.219241
H           3.459330       -1.366212        1.281132
H           2.310388       -2.684581        1.012652
H           2.052580        0.748583       -1.513657
H           3.347501        0.613607       -0.302990
H          -1.946096       -0.030643       -1.949964
H          -1.934951       -1.406345       -0.816188
H          -2.125006        1.541783       -0.027982
H          -4.176917        0.794821       -1.236825
H          -4.340759       -0.582875       -0.129914
H          -4.527597        1.070416        0.479846
H          -2.668495        0.719201        2.246170
H          -2.540130       -0.964182        1.697685
H          -1.098535        0.062628        1.745273
N           1.560496        1.561786        0.339941
H           1.733645        1.382963        1.332798
H           0.562487        1.363669        0.174176
C           1.895660        2.968456       -0.015123
H           1.655351        3.125613       -1.067119
H           1.310006        3.645416        0.608039
H           2.961547        3.127088        0.152874
```

---

### Compound_24_HEI_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Energy | -559.648309 |
| B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Free Energy (Quasiharmonic) | -559.408957 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      27.9654 cm-1
2.      50.8049 cm-1
3.      62.0734 cm-1
```

### B3LYP-D3(BJ)/6-31+G(d)-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.274055       -1.270036       -0.420954
C           1.423539       -1.002275        0.308361
C           2.405918       -2.095796        0.652660
C           1.698447        0.382934        0.757833
O          -0.191250       -2.365608       -0.829384
O          -0.407391       -0.062225       -0.786019
C          -1.798663       -0.136502       -1.118406
C          -2.685712        0.324620        0.043852
C          -2.542184       -0.594178        1.264404
C          -2.415311        1.788285        0.415782
H           2.391152       -2.380771        1.718854
H           2.184758       -3.001911        0.078485
H           3.444256       -1.808135        0.424318
H           0.873918        0.875206        1.285537
H           2.600274        0.451291        1.371480
H          -1.942592        0.519640       -1.984870
H          -2.036001       -1.163370       -1.410203
H          -3.720677        0.250347       -0.325276
H          -2.778506       -1.634262        1.010842
H          -1.516370       -0.567694        1.650862
H          -3.214752       -0.277855        2.070864
H          -3.102934        2.127012        1.200076
H          -1.392297        1.909195        0.790910
H          -2.537689        2.449401       -0.451499
N           1.942083        1.328714       -0.446263
H           1.083378        1.224995       -1.007041
H           2.705897        0.940628       -1.006445
C           2.201398        2.757156       -0.114964
H           1.349817        3.142546        0.446585
H           3.106342        2.816850        0.490881
H           2.327652        3.323304       -1.038700
```

---

### Methylamine

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -95.914405 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -95.871383 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 15)

```
  1.     300.4720 cm-1
  2.     879.3801 cm-1
```

```
  3.     977.4742 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.706643        0.000001        0.016444
H          -1.123193        0.878347       -0.475592
H          -1.055861        0.000371        1.054202
H          -1.123101       -0.878758       -0.474928
N           0.754103        0.000002       -0.130249
H           1.131638        0.806547        0.354694
H           1.131655       -0.806531        0.354703
```

---

### Compound_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -730.316857 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -730.240513 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      56.6682 cm-1
  2.      99.2792 cm-1
  3.     152.3673 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.072867        1.268052       -0.000010
H          -0.567247        2.239633       -0.000054
C          -0.190141        0.116329       -0.000002
C           1.160914        0.167459       -0.000037
C           1.943859        1.440065       -0.000055
H           2.599240        1.444566        0.874493
H           2.599132        1.444615       -0.874684
H           1.353911        2.349153        0.000009
C           1.983646       -1.080678       -0.000041
H           1.756208       -1.691307        0.875873
H           1.755887       -1.691549       -0.875698
H           3.045393       -0.847932       -0.000256
O          -2.294742        1.217737        0.000022
Cl         -1.008062       -1.438614        0.000059
```

## Compound_12_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -826.238362 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -826.093086 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      57.8944 cm-1
  2.     141.0058 cm-1
  3.     177.1993 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.450626        1.738699        0.086170
H          -1.280933        2.399625       -0.187693
C          -0.674145        0.402099        0.014670
C           0.353377       -0.641681        0.394701
C           0.462031       -0.774127        1.916453
H           1.237771       -1.491673        2.191677
H           0.688458        0.187670        2.375047
H          -0.490038       -1.127760        2.308017
C           0.149968       -2.009982       -0.238242
H          -0.004270       -1.949364       -1.313132
H           1.018435       -2.638083       -0.037614
H          -0.721454       -2.487053        0.203155
O           0.681116        2.294261        0.433368
C           1.964086       -0.078631       -1.523407
H           1.116975        0.366071       -2.036554
H           2.855843        0.514745       -1.705146
H           2.123447       -1.094185       -1.868901
N           1.696397       -0.069163       -0.066542
H           1.639976        0.937959        0.247842
H           2.442600       -0.555446        0.426967
Cl         -2.281098       -0.161807       -0.441582
```

## Compound_12_HEI_3

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -826.234438 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -826.088949 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      42.4560 cm-1
  2.      90.9075 cm-1
  3.     133.8854 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.752441        1.082512       -0.227243
H           1.364909        2.110066       -0.232885
C           0.802853        0.138965        0.044583
C          -0.649882        0.357595        0.321953
C          -1.031837        1.834639        0.339632
H          -2.093471        1.944621        0.550716
H          -0.482540        2.339640        1.130365
H          -0.809683        2.322624       -0.608042
C          -1.133423       -0.325696        1.600606
H          -1.009094       -1.405771        1.556097
H          -0.538523        0.052700        2.429858
H          -2.178937       -0.098739        1.800875
O           3.002211        0.920253       -0.458411
C          -2.893673       -0.372934       -0.842231
H          -3.310334        0.622178       -0.737784
H          -3.225489       -0.813873       -1.778035
H          -3.196767       -1.002466       -0.013643
N          -1.408849       -0.290535       -0.879664
H          -1.117328        0.227604       -1.708714
H          -1.032788       -1.234243       -0.982852
Cl          1.317378       -1.569595        0.058540
```

---

### Compound_12_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -826.233332 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -826.086975 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 57)

```
1.     -15.3888 cm-1
2.      99.4366 cm-1
3.     144.0350 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.492158        1.102459        0.416054
H          -1.025508        2.065528        0.669240
C          -0.625349        0.206478       -0.148589
C           0.838692        0.429352       -0.356078
C           1.193099        1.893820       -0.633144
H           2.272001        1.993053       -0.759883
H           0.706294        2.213861       -1.551145
H           0.883470        2.553892        0.174225
C           1.464825       -0.440299       -1.440804
H           1.326010       -1.502099       -1.262589
H           1.000917       -0.196463       -2.394706
H           2.532009       -0.229973       -1.513654
O          -2.738764        0.969025        0.676812
C           1.404249       -1.225528        1.582473
H           1.741182       -1.992551        0.894461
H           0.349966       -1.347522        1.803065
H           1.983759       -1.273608        2.499953
N           1.611850        0.112086        0.974619
H           2.607844        0.254582        0.800072
H           1.321441        0.822243        1.646511
Cl         -1.280728       -1.393849       -0.574227
```

---

### Compound_19

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -231.35349 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -231.290992 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.     128.7451 cm-1
2.     201.5906 cm-1
3.     217.8564 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.378812        0.331136        0.000003
O           2.462581       -0.243865       -0.000026
C           0.094076       -0.333475       -0.000013
C          -1.035909        0.388064        0.000022
H           0.081055       -1.417623       -0.000054
H           1.341678        1.433588        0.000046
C          -2.410341       -0.164927        0.000010
H          -2.959783        0.196261        0.873825
H          -2.959793        0.196325       -0.873773
H          -2.415566       -1.253581       -0.000030
H          -0.948059        1.471167        0.000063
```

---

## Compound_19_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -231.348871 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -231.286708 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.     136.5441 cm-1
2.     200.6098 cm-1
3.     206.5125 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.501308        0.420623       -0.000003
O          -2.031840       -0.684401       -0.000005
C          -0.065081        0.673728        0.000000
C           0.845141       -0.309212        0.000002
H           0.491239       -1.335542        0.000001
H           0.239988        1.713372        0.000001
H          -2.135164        1.322014       -0.000004
C           2.313713       -0.112938        0.000005
H           2.757426       -0.599152        0.873521
H           2.757431       -0.599154       -0.873508
H           2.589003        0.940471        0.000005
```

### Compound_19_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -327.273943 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -327.144767 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      70.9538 cm-1
2.     125.7857 cm-1
3.     182.2642 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           2.039497        0.199208       -0.063607
O           1.965929       -1.088544        0.159633
C           0.996916        1.070460       -0.021019
C          -0.386351        0.613380        0.328966
H          -0.465672        0.337884        1.384558
H           1.152007        2.115030       -0.250665
H           3.025403        0.604004       -0.331021
C          -1.468744        1.615879       -0.018492
H          -2.459419        1.265217        0.267038
H          -1.274490        2.545894        0.514960
H          -1.463514        1.830869       -1.088706
N          -0.622372       -0.704838       -0.394232
H          -0.736452       -0.507829       -1.387769
H           0.294731       -1.201363       -0.264214
C          -1.747929       -1.526056        0.102485
H          -1.587027       -1.731881        1.156979
H          -2.684216       -0.994279       -0.034095
H          -1.772520       -2.458556       -0.454500
```

### Compound_19_HEI_4_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -327.273943 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -327.144767 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      70.9531 cm-1
2.     125.7856 cm-1
3.     182.2631 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           2.039498        0.199208       -0.063607
O           1.965930       -1.088544        0.159634
C           0.996916        1.070460       -0.021020
C          -0.386351        0.613379        0.328966
H          -0.465671        0.337883        1.384558
H           1.152007        2.115030       -0.250667
H           3.025403        0.604004       -0.331021
C          -1.468743        1.615879       -0.018491
H          -2.459418        1.265216        0.267038
H          -1.274490        2.545893        0.514962
H          -1.463513        1.830870       -1.088705
N          -0.622373       -0.704838       -0.394233
H           0.294730       -1.201364       -0.264215
H          -0.736454       -0.507828       -1.387770
C          -1.747930       -1.526055        0.102485
H          -1.772524       -2.458553       -0.454503
H          -1.587025       -1.731883        1.156978
H          -2.684216       -0.994276       -0.034091
```

---

### Compound_19_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -327.273943 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -327.144767 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      70.9518 cm-1
2.     125.7853 cm-1
```

```
   3.     182.2615 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           2.039498        0.199208       -0.063607
O           1.965933       -1.088543        0.159633
C           0.996916        1.070459       -0.021020
C          -0.386352        0.613379        0.328966
H          -0.465672        0.337882        1.384558
H           1.152006        2.115029       -0.250668
H           3.025402        0.604006       -0.331022
C          -1.468744        1.615879       -0.018491
H          -2.459419        1.265214        0.267035
H          -1.274492        2.545892        0.514964
H          -1.463512        1.830872       -1.088704
N          -0.622374       -0.704838       -0.394233
H           0.294729       -1.201364       -0.264216
H          -0.736456       -0.507827       -1.387770
C          -1.747930       -1.526055        0.102486
H          -1.772528       -2.458551       -0.454505
H          -1.587022       -1.731887        1.156977
H          -2.684216       -0.994273       -0.034085
```

---

### Compound_26_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.62272 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477426 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
   1.      36.1327 cm-1
   2.      55.7175 cm-1
   3.      72.3693 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.789413       -0.425146       -0.098111
C          -2.700438        0.735120       -0.086345
C          -2.331303        1.979711        0.198726
```

```
O          -2.165362       -1.553164       -0.378012
O          -0.529455       -0.131696        0.220706
C           0.430830       -1.222599        0.225628
C           1.787681       -0.647075        0.555530
C           2.331631        0.307063       -0.504744
C           3.716049        0.838958       -0.152815
H          -3.724129        0.491964       -0.337637
H          -1.309848        2.230070        0.449913
H          -3.051740        2.786560        0.186759
H           0.421107       -1.691775       -0.758039
H           0.110442       -1.953545        0.966635
H           1.739345       -0.144187        1.525129
H           2.472430       -1.491110        0.674233
H           1.640536        1.143077       -0.632298
H           2.368901       -0.214563       -1.465365
H           3.696479        1.386992        0.791791
H           4.434845        0.023318       -0.047365
H           4.089949        1.515883       -0.922527
```

---

### Compound_26_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622937 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477172 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      40.1120 cm-1
  2.      60.9122 cm-1
  3.      76.3455 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.425890       -0.264952        0.042374
C          -2.422340        0.670020       -0.518472
C          -3.480276        1.062657        0.182286
O          -1.474936       -0.764138        1.152737
O          -0.446601       -0.505594       -0.839061
C           0.639487       -1.383279       -0.430559
C           1.698911       -0.638243        0.356298
C           2.363506        0.495183       -0.420270
C           3.446000        1.197372        0.391393
H          -2.243172        1.018718       -1.526197
```

```
H          -3.649462        0.709114        1.191162
H          -4.204208        1.748660       -0.235454
H           1.038614       -1.758922       -1.370176
H           0.222848       -2.210978        0.138316
H           1.263304       -0.252729        1.280643
H           2.452486       -1.375332        0.648252
H           1.605859        1.221359       -0.723002
H           2.794435        0.092896       -1.341527
H           4.232679        0.498512        0.684221
H           3.910889        2.003454       -0.178374
H           3.031637        1.630554        1.304430
```

---

### Compound_26_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.623397 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477914 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      39.0579 cm-1
  2.      64.0393 cm-1
  3.      72.9442 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.626255        0.237116        0.017625
C          -2.444530       -0.973901       -0.193717
C          -3.750958       -0.982123        0.046300
O          -2.042879        1.311659        0.414623
O          -0.343475        0.012465       -0.284194
C           0.583324        1.120480       -0.121271
C           1.967268        0.630744       -0.476635
C           2.514609       -0.431548        0.473153
C           3.925349       -0.872471        0.100397
H          -1.924038       -1.851220       -0.552478
H          -4.262306       -0.098439        0.405608
H          -4.342406       -1.873588       -0.110590
H           0.529287        1.461304        0.912603
H           0.261050        1.930103       -0.774553
H           1.962593        0.252180       -1.502320
H           2.626194        1.503163       -0.468271
H           2.508497       -0.033650        1.491924
```

```
H           1.849482       -1.297803        0.474518
H           3.949745       -1.297776       -0.905343
H           4.618206       -0.028290        0.119406
H           4.301690       -1.628750        0.790955
```

---

### Compound_26_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622464 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.476228 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      32.5522 cm-1
  2.      61.7889 cm-1
  3.      71.6841 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.361189        0.244317       -0.153692
C           2.318295       -0.879658       -0.203827
C           3.514169       -0.801953        0.369170
O           1.565546        1.320122        0.380499
O           0.222854       -0.067847       -0.785144
C          -0.847506        0.917006       -0.793073
C          -1.653234        0.885780        0.492588
C          -2.234608       -0.483120        0.850674
C          -3.200020       -1.042300       -0.190015
H           1.992400       -1.767908       -0.727275
H           3.830141        0.090975        0.892898
H           4.207801       -1.630516        0.329404
H          -1.449146        0.638397       -1.653584
H          -0.416446        1.900388       -0.965528
H          -1.031904        1.245906        1.313631
H          -2.463837        1.609697        0.368221
H          -2.750532       -0.390290        1.808797
H          -1.418011       -1.190924        1.011518
H          -2.701826       -1.240338       -1.140228
H          -3.638783       -1.981237        0.151037
H          -4.016766       -0.342788       -0.382685
```

---

### Compound_26_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622851 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477116 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      50.8755 cm-1
  2.      60.9917 cm-1
  3.      69.2937 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.571354        0.040354        0.190064
C          -2.849538        0.192567       -0.533833
C          -3.852664       -0.660962       -0.361271
O          -1.317925       -0.836588        0.996530
O          -0.708579        1.007916       -0.152316
C           0.613319        0.984480        0.450029
C           1.553817        0.078832       -0.318808
C           2.960238        0.100555        0.275210
C           3.928412       -0.794923       -0.489495
H          -2.923362        1.031575       -1.211945
H          -3.767730       -1.498687        0.318773
H          -4.784982       -0.543091       -0.896092
H           0.520631        0.679500        1.490353
H           0.942917        2.020064        0.409791
H           1.165467       -0.941686       -0.309551
H           1.587163        0.404464       -1.361380
H           2.914395       -0.216509        1.320561
H           3.334638        1.127900        0.278961
H           4.012738       -0.480366       -1.531858
H           4.926747       -0.766019       -0.050288
H           3.590034       -1.833184       -0.482413
```

---

### Compound_26_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.623221 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477928 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      40.6007 cm-1
2.      61.8116 cm-1
3.      87.0971 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.769222        0.196380       -0.000001
C           2.855783       -0.803380        0.000001
C           4.133880       -0.441541       -0.000000
O           1.920033        1.405583       -0.000003
O           0.568250       -0.394253        0.000000
C          -0.596665        0.472106       -0.000001
C          -1.826912       -0.404323        0.000001
C          -3.107464        0.427178        0.000000
C          -4.362286       -0.438310        0.000002
H           2.555675       -1.842175        0.000002
H           4.422942        0.601471       -0.000002
H           4.924038       -1.179712        0.000001
H          -0.553561        1.106393        0.885139
H          -0.553561        1.106390       -0.885143
H          -1.807870       -1.052256        0.879838
H          -1.807871       -1.052259       -0.879833
H          -3.112544        1.081696       -0.875820
H          -3.112544        1.081699        0.875818
H          -5.265887        0.173092        0.000001
H          -4.394217       -1.081820       -0.881760
H          -4.394217       -1.081817        0.881767
```

---

## Compound_26_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622936 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.477192 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      31.5785 cm-1
2.      46.4307 cm-1
3.      76.9848 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.447793        0.270375        0.072924
C           2.387390       -0.765360       -0.401732
C           3.644757       -0.813271        0.023878
O           1.713275        1.155019        0.868548
O           0.242399        0.120727       -0.485321
C          -0.792759        1.065980       -0.102085
C          -2.076025        0.659950       -0.790907
C          -2.601772       -0.725653       -0.409288
C          -2.922762       -0.880534        1.074325
H           1.996985       -1.481431       -1.111766
H           4.025927       -0.091892        0.735065
H           4.325328       -1.576028       -0.328504
H          -0.475063        2.061400       -0.409491
H          -0.883123        1.051719        0.982400
H          -2.821840        1.417724       -0.535779
H          -1.928714        0.714631       -1.871789
H          -1.875301       -1.484831       -0.707488
H          -3.502899       -0.918341       -0.995451
H          -2.028906       -0.793627        1.693857
H          -3.631375       -0.117407        1.404396
H          -3.366138       -1.856810        1.276045
```

---

### Compound_26_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622829 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.476906 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      46.3738 cm-1
2.      60.2010 cm-1
3.      88.7067 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.334663        0.227905        0.179353
C          -2.434970       -0.254235       -0.680739
C          -3.388334       -1.050766       -0.210585
O          -1.200766       -0.034627        1.360978
O          -0.494847        1.005540       -0.517940
C           0.681846        1.550583        0.141781
C           1.922483        0.783108       -0.265636
C           1.957905       -0.665808        0.212962
C           3.237057       -1.380819       -0.207552
H          -2.420604        0.072704       -1.711241
H          -3.393133       -1.374187        0.822217
H          -4.188955       -1.400329       -0.847787
H           0.525929        1.530248        1.217189
H           0.731928        2.583320       -0.195178
H           2.021361        0.817715       -1.353963
H           2.779228        1.325909        0.144004
H           1.094911       -1.204715       -0.185474
H           1.861830       -0.687153        1.301479
H           3.339158       -1.393532       -1.294940
H           4.118328       -0.882108        0.201815
H           3.246976       -2.414984        0.140068
```

---

### Compound_26_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622196 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.476518 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      38.3357 cm-1
  2.      47.4133 cm-1
  3.      69.6869 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.488722       -0.465847       -0.253497
C           2.563969        0.528305       -0.433452
C           2.690723        1.640751        0.282705
```

```
O           1.387348       -1.454636       -0.962253
O           0.653522       -0.184887        0.749105
C          -0.472774       -1.078433        0.971401
C          -1.636948       -0.754068        0.057609
C          -2.182081        0.661139        0.229556
C          -3.375295        0.936879       -0.678090
H           3.260605        0.281988       -1.223557
H           1.996179        1.895904        1.071051
H           3.501772        2.330802        0.092698
H          -0.733341       -0.912877        2.014477
H          -0.134443       -2.104000        0.844724
H          -1.342400       -0.916734       -0.981383
H          -2.424063       -1.481031        0.277849
H          -1.389712        1.383096        0.019998
H          -2.469616        0.809521        1.274343
H          -3.102939        0.818194       -1.729156
H          -4.195565        0.246593       -0.469024
H          -3.751335        1.952369       -0.544229
```

---

### Compound_26_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -424.622139 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -424.476155 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      38.7112 cm-1
  2.      53.9180 cm-1
  3.      70.3362 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.462321        0.076473       -0.161289
C          -2.836215       -0.405820        0.085540
C          -3.829775        0.433158        0.356669
O          -1.112257        1.243182       -0.150139
O          -0.632379       -0.946661       -0.409339
C           0.768356       -0.642369       -0.648681
C           1.533696       -0.550181        0.657823
C           3.034112       -0.341694        0.441740
C           3.389573        1.005849       -0.181653
H          -2.989215       -1.475036        0.035204
```

```
H          -3.665731        1.501837        0.405992
H          -4.833079        0.072135        0.536148
H           0.829028        0.272564       -1.231430
H           1.124319       -1.474859       -1.251692
H           1.130415        0.269124        1.256957
H           1.368838       -1.473763        1.216425
H           3.423742       -1.150800       -0.182593
H           3.533174       -0.432349        1.408613
H           4.471420        1.130773       -0.248598
H           2.984546        1.107477       -1.189349
H           2.995081        1.828229        0.419259
```

---

### Compound_26_HEI_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535163 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323998 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.6429 cm-1
  2.      36.9433 cm-1
  3.      47.4519 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.356423       -1.477500        0.095088
C          -2.361148       -0.603985        0.459882
C          -2.095970        0.825884        0.711243
O          -1.422407       -2.717983       -0.118852
O          -0.124161       -0.831139       -0.071431
C           1.043535       -1.629084       -0.294407
C           2.201579       -0.692312       -0.572915
C           2.536720        0.252378        0.578784
C           3.735235        1.143217        0.271620
H          -3.374299       -0.973175        0.506572
H          -1.282397        1.019130        1.411313
H          -2.980905        1.354256        1.056985
H           1.241016       -2.240709        0.590299
H           0.879820       -2.298600       -1.138974
H           1.979081       -0.111040       -1.472878
H           3.075025       -1.308078       -0.805572
H           2.735949       -0.337946        1.478083
```

```
H           1.668622        0.875865        0.803300
H           3.546688        1.762264       -0.608504
H           3.960887        1.810666        1.104947
H           4.627855        0.546593        0.070537
N          -1.644406        1.567379       -0.557052
H          -2.386177        1.490567       -1.251146
H          -0.842521        1.041514       -0.910260
C          -1.272591        2.985966       -0.341225
H          -2.134493        3.517477        0.051562
H          -0.961757        3.423094       -1.285647
H          -0.454626        3.022070        0.372592
```

---

### Compound_26_HEI_11_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.5349 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323573 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.4243 cm-1
  2.      42.7224 cm-1
  3.      55.7085 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.622493       -0.449925        0.232688
C           1.664248       -1.244334       -0.189984
C           3.042119       -0.824134        0.134257
O           0.727803        0.640678        0.871967
O          -0.648539       -0.914027       -0.107086
C          -1.767878       -0.102544        0.274532
C          -3.020374       -0.754021       -0.278132
C          -4.304103       -0.045143        0.157505
C          -4.430698        1.387917       -0.354047
H           1.490974       -2.109428       -0.810415
H           3.226074       -0.665417        1.198950
H           3.792463       -1.511450       -0.247317
H          -1.821875       -0.034724        1.364039
H          -1.638928        0.906043       -0.117824
H          -3.049487       -1.792975        0.058698
H          -2.962445       -0.772549       -1.370188
H          -4.363292       -0.049674        1.249715
```

```
H          -5.156175       -0.628504       -0.198140
H          -5.397009        1.815465       -0.081529
H          -3.656704        2.035977        0.059056
H          -4.346168        1.422279       -1.442775
N           3.359715        0.542136       -0.481165
H           3.282214        0.460534       -1.493609
H           2.599529        1.151478       -0.164934
C           4.675305        1.106785       -0.099280
H           5.456194        0.427013       -0.427904
H           4.705516        1.213994        0.980951
H           4.800331        2.076174       -0.572908
```

---

### Compound_26_HEI_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535715 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323422 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      43.4518 cm-1
  2.      54.1041 cm-1
  3.      64.1914 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.532792       -1.650956       -0.242757
C          -1.828433       -1.283579       -0.550850
C          -2.523348       -0.170408        0.115034
O           0.153926       -2.576015       -0.752812
O           0.035788       -0.866615        0.772754
C           1.421099       -1.069021        1.085521
C           2.354838       -0.328073        0.142984
C           2.183764        1.188426        0.157036
C           3.176245        1.896733       -0.758280
H          -2.321935       -1.805068       -1.357482
H          -2.399730       -0.141216        1.196879
H          -3.586312       -0.151212       -0.112778
H           1.533451       -0.689453        2.101878
H           1.645948       -2.134251        1.090725
H           2.219253       -0.706423       -0.872883
H           3.379321       -0.578705        0.435998
H           2.299983        1.553930        1.181561
```

```
H           1.167112        1.446091       -0.148840
H           3.060403        1.563893       -1.792195
H           3.035971        2.978801       -0.739289
H           4.205389        1.687915       -0.457636
N          -1.996934        1.206918       -0.337735
H          -2.115754        1.271043       -1.347716
H          -0.993342        1.205399       -0.156588
C          -2.635604        2.364211        0.334246
H          -3.700812        2.344043        0.123403
H          -2.197219        3.284048       -0.041533
H          -2.465513        2.279776        1.403500
```

---

### Compound_26_HEI_13

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535248 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323152 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.0690 cm-1
  2.      42.8954 cm-1
  3.      49.6877 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.299616        1.509004       -0.300007
C          -1.305518        1.007667       -1.099404
C          -1.866434       -0.341614       -0.922222
O           0.286413        2.621976       -0.386247
O           0.050865        0.646922        0.753265
C           1.372527        0.776195        1.299290
C           2.435938        0.198868        0.380614
C           2.247519       -1.284416        0.074787
C           3.340840       -1.839159       -0.831382
H          -1.730922        1.659299       -1.848653
H          -1.120961       -1.114454       -0.740227
H          -2.485018       -0.644938       -1.763578
H           1.579617        1.821590        1.524618
H           1.338590        0.223173        2.238263
H           3.407184        0.354778        0.860150
H           2.454117        0.768310       -0.552491
H           1.273325       -1.435909       -0.395634
```

```
H           2.227786       -1.844204        1.014700
H           4.326078       -1.728149       -0.372842
H           3.187674       -2.899448       -1.039649
H           3.360499       -1.311545       -1.787659
N          -2.794064       -0.446258        0.304789
H          -3.535883        0.244129        0.197092
H          -2.240612       -0.162763        1.113049
C          -3.370036       -1.795179        0.524912
H          -3.960833       -2.066356       -0.345125
H          -2.555388       -2.501089        0.656751
H          -3.996349       -1.778004        1.412043
```

---

### Compound_26_HEI_14

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535091 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322801 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.7298 cm-1
  2.      40.9698 cm-1
  3.      53.5284 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.553420       -0.849341        0.253763
C           1.601931       -1.281914       -0.519950
C           2.950615       -0.742895       -0.235611
O           0.618276        0.021710        1.176695
O          -0.679035       -1.451686       -0.022745
C          -1.860357       -0.746219        0.389714
C          -2.177956        0.419502       -0.533703
C          -3.398584        1.224298       -0.083679
C          -4.708131        0.439767       -0.117566
H           1.446402       -1.950893       -1.351167
H           3.306145       -0.930748        0.780365
H           3.702947       -1.098201       -0.934620
H          -2.649468       -1.495201        0.364776
H          -1.749957       -0.401810        1.417963
H          -2.339032        0.038024       -1.545988
H          -1.307498        1.077673       -0.573544
H          -3.491013        2.102456       -0.726641
```

```
H          -3.224461        1.601988        0.928141
H          -5.553443        1.078180        0.144518
H          -4.893295        0.034427       -1.115071
H          -4.698857       -0.396223        0.583090
N           2.946096        0.780673       -0.333644
H           2.155492        1.066327        0.257075
H           2.720291        1.038220       -1.293076
C           4.197968        1.440765        0.103806
H           4.090919        2.516195       -0.004559
H           5.017739        1.082965       -0.512663
H           4.377059        1.187934        1.144658
```

---

### Compound_26_HEI_15

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534637 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322907 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      21.4454 cm-1
  2.      34.0345 cm-1
  3.      44.6615 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.527917        0.399261       -0.060119
C          -1.566753        1.216281        0.321100
C          -2.846200        0.591993        0.715217
O          -0.553063       -0.867219       -0.110059
O           0.631163        1.073591       -0.461848
C           1.820643        0.293304       -0.649721
C           2.521533       -0.001078        0.667531
C           3.778046       -0.857544        0.500393
C           4.894795       -0.177852       -0.288796
H          -1.484017        2.289777        0.256589
H          -2.760506       -0.133956        1.526391
H          -3.604857        1.322025        0.984354
H           1.580635       -0.633115       -1.171405
H           2.447600        0.899688       -1.300901
H           1.818725       -0.514771        1.326385
H           2.781835        0.945470        1.149923
H           3.507515       -1.799545        0.014341
```

```
H           4.151422       -1.121375        1.492404
H           5.790695       -0.800434       -0.313718
H           4.602658        0.017418       -1.321452
H           5.166052        0.778023        0.165477
N          -3.434264       -0.233671       -0.432129
H          -3.616519        0.391643       -1.215571
H          -2.678036       -0.863386       -0.715582
C          -4.652098       -1.003572       -0.085009
H          -5.426686       -0.309749        0.228623
H          -4.411808       -1.684465        0.726141
H          -4.981955       -1.563294       -0.955407
```

---

### Compound_26_HEI_16

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535667 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323956 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.2841 cm-1
  2.      47.2659 cm-1
  3.      76.1273 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.803062       -0.258863        0.428713
C          -1.808944       -1.059997       -0.078359
C          -3.202022       -0.912189        0.350288
O          -0.888854        0.661089        1.285563
O           0.458719       -0.557932       -0.101006
C           1.568318        0.205910        0.386625
C           2.821128       -0.283567       -0.309940
C           4.063256        0.477097        0.146906
C           5.334395       -0.007975       -0.541018
H          -1.561760       -1.816278       -0.809394
H          -3.301529       -0.435096        1.323228
H          -3.750863       -1.852336        0.358728
H           1.406440        1.267016        0.184615
H           1.658390        0.082066        1.468041
H           2.699436       -0.172684       -1.391025
H           2.950409       -1.350993       -0.110663
H           4.171235        0.373709        1.230260
```

```
H           3.925084        1.544130       -0.048852
H           6.208925        0.548790       -0.200563
H           5.511785       -1.065889       -0.335520
H           5.263922        0.111616       -1.624353
N          -4.053127       -0.016588       -0.593352
H          -5.028474       -0.059340       -0.297822
H          -4.000906       -0.420226       -1.527885
C          -3.610401        1.397965       -0.645265
H          -4.226108        1.935681       -1.360430
H          -3.718389        1.829890        0.344790
H          -2.570651        1.420520       -0.953841
```

---

## Compound_26_HEI_17

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.536244 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323832 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.1616 cm-1
  2.      44.1759 cm-1
  3.      84.1915 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.490970       -1.213923        0.015397
C           1.488921       -0.937027       -0.884309
C           2.774530       -0.412657       -0.370063
O           0.556457       -1.049342        1.274265
O          -0.684847       -1.727868       -0.542315
C          -1.912648       -1.567152        0.187901
C          -2.636890       -0.284845       -0.186700
C          -1.922781        0.998864        0.230667
C          -2.703146        2.250170       -0.156277
H           1.305406       -0.978807       -1.945826
H           3.309828       -1.099953        0.288854
H           3.448546       -0.103964       -1.164924
H          -2.519613       -2.432070       -0.078668
H          -1.713681       -1.606496        1.257699
H          -3.625991       -0.318403        0.281626
H          -2.804506       -0.276273       -1.267987
H          -0.933452        1.034369       -0.229952
```

```
H          -1.759486        0.984636        1.311418
H          -3.688444        2.261325        0.315329
H          -2.177826        3.157386        0.147167
H          -2.853913        2.298858       -1.237139
N           2.546604        0.814534        0.516846
H           3.393073        1.021027        1.043842
H           1.821023        0.502097        1.176991
C           2.094342        2.024262       -0.208283
H           1.840350        2.796087        0.512221
H           2.897892        2.364786       -0.855162
H           1.221891        1.765199       -0.798995
```

---

### Compound_26_HEI_18

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53495 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323081 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.4913 cm-1
  2.      32.1437 cm-1
  3.      62.7893 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.424107        0.237792        0.114145
C          -1.288577       -0.307434        1.032173
C          -2.345067       -1.222292        0.548661
O          -0.430841        0.018170       -1.135729
O           0.494525        1.149302        0.646480
C           1.586432        1.593236       -0.173264
C           2.857485        0.810372        0.109127
C           2.792115       -0.665314       -0.275908
C           4.093980       -1.401613        0.021080
H          -1.280104        0.015391        2.061000
H          -1.968658       -2.126023        0.064381
H          -3.034861       -1.516239        1.335462
H           1.309973        1.524285       -1.223835
H           1.730619        2.644903        0.075617
H           3.100976        0.901253        1.172061
H           3.671510        1.294769       -0.439733
H           2.554926       -0.749253       -1.339635
```

```
H           1.972298       -1.146845        0.262325
H           4.335563       -1.356401        1.085470
H           4.031104       -2.453939       -0.261137
H           4.929353       -0.958840       -0.526152
N          -3.191312       -0.570516       -0.551283
H          -2.500355       -0.241905       -1.236003
H          -3.772116       -1.277431       -0.998795
C          -4.032576        0.559136       -0.093593
H          -3.392346        1.290924        0.388300
H          -4.527692        1.003292       -0.952049
H          -4.768584        0.182602        0.611164
```

---

### Compound_26_HEI_19

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53569 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323504 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.4436 cm-1
  2.      47.6654 cm-1
  3.      70.2342 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.734168       -0.980830        0.190746
C          -1.885529       -0.949498       -0.570257
C          -3.151889       -0.442999       -0.032355
O          -0.564190       -0.579820        1.372445
O           0.348159       -1.579525       -0.476702
C           1.657558       -1.344025        0.057603
C           2.201452        0.019185       -0.334663
C           3.615947        0.247188        0.190744
C           4.183921        1.602020       -0.217731
H          -1.858949       -1.327139       -1.582091
H          -3.199347       -0.476976        1.054317
H          -4.024160       -0.950108       -0.441155
H           1.645078       -1.457942        1.141188
H           2.279577       -2.135686       -0.360815
H           1.536570        0.796351        0.050891
H           2.195039        0.103632       -1.425020
H           4.270010       -0.549242       -0.175963
```

```
H           3.612416        0.165219        1.281317
H           5.193836        1.744984        0.170208
H           4.227737        1.696355       -1.304988
H           3.562770        2.417006        0.160270
N          -3.417676        1.048556       -0.371493
H          -4.364511        1.289413       -0.077945
H          -3.379904        1.145016       -1.385586
C          -2.450062        1.990091        0.243557
H          -2.686597        3.000265       -0.077788
H          -2.529256        1.910025        1.323192
H          -1.451713        1.716906       -0.081386
```

---

### Compound_26_HEI_1_reopt_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535687 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.325146 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      22.4738 cm-1
  2.      24.9401 cm-1
  3.      47.9423 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.702388        0.243376       -0.320473
C          -1.669147        1.192060       -0.068955
C          -3.079991        0.845303       -0.320884
O          -0.899371       -0.933799       -0.744591
O           0.605454        0.658461       -0.062464
C           1.645242       -0.316387       -0.216090
C           2.962446        0.336810        0.147139
C           4.136978       -0.627691        0.004003
C           5.470978        0.014336        0.368084
H          -1.414624        2.139980        0.378605
H          -3.274697        0.451571       -1.320218
H          -3.757221        1.675215       -0.136940
H           1.448604       -1.172508        0.433265
H           1.667220       -0.676442       -1.246798
H           2.911363        0.703867        1.175929
H           3.121918        1.207185       -0.495351
H           4.176925       -0.996781       -1.024641
```

```
H           3.965776       -1.501549        0.638858
H           5.467934        0.364829        1.402491
H           6.295789       -0.691499        0.257725
H           5.679825        0.874125       -0.272234
N          -3.549210       -0.291239        0.598057
H          -2.877593       -1.048703        0.454055
H          -3.449488        0.019353        1.563247
C          -4.929981       -0.766744        0.343701
H          -5.617012        0.060231        0.497921
H          -4.992105       -1.115921       -0.682691
H          -5.161622       -1.577958        1.027666
```

---

### Compound_26_HEI_22

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53431 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.321911 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.5873 cm-1
  2.      49.7645 cm-1
  3.      61.6297 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.712053       -1.609312        0.030557
C           2.040509       -1.325234       -0.200500
C           2.685247       -0.092249        0.288381
O           0.035147       -2.589059       -0.382686
O           0.080694       -0.656863        0.854673
C          -1.340886       -0.515998        0.727297
C          -1.710708        0.258182       -0.528047
C          -3.219803        0.424688       -0.712815
C          -3.888144        1.275152        0.364903
H           2.605895       -2.002650       -0.823055
H           2.505333        0.133748        1.338782
H           3.758620       -0.094852        0.116021
H          -1.817888       -1.496244        0.730721
H          -1.648609        0.015797        1.625559
H          -1.296147       -0.265769       -1.392037
H          -1.231474        1.241636       -0.490189
H          -3.687697       -0.563678       -0.742063
```

```
H          -3.401205        0.878156       -1.689809
H          -3.815621        0.812821        1.350189
H          -3.422648        2.261649        0.426499
H          -4.947644        1.420096        0.147649
N           2.163070        1.158219       -0.438580
H           2.330546        1.033623       -1.436019
H           1.150963        1.165245       -0.305778
C           2.751133        2.436336        0.031036
H           2.313472        3.258464       -0.527624
H           2.534668        2.547653        1.089417
H           3.824814        2.404760       -0.128966
```

---

### Compound_26_HEI_23

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.533886 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.321638 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.8604 cm-1
  2.      39.9718 cm-1
  3.      55.0454 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.513106        1.344660       -0.147082
C          -1.774155        1.358214        0.416325
C          -2.492063        0.137175        0.809760
O           0.189362        2.329869       -0.498804
O          -0.010749        0.050453       -0.359728
C           1.393693       -0.085006       -0.620322
C           2.215856       -0.016099        0.656762
C           3.721075       -0.127557        0.407815
C           4.159583       -1.474963       -0.161371
H          -2.272844        2.312206        0.506808
H          -1.866179       -0.615199        1.286622
H          -3.341886        0.345060        1.456000
H           1.492181       -1.057150       -1.099810
H           1.716483        0.679532       -1.326790
H           1.892800       -0.815530        1.329791
H           2.000895        0.930649        1.156346
H           4.241896        0.048013        1.351733
```

```
H           4.032699        0.674268       -0.267950
H           5.245987       -1.527036       -0.249880
H           3.838553       -2.294147        0.486372
H           3.741123       -1.653214       -1.152837
N          -3.098603       -0.616822       -0.395179
H          -3.734331        0.019805       -0.873608
H          -2.331586       -0.808422       -1.038901
C          -3.796440       -1.876614       -0.040234
H          -4.180606       -2.342228       -0.943084
H          -3.087041       -2.538187        0.448126
H          -4.613494       -1.642099        0.635664
```

---

### Compound_26_HEI_24_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535976 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323509 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      21.0068 cm-1
  2.      39.8926 cm-1
  3.      68.2676 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.535940       -1.173524       -0.021469
C           1.444653       -0.687960       -0.938067
C           2.811368       -0.322845       -0.550841
O           0.686870       -1.347939        1.217815
O          -0.687739       -1.546005       -0.603800
C          -1.838749       -1.543390        0.254350
C          -2.296593       -0.139177        0.613911
C          -2.660358        0.721765       -0.592646
C          -3.129126        2.116825       -0.194682
H           1.146071       -0.582718       -1.970931
H           3.137810       -0.808166        0.366722
H           3.544722       -0.511934       -1.332891
H          -2.609562       -2.059954       -0.318266
H          -1.635460       -2.124277        1.153466
H          -1.515966        0.356721        1.196777
H          -3.165135       -0.233477        1.273073
H          -3.442908        0.219634       -1.169282
```

```
H          -1.793777        0.803621       -1.252316
H          -2.350519        2.647289        0.358270
H          -3.384144        2.717989       -1.069112
H          -4.013003        2.067335        0.445313
N           2.983096        1.190536       -0.259950
H           3.973984        1.389326       -0.121203
H           2.684868        1.699401       -1.091403
C           2.210038        1.674579        0.910536
H           2.562497        1.154798        1.795904
H           1.160225        1.459826        0.740997
H           2.362545        2.744741        1.015867
```

---

### Compound_26_HEI_25

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535659 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322353 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      38.3912 cm-1
  2.      49.8327 cm-1
  3.      82.0977 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.770894        1.568725        0.169006
C          -1.987289        1.028549       -0.197252
C          -2.097926       -0.160868       -1.057558
O          -0.545143        2.536247        0.945541
O           0.321336        0.919110       -0.421423
C           1.620459        1.202162        0.112268
C           2.633171        0.313406       -0.584400
C           2.350274       -1.189065       -0.496475
C           2.142612       -1.706528        0.923879
H          -2.876674        1.434413        0.260301
H          -1.507878       -0.115281       -1.972418
H          -3.129166       -0.381421       -1.321928
H           1.870316        2.252194       -0.045705
H           1.614922        1.020662        1.188235
H           3.605545        0.529118       -0.132287
H           2.703853        0.605805       -1.635040
H           3.186806       -1.720113       -0.956629
```

```
H           1.473101       -1.428537       -1.101687
H           2.991038       -1.454828        1.564447
H           1.246471       -1.282524        1.380878
H           2.030641       -2.791851        0.929674
N          -1.575240       -1.449982       -0.378701
H          -1.573237       -2.208189       -1.059918
H          -0.603994       -1.265447       -0.126393
C          -2.335242       -1.860221        0.824440
H          -1.865577       -2.737553        1.259138
H          -2.324094       -1.039354        1.533967
H          -3.355930       -2.087034        0.529873
```

---

### Compound_26_HEI_26

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53552 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323194 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      22.7733 cm-1
  2.      46.3178 cm-1
  3.      67.0427 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.468310       -0.240113       -0.021849
C          -1.256052        0.781539       -0.515394
C          -2.399738        1.308993        0.234375
O          -0.561840       -0.836061        1.084270
O           0.540957       -0.630853       -0.915574
C           1.607291       -1.442088       -0.402448
C           2.627276       -0.644230        0.393520
C           3.307210        0.464632       -0.404888
C           4.340094        1.227200        0.417537
H          -1.028164        1.199470       -1.485303
H          -2.326273        1.132279        1.305665
H          -2.571399        2.369822        0.060628
H           1.200038       -2.254256        0.198579
H           2.074071       -1.873959       -1.288476
H           3.382412       -1.347687        0.758300
H           2.144622       -0.218996        1.276931
H           2.550997        1.160319       -0.775259
```

```
H           3.786581        0.029461       -1.286907
H           5.126025        0.559590        0.778034
H           4.815485        2.015746       -0.168321
H           3.877655        1.693900        1.290263
N          -3.755802        0.661467       -0.159438
H          -4.510956        1.168550        0.302398
H          -3.875967        0.786322       -1.164023
C          -3.852450       -0.781866        0.169663
H          -3.761529       -0.897383        1.245218
H          -3.045448       -1.303274       -0.333984
H          -4.812395       -1.159259       -0.170343
```

---

### Compound_26_HEI_27

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53356 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.321792 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.0830 cm-1
  2.      42.6510 cm-1
  3.      65.4557 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.842884        1.365292        0.046669
C          -2.165624        1.114174       -0.261516
C          -2.597014       -0.105585       -0.962188
O          -0.353556        2.361143        0.645163
O           0.021773        0.343143       -0.367929
C           1.425052        0.529248       -0.143742
C           2.138170       -0.718874       -0.625314
C           3.660158       -0.622636       -0.503988
C           4.166274       -0.523530        0.933168
H          -2.909016        1.801054        0.113452
H          -2.016636       -0.340959       -1.853809
H          -3.649944       -0.075032       -1.231256
H           1.774591        1.406599       -0.693533
H           1.603896        0.704726        0.916653
H           1.868119       -0.892827       -1.669622
H           1.777911       -1.579105       -0.053631
H           4.012336        0.240293       -1.076493
```

```
H           4.098715       -1.503905       -0.977102
H           3.805782       -1.363481        1.531652
H           5.256994       -0.536477        0.964564
H           3.834763        0.395307        1.418326
N          -2.442930       -1.387167       -0.106451
H          -1.460498       -1.430226        0.165650
H          -2.636568       -2.202252       -0.687235
C          -3.300309       -1.418061        1.101173
H          -4.340254       -1.411235        0.787512
H          -3.084654       -2.318708        1.668420
H          -3.083691       -0.538066        1.698160
```

---

### Compound_26_HEI_28

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53453 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322015 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.3478 cm-1
  2.      58.0929 cm-1
  3.      83.8667 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.584590        1.821073        0.094576
C          -1.850190        1.349062        0.379537
C          -2.123389       -0.078387        0.634256
O          -0.213228        3.010265       -0.099112
O           0.360233        0.791260       -0.013178
C           1.743093        1.142029       -0.139417
C           2.530300       -0.057545       -0.632487
C           2.677921       -1.230260        0.341023
C           1.417319       -2.065020        0.558575
H          -2.671053        2.050091        0.373536
H          -1.480236       -0.537540        1.385889
H          -3.159011       -0.250709        0.916534
H           1.844551        1.966965       -0.843178
H           2.119460        1.479543        0.831442
H           3.527836        0.314385       -0.881095
H           2.087773       -0.408016       -1.570036
H           3.038862       -0.851715        1.302127
```

```
H           3.464932       -1.884436       -0.042663
H           0.646555       -1.508483        1.088388
H           0.995480       -2.388793       -0.395996
H           1.641883       -2.960190        1.141705
N          -1.885540       -0.956360       -0.603976
H          -2.457568       -0.594775       -1.365488
H          -0.908112       -0.809060       -0.862865
C          -2.149163       -2.399704       -0.391862
H          -1.899186       -2.946762       -1.296259
H          -1.536005       -2.746090        0.434151
H          -3.201222       -2.529579       -0.155246
```

---

### Compound_26_HEI_29_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535248 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323152 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.0806 cm-1
  2.      42.9001 cm-1
  3.      49.6852 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.299659        1.508915       -0.299951
C          -1.305683        1.007713       -1.099286
C          -1.866650       -0.341550       -0.922156
O           0.286418        2.621869       -0.386157
O           0.050888        0.646712        0.753189
C           1.372518        0.776020        1.299283
C           2.436023        0.198903        0.380584
C           2.247726       -1.284350        0.074533
C           3.341148       -1.838886       -0.831642
H          -1.731135        1.659442       -1.848422
H          -1.121203       -1.114449       -0.740311
H          -2.485351       -0.644768       -1.763464
H           1.579511        1.821401        1.524763
H           1.338585        0.222866        2.238178
H           3.407228        0.354810        0.860202
H           2.454216        0.768480       -0.552438
H           1.273573       -1.435844       -0.395973
```

```
H           2.227971       -1.844274        1.014365
H           4.326347       -1.727863       -0.373021
H           3.188077       -2.899160       -1.040061
H           3.360829       -1.311142       -1.787846
N          -2.794153       -0.446248        0.304955
H          -3.535958        0.244169        0.197364
H          -2.240632       -0.162822        1.113190
C          -3.370163       -1.795159        0.525047
H          -3.961043       -2.066258       -0.344957
H          -2.555537       -2.501116        0.656776
H          -3.996402       -1.778009        1.412232
```

---

### Compound_26_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535762 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324553 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.2070 cm-1
  2.      44.7923 cm-1
  3.      53.0695 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.589684        0.336354       -0.447164
C           1.355961       -0.692738       -0.944129
C           2.826010       -0.580379       -0.844993
O           1.027672        1.381453        0.125762
O          -0.785976        0.176627       -0.595900
C          -1.633882        1.121380        0.073082
C          -3.074007        0.698090       -0.131663
C          -3.434635       -0.631052        0.527268
C          -4.900857       -1.001075        0.332768
H           0.902963       -1.593202       -1.327619
H           3.243570        0.311034       -1.318342
H           3.342865       -1.452620       -1.236186
H          -1.388214        1.145092        1.137516
H          -1.465654        2.119800       -0.333693
H          -3.286143        0.651272       -1.203885
H          -3.708507        1.489437        0.277691
H          -3.208427       -0.570034        1.595944
```

```
H          -2.801989       -1.423487        0.122002
H          -5.144014       -1.092590       -0.728247
H          -5.139795       -1.952090        0.811687
H          -5.558265       -0.239119        0.757682
N           3.262720       -0.437049        0.614180
H           2.978997       -1.276564        1.116617
H           2.698238        0.340053        0.973548
C           4.707096       -0.172914        0.810443
H           5.273820       -1.000047        0.392539
H           4.963012        0.749833        0.298135
H           4.912714       -0.078064        1.872779
```

---

### Compound_26_HEI_30

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534834 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322924 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      31.7512 cm-1
  2.      42.6270 cm-1
  3.      84.2220 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.712050       -0.429310        0.360204
C           1.807573       -1.059049       -0.200709
C           3.167995       -0.825134        0.290760
O           0.685565        0.406343        1.302939
O          -0.500801       -0.809933       -0.227309
C          -1.694718       -0.204441        0.284550
C          -2.859236       -0.702697       -0.549225
C          -4.214028       -0.201468       -0.045573
C          -4.392495        1.312338       -0.134935
H           1.655428       -1.757279       -1.011101
H           3.196327       -0.468023        1.318454
H           3.810104       -1.699641        0.201520
H          -1.831596       -0.479969        1.333419
H          -1.605812        0.880629        0.233190
H          -2.851675       -1.795276       -0.539366
H          -2.715178       -0.390874       -1.587683
H          -4.354823       -0.525765        0.989564
```

```
H          -4.998641       -0.688625       -0.628620
H          -3.694120        1.842690        0.513620
H          -4.229394        1.664299       -1.156297
H          -5.401569        1.604455        0.160532
N           3.942744        0.264008       -0.502684
H           4.914144        0.270513       -0.191443
H           3.939229       -0.010516       -1.484384
C           3.370464        1.626326       -0.373506
H           3.947776        2.312910       -0.985869
H           2.339912        1.599129       -0.710996
H           3.416943        1.922604        0.669811
```

---

### Compound_26_HEI_31

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534482 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322376 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.8696 cm-1
  2.      40.8937 cm-1
  3.      49.7718 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.194277       -0.894295        0.404471
C          -0.999623       -0.217148        1.287231
C          -2.432739       -0.063771        0.953897
O          -0.556497       -1.379905       -0.713163
O           1.130749       -1.052458        0.813296
C           2.109921       -1.297897       -0.209045
C           2.419954       -0.088451       -1.079475
C           3.142908        1.069432       -0.387695
C           2.295333        1.865049        0.603021
H          -0.591620        0.256096        2.165917
H          -2.964960       -1.006388        0.807050
H          -2.975190        0.527949        1.686353
H           3.001757       -1.607109        0.336914
H           1.786640       -2.132864       -0.830033
H           1.496091        0.272678       -1.538465
H           3.047226       -0.454744       -1.897359
H           3.504318        1.750999       -1.162037
```

```
H           4.033317        0.683206        0.117776
H           2.835102        2.747296        0.952619
H           1.368027        2.205167        0.136345
H           2.024917        1.271572        1.474857
N          -2.595105        0.646566       -0.388247
H          -2.194962        1.579737       -0.306443
H          -1.996720        0.111899       -1.028774
C          -3.984515        0.716262       -0.897151
H          -3.989649        1.232142       -1.852909
H          -4.359935       -0.295494       -1.018565
H          -4.594407        1.255719       -0.178098
```

---

### Compound_26_HEI_33_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.533887 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322143 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      27.0363 cm-1
  2.      36.8101 cm-1
  3.      41.1120 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.229584       -0.229868        0.318635
C           0.989686        0.858678        0.675449
C           2.284883        1.063195       -0.007706
O           0.533012       -1.091733       -0.563500
O          -0.949261       -0.389708        1.047347
C          -1.919391       -1.322013        0.547683
C          -2.698635       -0.828049       -0.662688
C          -3.615199        0.374335       -0.423799
C          -2.896535        1.710319       -0.244082
H           0.697447        1.500850        1.491096
H           2.210502        1.157089       -1.093352
H           2.832204        1.920513        0.374950
H          -1.431456       -2.269088        0.318010
H          -2.597047       -1.484070        1.386690
H          -3.307318       -1.673729       -0.996122
H          -2.004112       -0.607467       -1.476771
H          -4.246780        0.175504        0.447528
```

```
H          -4.292341        0.456515       -1.277832
H          -3.612631        2.533661       -0.208612
H          -2.310370        1.736801        0.672912
H          -2.214026        1.898679       -1.076067
N           3.195174       -0.151235        0.178063
H           2.616290       -0.948989       -0.105784
H           3.390911       -0.255072        1.172396
C           4.454818       -0.113610       -0.600959
H           5.026302        0.759794       -0.299879
H           5.023453       -1.018098       -0.405047
H           4.207479       -0.050638       -1.656538
```

---

### Compound_26_HEI_34

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534139 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322815 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.8350 cm-1
  2.      38.4055 cm-1
  3.      60.0577 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.736513        1.575892       -0.045756
C           2.071870        1.422018        0.272001
C           2.635162        0.130645        0.703532
O           0.132714        2.615959       -0.422881
O           0.008975        0.382569        0.065922
C          -1.396515        0.430154       -0.209263
C          -1.942929       -0.974126       -0.041248
C          -3.429057       -1.084779       -0.386329
C          -4.345750       -0.299108        0.548375
H           2.730018        2.265933        0.130446
H           2.073195       -0.369543        1.492490
H           3.671320        0.218431        1.020434
H          -1.877383        1.131414        0.473108
H          -1.562764        0.784956       -1.228760
H          -1.779547       -1.301961        0.989291
H          -1.369753       -1.645856       -0.685105
H          -3.710338       -2.139742       -0.358934
```

```
H          -3.584588       -0.752237       -1.416719
H          -4.168997        0.775138        0.482274
H          -5.394912       -0.475187        0.305365
H          -4.189900       -0.597684        1.587694
N           2.646388       -0.910976       -0.430663
H           1.682986       -0.975250       -0.761964
H           3.202395       -0.535820       -1.197577
C           3.143511       -2.250031       -0.033391
H           2.512695       -2.629877        0.764900
H           3.103255       -2.916672       -0.889864
H           4.167255       -2.151414        0.315711
```

---

### Compound_26_HEI_36

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534412 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323287 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      23.7996 cm-1
  2.      35.0331 cm-1
  3.      49.4243 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.001478        1.419534       -0.220418
C          -2.034521        0.709878       -0.801156
C          -1.929949       -0.727223       -1.102037
O          -0.960370        2.643893        0.077934
O           0.111789        0.621902        0.070145
C           1.284972        1.269656        0.578135
C           2.358157        0.219145        0.777031
C           2.833261       -0.441025       -0.514868
C           3.942563       -1.459394       -0.276900
H          -2.974636        1.217615       -0.953759
H          -1.018737       -1.010042       -1.628765
H          -2.784943       -1.093740       -1.664807
H           1.618280        2.032749       -0.129079
H           1.051131        1.764115        1.522205
H           1.989739       -0.543121        1.470141
H           3.205508        0.705228        1.268996
H           3.185935        0.334952       -1.200674
```

```
H           1.989704       -0.929109       -1.007596
H           3.603859       -2.259969        0.384690
H           4.271809       -1.917254       -1.211134
H           4.812200       -0.991221        0.189832
N          -1.879724       -1.613202        0.166688
H          -1.667292       -2.572915       -0.103773
H          -1.094930       -1.269001        0.720736
C          -3.120020       -1.585645        0.976260
H          -3.931172       -1.994272        0.380393
H          -2.974229       -2.181983        1.872083
H          -3.333417       -0.555532        1.242779
```

---

### Compound_26_HEI_37

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534697 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322197 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.3420 cm-1
  2.      35.6279 cm-1
  3.      54.1751 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.546962       -0.302896        0.016528
C          -1.691383       -1.060505       -0.142792
C          -2.834153       -0.576820       -0.921949
O          -0.290999        0.835982       -0.456420
O           0.416723       -0.931336        0.821281
C           1.719333       -0.335208        0.886486
C           2.590104       -0.734464       -0.294632
C           4.019343       -0.197877       -0.193446
C           4.119823        1.322635       -0.294844
H          -1.748248       -2.033643        0.323205
H          -2.562962        0.186680       -1.648399
H          -3.374436       -1.373904       -1.429608
H           1.623480        0.745577        0.964461
H           2.154338       -0.707810        1.814755
H           2.128682       -0.376575       -1.218339
H           2.612981       -1.825661       -0.348549
H           4.615837       -0.648356       -0.989913
```

```
H           4.463964       -0.532502        0.748650
H           3.614918        1.819797        0.534299
H           5.161689        1.647314       -0.287046
H           3.665952        1.680974       -1.221611
N          -3.934032        0.102721       -0.059745
H          -4.742772        0.298181       -0.649824
H          -4.229372       -0.569010        0.647835
C          -3.491593        1.351959        0.606691
H          -3.223444        2.074605       -0.157617
H          -4.304053        1.733641        1.218151
H          -2.631190        1.123549        1.226627
```

---

### Compound_26_HEI_38

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534796 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322718 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      22.7313 cm-1
  2.      34.5411 cm-1
  3.      45.7355 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.654592       -0.822400        0.259499
C           1.812222       -1.070723       -0.451460
C           3.132779       -0.712880        0.074256
O           0.530091       -0.270287        1.384660
O          -0.497196       -1.298679       -0.388499
C          -1.767504       -0.861576        0.113132
C          -2.112384        0.544503       -0.353812
C          -3.445519        1.049977        0.200660
C          -4.660693        0.264188       -0.286826
H           1.744914       -1.554856       -1.415000
H           3.148669       -0.612180        1.157694
H           3.917307       -1.403733       -0.229699
H          -2.480064       -1.588362       -0.272862
H          -1.780038       -0.917502        1.201826
H          -2.137958        0.559022       -1.447268
H          -1.312387        1.218867       -0.042289
H          -3.562438        2.099113       -0.080022
```

```
H          -3.409842        1.027472        1.293856
H          -4.705869        0.255054       -1.378407
H          -4.637272       -0.772270        0.052315
H          -5.587075        0.708611        0.080815
N           3.651983        0.658711       -0.437817
H           3.651432        0.624217       -1.456392
H           4.619720        0.777733       -0.138137
C           2.843849        1.818063        0.013081
H           1.819809        1.669533       -0.313064
H           2.889723        1.870438        1.096402
H           3.250277        2.724682       -0.425513
```

---

### Compound_26_HEI_39_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.533985 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.321893 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      26.8351 cm-1
  2.      39.0947 cm-1
  3.      59.9534 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.350504        1.170148       -0.044480
C           1.612739        1.347345        0.488992
C           2.524555        0.236890        0.795438
O          -0.497760        2.057029       -0.331024
O           0.032691       -0.172498       -0.299579
C          -1.337729       -0.491652       -0.579859
C          -2.166117       -0.602740        0.690035
C          -3.604707       -1.053692        0.429531
C          -4.441076       -0.041493       -0.350297
H           1.960577        2.361752        0.620862
H           2.032970       -0.644626        1.202431
H           3.328555        0.530949        1.466431
H          -1.751326        0.244750       -1.265298
H          -1.303313       -1.454176       -1.091428
H          -2.171415        0.363225        1.201106
H          -1.675259       -1.316231        1.356413
H          -4.085677       -1.248741        1.390604
```

```
H          -3.591640       -2.007862       -0.105801
H          -4.051751        0.118111       -1.356567
H          -5.473936       -0.380122       -0.447576
H          -4.453627        0.925592        0.157494
N           3.254100       -0.305213       -0.456307
H           2.535754       -0.592042       -1.120187
H           3.756581        0.471646       -0.883495
C           4.178264       -1.433404       -0.184974
H           3.609045       -2.247769        0.253513
H           4.635725       -1.756098       -1.115655
H           4.941992       -1.096514        0.509810
```

---

### Compound_26_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535708 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324698 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      16.2730 cm-1
  2.      30.0962 cm-1
  3.      56.3946 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.571936        0.002605        0.179846
C           1.351454        1.107311       -0.078759
C           2.782193        1.055498        0.283523
O           0.971144       -1.089201        0.688751
O          -0.769235        0.131618       -0.175686
C          -1.596476       -1.035321       -0.065358
C          -2.998414       -0.670032       -0.508205
C          -3.693767        0.345992        0.394622
C          -5.118088        0.650039       -0.056439
H           0.953474        1.961400       -0.603534
H           2.973569        0.821289        1.332835
H           3.314193        1.968859        0.030984
H          -1.189903       -1.831381       -0.692449
H          -1.601898       -1.389311        0.967647
H          -3.584180       -1.593480       -0.532050
H          -2.965726       -0.294123       -1.535046
H          -3.113763        1.270897        0.418705
```

```
H          -3.705743       -0.039138        1.418557
H          -5.129171        1.059938       -1.068924
H          -5.730639       -0.254457       -0.059693
H          -5.598957        1.375973        0.601311
N           3.494293       -0.076746       -0.461991
H           2.930353       -0.909378       -0.265767
H           3.424804        0.108239       -1.461412
C           4.905828       -0.293744       -0.067164
H           5.314454       -1.122015       -0.638761
H           5.468526        0.613225       -0.269287
H           4.937287       -0.522740        0.993907
```

---

### Compound_26_HEI_40

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.53497 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322399 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.6520 cm-1
  2.      35.8174 cm-1
  3.      48.2736 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.123479       -1.614305        0.060941
C          -1.247407       -1.346154        0.814343
C          -1.861260       -0.010249        0.880005
O           0.511358       -2.699363       -0.037599
O           0.301943       -0.517955       -0.707017
C           1.689909       -0.461468       -1.068777
C           2.585357       -0.115936        0.112169
C           2.173481        1.143282        0.877708
C           2.147453        2.410036        0.027760
H          -1.721090       -2.168644        1.330285
H          -1.144447        0.805319        0.965634
H          -2.584657        0.074214        1.687619
H           1.997892       -1.405870       -1.516596
H           1.741225        0.308914       -1.836349
H           3.601520        0.003833       -0.276183
H           2.610115       -0.963743        0.799906
H           2.868665        1.280822        1.709262
```

```
H           1.189654        0.985794        1.325653
H           1.393394        2.352535       -0.758516
H           1.918146        3.285187        0.638012
H           3.114060        2.582110       -0.451702
N          -2.654409        0.344251       -0.393756
H          -2.006844        0.252339       -1.176005
H          -3.376241       -0.363634       -0.522006
C          -3.254556        1.700572       -0.382987
H          -2.457067        2.429462       -0.273052
H          -3.785934        1.866147       -1.315632
H          -3.940934        1.769340        0.455923
```

---

### Compound_26_HEI_41

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535266 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.322215 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      50.4081 cm-1
  2.      58.0442 cm-1
  3.      73.9651 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.006343        1.540014       -0.004600
C           1.273150        1.595653       -0.547757
C           2.365032        0.710758       -0.099943
O          -1.013122        2.206246       -0.324385
O          -0.091121        0.608551        1.046132
C          -1.384857        0.125175        1.437238
C          -1.631587       -1.264672        0.872190
C          -1.785632       -1.320282       -0.649248
C          -3.074903       -0.684471       -1.160830
H           1.444515        2.268867       -1.374131
H           2.516797        0.680391        0.978982
H           3.312607        0.956820       -0.572788
H          -1.377912        0.089995        2.526941
H          -2.149469        0.832395        1.124501
H          -2.533708       -1.665243        1.345285
H          -0.803171       -1.908360        1.180971
H          -1.754301       -2.366590       -0.962370
```

```
H          -0.926457       -0.836914       -1.121237
H          -3.128171        0.375460       -0.910839
H          -3.150109       -0.769789       -2.246244
H          -3.949308       -1.174695       -0.726496
N           2.099588       -0.760067       -0.459168
H           1.186309       -0.985331       -0.062063
H           2.003363       -0.826376       -1.471397
C           3.123397       -1.712338        0.032674
H           3.176256       -1.634373        1.114575
H           4.081862       -1.451987       -0.406896
H           2.842067       -2.721188       -0.254937
```

---

### Compound_26_HEI_42

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.533546 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.320823 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      30.8040 cm-1
  2.      35.7085 cm-1
  3.      75.7424 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.013237        1.498424       -0.219850
C          -1.158336        1.229345       -0.943821
C          -1.894891       -0.040004       -0.849351
O           0.689271        2.545442       -0.246186
O           0.348747        0.466830        0.657536
C           1.694472        0.466764        1.159259
C           2.725296       -0.000748        0.140347
C           2.758363       -1.505819       -0.132726
C           1.499461       -2.077383       -0.780718
H          -1.567439        2.026826       -1.547133
H          -1.262906       -0.924888       -0.819442
H          -2.620436       -0.156639       -1.651068
H           1.944363        1.464106        1.518139
H           1.671232       -0.207517        2.016115
H           3.705280        0.305896        0.516685
H           2.570347        0.544397       -0.794232
H           2.954134       -2.032126        0.806472
```

```
H           3.613899       -1.712090       -0.781100
H           1.228515       -1.514191       -1.676599
H           1.653394       -3.117809       -1.073253
H           0.647800       -2.046830       -0.102593
N          -2.728559       -0.153705        0.445607
H          -3.357206        0.647500        0.483803
H          -2.077909       -0.055347        1.224344
C          -3.492917       -1.418536        0.572262
H          -4.186549       -1.488519       -0.260564
H          -2.793729       -2.249149        0.545383
H          -4.036288       -1.418111        1.512579
```

---

### Compound_26_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535931 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324261 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      29.8727 cm-1
  2.      45.9439 cm-1
  3.      64.2272 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.606768       -1.026565        0.137324
C          -1.625920       -1.131603       -0.775630
C          -2.922128       -0.491559       -0.456677
O          -0.650431       -0.384615        1.233532
O           0.565512       -1.715527       -0.195562
C           1.788214       -1.236420        0.385199
C           2.292882        0.019974       -0.302420
C           3.613599        0.508047        0.286140
C           4.145354        1.752497       -0.416390
H          -1.475592       -1.610504       -1.729905
H          -3.390619       -0.855028        0.460837
H          -3.642489       -0.572774       -1.266281
H           1.651960       -1.066071        1.452907
H           2.498716       -2.053192        0.258751
H           1.538991        0.806663       -0.213326
H           2.417677       -0.184655       -1.369374
H           4.355406       -0.293279        0.222215
```

```
H           3.477530        0.717973        1.350762
H           3.432564        2.576997       -0.345205
H           5.086985        2.087015        0.022069
H           4.321573        1.558072       -1.476603
N          -2.728367        0.998370       -0.189579
H          -1.973743        1.030295        0.507193
H          -2.375071        1.433122       -1.040585
C          -3.933064        1.708025        0.299329
H          -4.719516        1.617955       -0.444707
H          -4.249323        1.251288        1.232494
H          -3.690135        2.754287        0.460809
```

---

### Compound_26_HEI_5_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535582 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324513 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      19.5980 cm-1
  2.      23.0101 cm-1
  3.      60.9056 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.546095        0.485751        0.002868
C          -1.601064        1.039427        0.692148
C          -2.795075        0.209733        0.942263
O          -0.489429       -0.691708       -0.460027
O           0.528751        1.356501       -0.211646
C           1.722408        0.814656       -0.792866
C           2.611912        0.136236        0.234609
C           3.903158       -0.391711       -0.384660
C           4.817042       -1.057047        0.638559
H          -1.594915        2.080260        0.975306
H          -2.585072       -0.743878        1.430507
H          -3.557048        0.731472        1.515237
H           1.466481        0.126042       -1.597754
H           2.235880        1.671772       -1.229520
H           2.063986       -0.686945        0.699077
H           2.848550        0.851945        1.026990
H           4.434795        0.432235       -0.869480
```

```
H           3.656823       -1.106556       -1.174931
H           4.317717       -1.901439        1.118733
H           5.731238       -1.430505        0.174184
H           5.104632       -0.353381        1.422794
N          -3.468825       -0.212372       -0.369328
H          -2.728275       -0.650818       -0.922239
H          -3.756061        0.629964       -0.865240
C          -4.614870       -1.138332       -0.207322
H          -5.376840       -0.648128        0.391749
H          -5.013268       -1.390577       -1.185710
H          -4.265918       -2.035487        0.295370
```

---

### Compound_26_HEI_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.534939 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.323691 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      32.6837 cm-1
  2.      47.8697 cm-1
  3.      56.4165 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.089878       -1.592708        0.001984
C           2.373675       -1.138756        0.231202
C           2.656728        0.252577        0.626853
O           0.711793       -2.742882       -0.347482
O           0.120112       -0.595376        0.180038
C          -1.247063       -0.945067       -0.064006
C          -2.088264        0.297964        0.138546
C          -3.571134        0.035603       -0.109925
C          -4.428075        1.279988        0.093948
H           3.195019       -1.812957        0.041141
H           2.057284        0.620459        1.459929
H           3.706562        0.408289        0.862369
H          -1.355235       -1.322247       -1.082831
H          -1.555670       -1.737232        0.621458
H          -1.735210        1.082607       -0.536716
H          -1.945904        0.666617        1.158136
H          -3.914052       -0.758831        0.558787
```

```
H          -3.705555       -0.339001       -1.128492
H          -4.335065        1.656815        1.114844
H          -4.123524        2.080783       -0.583488
H          -5.483296        1.071557       -0.089591
N           2.341133        1.252934       -0.499411
H           2.901338        0.998745       -1.311589
H           1.363451        1.095471       -0.748112
C           2.557533        2.675488       -0.141609
H           2.297055        3.302300       -0.989447
H           1.927012        2.917972        0.708664
H           3.602951        2.813638        0.118402
```

---

### Compound_26_HEI_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.536267 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324523 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      33.3291 cm-1
  2.      36.1183 cm-1
  3.      62.1746 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.454994       -1.411677       -0.052144
C          -2.466678       -0.484717        0.105412
C          -2.200403        0.889398        0.568667
O          -1.529192       -2.596790       -0.474422
O          -0.197149       -0.906909        0.307519
C           0.948884       -1.727390        0.052297
C           2.189701       -0.951159        0.444290
C           2.423848        0.317700       -0.372507
C           3.749767        0.991442       -0.036542
H          -3.463652       -0.756929       -0.206257
H          -1.597430        0.955105        1.474432
H          -3.113066        1.459901        0.720408
H           0.876777       -2.651966        0.627327
H           0.979972       -1.990703       -1.007509
H           3.043716       -1.623201        0.319603
H           2.140504       -0.703025        1.508530
H           1.609733        1.024493       -0.198232
```

```
H           2.396313        0.067190       -1.437058
H           3.791109        1.269341        1.019049
H           4.590979        0.323874       -0.235905
H           3.896646        1.898628       -0.624960
N          -1.381466        1.691977       -0.458045
H          -0.562090        1.119784       -0.666286
H          -1.927255        1.758537       -1.315799
C          -0.957909        3.037776       -0.002655
H          -0.344923        2.924496        0.886495
H          -0.386136        3.518936       -0.790714
H          -1.843505        3.623051        0.227502
```

---

### Compound_26_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.536141 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324226 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.4750 cm-1
  2.      42.5441 cm-1
  3.      68.7650 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.383938       -1.072050        0.142089
C           1.159233       -0.634613        1.186290
C           2.549280       -0.213161        0.900552
O           0.730456       -1.109690       -1.080582
O          -0.890695       -1.526788        0.495502
C          -1.915835       -1.427107       -0.507616
C          -2.352223        0.006473       -0.758585
C          -2.904381        0.711558        0.477209
C          -3.354666        2.138154        0.183122
H           0.754735       -0.538284        2.181112
H           3.172692       -0.990464        0.452705
H           3.060371        0.175846        1.777081
H          -1.577546       -1.895246       -1.431450
H          -2.744235       -2.014095       -0.110723
H          -3.116464       -0.014669       -1.541646
H          -1.510305        0.575656       -1.161353
H          -2.140301        0.724541        1.257510
```

```
H          -3.744179        0.133866        0.874616
H          -2.523662        2.740963       -0.190287
H          -4.140787        2.153953       -0.575192
H          -3.744436        2.627167        1.077507
N           2.563171        0.898639       -0.144085
H           1.988328        0.528373       -0.911063
H           2.074605        1.705235        0.241470
C           3.908733        1.284930       -0.627399
H           3.809471        2.073206       -1.368049
H           4.496922        1.636490        0.215531
H           4.380029        0.413708       -1.072511
```

---

### Compound_26_HEI_9_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -520.535529 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -520.324175 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      18.5549 cm-1
  2.      34.5066 cm-1
  3.      48.6867 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.389241       -0.321340        0.254844
C          -1.180973        0.535538        0.984074
C          -2.424898        1.039468        0.368571
O          -0.613211       -0.720699       -0.927005
O           0.732284       -0.804257        0.936646
C           1.740801       -1.475275        0.166306
C           2.638284       -0.513444       -0.594666
C           3.389850        0.469339        0.299068
C           4.301971        1.400122       -0.492269
H          -0.955238        0.760602        2.014570
H          -2.281295        1.536165       -0.593021
H          -2.978079        1.707306        1.023587
H           2.322067       -2.031951        0.902195
H           1.275861       -2.188921       -0.512507
H           2.041342        0.035609       -1.327063
H           3.356060       -1.113673       -1.162674
H           3.980032       -0.090648        1.030675
```

```
H           2.671569        1.062110        0.869731
H           5.052019        0.834832       -1.050128
H           3.729638        1.989313       -1.212381
H           4.828606        2.096172        0.162875
N          -3.378124       -0.110690        0.029512
H          -2.823098       -0.754680       -0.540669
H          -3.609203       -0.597092        0.894322
C          -4.610949        0.292148       -0.687504
H          -5.208223       -0.590577       -0.896675
H          -5.168929        0.981875       -0.060819
H          -4.327903        0.778698       -1.616278
```

---

### Compound_20_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -270.683392 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -270.593765 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      91.0150 cm-1
  2.     179.9968 cm-1
  3.     217.2013 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.585491        0.176917       -0.000007
O           2.109896       -0.926579       -0.000027
C           0.136111        0.407627        0.000005
H           2.207580        1.086920        0.000004
C          -0.258745        1.685450        0.000027
H          -1.300285        1.973704        0.000037
H           0.472862        2.483934        0.000034
C          -0.763818       -0.793964       -0.000008
H          -0.507240       -1.407948       -0.868015
H          -0.507229       -1.407975        0.867977
C          -2.253865       -0.488009        0.000007
H          -2.827797       -1.414679       -0.000004
H          -2.544045        0.085262        0.881893
H          -2.544057        0.085290       -0.881858
```

---

### Compound_20_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -270.677814 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -270.588975 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      66.9592 cm-1
2.     102.0228 cm-1
3.     231.8921 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.411393       -0.615099       -0.000009
O           2.516009       -0.098449       -0.000015
C           0.120389        0.110720        0.000000
H           1.326756       -1.714756       -0.000012
C           0.121621        1.445284        0.000004
H          -0.791955        2.022237        0.000011
H           1.054195        1.993801        0.000000
C          -1.102941       -0.765115        0.000004
H          -1.044568       -1.428849       -0.868847
H          -1.044560       -1.428852        0.868852
C          -2.433000       -0.029720        0.000012
H          -2.537268        0.604694       -0.881715
H          -3.258182       -0.741796        0.000015
H          -2.537259        0.604690        0.881743
```

---

### Compound_20_HEI_1_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.601643 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.445597 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      67.1803 cm-1
2.      90.3454 cm-1
3.      97.6456 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.288778       -1.332571       -0.133067
O          -2.549472       -1.326944       -0.415743
C          -0.544852       -0.309078        0.392448
H          -0.737596       -2.272927       -0.317651
C           0.891661       -0.533602        0.648595
H           1.242534       -0.089300        1.580504
H           1.153300       -1.589890        0.638270
C           3.255213       -0.091905       -0.164553
H           3.463513       -1.156712       -0.116934
H           3.501317        0.379760        0.782117
H           3.822846        0.365592       -0.969393
N           1.805266        0.094002       -0.422102
H           1.549631       -0.317626       -1.319204
H           1.589331        1.088047       -0.486174
C          -1.165478        1.024393        0.729625
H          -2.159136        0.857687        1.156861
H          -0.572661        1.514016        1.508061
C          -1.317548        1.988462       -0.455449
H          -0.348487        2.260201       -0.879172
H          -1.910420        1.532140       -1.249674
H          -1.816571        2.912349       -0.152548
```

---

## Compound_20_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.601636 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.446031 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      41.6435 cm-1
2.      71.4429 cm-1
3.      94.5013 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.198198       -1.385545       -0.217598
O           2.398065       -1.678032        0.166297
C           0.517826       -0.210161       -0.045160
H           0.642547       -2.171872       -0.761150
C          -0.840957       -0.081063       -0.610895
H          -1.023394        0.875800       -1.101824
H          -1.079853       -0.883472       -1.305765
C          -3.313994        0.021321       -0.055506
H          -3.384329        1.001266       -0.517714
H          -4.019148       -0.056210        0.766732
H          -3.508648       -0.753557       -0.790841
N          -1.935400       -0.157511        0.465797
H          -1.847803       -1.062374        0.927174
H          -1.739894        0.551191        1.172439
C           1.127886        0.987451        0.638050
H           0.383710        1.491602        1.264627
H           1.914904        0.651789        1.316541
C           1.715787        2.012472       -0.339530
H           2.520000        1.564669       -0.926134
H           0.954896        2.370337       -1.036246
H           2.121810        2.880818        0.185035
```

---

### Compound_20_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.601636 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.446031 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      41.6436 cm-1
  2.      71.4429 cm-1
  3.      94.5012 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.198198       -1.385545       -0.217598
O           2.398065       -1.678032        0.166297
C           0.517826       -0.210161       -0.045160
H           0.642547       -2.171872       -0.761150
C          -0.840957       -0.081063       -0.610895
H          -1.023394        0.875801       -1.101824
```

```
H          -1.079853       -0.883472       -1.305765
C          -3.313994        0.021321       -0.055506
H          -3.508648       -0.753557       -0.790841
H          -3.384329        1.001267       -0.517714
H          -4.019148       -0.056210        0.766732
N          -1.935400       -0.157511        0.465797
H          -1.847803       -1.062374        0.927174
H          -1.739894        0.551191        1.172439
C           1.127886        0.987451        0.638050
H           0.383710        1.491602        1.264626
H           1.914904        0.651789        1.316541
C           1.715788        2.012471       -0.339530
H           2.520002        1.564668       -0.926133
H           0.954898        2.370337       -1.036247
H           2.121811        2.880817        0.185035
```

---

### Compound_20_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.599581 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.44397 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      37.8161 cm-1
2.      57.3738 cm-1
3.     108.3470 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.048940       -1.390770        0.094530
O          -2.130802       -1.644549       -0.564770
C          -0.358138       -0.209557        0.160014
H          -0.618044       -2.220610        0.685544
C           0.846497       -0.143089        1.015543
H           1.013033        0.842204        1.449644
H           0.830358       -0.880469        1.816174
C           2.500127        0.473082       -0.837319
H           2.547694        1.482904       -0.441314
H           1.732631        0.400606       -1.599684
H           3.462487        0.187318       -1.251699
N           2.163096       -0.455823        0.270263
H           2.925348       -0.461982        0.948388
```

```
H           2.080161       -1.401442       -0.102073
C          -0.861876        1.040654       -0.518864
H          -0.027565        1.683275       -0.807440
H          -1.374826        0.770006       -1.445223
C          -1.822126        1.856214        0.356671
H          -2.162472        2.760308       -0.154644
H          -2.701205        1.265078        0.619030
H          -1.336123        2.160748        1.286166
```

---

### Compound_20_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.599581 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.44397 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      37.8225 cm-1
  2.      57.3777 cm-1
  3.     108.3440 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.048975       -1.390766        0.094547
O          -2.130844       -1.644564       -0.564732
C          -0.358158       -0.209559        0.159987
H          -0.618077       -2.220588        0.685585
C           0.846472       -0.143074        1.015527
H           1.013014        0.842234        1.449590
H           0.830310       -0.880419        1.816191
C           2.500135        0.473020       -0.837318
H           2.547698        1.482851       -0.441336
H           1.732660        0.400529       -1.599702
H           3.462505        0.187239       -1.251664
N           2.163068       -0.455854        0.270279
H           2.925310       -0.462010        0.948415
H           2.080122       -1.401481       -0.102036
C          -0.861886        1.040644       -0.518910
H          -0.027568        1.683202       -0.807607
H          -1.374947        0.769969       -1.445198
C          -1.821997        1.856311        0.356677
H          -2.701095        1.265247        0.619143
```

```
H          -1.335888        2.160851        1.286114
H          -2.162327        2.760406       -0.154646
```

---

### Compound_20_HEI_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.608104 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.453323 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      65.9641 cm-1
  2.      98.0562 cm-1
  3.     103.4754 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.530318        1.598126       -0.019325
O           0.696983        2.196041       -0.216548
C          -0.706970        0.318318        0.315899
H          -1.357069        2.282549       -0.163888
C           0.465362       -0.601121        0.553346
H           0.146914       -1.646539        0.473920
H           0.827234       -0.470779        1.578835
C           2.768756       -1.137574       -0.015490
H           3.153087       -0.847331        0.962575
H           3.552406       -0.972019       -0.753374
H           2.540378       -2.209896        0.013739
N           1.600191       -0.322484       -0.344499
H           1.304196       -0.543547       -1.289541
H           1.342883        1.440108       -0.264868
C          -2.087349       -0.251095        0.497711
H          -2.135160       -0.778140        1.456504
H          -2.810759        0.564599        0.554005
C          -2.497956       -1.217087       -0.617784
H          -3.481963       -1.646234       -0.420158
H          -2.539549       -0.699867       -1.577856
H          -1.788956       -2.041244       -0.712158
```

---

### Compound_20_HEI_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.608253 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.453554 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      78.4565 cm-1
2.      88.2957 cm-1
3.      96.9097 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.477266        1.595815        0.024419
O          -0.722531        2.161236       -0.353155
C           0.689860        0.288938        0.195670
H           1.255930        2.333495        0.173547
C          -0.392223       -0.734663       -0.044256
H          -0.169488       -1.646452        0.524192
H          -0.398942       -1.029491       -1.098211
C          -2.782083       -1.182082       -0.104315
H          -2.619030       -2.177230        0.326850
H          -2.809812       -1.284267       -1.189309
H          -3.752131       -0.816636        0.229483
N          -1.739187       -0.228422        0.272212
H          -1.783070       -0.079281        1.274942
H          -1.384953        1.421298       -0.283915
C           2.050418       -0.223621        0.580327
H           2.709135        0.621613        0.788637
H           1.970988       -0.799030        1.508904
C           2.687200       -1.113489       -0.491707
H           3.666614       -1.470086       -0.168363
H           2.069283       -1.987732       -0.702763
H           2.817402       -0.562527       -1.425067
```

---

### Compound_20_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -366.608104 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -366.453324 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      65.9509 cm-1
2.      98.0503 cm-1
3.     103.4592 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.530286        1.598136       -0.019365
O           0.697036        2.196052       -0.216536
C          -0.706972        0.318343        0.315885
H          -1.357018        2.282566       -0.163981
C           0.465349       -0.601088        0.553418
H           0.146888       -1.646514        0.474158
H           0.827270       -0.470594        1.578869
C           2.768713       -1.137607       -0.015509
H           2.540356       -2.209932        0.013824
H           3.153108       -0.847280        0.962505
H           3.552310       -0.972109       -0.753461
N           1.600122       -0.322560       -0.344502
H           1.304077       -0.543599       -1.289530
H           1.342949        1.440148       -0.264927
C          -2.087368       -0.251040        0.497669
H          -2.135238       -0.777999        1.456505
H          -2.810780        0.564661        0.553838
C          -2.497903       -1.217129       -0.617759
H          -3.481908       -1.646282       -0.420137
H          -2.539478       -0.699980       -1.577871
H          -1.788874       -2.041272       -0.712028
```

---

## Compound_28_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.960132 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.788849 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      37.1279 cm-1
2.      50.5467 cm-1
3.      95.8958 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.712968        0.311183       -0.000058
C          -2.743610       -0.746496        0.000106
C          -4.039678       -0.455741        0.000051
O          -1.930664        1.510658       -0.000251
O          -0.484811       -0.213159        0.000031
C           0.633047        0.709743       -0.000109
C           1.937776       -0.078344        0.000022
C           2.034573       -0.949416       -1.256278
H          -4.385542        0.569814       -0.000118
H          -4.787809       -1.236490        0.000174
H           0.556756        1.338390       -0.886976
H           0.556747        1.338668        0.886561
H           1.960579       -0.340367       -2.159378
H           2.991638       -1.472841       -1.278685
H           1.242291       -1.697724       -1.284728
C           2.034547       -0.949042        1.256584
H           1.960526       -0.339725        2.159501
H           1.242268       -1.697346        1.285236
H           2.991614       -1.472455        1.279170
C           3.071909        0.952828       -0.000119
H           4.038118        0.446684       -0.000032
H           3.024927        1.591039       -0.884460
H           3.024906        1.591304        0.884029
H          -2.386806       -1.767230        0.000275
```

---

## Compound_28_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.959809 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.787677 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      53.6424 cm-1
2.      57.4777 cm-1
3.      74.3011 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.540651       -0.206628       -0.286019
C          -2.690125        0.681761       -0.017982
C          -3.846390        0.207555        0.432106
O          -1.540974       -1.416229       -0.146168
O          -0.486350        0.501798       -0.712373
C           0.762824       -0.180671       -0.991007
C           1.793474        0.049947        0.115530
C           1.300635       -0.529951        1.444509
H          -3.987556       -0.849598        0.616218
H          -4.681583        0.865507        0.628856
H           0.565912       -1.240223       -1.129259
H           1.110751        0.248860       -1.928490
H           1.103182       -1.599308        1.358652
H           2.056758       -0.384879        2.217674
H           0.385829       -0.039302        1.779942
C           2.075633        1.547185        0.271486
H           2.425540        1.978657       -0.668379
H           1.182507        2.089355        0.583404
H           2.846939        1.708808        1.026198
C           3.070990       -0.674321       -0.322820
H           3.854253       -0.539752        0.424396
H           2.896111       -1.745386       -0.440235
H           3.439798       -0.282819       -1.272805
H          -2.538185        1.736251       -0.202658
```

---

### Compound_28_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.959575 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.78826 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      24.3449 cm-1
  2.      51.1129 cm-1
  3.      98.7245 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.793006        0.654981        0.000002
C          -2.970257       -0.234106       -0.000047
C          -2.910040       -1.561840        0.000023
```

```
O          -1.888560        1.872824        0.000025
O          -0.628067        0.011638        0.000018
C           0.579474        0.812609        0.000091
C           1.791099       -0.112171       -0.000004
C           1.791342       -0.989080        1.256048
H          -1.967520       -2.091706        0.000113
H          -3.813887       -2.156081       -0.000006
H           0.570995        1.445797       -0.886792
H           0.570998        1.445622        0.887100
H           0.922726       -1.647410        1.282458
H           2.686298       -1.612785        1.279660
H           1.781975       -0.376096        2.159475
C           3.030766        0.789044        0.000097
H           3.053150        1.428838       -0.884101
H           3.053152        1.428635        0.884442
H           3.936430        0.181133        0.000026
C           1.791347       -0.988803       -1.256250
H           2.686297       -1.612511       -1.279994
H           0.922725       -1.647119       -1.282814
H           1.781992       -0.375619       -2.159542
H          -3.916669        0.289797       -0.000126
```

---

### Compound_28_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.959118 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.787293 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      34.3021 cm-1
  2.      62.2823 cm-1
  3.      72.6537 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.583322       -0.633132       -0.134673
C          -2.854271        0.037444        0.201890
C          -3.069490        1.344215        0.090519
O          -1.409312       -1.827289        0.046632
O          -0.666749        0.188502       -0.650921
C           0.655945       -0.319910       -0.958938
C           1.687859        0.137742        0.072614
```

```
C           1.742217        1.667611        0.121546
H          -2.307328        2.020248       -0.271511
H          -4.024124        1.772356        0.365309
H           0.615495       -1.403885       -1.020782
H           0.890848        0.090664       -1.939132
H           0.790360        2.087980        0.447496
H           2.511772        1.995665        0.822082
H           1.979170        2.081618       -0.860491
C           1.348570       -0.416800        1.459419
H           0.387871       -0.042185        1.815759
H           1.308198       -1.506907        1.448893
H           2.109758       -0.111880        2.179258
C           3.040710       -0.414622       -0.388846
H           3.826567       -0.110983        0.304084
H           3.028040       -1.505412       -0.428867
H           3.301682       -0.039941       -1.380449
H          -3.619128       -0.632326        0.571474
```

---

### Compound_28_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.95353 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.782122 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      27.9958 cm-1
  2.      55.7005 cm-1
  3.     101.2630 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.760110       -0.498337        0.000018
C          -2.380740        0.844845       -0.000033
C          -3.703160        0.982646       -0.000068
O          -2.401064       -1.537743        0.000051
O          -0.426574       -0.595945        0.000030
C           0.444164        0.567149       -0.000008
C           1.896028        0.100001        0.000003
C           2.759151        1.366955       -0.000033
H          -4.361629        0.124178       -0.000062
H          -4.158457        1.963508       -0.000105
H           0.236596        1.158176       -0.891083
```

```
H           0.236599        1.158230        0.891031
H           2.564823        1.976667        0.884323
H           3.816470        1.099332       -0.000029
H           2.564819        1.976620       -0.884421
C           2.191483       -0.724138        1.256684
H           1.976041       -0.148924        2.159300
H           1.596051       -1.636802        1.284289
H           3.244382       -1.009063        1.280110
C           2.191479       -0.724207       -1.256635
H           3.244377       -1.009135       -1.280047
H           1.596044       -1.636870       -1.284190
H           1.976036       -0.149040       -2.159281
H          -1.740810        1.713142       -0.000041
```

---

### Compound_28_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.952582 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.780323 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      38.0950 cm-1
  2.      56.2250 cm-1
  3.      75.2219 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.622165       -0.599370       -0.122716
C           1.991162        0.828375       -0.243228
C           3.196392        1.248651        0.128413
O           2.383062       -1.447209        0.317287
O           0.413306       -1.017382       -0.519905
C          -0.660267       -0.170977       -1.007379
C          -1.697527        0.130897        0.075652
C          -2.270290       -1.175412        0.633523
H           3.936386        0.568117        0.527658
H           3.469528        2.291372        0.041389
H          -0.262570        0.741318       -1.441499
H          -1.114988       -0.757551       -1.803259
H          -1.501061       -1.765808        1.131795
H          -3.053683       -0.961054        1.361995
H          -2.704465       -1.783181       -0.162698
```

```
C          -1.087923        0.958908        1.210162
H          -0.284245        0.421356        1.715454
H          -0.688524        1.904094        0.840060
H          -1.851702        1.183738        1.956132
C          -2.810762        0.934300       -0.606315
H          -3.592742        1.176673        0.114392
H          -2.427030        1.870302       -1.016525
H          -3.265390        0.365905       -1.419800
H           1.271841        1.529216       -0.632823
```

---

### Compound_28_HEI_1_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.872289 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.635943 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.       8.4258 cm-1
2.      29.7626 cm-1
3.      42.6088 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.752307        0.134021       -0.356641
C          -1.647686        1.145136       -0.086084
C          -3.081908        0.898152       -0.329470
O          -1.039967       -1.023611       -0.786787
O           0.580648        0.451468       -0.114152
C           1.539538       -0.603816       -0.231603
C           2.932242       -0.075524        0.114139
C           3.904361       -1.251807       -0.027445
H          -3.315855        0.560200       -1.341172
H          -3.702696        1.760252       -0.100411
H           1.273372       -1.418340        0.446096
H           1.536276       -0.995088       -1.250888
H           3.900483       -1.645858       -1.045669
H           4.921521       -0.933655        0.206492
H           3.641007       -2.064762        0.652158
C           2.966657        0.443395        1.555169
H           2.296854        1.292779        1.689741
H           2.669145       -0.338226        2.257442
H           3.975496        0.766625        1.818273
```

```
C           3.336655        1.039508       -0.855594
H           4.351904        1.378848       -0.642136
H           3.309348        0.685805       -1.888425
H           2.671625        1.899410       -0.774224
N          -3.602583       -0.246191        0.548601
H          -2.966376       -1.027282        0.367268
H          -3.482070        0.021374        1.524210
C          -5.005686       -0.644863        0.286313
H          -5.272736       -1.467899        0.942782
H          -5.651735        0.207844        0.473985
H          -5.089423       -0.954284       -0.751253
H          -1.324701        2.067529        0.370329
```

---

### Compound_28_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.87307 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.634862 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      30.3025 cm-1
  2.      51.0328 cm-1
  3.      60.1315 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.911715        1.732738       -0.031806
C           2.214883        1.376303        0.255983
C           2.573788        0.001188        0.649028
O           0.460994        2.851010       -0.399262
O           0.020401        0.661238        0.103906
C          -1.356519        0.889629       -0.198983
C          -2.151585       -0.395673        0.033947
C          -1.634444       -1.522914       -0.866432
H           1.969311       -0.412875        1.456468
H           3.622343       -0.092955        0.919672
H          -1.747153        1.687108        0.436173
H          -1.455566        1.204350       -1.240251
H          -2.274923       -2.402154       -0.775588
H          -1.629765       -1.216012       -1.914309
H          -0.622379       -1.824447       -0.594886
C          -3.609843       -0.088048       -0.323190
```

```
H          -4.004129        0.721029        0.294834
H          -3.705134        0.207250       -1.370007
H          -4.233623       -0.968811       -0.163367
C          -2.062440       -0.818997        1.503515
H          -2.428486       -0.026908        2.160082
H          -2.667995       -1.709860        1.679807
H          -1.035800       -1.049040        1.789081
N           2.353432       -0.998675       -0.499790
H           2.957720       -0.730724       -1.274803
H           1.389602       -0.854556       -0.804621
C           2.564922       -2.420350       -0.137278
H           2.367995       -3.044539       -1.003933
H           3.592655       -2.548337        0.189999
H           1.883191       -2.675758        0.668430
H           2.994090        2.106724        0.099900
```

---

### Compound_28_HEI_3_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.872956 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.635146 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      27.2717 cm-1
  2.      35.5592 cm-1
  3.      54.6589 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.569871       -0.858752       -0.395270
C          -1.515954       -1.290606        0.503142
C          -2.914366       -0.851846        0.308836
O          -0.778858       -0.086581       -1.379340
O           0.719800       -1.350208       -0.170652
C           1.827454       -0.683726       -0.787998
C           2.503768        0.343676        0.129135
C           3.696579        0.916735       -0.642919
H          -3.340156       -1.117034       -0.661438
H          -3.581396       -1.210758        1.088065
H           2.540748       -1.470991       -1.036064
H           1.502417       -0.209067       -1.711878
H           4.225459        1.653610       -0.036071
```

```
H           4.405876        0.131254       -0.911994
H           3.370776        1.408473       -1.561806
C           2.998615       -0.337571        1.408364
H           3.691439       -1.149162        1.175931
H           3.520095        0.379515        2.045201
H           2.169509       -0.753770        1.981354
C           1.533889        1.474102        0.488211
H           1.175847        1.985164       -0.406597
H           0.667577        1.097738        1.033822
H           2.032541        2.209957        1.122074
N          -3.005739        0.674429        0.328767
H          -2.299659        0.979762       -0.350113
H          -2.706077        0.999472        1.246623
C          -4.337102        1.226965       -0.012752
H          -4.295237        2.311539        0.028248
H          -4.599942        0.903068       -1.015471
H          -5.065162        0.853800        0.701841
H          -1.240082       -1.863116        1.374358
```

---

### Compound_28_HEI_6_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.872199 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.634858 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      20.0843 cm-1
2.      30.3853 cm-1
3.      82.9153 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.831557        0.193510       -0.493367
C          -1.776170        1.021092        0.085196
C          -3.181382        0.991647       -0.327093
O          -0.994637       -0.669370       -1.397504
O           0.454175        0.387544        0.018289
C           1.504475       -0.414457       -0.526649
C           2.828944       -0.060659        0.150625
C           3.180587        1.409638       -0.097287
H          -3.323639        0.592767       -1.329621
H          -3.668060        1.963020       -0.258787
```

```
H           1.280716       -1.472056       -0.369753
H           1.582117       -0.240573       -1.602133
H           4.152357        1.646779        0.339682
H           3.230935        1.622450       -1.167250
H           2.441450        2.076801        0.346409
C           3.904323       -0.954937       -0.475943
H           3.982211       -0.782959       -1.551335
H           4.878311       -0.746681       -0.030307
H           3.680016       -2.011529       -0.316528
C           2.750708       -0.335588        1.655637
H           2.003138        0.294540        2.137659
H           2.490424       -1.378706        1.847584
H           3.713844       -0.136107        2.129036
N          -4.076787        0.085472        0.564249
H          -3.979286        0.408474        1.526108
H          -5.051991        0.217749        0.295896
C          -3.734327       -1.356164        0.495586
H          -3.885762       -1.698905       -0.523191
H          -2.694738       -1.475668        0.781708
H          -4.376891       -1.905525        1.177522
H          -1.467552        1.717936        0.851032
```

---

### Compound_28_HEI_8_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.872969 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.634161 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      37.1104 cm-1
  2.      48.7317 cm-1
  3.      64.2364 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.678382       -0.974196       -0.300664
C           1.723049       -1.045819        0.599104
C           3.106293       -0.774185        0.197615
O           0.719507       -0.675999       -1.522670
O          -0.555898       -1.328197        0.270791
C          -1.757583       -0.981670       -0.423971
C          -2.404719        0.306231        0.103284
```

```
C          -2.762493        0.146917        1.583935
H           3.274238       -0.904274       -0.869686
H           3.837832       -1.364239        0.747255
H          -1.553951       -0.891755       -1.489072
H          -2.442241       -1.818006       -0.272977
H          -3.253797        1.047244        1.957854
H          -3.442093       -0.695011        1.732664
H          -1.872254       -0.025452        2.189690
C          -3.680931        0.536209       -0.712189
H          -4.369181       -0.305967       -0.613845
H          -4.197630        1.433736       -0.367852
H          -3.452349        0.664946       -1.772121
C          -1.459230        1.498466       -0.073842
H          -0.539564        1.364219        0.496749
H          -1.190945        1.637456       -1.122060
H          -1.938281        2.414293        0.277853
N           3.553125        0.687726        0.472217
H           3.415512        0.868825        1.465957
H           4.552416        0.768241        0.283791
C           2.815465        1.705361       -0.316230
H           3.004589        1.528826       -1.370461
H           1.756778        1.605708       -0.102023
H           3.164577        2.693647       -0.031333
H           1.516208       -1.306841        1.626876
```

---

### Compound_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -247.430487 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -247.378234 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      49.9372 cm-1
2.     292.1380 cm-1
3.     318.7427 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.557504       -0.110931        0.016699
O           1.492212       -0.921406       -0.091030
C          -0.836930       -0.609671        0.111791
C          -1.938979        0.105717       -0.084695
```

```
H          -2.914947       -0.356747       -0.021013
H          -1.921397        1.160976       -0.325799
H          -0.897117       -1.670216        0.320796
N           0.767904        1.213300        0.047808
H           0.021114        1.871857        0.188138
H           1.709750        1.561584       -0.031310
```

---

### Compound_7_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -247.432401 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -247.379948 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      96.9075 cm-1
2.     281.6741 cm-1
3.     310.5682 cm-1
```

#### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.482533        0.118467        0.000016
O          -0.537949        1.356265       -0.000120
C           0.798073       -0.634021       -0.000035
C           1.975275       -0.020581       -0.000127
H           2.899672       -0.581679       -0.000156
H           2.045626        1.059520       -0.000171
H           0.731548       -1.715112        0.000013
N          -1.585619       -0.647118        0.000239
H          -2.495903       -0.214813        0.000211
H          -1.522910       -1.651403        0.000267
```

---

### Compound_7_HEI_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -343.335903 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -343.217477 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      79.1038 cm-1
2.      93.9188 cm-1
3.     106.3629 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.643718       -0.054309       -0.015708
O           2.804970       -0.441713       -0.398465
C           0.579369       -0.909059        0.241187
C          -0.756910       -0.485486        0.670646
H          -1.304711       -1.277529        1.177173
H          -0.777729        0.398231        1.308698
H           0.741295       -1.961547        0.050690
C          -3.055148        0.317602       -0.103583
H          -3.527036       -0.509956        0.417910
H          -3.631016        0.579579       -0.986466
H          -2.973413        1.175772        0.556990
N          -1.690535       -0.096520       -0.511080
H          -1.235519        0.655064       -1.027233
H          -1.735378       -0.897028       -1.140075
N           1.472879        1.338436        0.094557
H           2.340083        1.813415        0.299295
H           0.721078        1.651796        0.691142
```

---

### Compound_7_HEI_2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -343.338269 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -343.219949 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      74.0979 cm-1
2.     112.7293 cm-1
3.     128.7643 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.401522       -0.100675        0.065528
O          -0.920330       -1.261760        0.377774
C          -0.646750        1.052490        0.051252
C           0.788986        0.967253        0.405931
H           1.322128        1.900025        0.240336
H           0.985278        0.637804        1.429842
H          -1.058497        1.988440       -0.296190
C           2.864094       -0.420125       -0.045988
H           2.859271       -0.779528        0.978906
H           3.470618        0.478308       -0.120660
H           3.255538       -1.189082       -0.706022
N           1.475299       -0.098376       -0.441131
H           0.849778       -0.913277       -0.326848
H           1.435081        0.190701       -1.416660
N          -2.746838       -0.075393       -0.345453
H          -3.198115        0.821616       -0.235127
H          -3.286515       -0.818203        0.075981
```

---

### Compound_7_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -343.335281 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -343.216932 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      55.1681 cm-1
  2.      92.0403 cm-1
  3.     104.7866 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.494371       -0.187765        0.011003
O           2.443351       -1.012235       -0.244028
C           0.318566       -0.528498        0.668370
C          -0.783704        0.394532        0.948383
H          -1.413820        0.061343        1.770731
H          -0.477738        1.420573        1.151398
```

```
H           0.191821       -1.570856        0.925622
C          -2.537572       -0.682821       -0.552525
H          -1.820711       -1.462720       -0.788799
H          -3.188308       -0.502573       -1.403024
H          -3.124888       -0.965679        0.316564
N          -1.793836        0.558301       -0.233888
H          -1.262613        0.855691       -1.050945
H          -2.451305        1.304363       -0.007203
N           1.684688        1.123712       -0.462535
H           1.152005        1.847695       -0.002532
H           2.662826        1.363264       -0.536017
```

---

### Compound_7_HEI_4_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -343.337347 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -343.2188 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      74.9790 cm-1
  2.     101.1428 cm-1
  3.     129.8705 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.328147        0.030855        0.097776
O           1.250785        1.025540        0.902363
C           0.366053       -0.954867       -0.073503
C          -0.910456       -0.935412        0.641496
H          -1.289794       -1.927426        0.881748
H          -0.880318       -0.336218        1.549387
H           0.555602       -1.762548       -0.768769
C          -1.886499        1.128251       -0.497251
H          -1.855978        1.688447        0.432007
H          -2.712160        1.468788       -1.115462
H          -0.948538        1.236361       -1.031770
N          -2.078787       -0.306921       -0.178252
H          -2.949748       -0.430833        0.337812
H          -2.161044       -0.835516       -1.045833
N           2.488051       -0.030023       -0.700820
H           2.698775       -0.947089       -1.067987
H           3.288609        0.387355       -0.247639
```

### Compound_24_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962005 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.790211 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      27.6777 cm-1
2.      53.3909 cm-1
3.      68.9634 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.972488       -0.243371       -0.374085
C           2.285510        0.272691        0.103509
C           3.390420       -0.737739        0.164627
C           2.436585        1.547878        0.460868
O           0.785886       -1.420453       -0.631179
O           0.034112        0.700735       -0.495959
C          -1.309352        0.324083       -0.892400
C          -2.253416        0.341592        0.300209
C          -3.676889        0.100678       -0.200463
C          -1.859284       -0.679340        1.364728
H           4.309158       -0.274756        0.518957
H           3.131856       -1.559541        0.834513
H           3.574942       -1.175356       -0.818037
H           1.623194        2.256376        0.414227
H           3.392619        1.909710        0.815835
H          -1.602020        1.071629       -1.626746
H          -1.285035       -0.654436       -1.366103
H          -2.205151        1.341507        0.740696
H          -3.970610        0.844324       -0.943193
H          -3.764552       -0.887465       -0.658118
H          -4.386297        0.149995        0.626209
H          -1.896399       -1.693561        0.961553
H          -0.852449       -0.501763        1.744183
H          -2.545604       -0.627742        2.211169
```

### Compound_24_1

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962247 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.790317 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      34.9029 cm-1
2.      52.3045 cm-1
3.      56.5356 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.994027       -0.560531        0.125849
C          -2.322962        0.085320       -0.081315
C          -2.494490        1.522852        0.308036
C          -3.298110       -0.652596       -0.610334
O          -0.721645       -1.709569       -0.176109
O          -0.120095        0.275430        0.694598
C           1.234668       -0.195199        0.913723
C           2.100516       -0.042317       -0.328448
C           3.498498       -0.572991       -0.015992
C           2.146977        1.406768       -0.806200
H          -3.507961        1.853333        0.088307
H          -2.303864        1.668938        1.372276
H          -1.794517        2.162564       -0.231695
H          -3.138415       -1.686963       -0.880257
H          -4.280282       -0.233684       -0.783004
H           1.606442        0.432269        1.721925
H           1.197756       -1.229465        1.248096
H           1.664420       -0.658511       -1.118222
H           3.467764       -1.616878        0.300575
H           4.138824       -0.505350       -0.896095
H           3.964692        0.009155        0.782533
H           2.765743        1.494966       -1.700305
H           1.152323        1.781823       -1.048368
H           2.574573        2.053083       -0.035589
```

---

### Compound_24_2

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962321 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.79052 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      31.9501 cm-1
  2.      47.0137 cm-1
  3.      59.1019 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.984096       -0.428822       -0.177052
C           2.297244        0.244816        0.017469
C           3.388599       -0.619367        0.571881
C           2.458513        1.535488       -0.273957
O           0.781248       -1.583916        0.157948
O           0.057297        0.341377       -0.754253
C          -1.275958       -0.205648       -0.920063
C          -2.115709       -0.063398        0.340996
C          -3.487245       -0.686139        0.086790
C          -2.236388        1.395825        0.772968
H           4.309633       -0.048985        0.673612
H           3.113219       -1.016612        1.550345
H           3.577086       -1.476244       -0.077205
H           1.653407        2.139354       -0.665172
H           3.414098        2.019078       -0.119122
H          -1.702661        0.377725       -1.734190
H          -1.194200       -1.245566       -1.228171
H          -1.622142       -0.625533        1.137286
H          -3.402759       -1.737684       -0.192544
H          -4.107887       -0.622903        0.981233
H          -4.007449       -0.162796       -0.719079
H          -2.833495        1.477860        1.682270
H          -1.259777        1.837620        0.971924
H          -2.724344        1.988465       -0.004933
```

---

### Compound_24_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962251 |

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.790682 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      29.5455 cm-1
  2.      56.5286 cm-1
  3.      58.9788 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.156649       -0.645984       -0.000013
C          -2.199910        0.420665        0.000002
C          -1.759990        1.854058        0.000024
C          -3.477736        0.043762       -0.000003
O          -1.379108       -1.845376       -0.000032
O           0.073891       -0.136299       -0.000005
C           1.188886       -1.064541       -0.000018
C           2.479090       -0.265508        0.000001
C           2.623874        0.580408       -1.264354
C           2.623866        0.580360        1.264388
H          -2.625855        2.513566        0.000032
H          -1.150469        2.079031        0.876545
H          -1.150467        2.079056       -0.876490
H          -3.756136       -1.000642       -0.000019
H          -4.273476        0.776438        0.000007
H           1.109850       -1.692681        0.886606
H           1.109856       -1.692648       -0.886666
H           3.271633       -1.019737       -0.000011
H           1.857718        1.356257       -1.307107
H           3.596992        1.072582       -1.286180
H           2.534410       -0.032906       -2.162779
H           1.857710        1.356208        1.307166
H           2.534395       -0.032987        2.162790
H           3.596983        1.072534        1.286239
```

---

### Compound_24_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962557 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.791038 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      33.6815 cm-1
2.      52.9313 cm-1
3.      64.2519 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.193049       -0.627956        0.050819
C          -2.388300        0.258850       -0.053789
C          -2.181077        1.711635       -0.361257
C          -3.589010       -0.286969        0.134807
O          -1.224143       -1.820847        0.302505
O          -0.057724        0.037744       -0.164880
C           1.182707       -0.708178       -0.082575
C           2.334536        0.253967       -0.301030
C           2.380931        1.333527        0.777952
C           3.638555       -0.540888       -0.346777
H          -3.138273        2.228184       -0.400857
H          -1.558233        2.189603        0.396402
H          -1.674602        1.843465       -1.318575
H          -3.701933       -1.338945        0.355685
H          -4.487319        0.312191        0.071832
H           1.240149       -1.176723        0.900630
H           1.163398       -1.487961       -0.843137
H           2.185510        0.732574       -1.273087
H           2.524352        0.883355        1.763446
H           3.209828        2.019570        0.598307
H           1.460961        1.917566        0.804030
H           3.815553       -1.050443        0.603328
H           3.620078       -1.294279       -1.135959
H           4.483704        0.122736       -0.531947
```

---

### Compound_24_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962262 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.791029 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      26.1921 cm-1
2.      52.7775 cm-1
3.      58.7160 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -1.108670       -0.538736       -0.000080
C          -2.160246        0.515169        0.000024
C          -3.573521        0.017416       -0.000022
C          -1.836252        1.808226        0.000145
O          -1.367604       -1.731632       -0.000213
O           0.136534       -0.066811       -0.000013
C           1.219605       -1.031729       -0.000106
C           2.536172       -0.276916        0.000008
C           2.710404        0.563481       -1.264254
C           2.710353        0.563186        1.264474
H          -4.269964        0.853484        0.000061
H          -3.770207       -0.601868       -0.876900
H          -3.770203       -0.602040        0.876736
H          -0.809065        2.141365        0.000173
H          -2.606499        2.568322        0.000218
H           1.120971       -1.657294        0.886486
H           1.121003       -1.657086       -0.886848
H           3.302253       -1.058091       -0.000068
H           1.972746        1.366506       -1.306472
H           3.700666        1.020204       -1.286758
H           2.598285       -0.046070       -2.162704
H           1.972693        1.366202        1.306848
H           2.598194       -0.046576        2.162776
H           3.700614        1.019903        1.287125
```

---

### Compound_24_6

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.962615 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.79122 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      29.1027 cm-1
2.      52.4888 cm-1
3.      61.9682 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           1.160798       -0.502660        0.037891
C           2.353577        0.378834       -0.089764
C           3.676506       -0.291111        0.125095
C           2.223744        1.675231       -0.371543
O           1.240768       -1.686793        0.322761
O          -0.000795        0.112198       -0.185683
C          -1.208746       -0.680141       -0.066823
C          -2.400284        0.226624       -0.308544
C          -3.670868       -0.621857       -0.320982
C          -2.486055        1.337194        0.736026
H           4.487705        0.424782        0.009275
H           3.735796       -0.728453        1.123253
H           3.823098       -1.104738       -0.587402
H           1.258397        2.135953       -0.519570
H           3.096413        2.309083       -0.458713
H          -1.164639       -1.484675       -0.800216
H          -1.241540       -1.116133        0.932488
H          -2.275687        0.679524       -1.296240
H          -3.822150       -1.107621        0.645874
H          -4.543503        0.000353       -0.521854
H          -3.625405       -1.398696       -1.085970
H          -2.607734        0.913047        1.735887
H          -1.590138        1.958056        0.739437
H          -3.342436        1.983588        0.538988
```

---

## Compound_24_7

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.961649 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.78947 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      33.3216 cm-1
2.      50.9981 cm-1
3.      69.0277 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.940431       -0.528445       -0.317127
C           2.128273        0.258265        0.128604
C           2.052309        1.755346        0.104478
C           3.203694       -0.415066        0.535148
O           0.874343       -1.745001       -0.320069
O          -0.052039        0.269852       -0.720890
C          -1.320786       -0.312945       -1.122136
C          -2.369086       -0.127035       -0.034137
C          -2.018818       -0.893184        1.240498
C          -2.625394        1.350943        0.256361
H           2.983808        2.185091        0.468276
H           1.869866        2.124779       -0.905743
H           1.233902        2.117671        0.728463
H           3.222465       -1.495739        0.540475
H           4.090334        0.105268        0.871466
H          -1.599656        0.226945       -2.024635
H          -1.170845       -1.362407       -1.358675
H          -3.282430       -0.558695       -0.455198
H          -1.869939       -1.954861        1.040609
H          -1.106143       -0.502388        1.695133
H          -2.819518       -0.794055        1.974552
H          -1.740180        1.824322        0.684773
H          -2.892053        1.893014       -0.652660
H          -3.441779        1.464970        0.970706
```

---

### Compound_24_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.961673 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.789677 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      30.8543 cm-1
2.      55.1467 cm-1
3.      62.1533 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.914072       -0.390298       -0.348729
C          -2.085670        0.414716        0.096250
C          -3.303422       -0.373180        0.472322
C          -2.021893        1.744423        0.162872
O          -0.918445       -1.609529       -0.345917
O           0.123755        0.347631       -0.750916
C           1.364480       -0.308944       -1.124022
C           2.400946       -0.185167       -0.016115
C           2.732772        1.275595        0.285107
C           1.986093       -0.934782        1.248956
H          -4.107379        0.293383        0.777828
H          -3.650920       -0.980583       -0.365186
H          -3.086513       -1.058823        1.293232
H          -1.129058        2.289012       -0.105780
H          -2.875488        2.319717        0.496675
H           1.159131       -1.347959       -1.365283
H           1.693237        0.212871       -2.020381
H           3.296999       -0.665111       -0.421987
H           1.867802        1.794727        0.701528
H           3.542622        1.342561        1.012729
H           3.042974        1.805725       -0.617141
H           1.086258       -0.498290        1.687329
H           1.785998       -1.986741        1.042546
H           2.776450       -0.879475        1.998710
```

---

### Compound_24_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -463.961929 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -463.789818 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      34.1888 cm-1
2.      52.8775 cm-1
3.      69.0188 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.990396       -0.405698       -0.366308
C           2.314113        0.115377        0.086285
C           2.467060        1.586740        0.330206
```

```
C           3.303209       -0.761105        0.256359
O           0.741477       -1.579156       -0.579692
O           0.099614        0.580599       -0.515629
C          -1.261573        0.262289       -0.903996
C          -2.204921        0.390696        0.282421
C          -3.638849        0.205137       -0.211812
C          -1.868922       -0.598203        1.395906
H           3.480551        1.809599        0.658569
H           2.260356        2.160193       -0.574606
H           1.769336        1.933893        1.093693
H           3.159938       -1.816418        0.072430
H           4.281641       -0.436851        0.584309
H          -1.508598        0.989055       -1.674992
H          -1.290335       -0.738092       -1.329072
H          -2.101416        1.406479        0.674243
H          -3.780659       -0.797852       -0.621014
H          -4.345536        0.334262        0.608535
H          -3.889456        0.926652       -0.991248
H          -1.962337       -1.626892        1.041414
H          -0.853715       -0.459090        1.769169
H          -2.551588       -0.467873        2.236785
```

---

### Compound_24_HEI_10

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867735 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630366 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.6625 cm-1
  2.      36.1060 cm-1
  3.      58.5427 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.150388        0.316039        0.824228
C           0.948631        1.152972        0.093764
C           0.480554        2.373815       -0.645863
C           2.390383        0.779363        0.016689
O           0.530111       -0.773604        1.387948
O          -1.184495        0.706894        0.978462
C          -2.176747       -0.317847        1.135071
```

```
C          -2.750054       -0.801686       -0.195594
C          -3.379027        0.342746       -0.988824
C          -1.720538       -1.555076       -1.038524
H           0.844657        2.379446       -1.679120
H          -0.606451        2.421938       -0.684323
H           0.827391        3.311762       -0.193865
H           2.911224        0.788478        0.977259
H           2.943409        1.408680       -0.676784
H          -1.759834       -1.150871        1.698746
H          -2.968069        0.139377        1.729865
H          -3.544766       -1.504551        0.077485
H          -4.127824        0.872089       -0.396175
H          -2.621795        1.065779       -1.297186
H          -3.865981       -0.032959       -1.890274
H          -2.185651       -1.956370       -1.940701
H          -0.909805       -0.894373       -1.350734
H          -1.282571       -2.386522       -0.484776
N           2.534426       -0.651489       -0.466734
H           2.170889       -0.709719       -1.416082
H           1.882484       -1.165724        0.152968
C           3.904926       -1.204506       -0.394945
H           4.566166       -0.595673       -1.005482
H           4.232848       -1.184489        0.640221
H           3.896670       -2.227099       -0.761191
```

---

### Compound_24_HEI_11

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867472 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.631375 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      20.0131 cm-1
2.      30.3121 cm-1
3.      65.2207 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.425670       -0.069052       -0.461005
C          -1.329061        0.947975       -0.302640
C          -0.978581        2.398700       -0.127723
C          -2.768342        0.562241       -0.357684
```

```
O          -0.715010       -1.317425       -0.564547
O           0.918656        0.297650       -0.517012
C           1.883220       -0.712175       -0.200692
C           3.261602       -0.072688       -0.139927
C           3.351979        0.980480        0.962452
C           4.314194       -1.162794        0.054634
H           0.073855        2.527381        0.121273
H          -1.169530        3.001368       -1.025380
H          -1.562860        2.856210        0.677517
H          -3.089150        0.151646       -1.318855
H          -3.426326        1.390837       -0.105991
H           1.637037       -1.167839        0.763361
H           1.865270       -1.496732       -0.959030
H           3.441303        0.413438       -1.103877
H           2.624781        1.779311        0.818173
H           3.165653        0.527266        1.939748
H           4.345863        1.430570        0.986839
H           5.316870       -0.733619        0.070879
H           4.160496       -1.685125        1.002228
H           4.276465       -1.902553       -0.746941
N          -3.055098       -0.551246        0.631040
H          -2.306542       -1.237222        0.425688
H          -2.902963       -0.194987        1.572646
C          -4.398854       -1.160348        0.515727
H          -4.504830       -1.935811        1.269020
H          -5.151003       -0.390566        0.665215
H          -4.500797       -1.590690       -0.476177
```

---

### Compound_24_HEI_12

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868164 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.63081 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      36.0828 cm-1
2.      47.3089 cm-1
3.      52.7831 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.066836        1.107715       -0.320310
C          -1.238829        0.977781        0.392623
C          -2.008992        2.188578        0.849966
C          -1.849103       -0.341472        0.631774
O           0.576008        2.166901       -0.585309
O           0.434692       -0.105336       -0.835162
C           1.853887       -0.195864       -1.002179
C           2.609912       -0.298009        0.319098
C           2.150574       -1.499445        1.141069
C           4.109601       -0.358450        0.036737
H          -1.431305        3.101366        0.710350
H          -2.954953        2.323232        0.308831
H          -2.270393        2.125449        1.912018
H          -1.135497       -1.157941        0.683687
H          -2.471314       -0.354779        1.526347
H           2.009740       -1.102457       -1.589643
H           2.217942        0.652985       -1.581148
H           2.403166        0.611941        0.889415
H           1.086035       -1.445554        1.369317
H           2.332626       -2.430637        0.597822
H           2.693743       -1.552165        2.086278
H           4.679227       -0.399295        0.966313
H           4.358773       -1.249250       -0.545690
H           4.444954        0.514955       -0.525623
N          -2.817170       -0.760393       -0.497543
H          -2.276347       -0.789392       -1.360961
H          -3.509558       -0.020974       -0.608438
C          -3.492374       -2.062046       -0.272619
H          -2.732538       -2.831764       -0.173378
H          -4.076730       -1.995823        0.640301
H          -4.140022       -2.282394       -1.116180
```

---

### Compound_24_HEI_13

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867204 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630376 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      30.3404 cm-1
2.      34.5174 cm-1
3.      67.4764 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.449356       -0.213983       -0.474086
C          -1.448546        0.730352       -0.329604
C          -1.251707        2.031527        0.407699
C          -2.798039        0.410717       -0.810188
O          -0.510362       -1.345311       -1.041352
O           0.772776        0.169933        0.089799
C           1.901620       -0.672858       -0.153995
C           3.133457       -0.038347        0.473542
C           4.315310       -0.997584        0.341982
C           3.455930        1.317144       -0.152133
H          -0.258339        2.453060        0.248372
H          -1.977358        2.774190        0.063383
H          -1.384662        1.952111        1.495277
H          -2.815551       -0.401197       -1.531756
H          -3.320571        1.274145       -1.222938
H           1.725890       -1.661546        0.274442
H           2.051374       -0.795012       -1.230368
H           2.924111        0.108401        1.537677
H           4.105234       -1.958188        0.815652
H           4.547266       -1.184613       -0.709505
H           5.207364       -0.578627        0.809494
H           4.341450        1.756145        0.310671
H           3.657126        1.206073       -1.220973
H           2.632551        2.021703       -0.036456
N          -3.758583       -0.065945        0.320234
H          -4.699599       -0.151953       -0.062502
H          -3.788937        0.664050        1.030598
C          -3.353482       -1.346172        0.949081
H          -3.388334       -2.127306        0.196001
H          -2.342699       -1.236479        1.328216
H          -4.036673       -1.575096        1.761713
```

---

### Compound_24_HEI_14

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.86657 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630228 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      23.3769 cm-1
  2.      25.7921 cm-1
```

```
   3.      63.7032 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.402169       -0.259003       -0.636456
C           1.311160        0.750366       -0.377092
C           0.947373        2.004159        0.378983
C           2.719114        0.545712       -0.736252
O           0.595699       -1.361923       -1.229889
O          -0.885806        0.017558       -0.169955
C          -1.929685       -0.891973       -0.527693
C          -3.241383       -0.398830        0.068257
C          -3.205851       -0.387132        1.596230
C          -3.649813        0.963778       -0.491029
H           1.656029        2.804328        0.146476
H          -0.047968        2.369794        0.122530
H           0.962462        1.886506        1.471040
H           2.863453       -0.238148       -1.474320
H           3.213353        1.457431       -1.073176
H          -2.009671       -0.951820       -1.615734
H          -1.698298       -1.890060       -0.150664
H          -3.989387       -1.132805       -0.247657
H          -2.926137       -1.365374        1.992225
H          -2.486166        0.344378        1.966944
H          -4.184129       -0.125925        2.003071
H          -4.639397        1.248270       -0.129630
H          -2.948164        1.741013       -0.184048
H          -3.680526        0.950050       -1.582313
N           3.603452        0.100705        0.468661
H           3.516727        0.811538        1.193946
H           4.579670        0.087540        0.174716
C           3.229698       -1.219952        1.029433
H           2.184590       -1.185246        1.319257
H           3.380860       -1.975631        0.264940
H           3.852702       -1.428597        1.894244
```

---

### Compound_24_HEI_15_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867746 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630483 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      22.4780 cm-1
  2.      36.7809 cm-1
  3.      43.3818 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.332916       -0.628642       -0.788044
C           1.479725       -0.912051       -0.076276
C           1.481917       -1.774261        1.163612
C           2.737949       -0.266352       -0.474869
O           0.191900        0.124275       -1.797240
O          -0.799183       -1.317633       -0.318294
C          -2.077840       -0.755895       -0.629426
C          -2.391130        0.505058        0.172296
C          -3.771536        1.022402       -0.226526
C          -2.303521        0.255610        1.675593
H           0.914654       -2.698933        1.038630
H           2.505611       -2.060489        1.418170
H           1.069141       -1.274816        2.049121
H           2.722607        0.108719       -1.494383
H           3.611548       -0.903460       -0.336940
H          -2.151277       -0.552606       -1.697764
H          -2.795511       -1.539652       -0.380473
H          -1.649003        1.261485       -0.096643
H          -3.826518        1.227059       -1.297412
H          -4.545335        0.289323        0.015620
H          -4.009762        1.944913        0.304943
H          -2.522447        1.168587        2.232141
H          -3.025043       -0.505841        1.983706
H          -1.309932       -0.084921        1.967930
N           3.077452        0.982015        0.387767
H           4.013322        1.306950        0.145749
H           3.106043        0.684808        1.362505
C           2.107081        2.094396        0.244543
H           2.127052        2.440085       -0.784118
H           1.119443        1.721514        0.495354
H           2.388140        2.898441        0.918353
```

---

### Compound_24_HEI_16_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867236 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.629241 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      43.2603 cm-1
2.      57.0512 cm-1
3.      63.5674 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.423043       -1.190209       -0.173155
C          -1.713633       -0.699677       -0.233430
C          -2.820591       -1.402772        0.509831
C          -2.061714        0.541520       -0.936671
O          -0.037850       -2.236419        0.423487
O           0.526799       -0.438447       -0.886818
C           1.894825       -0.861133       -0.885632
C           2.776151        0.008176        0.008502
C           2.793048        1.464561       -0.453778
C           2.389600       -0.100977        1.482573
H          -3.006402       -0.998271        1.514595
H          -3.767058       -1.319655       -0.034016
H          -2.609106       -2.464994        0.637594
H          -1.298069        0.888720       -1.624297
H          -3.015200        0.475075       -1.463236
H           1.957381       -1.903029       -0.580680
H           2.234157       -0.781468       -1.920431
H           3.787118       -0.396463       -0.109903
H           3.087431        1.543342       -1.502268
H           1.808709        1.921983       -0.345587
H           3.497094        2.051138        0.138997
H           3.065954        0.491229        2.101527
H           1.377441        0.271123        1.650027
H           2.428886       -1.134050        1.829982
N          -2.291292        1.745095        0.025511
H          -2.995873        1.466307        0.706811
H          -2.679965        2.522208       -0.507542
C          -1.068528        2.187582        0.736683
H          -0.649512        1.334128        1.259094
H          -0.361525        2.563836        0.004651
H          -1.330699        2.969678        1.443217
```

---

### Compound_24_HEI_16

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867236 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.62924 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      43.2898 cm-1
  2.      57.0571 cm-1
  3.      63.6432 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.423031       -1.190210       -0.173165
C          -1.713621       -0.699677       -0.233435
C          -2.820564       -1.402773        0.509848
C          -2.061710        0.541515       -0.936678
O          -0.037845       -2.236405        0.423503
O           0.526810       -0.438484       -0.886867
C           1.894844       -0.861145       -0.885624
C           2.776127        0.008187        0.008530
C           2.793023        1.464563       -0.453780
C           2.389532       -0.100951        1.482591
H          -3.006268       -0.998369        1.514671
H          -3.767067       -1.319529       -0.033917
H          -2.609148       -2.465026        0.637479
H          -1.298073        0.888706       -1.624318
H          -3.015200        0.475065       -1.463235
H           1.957408       -1.903038       -0.580664
H           2.234211       -0.781483       -1.920411
H           3.787103       -0.396443       -0.109833
H           3.087522        1.543325       -1.502239
H           1.808657        1.921957       -0.345717
H           3.496985        2.051179        0.139056
H           3.065863        0.491269        2.101556
H           1.377366        0.271144        1.650009
H           2.428814       -1.134018        1.830015
N          -2.291277        1.745107        0.025493
H          -2.995882        1.466360        0.706785
H          -2.679910        2.522227       -0.507581
C          -1.068512        2.187569        0.736684
H          -0.649555        1.334110        1.259136
H          -0.361466        2.563765        0.004664
H          -1.330670        2.969698        1.443185
```

---

### Compound_24_HEI_18

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867112 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.629045 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      30.4026 cm-1
  2.      53.8059 cm-1
  3.      55.1559 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.224927       -0.502707        0.865662
C          -1.225128       -0.987257        0.048619
C          -0.943771       -1.891953       -1.128271
C          -2.616704       -0.600949        0.320186
O          -0.318097        0.303984        1.837034
O           1.038507       -1.038406        0.557904
C           2.210082       -0.348771        1.008684
C           2.783011        0.582992       -0.057998
C           3.207227       -0.184809       -1.309113
C           1.821797        1.717502       -0.411089
H          -0.551855       -2.874515       -0.841646
H          -1.862181       -2.072183       -1.691616
H          -0.221960       -1.466308       -1.832124
H          -2.768619       -0.226305        1.328805
H          -3.330040       -1.401678        0.124766
H           1.987584        0.202355        1.920343
H           2.937341       -1.126693        1.245839
H           3.679117        1.021036        0.394569
H           3.913958       -0.980642       -1.065654
H           2.343825       -0.639784       -1.798370
H           3.684029        0.481299       -2.030197
H           2.286765        2.408272       -1.116567
H           0.915958        1.328375       -0.879676
H           1.526419        2.283166        0.473326
N          -3.125199        0.548631       -0.593814
H          -4.127309        0.668863       -0.447316
H          -2.995208        0.253757       -1.560971
C          -2.429729        1.840720       -0.378098
H          -2.622850        2.171415        0.637608
H          -1.366182        1.686414       -0.525762
H          -2.806829        2.569506       -1.089652
```

### Compound_24_HEI_19_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.86673 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.629239 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      24.8326 cm-1
2.      36.1401 cm-1
3.      54.1591 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.230389       -0.383798       -0.044032
C           1.086485        0.651325        0.276469
C           0.898778        2.061547       -0.223626
C           2.299711        0.351398        1.047771
O           0.302887       -1.599072        0.302381
O          -0.827354        0.007461       -0.881830
C          -1.991284       -0.824652       -0.956388
C          -3.101876       -0.357740       -0.017388
C          -2.707060       -0.486930        1.453415
C          -3.553702        1.065172       -0.342986
H          -0.151952        2.353595       -0.253208
H           1.413035        2.767063        0.435337
H           1.298228        2.234422       -1.232003
H           2.241397       -0.589029        1.588352
H           2.575116        1.149879        1.737009
H          -2.333214       -0.759730       -1.990409
H          -1.719653       -1.857391       -0.746601
H          -3.942017       -1.034566       -0.206834
H          -2.418884       -1.509160        1.701692
H          -1.865870        0.167104        1.691295
H          -3.539144       -0.202685        2.099982
H          -4.402478        1.354670        0.278877
H          -2.749596        1.780730       -0.161235
H          -3.854592        1.156027       -1.388646
N           3.570758        0.203362        0.161199
H           4.387554        0.120033        0.765841
H           3.677753        1.065389       -0.372131
C           3.517920       -0.948197       -0.771662
H           3.471198       -1.862914       -0.189137
H           2.629326       -0.849979       -1.386500
H           4.408051       -0.942859       -1.393921
```

### Compound_24_HEI_2_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868267 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.631149 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      40.5440 cm-1
  2.      45.3079 cm-1
  3.      55.4145 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.688882       -1.361844        0.006762
C           1.932529       -0.811463       -0.218039
C           3.194152       -1.553717        0.130103
C           2.041081        0.587301       -0.683270
O           0.391081       -2.516877        0.431115
O          -0.364797       -0.471015       -0.275993
C          -1.696260       -0.914708       -0.014359
C          -2.664832        0.211263       -0.344504
C          -4.096272       -0.294385       -0.170998
C          -2.415915        1.451565        0.511991
H           3.904282       -1.580224       -0.703969
H           3.731967       -1.108249        0.977353
H           2.976703       -2.586924        0.399952
H           1.374604        0.846674       -1.503959
H           3.058197        0.848856       -0.967680
H          -1.921863       -1.794778       -0.620002
H          -1.795482       -1.195993        1.037772
H          -2.517550        0.477715       -1.395639
H          -4.283837       -0.578359        0.867491
H          -4.815121        0.481064       -0.438646
H          -4.290893       -1.166187       -0.798120
H          -3.152364        2.226100        0.291013
H          -2.496201        1.206611        1.574313
H          -1.427628        1.876839        0.337510
N           1.661158        1.594655        0.417290
H           2.297057        1.463962        1.202237
H           0.730202        1.322469        0.733895
C           1.654884        3.012651       -0.016075
H           1.361758        3.642111        0.819046
```

```
H           2.652617        3.278750       -0.352781
H           0.945677        3.120135       -0.831451
```

---

### Compound_24_HEI_3

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867472 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.631375 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      20.0135 cm-1
  2.      30.3120 cm-1
  3.      65.2212 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.425671       -0.069052       -0.461008
C          -1.329060        0.947976       -0.302639
C          -0.978579        2.398700       -0.127721
C          -2.768342        0.562243       -0.357681
O          -0.715012       -1.317424       -0.564551
O           0.918656        0.297649       -0.517017
C           1.883219       -0.712175       -0.200693
C           3.261601       -0.072689       -0.139926
C           3.351976        0.980482        0.962449
C           4.314192       -1.162795        0.054640
H           0.073859        2.527380        0.121273
H          -1.169529        3.001370       -1.025377
H          -1.562856        2.856210        0.677521
H          -3.089152        0.151651       -1.318852
H          -3.426324        1.390838       -0.105983
H           1.637034       -1.167837        0.763361
H           1.865270       -1.496735       -0.959029
H           3.441304        0.413434       -1.103878
H           2.624779        1.779313        0.818167
H           3.165648        0.527271        1.939746
H           4.345860        1.430571        0.986837
H           5.316869       -0.733621        0.070885
H           4.160492       -1.685123        1.002234
H           4.276464       -1.902557       -0.746933
N          -3.055095       -0.551247        0.631040
H          -2.902957       -0.194991        1.572647
```

```
H          -2.306539       -1.237222        0.425683
C          -4.398851       -1.160349        0.515728
H          -4.500798       -1.590686       -0.476177
H          -4.504825       -1.935815        1.269019
H          -5.151000       -0.390567        0.665222
```

---

### Compound_24_HEI_4

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868164 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630812 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      36.0892 cm-1
  2.      47.3081 cm-1
  3.      52.6055 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.066947        1.107747       -0.320302
C          -1.238954        0.977876        0.392621
C          -2.009055        2.188742        0.849886
C          -1.849176       -0.341382        0.631866
O           0.575886        2.166912       -0.585388
O           0.434587       -0.105364       -0.835026
C           1.853775       -0.195869       -1.002134
C           2.609868       -0.298012        0.319107
C           2.150757       -1.499599        1.140982
C           4.109561       -0.358182        0.036708
H          -2.954611        2.323919        0.308177
H          -2.271163        2.125279        1.911740
H          -1.431003        3.101420        0.711010
H          -1.135508       -1.157790        0.683948
H          -2.471468       -0.354629        1.526378
H           2.009624       -1.102448       -1.589622
H           2.217768        0.652998       -1.581112
H           2.402990        0.611857        0.889507
H           1.086186       -1.445993        1.369138
H           2.333089       -2.430717        0.597700
H           2.693857       -1.552234        2.086234
H           4.679207       -0.399070        0.966270
H           4.358860       -1.248863       -0.545846
```

```
H           4.444769        0.515353       -0.525534
N          -2.817099       -0.760516       -0.497501
H          -2.276210       -0.789384       -1.360884
H          -3.509668       -0.021267       -0.608401
C          -3.491983       -2.062351       -0.272646
H          -4.139601       -2.282796       -1.116206
H          -4.076327       -1.996338        0.640296
H          -2.731954       -2.831889       -0.173490
```

---

### Compound_24_HEI_5_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867313 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630967 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.9082 cm-1
  2.      32.9690 cm-1
  3.      66.4993 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.420865        0.020149        0.229117
C           1.359004        0.992967        0.002102
C           1.066509        2.381130       -0.493572
C           2.769201        0.628507        0.319397
O           0.670024       -1.181102        0.610278
O          -0.909662        0.379910        0.019335
C          -1.869877       -0.677991       -0.065677
C          -3.239982       -0.077409       -0.339884
C          -4.246384       -1.204984       -0.563652
C          -3.692117        0.843636        0.791524
H           1.153521        3.147791        0.287561
H           1.759088        2.675526       -1.289216
H           0.058079        2.456372       -0.898085
H           2.952226        0.406698        1.374225
H           3.473088        1.396598        0.007073
H          -1.588956       -1.363898       -0.868615
H          -1.891746       -1.243270        0.869056
H          -3.167139        0.509070       -1.260850
H          -3.947604       -1.849273       -1.392418
H          -4.336592       -1.826769        0.330529
```

```
H          -5.234494       -0.801647       -0.788967
H          -4.675783        1.264827        0.577222
H          -3.762729        0.288595        1.730720
H          -2.998258        1.670663        0.940906
N           3.159847       -0.651308       -0.395839
H           2.375887       -1.287780       -0.166187
H           3.140549       -0.479514       -1.399303
C           4.461852       -1.224647        0.011745
H           4.421411       -1.457051        1.071872
H           4.647673       -2.129824       -0.559328
H           5.245532       -0.496574       -0.178826
```

---

### Compound_24_HEI_5

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867313 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630967 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.9083 cm-1
  2.      32.9689 cm-1
  3.      66.5001 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.420865        0.020150        0.229117
C           1.359004        0.992967        0.002101
C           1.066509        2.381131       -0.493572
C           2.769202        0.628508        0.319395
O           0.670025       -1.181101        0.610278
O          -0.909663        0.379911        0.019335
C          -1.869877       -0.677991       -0.065677
C          -3.239982       -0.077409       -0.339883
C          -4.246384       -1.204984       -0.563652
C          -3.692117        0.843635        0.791524
H           1.153528        3.147792        0.287561
H           1.759084        2.675526       -1.289220
H           0.058078        2.456375       -0.898079
H           2.952228        0.406701        1.374223
H           3.473088        1.396597        0.007068
H          -1.588956       -1.363897       -0.868616
H          -1.891746       -1.243270        0.869055
```

```
H          -3.167139        0.509071       -1.260849
H          -3.947603       -1.849273       -1.392419
H          -4.336592       -1.826770        0.330528
H          -5.234493       -0.801647       -0.788967
H          -4.675783        1.264826        0.577223
H          -3.762728        0.288594        1.730721
H          -2.998258        1.670662        0.940907
N           3.159845       -0.651310       -0.395837
H           2.375886       -1.287782       -0.166180
H           3.140544       -0.479520       -1.399301
C           4.461852       -1.224647        0.011745
H           4.421414       -1.457046        1.071873
H           4.647671       -2.129826       -0.559325
H           5.245531       -0.496575       -0.178832
```

---

### Compound_24_HEI_6_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868636 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.629848 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      48.2462 cm-1
  2.      58.5778 cm-1
  3.      67.1650 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.144868       -1.434897       -0.298750
C          -1.459852       -1.028097       -0.205972
C          -2.455576       -1.871280        0.548622
C          -1.887593        0.298680       -0.677695
O           0.364173       -2.496527        0.162458
O           0.682562       -0.565237       -1.036191
C           2.097234       -0.616863       -0.825662
C           2.578684        0.428496        0.178997
C           2.249725        1.848953       -0.278958
C           2.052269        0.162742        1.588784
H          -3.467254       -1.714698        0.163751
H          -2.233951       -2.935882        0.456195
H          -2.495651       -1.654417        1.625017
H          -1.297018        0.691179       -1.499109
```

```
H          -2.941776        0.331445       -0.951048
H           2.386945       -1.616105       -0.505940
H           2.548214       -0.423450       -1.800151
H           3.668892        0.323571        0.199528
H           2.653359        2.046696       -1.273975
H           1.171265        2.013289       -0.318722
H           2.670654        2.584746        0.408262
H           2.463496        0.886110        2.294941
H           0.964661        0.247214        1.627548
H           2.320706       -0.837106        1.932427
N          -1.758566        1.382347        0.422227
H          -0.788032        1.373319        0.733616
H          -2.325896        1.093232        1.217481
C          -2.141227        2.746364       -0.014492
H          -1.501029        3.033793       -0.843411
H          -3.179063        2.731161       -0.333960
H          -2.015209        3.439004        0.812581
```

---

### Compound_24_HEI_6_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868636 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.629848 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      48.2214 cm-1
  2.      58.5712 cm-1
  3.      67.1586 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C          -0.144929       -1.434948       -0.298632
C          -1.459899       -1.028064       -0.206005
C          -2.455750       -1.871110        0.548573
C          -1.887508        0.298720       -0.677830
O           0.364018       -2.496570        0.162694
O           0.682599       -0.565383       -1.036065
C           2.097255       -0.617050       -0.825457
C           2.578689        0.428427        0.179087
C           2.249778        1.848833       -0.279063
C           2.052199        0.162868        1.588883
H          -3.467380       -1.714501        0.163588
```

```
H          -2.234178       -2.935731        0.456260
H          -2.495921       -1.654151        1.624946
H          -1.296841        0.691137       -1.499215
H          -2.941667        0.331543       -0.951269
H           2.386906       -1.616260       -0.505579
H           2.548299       -0.423791       -1.799948
H           3.668893        0.323478        0.199681
H           2.653444        2.046440       -1.274094
H           1.171321        2.013183       -0.318876
H           2.670704        2.584706        0.408075
H           2.463409        0.886317        2.294967
H           0.964591        0.247373        1.627580
H           2.320595       -0.836942        1.932667
N          -1.758496        1.382434        0.422049
H          -0.787990        1.373357        0.733526
H          -2.325910        1.093396        1.217270
C          -2.141026        2.746457       -0.014768
H          -1.500749        3.033793       -0.843658
H          -3.178841        2.731315       -0.334307
H          -2.015013        3.439130        0.812277
```

---

### Compound_24_HEI_8

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.868112 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630778 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      29.4347 cm-1
  2.      49.3972 cm-1
  3.      57.8746 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.433766       -1.306503       -0.334389
C           1.727186       -0.907005       -0.093140
C           2.693225       -1.778892        0.661718
C           2.178013        0.442495       -0.506484
O          -0.136858       -2.393548       -0.029275
O          -0.317854       -0.330807       -1.034393
C          -1.745821       -0.383992       -0.969835
C          -2.307037        0.532427        0.113473
```

```
C          -3.826426        0.609909       -0.023461
C          -1.904046        0.082925        1.516642
H           3.587554       -2.025733        0.077114
H           3.050534       -1.303398        1.583366
H           2.226934       -2.721030        0.947809
H           1.941998        0.711807       -1.535058
H           3.246875        0.576723       -0.354555
H          -2.099954       -0.057698       -1.948643
H          -2.073256       -1.411213       -0.811462
H          -1.891791        1.530867       -0.062015
H          -4.120884        0.968489       -1.011497
H          -4.278547       -0.373863        0.125575
H          -4.249565        1.286119        0.720742
H          -2.287642        0.777583        2.266107
H          -2.311009       -0.906671        1.735898
H          -0.821279        0.032144        1.633412
N           1.509557        1.548967        0.318386
H           1.704828        1.373600        1.302977
H           0.504625        1.422071        0.188990
C           1.907042        2.927693       -0.054804
H           1.657649        3.087640       -1.099635
H           1.370642        3.636446        0.569462
H           2.977676        3.033837        0.093732
```

---

### Compound_24_HEI_9

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-SMD Energy | -559.867304 |
| B3LYP-D3(BJ)/def2tzvpp-SMD (Quasiharmonic) | -559.630074 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      16.5146 cm-1
2.      37.4950 cm-1
3.      62.4171 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-SMD Molecular Geometry in Cartesian Coordinates

```
C           0.103170       -1.235929       -0.438261
C           1.238684       -1.077472        0.321337
C           2.101257       -2.248566        0.706798
C           1.673903        0.276614        0.729180
O          -0.453173       -2.302516       -0.832457
```

```
O          -0.445864       -0.002970       -0.864632
C          -1.848412        0.070190       -1.146046
C          -2.660588        0.552188        0.053753
C          -2.609115       -0.437650        1.217230
C          -2.234904        1.950746        0.498232
H           2.178180       -2.376292        1.793132
H           1.702362       -3.178478        0.302627
H           3.128598       -2.149752        0.335630
H           0.876830        0.907865        1.118823
H           2.478944        0.242977        1.460543
H          -1.947774        0.780579       -1.967998
H          -2.205418       -0.899954       -1.487278
H          -3.694778        0.607634       -0.302917
H          -2.932444       -1.432875        0.908642
H          -1.595810       -0.521946        1.614295
H          -3.256881       -0.107908        2.031293
H          -2.875288        2.313659        1.303893
H          -1.207426        1.947474        0.867041
H          -2.293485        2.663536       -0.326834
N           2.234667        1.090640       -0.445952
H           1.494242        1.109347       -1.148061
H           3.017957        0.576731       -0.846338
C           2.645759        2.472000       -0.096408
H           1.781827        2.998148        0.298896
H           3.428296        2.422668        0.655183
H           3.013168        2.973272       -0.987098
```

---

### Methylamine

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -95.873439 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -95.82983 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 15)

```
1.     295.9720 cm-1
2.     869.8483 cm-1
3.     985.9654 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.704629       -0.000001        0.016948
H           1.118239       -0.878632       -0.478392
```

```
H           1.058522       -0.000083        1.053879
H           1.118218        0.878723       -0.478244
N          -0.749061       -0.000001       -0.125879
H          -1.139664       -0.806964        0.341112
H          -1.139660        0.806964        0.341112
```

---

### Compound_12_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -730.182807 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -730.105172 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      59.8789 cm-1
  2.     104.4859 cm-1
  3.     157.4103 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.086521        1.265579       -0.000013
H          -0.586823        2.243203       -0.000054
C          -0.187646        0.110003       -0.000005
C           1.155898        0.168557       -0.000030
C           1.937683        1.445485       -0.000025
H           2.590063        1.455472        0.875295
H           2.589937        1.455563       -0.875438
H           1.346734        2.353992        0.000069
C           1.988173       -1.077078       -0.000033
H           1.765523       -1.687163        0.876561
H           1.765062       -1.687516       -0.876258
H           3.048720       -0.837866       -0.000344
O          -2.293811        1.200390        0.000013
Cl         -1.000838       -1.433770        0.000042
```

---

### Compound_12_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -730.179418 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -730.101613 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      94.6129 cm-1
2.     131.6268 cm-1
3.     148.9776 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.349216       -1.639823       -0.010516
H           0.415943       -2.434037       -0.045333
C           0.203794       -0.275918       -0.003114
C          -0.500373        0.868823       -0.002275
C          -2.002486        0.868348       -0.012115
H          -2.396379        0.414720        0.897390
H          -2.373077        1.888706       -0.083174
H          -2.395018        0.286213       -0.844100
C           0.128410        2.221741        0.008767
H          -0.250682        2.782979        0.865623
H           1.212170        2.200024        0.047126
H          -0.187673        2.767785       -0.883064
O          -1.525188       -1.917850        0.019674
Cl          1.958556       -0.283683        0.000215
```

---

### Compound_12_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -826.063167 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -825.91639 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      58.3305 cm-1
2.     159.5912 cm-1
3.     181.5906 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.414849        1.736911        0.091416
H          -1.227989        2.427319       -0.164377
C          -0.674986        0.407679       -0.004245
C           0.338467       -0.651738        0.376227
C           0.396414       -0.827021        1.896409
H           1.144854       -1.568350        2.184793
H           0.624345        0.120438        2.384081
H          -0.575153       -1.169170        2.248403
C           0.140652       -1.999836       -0.301813
H           0.008499       -1.904499       -1.377918
H           0.995768       -2.647227       -0.103789
H          -0.746121       -2.481684        0.103145
O           0.724726        2.240354        0.436885
C           2.016995       -0.078013       -1.460256
H           1.187130        0.357170       -2.010527
H           2.908668        0.524721       -1.607114
H           2.201167       -1.092185       -1.800602
N           1.681698       -0.063797       -0.024949
H           1.566993        0.973473        0.276727
H           2.418930       -0.510817        0.510395
Cl         -2.287820       -0.119608       -0.444122
```

---

### Compound_12_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -826.053186 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -825.905822 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      47.2143 cm-1
  2.     101.4579 cm-1
  3.     127.9157 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.771111        1.074925       -0.231119
H           1.386966        2.109781       -0.236682
C           0.803963        0.140859        0.055672
```

```
C          -0.646510        0.365536        0.323166
C          -1.033826        1.840648        0.318730
H          -2.098400        1.956141        0.514136
H          -0.498356        2.353052        1.114344
H          -0.797550        2.327563       -0.626200
C          -1.147181       -0.299823        1.605005
H          -1.010981       -1.379720        1.582659
H          -0.566424        0.097034        2.435269
H          -2.197198       -0.079550        1.792857
O           2.992557        0.895955       -0.465313
C          -2.872104       -0.383547       -0.859285
H          -3.288524        0.614717       -0.783286
H          -3.193183       -0.844001       -1.788813
H          -3.192189       -0.992099       -0.021211
N          -1.393100       -0.303391       -0.869308
H          -1.078575        0.183934       -1.705780
H          -1.005256       -1.244403       -0.942312
Cl          1.299894       -1.563409        0.070568
```

---

### Compound_19

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -231.254926 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.191584 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
1.     127.4784 cm-1
2.     199.9986 cm-1
3.     216.6789 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.388896        0.329467        0.000003
O           2.456565       -0.245077       -0.000025
C           0.090183       -0.332865       -0.000013
C          -1.032715        0.387265        0.000022
H           0.077238       -1.417130       -0.000054
H           1.350668        1.435219        0.000045
C          -2.412793       -0.162325        0.000010
H          -2.958973        0.196439        0.874839
H          -2.958983        0.196503       -0.874787
```

```
H          -2.418559       -1.250678       -0.000030
H          -0.945341        1.471007        0.000062
```

---

### Compound_19_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -231.251022 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -231.187991 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 27)

```
  1.     133.1914 cm-1
  2.     201.1011 cm-1
  3.     208.8759 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.507836        0.414327       -0.000003
O          -2.018078       -0.685626       -0.000004
C          -0.063215        0.679219       -0.000000
C           0.838849       -0.302673        0.000002
H           0.474140       -1.325708        0.000001
H           0.241465        1.719569        0.000001
H          -2.148663        1.313568       -0.000005
C           2.312481       -0.116635        0.000005
H           2.751653       -0.601546        0.874502
H           2.751658       -0.601547       -0.874489
H           2.592703        0.935243        0.000005
```

---

### Compound_19_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -327.13249 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.001894 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      81.6894 cm-1
2.     142.4929 cm-1
3.     200.1028 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.012652        0.213732       -0.048736
O           1.910538       -1.066963        0.114685
C           0.980687        1.096772        0.012995
C          -0.404641        0.618944        0.329412
H          -0.507101        0.360673        1.389018
H           1.141606        2.150177       -0.165323
H           3.009806        0.614009       -0.281094
C          -1.495975        1.598554       -0.055566
H          -2.490087        1.229879        0.194268
H          -1.340788        2.531101        0.485346
H          -1.457233        1.819280       -1.123687
N          -0.580830       -0.705446       -0.373631
H          -0.674143       -0.534166       -1.370917
H           0.391956       -1.153391       -0.214553
C          -1.673486       -1.562915        0.110399
H          -1.506190       -1.777951        1.162344
H          -2.631173       -1.065474       -0.014268
H          -1.670565       -2.490830       -0.454223
```

---

### Compound_19_HEI_4_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -327.13249 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -327.001895 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 48)

```
1.      81.6881 cm-1
2.     142.4957 cm-1
3.     200.1018 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.012648        0.213737       -0.048735
O           1.910528       -1.066960        0.114683
C           0.980684        1.096776        0.012998
C          -0.404644        0.618941        0.329411
H          -0.507103        0.360673        1.389018
H           1.141601        2.150181       -0.165321
H           3.009803        0.614009       -0.281091
C          -1.495980        1.598549       -0.055568
H          -2.490091        1.229867        0.194260
H          -1.340800        2.531095        0.485349
H          -1.457234        1.819279       -1.123687
N          -0.580824       -0.705445       -0.373630
H           0.391981       -1.153384       -0.214547
H          -0.674136       -0.534166       -1.370916
C          -1.673474       -1.562918        0.110399
H          -1.670559       -2.490827       -0.454234
H          -1.506168       -1.777968        1.162339
H          -2.631163       -1.065477       -0.014251
```

---

### Compound_26_10

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452576 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.305115 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      41.1640 cm-1
  2.      57.4354 cm-1
  3.      71.0720 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.786565       -0.427985       -0.094270
C          -2.683349        0.751068       -0.076882
C          -2.289203        1.987031        0.193587
O          -2.173035       -1.541720       -0.368888
O          -0.528063       -0.141461        0.217489
C           0.415766       -1.224788        0.210058
C           1.778136       -0.662811        0.543095
C           2.316834        0.310810       -0.499075
C           3.701675        0.834209       -0.142825
```

```
H          -3.714286        0.523194       -0.313237
H          -1.257899        2.214149        0.427827
H          -2.994050        2.807448        0.186313
H           0.406621       -1.689723       -0.777144
H           0.099349       -1.968452        0.941486
H           1.737095       -0.178756        1.522416
H           2.462083       -1.509751        0.641903
H           1.624293        1.148237       -0.605280
H           2.350225       -0.189823       -1.470726
H           3.685113        1.361501        0.813015
H           4.419375        0.015881       -0.057672
H           4.071088        1.526342       -0.899839
```

---

### Compound_26_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452696 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304988 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      40.2904 cm-1
2.      60.0430 cm-1
3.      79.1376 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.420628       -0.266227        0.042302
C          -2.417308        0.681427       -0.513033
C          -3.475797        1.055766        0.189465
O          -1.478771       -0.775645        1.136514
O          -0.443040       -0.490278       -0.835418
C           0.625527       -1.368804       -0.439369
C           1.693256       -0.638965        0.351243
C           2.367165        0.491428       -0.417893
C           3.448313        1.184759        0.400194
H          -2.234202        1.049854       -1.513337
H          -3.640478        0.676572        1.190029
H          -4.201485        1.747563       -0.215333
H           1.025762       -1.746690       -1.378565
H           0.209298       -2.196801        0.131219
H           1.257341       -0.255518        1.276623
H           2.440791       -1.381803        0.643078
```

```
H          1.614910        1.221872       -0.722956
H          2.800960        0.090229       -1.338033
H          4.228535        0.480119        0.694678
H          3.919433        1.989062       -0.165309
H          3.030447        1.616621        1.311682
```

---

### Compound_26_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.453182 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.30572 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      39.2991 cm-1
  2.      62.5542 cm-1
  3.      73.7087 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C         -1.616914        0.242175        0.020562
C         -2.434767       -0.975965       -0.195093
C         -3.737230       -0.981392        0.044763
O         -2.035085        1.303268        0.420803
O         -0.341425        0.019191       -0.287030
C          0.573455        1.116158       -0.125936
C          1.960702        0.631074       -0.476828
C          2.503448       -0.431878        0.471708
C          3.913907       -0.871975        0.103368
H         -1.915212       -1.853323       -0.556088
H         -4.239209       -0.092649        0.405618
H         -4.332650       -1.870071       -0.112729
H          0.522263        1.464997        0.906733
H          0.257200        1.930565       -0.777793
H          1.960424        0.253719       -1.502814
H          2.619993        1.502867       -0.465396
H          2.494734       -0.037051        1.491448
H          1.836779       -1.296476        0.468150
H          3.940285       -1.294354       -0.903013
H          4.605740       -0.027697        0.126891
H          4.286133       -1.629391        0.793545
```

### Compound_26_3

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452154 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304144 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      33.1034 cm-1
2.      56.8614 cm-1
3.      63.9966 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.365403        0.243185       -0.150878
C           2.320550       -0.890982       -0.185066
C           3.522849       -0.793772        0.361753
O           1.582816        1.321566        0.349096
O           0.224094       -0.083302       -0.756312
C          -0.827966        0.897440       -0.782283
C          -1.649400        0.879659        0.493775
C          -2.259265       -0.476394        0.844287
C          -3.227001       -1.013458       -0.203639
H           1.985096       -1.795372       -0.674396
H           3.839147        0.120224        0.848170
H           4.218528       -1.621116        0.337667
H          -1.427219        0.626089       -1.648290
H          -0.393093        1.881150       -0.948758
H          -1.026129        1.226764        1.319266
H          -2.444778        1.619479        0.367248
H          -2.780505       -0.375385        1.798164
H          -1.458981       -1.201145        1.009676
H          -2.722818       -1.232462       -1.145979
H          -3.695584       -1.936856        0.137290
H          -4.019955       -0.291541       -0.410030
```

---

### Compound_26_4

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452632 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304792 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      52.3425 cm-1
2.      60.1734 cm-1
3.      79.0869 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.561721        0.032940        0.189089
C          -2.846203        0.203170       -0.532439
C          -3.848657       -0.645144       -0.361062
O          -1.315749       -0.852514        0.973506
O          -0.704225        0.999074       -0.139772
C           0.600637        0.968137        0.459741
C           1.551826        0.082974       -0.320143
C           2.952915        0.097994        0.280683
C           3.927877       -0.776738       -0.496009
H          -2.920220        1.049599       -1.201746
H          -3.754859       -1.487123        0.312948
H          -4.784799       -0.520519       -0.887536
H           0.511542        0.635529        1.493212
H           0.933993        2.004149        0.447837
H           1.166338       -0.938851       -0.330935
H           1.589410        0.426729       -1.356740
H           2.904133       -0.240404        1.319001
H           3.324248        1.125937        0.307733
H           4.015695       -0.439190       -1.530333
H           4.922381       -0.753180       -0.050061
H           3.591881       -1.815154       -0.512421
```

---

### Compound_26_5

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.453013 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.305834 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      39.4263 cm-1
2.      63.2278 cm-1
3.      86.9013 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.759017        0.200901       -0.000001
C           2.848454       -0.805123        0.000001
C           4.121355       -0.439536        0.000000
O           1.914255        1.399391       -0.000003
O           0.565665       -0.389399        0.000000
C          -0.586566        0.466477       -0.000001
C          -1.820297       -0.405730        0.000001
C          -3.097727        0.426609        0.000000
C          -4.352632       -0.435924        0.000002
H           2.551161       -1.845111        0.000002
H           4.398426        0.607033       -0.000002
H           4.915555       -1.173234        0.000001
H          -0.550646        1.106064        0.883192
H          -0.550646        1.106061       -0.883197
H          -1.802354       -1.054540        0.879059
H          -1.802355       -1.054543       -0.879055
H          -3.103091        1.081258       -0.875438
H          -3.103090        1.081261        0.875437
H          -5.253942        0.177254        0.000002
H          -4.384004       -1.078744       -0.881629
H          -4.384003       -1.078741        0.881636
```

---

### Compound_26_6

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452685 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304845 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      35.2497 cm-1
2.      48.5686 cm-1
3.      78.5127 cm-1
```

## WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.439231        0.272411        0.076909
C           2.379391       -0.769981       -0.401199
C           3.633881       -0.810009        0.021430
O           1.708775        1.148235        0.865023
O           0.239390        0.122236       -0.479156
C          -0.780509        1.061982       -0.102743
C          -2.068054        0.661986       -0.788206
C          -2.593815       -0.722280       -0.410835
C          -2.918031       -0.880314        1.070174
H           1.989495       -1.490256       -1.107702
H           4.004722       -0.079305        0.728991
H           4.319217       -1.570235       -0.327022
H          -0.465784        2.059898       -0.408511
H          -0.875661        1.057986        0.983120
H          -2.812999        1.419652       -0.531116
H          -1.923587        0.718563       -1.869071
H          -1.866373       -1.479677       -0.709778
H          -3.493678       -0.913382       -0.998613
H          -2.024346       -0.803909        1.691243
H          -3.620386       -0.112549        1.401410
H          -3.368509       -1.853333        1.266946
```

### Compound_26_7

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452429 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304514 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      47.6263 cm-1
2.      58.2448 cm-1
3.      92.5188 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.340178        0.231551        0.176990
C          -2.429366       -0.283706       -0.688479
C          -3.394758       -1.046028       -0.197663
O          -1.239539        0.022890        1.362543
O          -0.483757        0.962626       -0.537169
C           0.665642        1.529730        0.117336
C           1.923882        0.781674       -0.272615
C           1.973600       -0.659630        0.220496
C           3.264765       -1.362458       -0.176976
H          -2.392180       -0.008491       -1.733799
H          -3.413374       -1.311459        0.851706
H          -4.187472       -1.422745       -0.829140
H           0.507812        1.510602        1.193840
H           0.707088        2.563097       -0.221053
H           2.032385        0.806827       -1.360190
H           2.769847        1.339408        0.138447
H           1.121934       -1.213418       -0.181992
H           1.863967       -0.671315        1.307675
H           3.378981       -1.383776       -1.262521
H           4.133511       -0.847755        0.238025
H           3.282346       -2.391906        0.181473
```

---

### Compound_26_8

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.452019 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.304256 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      38.3095 cm-1
2.      48.8263 cm-1
3.      77.6604 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.493797       -0.472250       -0.247571
C           2.559902        0.541948       -0.420805
C           2.643298        1.667731        0.273203
O           1.415070       -1.460040       -0.942194
O           0.649733       -0.186750        0.739515
C          -0.457645       -1.078512        0.957129
C          -1.626462       -0.756888        0.047441
C          -2.186227        0.648341        0.236701
C          -3.371864        0.927850       -0.677039
H           3.281276        0.294283       -1.188227
H           1.918853        1.917644        1.036435
H           3.443455        2.372477        0.091400
H          -0.723449       -0.926994        2.001855
H          -0.119921       -2.103813        0.819173
H          -1.324750       -0.903598       -0.992256
H          -2.406918       -1.494815        0.252716
H          -1.398529        1.380899        0.048162
H          -2.486208        0.777279        1.280373
H          -3.086518        0.830587       -1.726336
H          -4.185631        0.224906       -0.488251
H          -3.758870        1.936144       -0.527966
```

---

### Compound_26_9

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -424.451807 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -424.303913 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      37.4143 cm-1
2.      55.7808 cm-1
3.      66.1045 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.454417        0.081686       -0.160633
C          -2.832557       -0.411549        0.077981
C          -3.822741        0.422802        0.356197
O          -1.115937        1.241411       -0.136817
O          -0.627446       -0.932989       -0.413351
C           0.756777       -0.625641       -0.647174
C           1.528153       -0.547969        0.656838
C           3.027533       -0.348301        0.442768
C           3.392484        0.992874       -0.185346
H          -2.984903       -1.480521        0.015145
H          -3.649684        1.489778        0.415999
H          -4.827192        0.062590        0.530504
H           0.819873        0.301732       -1.212859
H           1.121822       -1.444692       -1.264545
H           1.129951        0.270505        1.260866
H           1.357972       -1.473068        1.210978
H           3.416313       -1.162397       -0.175187
H           3.523738       -0.436561        1.410776
H           4.474467        1.116679       -0.235040
H           3.006246        1.086029       -1.201082
H           2.987076        1.819138        0.402011
```

---

### Compound_26_HEI_10_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317833 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.10307 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      34.8811 cm-1
2.      50.7799 cm-1
3.      67.2214 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.415303       -1.431602        0.107338
C          -2.384340       -0.514882        0.485810
C          -2.046884        0.899111        0.726161
O          -1.505753       -2.651222       -0.095000
O          -0.174622       -0.807178       -0.087617
C           0.949649       -1.626854       -0.358049
C           2.140796       -0.722919       -0.601661
C           2.522583        0.136119        0.598616
C           3.730024        1.022167        0.323108
H          -3.410114       -0.840203        0.562349
H          -1.226350        1.061971        1.428997
H          -2.904998        1.480089        1.057167
H           1.136115       -2.289635        0.492224
H           0.754430       -2.253849       -1.229389
H           1.929746       -0.080525       -1.462174
H           2.988200       -1.353854       -0.884027
H           2.730113       -0.515844        1.452047
H           1.670537        0.756273        0.884315
H           3.532622        1.701599       -0.508665
H           3.987749        1.626459        1.193461
H           4.604360        0.423120        0.060458
N          -1.542450        1.583128       -0.547906
H          -2.272689        1.516071       -1.251625
H          -0.773944        0.984237       -0.861488
C          -1.090248        2.978109       -0.383885
H          -1.922328        3.577928       -0.026833
H          -0.738044        3.359034       -1.337679
H          -0.282914        2.996935        0.342518
```

---

### Compound_26_HEI_11_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.319298 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.104912 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      34.5508 cm-1
2.      37.0601 cm-1
3.      74.0338 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.648275       -0.512709        0.186993
C           1.668919       -1.310142       -0.279611
C           3.057024       -0.868376       -0.004662
O           0.804701        0.593007        0.781710
O          -0.625058       -0.968980       -0.046827
C          -1.696764       -0.096844        0.279038
C          -2.986581       -0.767763       -0.149352
C          -4.233308        0.027194        0.233822
C          -4.345775        1.382843       -0.456400
H           1.480090       -2.195456       -0.864756
H           3.332579       -0.864931        1.055075
H           3.802198       -1.446291       -0.546919
H          -1.710794        0.100831        1.354661
H          -1.561204        0.860781       -0.227428
H          -3.031956       -1.756675        0.312446
H          -2.967414       -0.922741       -1.231825
H          -4.252949        0.166418        1.318420
H          -5.112039       -0.572076       -0.012467
H          -5.294034        1.864986       -0.216940
H          -3.547414        2.060648       -0.151998
H          -4.291408        1.271496       -1.541448
N           3.212850        0.580999       -0.413586
H           3.081344        0.645599       -1.418598
H           2.375486        1.012830        0.033484
C           4.466061        1.235435       -0.001446
H           5.308039        0.702376       -0.434651
H           4.532576        1.209160        1.082474
H           4.462697        2.266017       -0.343782
```

---

### Compound_26_HEI_12_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317127 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102182 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      28.8837 cm-1
2.      45.5327 cm-1
3.      72.8591 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.648248       -1.609317       -0.244793
C          -1.919512       -1.210738       -0.627447
C          -2.587616       -0.051519       -0.010210
O           0.023471       -2.580878       -0.619622
O          -0.094199       -0.722696        0.697832
C           1.217531       -0.989505        1.172089
C           2.303650       -0.438430        0.263791
C           2.212315        1.063764        0.023301
C           3.387084        1.599097       -0.784992
H          -2.422864       -1.760479       -1.407367
H          -2.637580       -0.073605        1.081095
H          -3.593401        0.098831       -0.396738
H           1.269471       -0.508335        2.150623
H           1.346933       -2.063077        1.304431
H           2.274949       -0.968708       -0.690463
H           3.267215       -0.672622        0.727000
H           2.157530        1.583879        0.984003
H           1.285014        1.291789       -0.507759
H           3.447638        1.105145       -1.756794
H           3.295571        2.671517       -0.959890
H           4.330579        1.423117       -0.264670
N          -1.829503        1.247261       -0.290506
H          -1.768835        1.364254       -1.298333
H          -0.880740        1.052577        0.040865
C          -2.376907        2.456900        0.353454
H          -3.392587        2.612747        0.001796
H          -1.758697        3.312677        0.099862
H          -2.377639        2.306551        1.429042
```

---

### Compound_26_HEI_13_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317339 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102575 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      24.5140 cm-1
2.      42.6616 cm-1
3.      66.3593 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.438764        1.553016       -0.258311
C          -1.472849        1.109524       -1.066267
C          -1.947781       -0.283821       -1.011418
O           0.119412        2.658830       -0.216245
O          -0.043285        0.557927        0.656864
C           1.212529        0.712428        1.299442
C           2.364528        0.259883        0.418659
C           2.277319       -1.202740        0.000277
C           3.439849       -1.630318       -0.885556
H          -1.961942        1.813992       -1.721237
H          -1.163736       -1.037427       -1.115792
H          -2.723043       -0.487072       -1.747337
H           1.345920        1.750839        1.600932
H           1.155798        0.093403        2.196460
H           3.295926        0.431339        0.966753
H           2.401724        0.897288       -0.468935
H           1.334754       -1.368634       -0.526254
H           2.245577       -1.830876        0.895463
H           4.393789       -1.498879       -0.370669
H           3.357431       -2.678719       -1.174303
H           3.472479       -1.033470       -1.799343
N          -2.563571       -0.620011        0.349154
H          -3.334842        0.021244        0.513751
H          -1.830922       -0.377144        1.020480
C          -2.995491       -2.021028        0.518708
H          -3.754817       -2.245732       -0.224634
H          -2.135245       -2.668257        0.375072
H          -3.398899       -2.157529        1.517359
```

---

### Compound_26_HEI_14_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.319286 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.104113 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      35.3526 cm-1
2.      37.2695 cm-1
3.      59.2693 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.573976       -0.814803        0.243810
C           1.622479       -1.341405       -0.472923
C           2.969216       -0.767912       -0.234289
O           0.658492        0.164073        1.041523
O          -0.646998       -1.420460        0.051169
C          -1.803798       -0.696755        0.446573
C          -2.186609        0.363918       -0.573369
C          -3.403320        1.188358       -0.158311
C          -4.696340        0.384541       -0.062771
H           1.477687       -2.112311       -1.212098
H           3.367391       -0.943477        0.770428
H           3.708816       -1.106925       -0.956496
H          -2.586334       -1.449065        0.540472
H          -1.646967       -0.239441        1.424619
H          -2.378352       -0.119607       -1.535572
H          -1.330334        1.027345       -0.711408
H          -3.538163        1.995654       -0.881037
H          -3.200122        1.669860        0.802582
H          -5.544722        1.033420        0.156785
H          -4.903159       -0.130122       -1.003532
H          -4.648586       -0.369226        0.724114
N           2.892905        0.740628       -0.326024
H           2.065183        0.942581        0.276768
H           2.637009        0.990914       -1.276618
C           4.094895        1.472891        0.107358
H           3.921517        2.540202        0.007471
H           4.938620        1.174609       -0.509085
H           4.295231        1.229296        1.146767
```

---

### Compound_26_HEI_15_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.318917 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.10401 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      30.8914 cm-1
2.      42.6809 cm-1
3.      46.9139 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.563675        0.523478       -0.041374
C          -1.629311        1.351095        0.230300
C          -2.913688        0.708403        0.597255
O          -0.610040       -0.740521       -0.038911
O           0.611635        1.155114       -0.377045
C           1.756789        0.346000       -0.601367
C           2.481299        0.013547        0.693453
C           3.684728       -0.904835        0.491792
C           4.803963       -0.291915       -0.344254
H          -1.561360        2.421921        0.127312
H          -2.894410        0.162963        1.546493
H          -3.746384        1.407982        0.624902
H           1.474296       -0.571609       -1.119160
H           2.392769        0.933830       -1.263112
H           1.767996       -0.465748        1.366324
H           2.801896        0.943707        1.171574
H           3.350616       -1.837170        0.027435
H           4.080524       -1.177751        1.472174
H           5.669005       -0.954552       -0.384934
H           4.487293       -0.103858       -1.370925
H           5.130515        0.659064        0.082012
N          -3.248549       -0.364587       -0.417312
H          -3.396226        0.080728       -1.318224
H          -2.346235       -0.883039       -0.475448
C          -4.376888       -1.246224       -0.072346
H          -5.275754       -0.647240        0.046320
H          -4.148419       -1.755480        0.859587
H          -4.518346       -1.975686       -0.864257
```

---

### Compound_26_HEI_16_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.316119 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102059 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.0491 cm-1
2.      46.1571 cm-1
3.      77.8936 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.792160       -0.253022        0.420410
C          -1.797843       -1.072712       -0.082071
C          -3.181755       -0.912123        0.353266
O          -0.900384        0.694565        1.218352
O           0.463132       -0.586795       -0.058811
C           1.550826        0.203903        0.385931
C           2.810863       -0.299688       -0.286802
C           4.043353        0.492376        0.133631
C           5.316518       -0.001880       -0.540355
H          -1.544751       -1.875498       -0.759236
H          -3.269886       -0.415560        1.319075
H          -3.742693       -1.845717        0.374896
H           1.380170        1.255359        0.138707
H           1.647085        0.138786        1.473443
H           2.687861       -0.239178       -1.371762
H           2.952192       -1.356150       -0.042327
H           4.157948        0.433369        1.219497
H           3.891614        1.549289       -0.102354
H           6.184669        0.577818       -0.225320
H           5.506033       -1.048873       -0.295796
H           5.238002        0.075805       -1.626512
N          -4.032093       -0.017019       -0.595637
H          -5.013085       -0.073277       -0.332405
H          -3.953855       -0.414579       -1.528119
C          -3.601872        1.396263       -0.627541
H          -4.176748        1.930951       -1.377639
H          -3.766408        1.827884        0.354832
H          -2.543056        1.417832       -0.864648
```

---

### Compound_26_HEI_17_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.320601 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.105849 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      27.7510 cm-1
2.      36.8681 cm-1
3.      90.3377 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.544436       -1.135827       -0.026322
C           1.500219       -0.850118       -0.970250
C           2.807869       -0.333249       -0.495997
O           0.673125       -0.945534        1.218762
O          -0.633795       -1.659877       -0.510222
C          -1.795265       -1.581167        0.306754
C          -2.672653       -0.403509       -0.083172
C          -2.030224        0.957314        0.160195
C          -2.931485        2.112805       -0.253739
H           1.287117       -0.910420       -2.024958
H           3.412883       -1.065469        0.046957
H           3.414199        0.077380       -1.300861
H          -2.335423       -2.516616        0.155371
H          -1.501973       -1.515599        1.354024
H          -3.604804       -0.475724        0.486038
H          -2.943973       -0.496218       -1.139158
H          -1.089231        1.012948       -0.392370
H          -1.771128        1.048924        1.217983
H          -3.870671        2.095765        0.303132
H          -2.453044        3.076087       -0.073162
H          -3.176208        2.055248       -1.316391
N           2.589311        0.769241        0.524460
H           3.436221        0.933693        1.058408
H           1.874014        0.327208        1.146854
C           2.079851        2.035376       -0.031212
H           1.830423        2.709355        0.782890
H           2.842240        2.480342       -0.665019
H           1.193046        1.811952       -0.616820
```

---

### Compound_26_HEI_18_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.319461 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.1046 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      26.9128 cm-1
2.      33.5496 cm-1
3.      80.6920 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.471050        0.191602        0.197978
C          -1.336267       -0.378487        1.101632
C          -2.427806       -1.231981        0.571785
O          -0.549078        0.065849       -1.058675
O           0.510902        0.987865        0.742688
C           1.509114        1.533752       -0.108674
C           2.842984        0.836737        0.095725
C           2.847258       -0.626436       -0.329980
C           4.187873       -1.304373       -0.079357
H          -1.289369       -0.144198        2.152685
H          -2.090778       -2.179684        0.140796
H          -3.189346       -1.451291        1.317546
H           1.187771        1.455821       -1.146494
H           1.595176        2.590501        0.151159
H           3.126905        0.913021        1.149726
H           3.600641        1.386131       -0.471685
H           2.592646       -0.691526       -1.390945
H           2.060382       -1.160391        0.208398
H           4.446276       -1.277328        0.981281
H           4.171919       -2.348900       -0.392489
H           4.988486       -0.802998       -0.627251
N          -3.112993       -0.542361       -0.594576
H          -2.290358       -0.240747       -1.162286
H          -3.656839       -1.209177       -1.132093
C          -3.943074        0.618905       -0.228181
H          -3.331354        1.297898        0.358278
H          -4.288392        1.111538       -1.132172
H          -4.791600        0.279845        0.359902
```

---

### Compound_26_HEI_19_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.316089 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101314 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.4189 cm-1
2.      50.1818 cm-1
3.      74.0481 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.718227       -0.913644        0.192924
C          -1.909805       -0.985668       -0.519356
C          -3.155369       -0.490049        0.058901
O          -0.526458       -0.416618        1.316122
O           0.344062       -1.503960       -0.479142
C           1.640023       -1.312125        0.060826
C           2.246849        0.018784       -0.349840
C           3.654061        0.206862        0.203507
C           4.276572        1.534606       -0.208072
H          -1.926752       -1.462156       -1.488682
H          -3.127556       -0.441270        1.146840
H          -4.036105       -1.048534       -0.255689
H           1.610538       -1.392053        1.148337
H           2.242740       -2.135126       -0.327783
H           1.599649        0.824542        0.005502
H           2.267876        0.080542       -1.441683
H           4.289968       -0.615758       -0.136168
H           3.623580        0.140496        1.294675
H           5.280895        1.648455        0.201280
H           4.346914        1.611982       -1.294829
H           3.673566        2.373306        0.145384
N          -3.496560        0.968293       -0.363285
H          -4.438845        1.201992       -0.058702
H          -3.501990        0.990332       -1.379595
C          -2.539757        1.974456        0.143041
H          -2.792234        2.948642       -0.264624
H          -2.599337        1.989262        1.226862
H          -1.543906        1.672579       -0.165560
```

---

### Compound_26_HEI_1_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.32014 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.106139 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      27.0288 cm-1
2.      45.1952 cm-1
3.      69.5699 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.730928        0.336776       -0.224672
C          -1.675786        1.307552        0.020458
C          -3.095655        0.947715       -0.206670
O          -0.985207       -0.853482       -0.569962
O           0.577150        0.714381       -0.050126
C           1.564869       -0.299134       -0.154456
C           2.917751        0.335315        0.089975
C           4.052537       -0.678313        0.001320
C           5.418940       -0.050093        0.241767
H          -1.410416        2.279474        0.403513
H          -3.350922        0.739582       -1.251000
H          -3.789057        1.697117        0.168865
H           1.373312       -1.087850        0.578590
H           1.530949       -0.759134       -1.145147
H           2.921464        0.806077        1.076873
H           3.077999        1.131636       -0.642077
H           4.036864       -1.153649       -0.983280
H           3.883263       -1.475431        0.730439
H           5.469390        0.406522        1.232142
H           6.215368       -0.791728        0.174141
H           5.624101        0.730062       -0.493855
N          -3.403512       -0.357874        0.495837
H          -2.604053       -0.951759        0.186407
H          -3.301924       -0.217326        1.496756
C          -4.706324       -0.966083        0.176937
H          -5.500748       -0.279200        0.456186
H          -4.747137       -1.160807       -0.890920
H          -4.811838       -1.898064        0.724255
```

---

### Compound_26_HEI_20_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.31716 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101664 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.0502 cm-1
2.      33.6605 cm-1
3.      70.4168 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.175506       -1.673567        0.057111
C          -1.326172       -1.443010        0.792707
C          -1.901506       -0.091817        0.914574
O           0.476845       -2.715864       -0.097941
O           0.230684       -0.513312       -0.629170
C           1.577084       -0.439749       -1.068927
C           2.535039       -0.103866        0.064743
C           2.117842        1.102304        0.904333
C           1.928677        2.384840        0.103182
H          -1.827641       -2.278834        1.255901
H          -1.197307        0.675586        1.244508
H          -2.769456       -0.068600        1.570132
H           1.866422       -1.378290       -1.541466
H           1.586215        0.342801       -1.827600
H           3.519686        0.074594       -0.377829
H           2.633429       -0.976857        0.713200
H           2.874596        1.263674        1.675106
H           1.190649        0.864736        1.430827
H           1.093383        2.299818       -0.593638
H           1.722828        3.229933        0.760860
H           2.823552        2.622002       -0.476572
N          -2.380961        0.445868       -0.435387
H          -3.076555       -0.197286       -0.803388
H          -1.558869        0.367308       -1.039369
C          -2.894052        1.829599       -0.417374
H          -3.192663        2.118406       -1.420465
H          -3.745709        1.879130        0.254844
H          -2.104495        2.485806       -0.062544
```

---

### Compound_26_HEI_21_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315895 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101555 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      30.4817 cm-1
2.      35.6825 cm-1
3.      59.9247 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.612909       -0.122641        0.188378
C          -1.677340       -0.992785        0.395077
C          -2.782048       -1.060120       -0.556719
O          -0.456989        0.688969       -0.740236
O           0.356561       -0.218436        1.177781
C           1.565332        0.493117        0.976757
C           2.555448       -0.278970        0.121535
C           3.875436        0.463179       -0.047646
C           4.879703       -0.307715       -0.894521
H          -1.661814       -1.665814        1.239874
H          -2.508936       -0.697981       -1.547362
H          -3.222989       -2.052523       -0.642141
H           1.359152        1.465630        0.527680
H           1.978583        0.654975        1.974222
H           2.106357       -0.462277       -0.857672
H           2.737209       -1.255244        0.580077
H           4.306578        0.664468        0.937275
H           3.684834        1.438456       -0.504271
H           4.482984       -0.495470       -1.894167
H           5.815359        0.241715       -1.003390
H           5.109521       -1.274592       -0.442488
N          -3.997377       -0.170372       -0.165229
H          -4.272107       -0.438477        0.776318
H          -4.785712       -0.380313       -0.773027
C          -3.710083        1.278758       -0.197830
H          -3.486579        1.561204       -1.221902
H          -4.574315        1.825821        0.166654
H          -2.844300        1.461822        0.430365
```

---

### Compound_26_HEI_22_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.316006 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.10135 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      33.1858 cm-1
2.      34.7521 cm-1
3.      60.4923 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.705374       -1.533919        0.047720
C           2.075477       -1.391659       -0.100293
C           2.780194       -0.172747        0.334486
O          -0.027991       -2.486285       -0.253506
O           0.124922       -0.383119        0.617849
C          -1.291590       -0.321813        0.677162
C          -1.882625        0.217808       -0.615283
C          -3.408846        0.268718       -0.608398
C          -3.994480        1.240335        0.411455
H           2.628324       -2.180272       -0.586551
H           2.607805        0.117004        1.373670
H           3.853723       -0.236037        0.169350
H          -1.695680       -1.311848        0.890819
H          -1.517832        0.335231        1.516796
H          -1.543303       -0.420641       -1.433251
H          -1.482175        1.219578       -0.799804
H          -3.800450       -0.735707       -0.423902
H          -3.750831        0.550382       -1.606327
H          -3.768806        0.939509        1.435257
H          -3.593027        2.245259        0.264333
H          -5.079450        1.297068        0.318743
N           2.305683        1.054358       -0.446681
H           2.461233        0.875549       -1.434963
H           1.292210        1.059492       -0.306727
C           2.904417        2.340256       -0.038848
H           2.490704        3.140124       -0.645402
H           2.674393        2.512534        1.008551
H           3.980403        2.285620       -0.176574
```

---

### Compound_26_HEI_23_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315838 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101446 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      26.8578 cm-1
2.      36.3303 cm-1
3.      48.4885 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.607429        1.418590       -0.149820
C          -1.901366        1.427667        0.346026
C          -2.572056        0.189172        0.776804
O           0.102148        2.361698       -0.527651
O          -0.103253        0.107363       -0.248515
C           1.271571       -0.050156       -0.561181
C           2.147206        0.042720        0.677780
C           3.638042       -0.089784        0.373911
C           4.043303       -1.455401       -0.172093
H          -2.443732        2.360377        0.362124
H          -2.011457       -0.410410        1.497425
H          -3.565342        0.374526        1.180244
H           1.350186       -1.034029       -1.023384
H           1.572457        0.701943       -1.291739
H           1.843925       -0.732799        1.387175
H           1.958457        1.006575        1.154503
H           4.197413        0.107595        1.290605
H           3.930729        0.689446       -0.335696
H           5.124889       -1.522485       -0.293323
H           3.732631       -2.252175        0.507126
H           3.592193       -1.654196       -1.145045
N          -2.769263       -0.779090       -0.393314
H          -3.308231       -0.299477       -1.109068
H          -1.827912       -0.904993       -0.772778
C          -3.381331       -2.077365       -0.050246
H          -3.454359       -2.690162       -0.943448
H          -2.755818       -2.571042        0.687708
H          -4.369991       -1.900207        0.363015
```

---

### Compound_26_HEI_24_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.31624 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101549 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      20.1849 cm-1
2.      39.0147 cm-1
3.      69.0670 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.558142       -1.087664        0.006002
C           1.520781       -0.712635       -0.923482
C           2.878033       -0.379913       -0.499005
O           0.671178       -1.151313        1.242628
O          -0.647394       -1.443269       -0.583953
C          -1.779683       -1.534082        0.266037
C          -2.358055       -0.172014        0.615540
C          -2.808606        0.634657       -0.596250
C          -3.376181        1.995918       -0.216440
H           1.277173       -0.710067       -1.975893
H           3.138468       -0.813736        0.465859
H           3.642415       -0.638913       -1.230716
H          -2.510521       -2.119307       -0.295332
H          -1.524505       -2.079707        1.174403
H          -1.611124        0.392957        1.179312
H          -3.206863       -0.328659        1.288547
H          -3.560310        0.063665       -1.149327
H          -1.961862        0.766657       -1.273081
H          -2.630793        2.594280        0.311696
H          -3.692065        2.557206       -1.096591
H          -4.241357        1.890309        0.441467
N           3.098610        1.144591       -0.286197
H           4.088330        1.331299       -0.143881
H           2.833208        1.608181       -1.151309
C           2.314603        1.710206        0.831686
H           2.657289        1.254844        1.755609
H           1.270925        1.462476        0.665758
H           2.456845        2.786197        0.862930
```

---

### Compound_26_HEI_25_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.316977 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101275 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      34.8005 cm-1
2.      47.9139 cm-1
3.      58.2372 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.882673        1.498799        0.231952
C          -2.100067        0.936234       -0.119570
C          -2.184655       -0.230040       -1.011221
O          -0.641448        2.465017        0.970185
O           0.195894        0.810619       -0.346060
C           1.499284        1.268449       -0.024959
C           2.512667        0.405656       -0.751401
C           2.409215       -1.093582       -0.471025
C           2.422866       -1.457009        1.008961
H          -2.993275        1.308199        0.357608
H          -1.673851       -0.111708       -1.968629
H          -3.212610       -0.530890       -1.202300
H           1.612272        2.312531       -0.321982
H           1.649656        1.222076        1.055864
H           3.503786        0.761286       -0.456251
H           2.425576        0.576807       -1.826825
H           3.240434       -1.592719       -0.973248
H           1.505795       -1.490678       -0.940145
H           3.304324       -1.045033        1.504498
H           1.543301       -1.071656        1.527883
H           2.436982       -2.538625        1.144289
N          -1.491049       -1.473287       -0.418682
H          -1.436259       -2.207181       -1.119458
H          -0.537130       -1.156232       -0.232359
C          -2.109001       -1.993942        0.815533
H          -1.491071       -2.789884        1.219553
H          -2.182939       -1.173872        1.523189
H          -3.099027       -2.371895        0.576460
```

---

### Compound_26_HEI_26_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315879 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101205 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.6993 cm-1
2.      44.0813 cm-1
3.      75.6122 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.479137       -0.182536       -0.054005
C          -1.312245        0.817871       -0.543147
C          -2.448748        1.294821        0.239004
O          -0.573860       -0.800521        1.020591
O           0.560015       -0.483884       -0.922761
C           1.566534       -1.368155       -0.456935
C           2.627394       -0.664617        0.374077
C           3.371421        0.432512       -0.377673
C           4.429819        1.115651        0.478394
H          -1.086935        1.285727       -1.490488
H          -2.341835        1.098789        1.305272
H          -2.670444        2.350138        0.085386
H           1.114933       -2.178212        0.115518
H           2.016811       -1.788787       -1.358493
H           3.340696       -1.420312        0.718062
H           2.156042       -0.247970        1.267831
H           2.653176        1.174033       -0.733754
H           3.839818        0.003404       -1.268480
H           5.176688        0.398066        0.824555
H           4.949586        1.897621       -0.076426
H           3.979494        1.575007        1.360797
N          -3.791944        0.599357       -0.128281
H          -4.565015        1.086639        0.318872
H          -3.916664        0.707039       -1.131536
C          -3.834889       -0.836450        0.218471
H          -3.783049       -0.930718        1.298724
H          -2.972412       -1.315182       -0.234026
H          -4.757418       -1.270119       -0.155600
```

---

### Compound_26_HEI_27_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315864 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101447 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      27.5457 cm-1
2.      38.2863 cm-1
3.      69.7993 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.909280        1.397505        0.067598
C          -2.235645        1.105307       -0.210741
C          -2.621957       -0.122439       -0.923870
O          -0.415948        2.380970        0.639358
O          -0.054019        0.371891       -0.363645
C           1.338278        0.558198       -0.173566
C           2.039600       -0.715896       -0.600488
C           3.562132       -0.619836       -0.525480
C           4.106473       -0.430533        0.886800
H          -3.000179        1.756094        0.183825
H          -2.119006       -0.270068       -1.881358
H          -3.696267       -0.186676       -1.083952
H           1.687622        1.405097       -0.771715
H           1.538281        0.791893        0.872777
H           1.741293       -0.949606       -1.625060
H           1.692490       -1.541381        0.028197
H           3.903034        0.201355       -1.162236
H           3.985288       -1.531632       -0.951466
H           3.748627       -1.221279        1.549615
H           5.196486       -0.458257        0.891408
H           3.801069        0.524847        1.314951
N          -2.241384       -1.399318       -0.149315
H          -1.236277       -1.301263        0.011138
H          -2.376286       -2.215991       -0.738742
C          -2.953759       -1.573208        1.130672
H          -4.009593       -1.724346        0.924362
H          -2.547967       -2.431873        1.656543
H          -2.814240       -0.669168        1.715667
```

---

### Compound_26_HEI_29_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317339 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102575 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      24.5140 cm-1
2.      42.6616 cm-1
3.      66.3592 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.438764        1.553016       -0.258311
C          -1.472849        1.109524       -1.066267
C          -1.947781       -0.283821       -1.011418
O           0.119412        2.658830       -0.216245
O          -0.043285        0.557927        0.656864
C           1.212529        0.712428        1.299442
C           2.364528        0.259883        0.418659
C           2.277319       -1.202740        0.000277
C           3.439849       -1.630318       -0.885556
H          -1.961942        1.813992       -1.721237
H          -1.163736       -1.037427       -1.115791
H          -2.723043       -0.487072       -1.747337
H           1.345920        1.750839        1.600932
H           1.155798        0.093403        2.196460
H           3.295926        0.431338        0.966753
H           2.401724        0.897288       -0.468935
H           1.334754       -1.368634       -0.526254
H           2.245577       -1.830876        0.895463
H           4.393789       -1.498879       -0.370669
H           3.357431       -2.678719       -1.174303
H           3.472479       -1.033470       -1.799343
N          -2.563572       -0.620011        0.349154
H          -3.334842        0.021244        0.513751
H          -1.830922       -0.377144        1.020480
C          -2.995491       -2.021028        0.518708
H          -3.754817       -2.245731       -0.224634
H          -2.135246       -2.668257        0.375072
H          -3.398899       -2.157529        1.517359
```

---

### Compound_26_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.320191 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.105744 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.3205 cm-1
2.      44.2151 cm-1
3.      65.0805 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.599276        0.128663       -0.470129
C           1.341684       -1.000984       -0.731119
C           2.816997       -0.878332       -0.653640
O           1.076938        1.243614       -0.109239
O          -0.760118       -0.003030       -0.598084
C          -1.562670        1.089446       -0.174038
C          -3.017811        0.688398       -0.298969
C          -3.429998       -0.446214        0.631863
C          -4.904536       -0.803999        0.500888
H           0.880016       -1.951585       -0.943029
H           3.259370       -0.221471       -1.409899
H           3.326403       -1.838490       -0.699047
H          -1.324581        1.346681        0.861834
H          -1.352714        1.967930       -0.787890
H          -3.226190        0.410979       -1.336407
H          -3.624724        1.572775       -0.084851
H          -3.212028       -0.156314        1.663915
H          -2.818191       -1.325521        0.421891
H          -5.139762       -1.120947       -0.517221
H          -5.179441       -1.615951        1.174949
H          -5.538018        0.054207        0.734614
N           3.198629       -0.215962        0.653359
H           2.927116       -0.829555        1.415887
H           2.548454        0.599849        0.668250
C           4.608018        0.192351        0.778962
H           5.245283       -0.682190        0.680110
H           4.835550        0.904138       -0.009387
H           4.762729        0.656552        1.748453
```

---

### Compound_26_HEI_30_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315239 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.100842 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.9175 cm-1
2.      39.9726 cm-1
3.      80.2265 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.702835       -0.422199        0.344048
C           1.800902       -1.062686       -0.221691
C           3.146682       -0.827603        0.292019
O           0.693406        0.414437        1.263945
O          -0.498724       -0.810473       -0.223227
C          -1.674023       -0.204432        0.285822
C          -2.849686       -0.712166       -0.525728
C          -4.196563       -0.196963       -0.022080
C          -4.376844        1.311921       -0.154964
H           1.651522       -1.788398       -1.007815
H           3.151073       -0.460616        1.317881
H           3.800483       -1.695455        0.215262
H          -1.806071       -0.459322        1.342044
H          -1.588960        0.882121        0.223169
H          -2.845630       -1.804156       -0.494834
H          -2.714011       -0.423587       -1.572015
H          -4.326689       -0.490106        1.023578
H          -4.988440       -0.700421       -0.580262
H          -3.675153        1.861545        0.473476
H          -4.218942        1.631667       -1.187221
H          -5.383563        1.611990        0.137532
N           3.929564        0.268469       -0.488993
H           4.900624        0.277248       -0.185950
H           3.928915       -0.005235       -1.468130
C           3.350589        1.621709       -0.359029
H           3.898323        2.310902       -0.994713
H           2.308016        1.568515       -0.655606
H           3.420731        1.926827        0.680440
```

---

### Compound_26_HEI_31_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.318725 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.103467 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      24.7436 cm-1
2.      45.8248 cm-1
3.      57.9891 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.221739       -0.786052        0.476989
C          -1.002811       -0.062631        1.346995
C          -2.435172        0.105902        1.002284
O          -0.617707       -1.270478       -0.624125
O           1.084108       -0.974198        0.861807
C           2.015188       -1.353218       -0.143093
C           2.438513       -0.214855       -1.060096
C           3.193867        0.932112       -0.387408
C           2.316990        1.888333        0.414863
H          -0.587149        0.417876        2.217567
H          -3.019822       -0.819716        1.018804
H          -2.940035        0.836623        1.630353
H           2.880679       -1.726243        0.407245
H           1.606144       -2.171865       -0.735472
H           1.558089        0.172270       -1.579589
H           3.078610       -0.661123       -1.826310
H           3.713800        1.501771       -1.161413
H           3.973547        0.516724        0.258371
H           2.907797        2.709328        0.824026
H           1.540376        2.320403       -0.220510
H           1.819246        1.376950        1.237181
N          -2.552201        0.571741       -0.432797
H          -2.132860        1.494046       -0.507985
H          -1.912216       -0.095994       -0.918192
C          -3.910672        0.560522       -1.001121
H          -3.872328        0.901862       -2.031318
H          -4.294833       -0.454813       -0.965012
H          -4.549827        1.216439       -0.416104
```

---

### Compound_26_HEI_32_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.318051 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.103386 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.9480 cm-1
2.      38.0247 cm-1
3.      70.7380 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.522548       -0.706698        0.317477
C           1.330504       -0.015979        1.190027
C           2.798367       -0.115813        1.001422
O           0.929589       -1.378393       -0.677164
O          -0.824847       -0.621522        0.554954
C          -1.698946       -1.126089       -0.444878
C          -3.120833       -0.707962       -0.118276
C          -3.467969        0.747646       -0.430879
C          -2.735989        1.787686        0.410342
H           0.919866        0.639486        1.940674
H           3.216935       -1.101038        1.229606
H           3.347575        0.626560        1.576977
H          -1.404639       -0.746625       -1.426900
H          -1.624548       -2.215710       -0.479747
H          -3.320254       -0.924612        0.935125
H          -3.785308       -1.353190       -0.698128
H          -4.544522        0.876898       -0.294997
H          -3.271640        0.934326       -1.490898
H          -2.897099        1.608976        1.475477
H          -1.661456        1.760956        0.233754
H          -3.095361        2.791847        0.180484
N           3.150734        0.082714       -0.461943
H           4.085720       -0.262514       -0.651292
H           2.455168       -0.548489       -0.922516
C           3.004221        1.463368       -0.955800
H           2.000724        1.801713       -0.714502
H           3.738939        2.097959       -0.467358
H           3.155409        1.476825       -2.031084
```

---

### Compound_26_HEI_33_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.318109 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102053 |
| Number of Imaginary Frequencies | 1 |

**Frequencies** (Top 3 out of 78)

```
1.      -2.5640 cm-1
2.      37.8092 cm-1
3.      47.2692 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.266968       -0.114496        0.381885
C           1.031369        0.983142        0.706004
C           2.339389        1.127621        0.023511
O           0.611786       -1.022553       -0.429160
O          -0.932818       -0.220617        1.042742
C          -1.819856       -1.254680        0.640290
C          -2.630740       -0.925395       -0.604784
C          -3.631016        0.221668       -0.461637
C          -3.006336        1.612284       -0.405076
H           0.728558        1.684311        1.466588
H           2.271720        1.302541       -1.055254
H           2.960784        1.909079        0.455498
H          -1.260905       -2.177256        0.482759
H          -2.488882       -1.396973        1.491128
H          -3.174588       -1.836669       -0.869364
H          -1.944837       -0.722148       -1.430869
H          -4.240220        0.055367        0.432116
H          -4.319818        0.181856       -1.309038
H          -3.776685        2.384586       -0.381236
H          -2.374425        1.728976        0.473715
H          -2.382835        1.789493       -1.284437
N           3.105068       -0.174579        0.120655
H           2.381110       -0.862518       -0.178314
H           3.303788       -0.357863        1.099785
C           4.330016       -0.261803       -0.692388
H           5.018777        0.521126       -0.386446
H           4.787842       -1.236016       -0.549179
H           4.064635       -0.130532       -1.737522
```

---

### Compound_26_HEI_34_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.316296 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102294 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      27.5162 cm-1
2.      32.9262 cm-1
3.      64.9082 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.786705        1.595135       -0.052612
C           2.122687        1.406635        0.267658
C           2.631641        0.093883        0.699446
O           0.190292        2.624125       -0.402138
O           0.065208        0.393869        0.025708
C          -1.327914        0.449054       -0.230247
C          -1.888501       -0.946808       -0.042853
C          -3.377433       -1.047406       -0.368109
C          -4.274852       -0.240220        0.564482
H           2.806815        2.232902        0.152482
H           2.086010       -0.361702        1.528946
H           3.688158        0.123020        0.957103
H          -1.797191        1.162234        0.449471
H          -1.510117        0.799369       -1.250023
H          -1.714509       -1.266770        0.988397
H          -1.331071       -1.632073       -0.686269
H          -3.668968       -2.098476       -0.321701
H          -3.543243       -0.729876       -1.401412
H          -4.096837        0.831759        0.472128
H          -5.327597       -0.417856        0.342891
H          -4.100593       -0.517470        1.606301
N           2.499230       -0.954117       -0.410524
H           1.509481       -0.920842       -0.666766
H           3.020890       -0.624320       -1.218020
C           2.902166       -2.325120       -0.041340
H           2.291139       -2.651192        0.795350
H           2.752605       -2.987100       -0.888779
H           3.949424       -2.317652        0.246464
```

---

### Compound_26_HEI_35_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.31696 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101878 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      40.4252 cm-1
2.      56.2417 cm-1
3.      66.5975 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.267950       -1.376092       -0.136483
C           2.354832       -0.603691        0.243880
C           2.191384        0.627167        1.032760
O           1.236270       -2.440951       -0.770838
O           0.053766       -0.794914        0.262106
C          -1.131219       -1.545617        0.047255
C          -2.320347       -0.702212        0.458489
C          -2.560306        0.514666       -0.427811
C          -3.789429        1.310060       -0.008640
H           3.331926       -0.874853       -0.124397
H           1.624907        0.502924        1.957680
H           3.144112        1.095853        1.270315
H          -1.207316       -1.829004       -1.004839
H          -1.093264       -2.465734        0.635185
H          -2.196879       -0.386786        1.498513
H          -3.205419       -1.343884        0.430491
H          -2.669405        0.184620       -1.464562
H          -1.686132        1.169197       -0.406368
H          -3.687946        1.672805        1.016108
H          -3.944822        2.173911       -0.655490
H          -4.687845        0.691338       -0.053546
N           1.374505        1.699950        0.286901
H           0.501560        1.221450        0.053776
H           1.144812        2.463103        0.917308
C           2.016321        2.223324       -0.933678
H           2.275975        1.377446       -1.562965
H           2.913331        2.766675       -0.650200
H           1.325465        2.882589       -1.450090
```

---

### Compound_26_HEI_36_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317118 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.102571 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      32.8217 cm-1
2.      45.8598 cm-1
3.      55.7716 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.167169        1.399526       -0.187788
C          -2.155482        0.605138       -0.748296
C          -1.899105       -0.796318       -1.118422
O          -1.199826        2.592685        0.148308
O           0.010217        0.670482        0.033866
C           1.148402        1.375306        0.500308
C           2.262993        0.375534        0.730105
C           2.713247       -0.353075       -0.531033
C           3.859514       -1.320756       -0.268792
H          -3.152163        1.007653       -0.839966
H          -1.043229       -0.941607       -1.780510
H          -2.769237       -1.270111       -1.568178
H           1.449344        2.122061       -0.240450
H           0.907046        1.904143        1.423682
H           1.941296       -0.351991        1.481694
H           3.110597        0.915050        1.162035
H           3.017405        0.384611       -1.279259
H           1.866307       -0.894220       -0.957795
H           3.568445       -2.081733        0.458249
H           4.166710       -1.831768       -1.181793
H           4.730310       -0.797298        0.131256
N          -1.529306       -1.671584        0.094186
H          -1.212971       -2.584264       -0.221163
H          -0.724283       -1.193128        0.505934
C          -2.604234       -1.823245        1.092762
H          -3.423998       -2.375461        0.641707
H          -2.221512       -2.358808        1.956089
H          -2.937035       -0.830036        1.378710
```

---

### Compound_26_HEI_37_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315031 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.100442 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.3427 cm-1
2.      36.4121 cm-1
3.      45.1979 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.550016       -0.338775        0.010289
C          -1.714961       -1.089208       -0.106176
C          -2.848833       -0.595510       -0.882072
O          -0.317093        0.789819       -0.455865
O           0.430256       -0.983673        0.751802
C           1.696240       -0.352978        0.848553
C           2.612513       -0.735377       -0.303148
C           4.022394       -0.163866       -0.167529
C           4.088085        1.357021       -0.268486
H          -1.765089       -2.071868        0.339665
H          -2.563944        0.147358       -1.626501
H          -3.424249       -1.386298       -1.361782
H           1.564941        0.727091        0.898760
H           2.125339       -0.695203        1.792890
H           2.163407       -0.392482       -1.238768
H           2.664454       -1.825743       -0.352264
H           4.650786       -0.599334       -0.947182
H           4.452640       -0.486069        0.785446
H           3.556546        1.841637        0.551257
H           5.120720        1.706649       -0.242106
H           3.641373        1.702301       -1.203229
N          -3.916407        0.141356       -0.022135
H          -4.749880        0.310970       -0.580371
H          -4.186371       -0.493093        0.724971
C          -3.436937        1.410965        0.562307
H          -3.228276        2.103769       -0.247119
H          -4.199817        1.815430        1.220652
H          -2.523939        1.202603        1.110697
```

---

### Compound_26_HEI_38_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.31516 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.099831 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      33.0515 cm-1
2.      41.6631 cm-1
3.      61.5072 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.647329       -0.798472        0.259833
C           1.809663       -1.084329       -0.446813
C           3.118208       -0.724440        0.091977
O           0.536951       -0.198566        1.343121
O          -0.493213       -1.287275       -0.364299
C          -1.743760       -0.845971        0.136516
C          -2.121457        0.523718       -0.407232
C          -3.437283        1.056372        0.155593
C          -4.659853        0.230514       -0.232462
H           1.749528       -1.624767       -1.380245
H           3.111829       -0.600130        1.174255
H           3.911869       -1.416204       -0.188009
H          -2.461685       -1.602250       -0.181188
H          -1.726750       -0.823548        1.227463
H          -2.181094        0.470063       -1.498270
H          -1.314902        1.218004       -0.162859
H          -3.574955        2.082009       -0.193105
H          -3.364950        1.111945        1.245656
H          -4.735153        0.136052       -1.317896
H          -4.618960       -0.775969        0.185862
H          -5.577531        0.697317        0.126840
N           3.646523        0.642814       -0.429438
H           3.646938        0.595193       -1.444990
H           4.613745        0.767741       -0.140470
C           2.838902        1.801156        0.006449
H           1.808604        1.617396       -0.281366
H           2.909344        1.880689        1.086862
H           3.218065        2.702200       -0.466212
```

---

### Compound_26_HEI_39_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315885 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101279 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      26.5629 cm-1
2.      36.9628 cm-1
3.      56.2189 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.398691        1.284835       -0.063317
C           1.675691        1.490520        0.434193
C           2.558560        0.365437        0.783057
O          -0.473620        2.110282       -0.369439
O           0.137302       -0.084418       -0.260080
C          -1.196884       -0.460988       -0.561489
C          -2.029885       -0.633030        0.697936
C          -3.458619       -1.094776        0.418147
C          -4.314203       -0.058001       -0.303370
H           2.042740        2.501632        0.519099
H           2.114242       -0.377458        1.449059
H           3.500578        0.696847        1.214723
H          -1.639298        0.278956       -1.226698
H          -1.123447       -1.409659       -1.096262
H          -2.049421        0.317652        1.237051
H          -1.529649       -1.358513        1.343844
H          -3.933710       -1.348621        1.367880
H          -3.432608       -2.019509       -0.165908
H          -3.932491        0.160644       -1.301259
H          -5.341311       -0.407162       -0.414210
H          -4.337710        0.879895        0.255371
N           2.934212       -0.463835       -0.449778
H           2.035240       -0.736930       -0.853305
H           3.377106        0.156661       -1.122322
C           3.777660       -1.645773       -0.184052
H           3.255665       -2.293178        0.514400
H           3.962279       -2.175779       -1.113458
H           4.716794       -1.314887        0.249956
```

---

### Compound_26_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.320151 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.10562 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      25.8076 cm-1
2.      43.8965 cm-1
3.      72.2977 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.580796        0.072557        0.059552
C           1.340439        1.186183       -0.220363
C           2.771558        1.147561        0.163423
O           1.023317       -0.999802        0.564878
O          -0.748731        0.156752       -0.267643
C          -1.529035       -1.022834       -0.139743
C          -2.962055       -0.685363       -0.495428
C          -3.622227        0.296590        0.465783
C          -5.068913        0.595263        0.095302
H           0.933423        2.039688       -0.737661
H           2.952643        1.101301        1.242418
H           3.342635        1.980675       -0.240475
H          -1.140701       -1.798759       -0.804450
H          -1.468343       -1.403845        0.882468
H          -3.529924       -1.620072       -0.506981
H          -2.996037       -0.286775       -1.513548
H          -3.048112        1.224868        0.483686
H          -3.578971       -0.114092        1.478749
H          -5.133365        1.031617       -0.903585
H          -5.670032       -0.316384        0.097273
H          -5.523213        1.296832        0.795720
N           3.396818       -0.131543       -0.351873
H           2.699296       -0.841906       -0.040872
H           3.374403       -0.114681       -1.367263
C           4.752332       -0.426748        0.142299
H           5.093838       -1.365702       -0.283216
H           5.422454        0.378266       -0.147191
H           4.718234       -0.505081        1.225212
```

---

### Compound_26_HEI_40_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.31716 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101664 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      29.0439 cm-1
2.      33.6566 cm-1
3.      70.4155 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.175511       -1.673566        0.057110
C          -1.326177       -1.443007        0.792706
C          -1.901508       -0.091813        0.914574
O           0.476838       -2.715865       -0.097942
O           0.230682       -0.513312       -0.629170
C           1.577082       -0.439752       -1.068926
C           2.535038       -0.103873        0.064743
C           2.117847        1.102299        0.904332
C           1.928693        2.384836        0.103180
H          -1.827647       -2.278831        1.255900
H          -1.197307        0.675589        1.244508
H          -2.769457       -0.068595        1.570133
H           1.866418       -1.378293       -1.541467
H           1.586216        0.342799       -1.827599
H           3.519686        0.074581       -0.377828
H           2.633423       -0.976864        0.713201
H           2.874600        1.263664        1.675108
H           1.190651        0.864738        1.430824
H           1.093401        2.299821       -0.593641
H           1.722849        3.229932        0.760859
H           2.823572        2.621992       -0.476571
N          -2.380963        0.445873       -0.435386
H          -1.558870        0.367313       -1.039369
H          -3.076557       -0.197280       -0.803388
C          -2.894053        1.829604       -0.417373
H          -2.104495        2.485810       -0.062543
H          -3.192664        2.118412       -1.420463
H          -3.745710        1.879136        0.254846
```

---

### Compound_26_HEI_41_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317125 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.101494 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      40.2336 cm-1
2.      49.5254 cm-1
3.      57.0186 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.104493        1.520074        0.022853
C           1.403474        1.610361       -0.451898
C           2.449861        0.664135       -0.028809
O          -0.874014        2.240948       -0.215413
O          -0.048540        0.412438        0.880299
C          -1.338553        0.103178        1.386030
C          -1.798161       -1.248441        0.865030
C          -2.008448       -1.302939       -0.646892
C          -3.164069       -0.438844       -1.137851
H           1.637532        2.372939       -1.178313
H           2.565025        0.555927        1.051967
H           3.421342        0.903431       -0.456106
H          -1.264549        0.077699        2.475153
H          -2.028966        0.896539        1.105795
H          -2.731826       -1.506865        1.373572
H          -1.063881       -2.002838        1.160967
H          -2.182952       -2.341433       -0.936249
H          -1.088754       -0.996487       -1.153263
H          -2.976904        0.616609       -0.938419
H          -3.308744       -0.553736       -2.212734
H          -4.096526       -0.719111       -0.642949
N           2.130945       -0.763485       -0.481726
H           1.197541       -0.939067       -0.101899
H           2.038510       -0.758953       -1.493983
C           3.085174       -1.799635       -0.041658
H           3.128773       -1.792034        1.043439
H           4.064386       -1.571357       -0.452222
H           2.751182       -2.771292       -0.392594
```

---

### Compound_26_HEI_42_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.315867 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.100445 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      36.8053 cm-1
2.      50.9420 cm-1
3.      67.0187 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.101849        1.605227       -0.185278
C          -1.270637        1.384183       -0.896245
C          -1.937116        0.070563       -0.897334
O           0.598664        2.625106       -0.110631
O           0.260360        0.475827        0.572602
C           1.569138        0.447968        1.123256
C           2.626656       -0.003581        0.125358
C           2.648793       -1.499619       -0.183010
C           1.388513       -2.039466       -0.850130
H          -1.729491        2.213580       -1.412153
H          -1.292711       -0.768377       -1.166907
H          -2.815143        0.052238       -1.539398
H           1.815734        1.437589        1.506266
H           1.516958       -0.246967        1.963548
H           3.600862        0.282772        0.530527
H           2.495864        0.568323       -0.797214
H           2.830510       -2.049769        0.745122
H           3.506975       -1.702222       -0.828416
H           1.145058       -1.465335       -1.746875
H           1.519369       -3.082294       -1.142088
H           0.530955       -1.981199       -0.181061
N          -2.431526       -0.313819        0.500144
H          -3.071069        0.409056        0.818542
H          -1.596042       -0.244281        1.086564
C          -3.046109       -1.651312        0.608953
H          -3.915044       -1.691818       -0.041414
H          -2.317433       -2.393886        0.296707
H          -3.341190       -1.831924        1.638061
```

---

### Compound_26_HEI_4_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.320216 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.105833 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      25.4256 cm-1
  2.      39.2152 cm-1
  3.      64.9713 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.635740       -0.959687        0.137633
C          -1.678384       -1.204807       -0.724116
C          -2.967974       -0.526248       -0.447113
O          -0.671386       -0.148227        1.108476
O           0.521260       -1.664750       -0.106683
C           1.719113       -1.177355        0.479996
C           2.320674       -0.027901       -0.309666
C           3.626052        0.468467        0.300077
C           4.245203        1.614869       -0.488695
H          -1.564527       -1.833629       -1.592008
H          -3.459367       -0.843769        0.478462
H          -3.682787       -0.624263       -1.261269
H           1.535985       -0.874195        1.511361
H           2.402609       -2.027666        0.487912
H           1.598758        0.792031       -0.350047
H           2.493759       -0.353547       -1.339215
H           4.336762       -0.360838        0.358427
H           3.443667        0.789517        1.329391
H           3.564452        2.467066       -0.536215
H           5.176038        1.954934       -0.033732
H           4.465189        1.308912       -1.513334
N          -2.718571        0.949799       -0.227403
H          -1.918305        0.926218        0.442812
H          -2.371135        1.349625       -1.094270
C          -3.859651        1.723069        0.290800
H          -4.687974        1.653063       -0.409136
H          -4.153733        1.308590        1.250776
H          -3.564152        2.760732        0.414063
```

---

### Compound_26_HEI_5_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.319912 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.105496 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      33.3714 cm-1
2.      35.5595 cm-1
3.      67.1649 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.597810       -0.595093       -0.005795
C           1.670846       -1.246488        0.559030
C           2.873377       -0.436232        0.865064
O           0.578854        0.629103       -0.321807
O          -0.503858       -1.376868       -0.265920
C          -1.645913       -0.746897       -0.825914
C          -2.558657       -0.155574        0.233940
C          -3.815684        0.460021       -0.368782
C          -4.747317        1.044916        0.684660
H           1.669937       -2.311623        0.724346
H           2.724285        0.325318        1.637462
H           3.732980       -1.040671        1.146272
H          -1.339166        0.024385       -1.533084
H          -2.169096       -1.531469       -1.375540
H          -2.006330        0.603579        0.792840
H          -2.836093       -0.940100        0.943707
H          -4.349399       -0.299649       -0.947070
H          -3.530020        1.241499       -1.078451
H          -4.245422        1.827389        1.257107
H          -5.638216        1.480762        0.231405
H          -5.071476        0.275713        1.388352
N           3.261440        0.373174       -0.354793
H           2.347637        0.795610       -0.622937
H           3.522157       -0.269898       -1.096622
C           4.306717        1.389161       -0.144071
H           5.214315        0.901718        0.201395
H           4.496772        1.909598       -1.078035
H           3.960017        2.094851        0.605421
```

---

### Compound_26_HEI_6_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317189 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.103107 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      39.2363 cm-1
2.      48.0205 cm-1
3.      63.2900 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.164752       -1.582258       -0.012567
C           2.436732       -1.077030        0.210057
C           2.649693        0.324450        0.610162
O           0.807757       -2.727653       -0.324552
O           0.184139       -0.587473        0.127234
C          -1.169148       -0.974466       -0.037668
C          -2.033743        0.260521        0.104230
C          -3.516670       -0.053259       -0.055324
C          -4.394964        1.183252        0.082241
H           3.287868       -1.717792        0.039854
H           2.078219        0.646190        1.483928
H           3.699897        0.550325        0.783025
H          -1.311271       -1.433192       -1.018984
H          -1.438413       -1.720562        0.714667
H          -1.732025        0.997580       -0.645689
H          -1.856519        0.713461        1.083574
H          -3.810976       -0.795940        0.691196
H          -3.685297       -0.515057       -1.031952
H          -4.265580        1.646293        1.062388
H          -4.139665        1.928868       -0.673238
H          -5.450511        0.936268       -0.034572
N           2.184680        1.297803       -0.477407
H           2.699801        1.087909       -1.328022
H           1.212069        1.032045       -0.650060
C           2.287810        2.729741       -0.135542
H           1.916809        3.326968       -0.962815
H           1.692130        2.917686        0.752987
H           3.328756        2.969630        0.060584
```

---

### Compound_26_HEI_7_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.317537 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.103686 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.       8.6560 cm-1
2.      57.4320 cm-1
3.      58.5704 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.461304       -1.404457       -0.090060
C          -2.492047       -0.490472        0.069942
C          -2.239231        0.876791        0.553862
O          -1.499910       -2.586045       -0.462821
O          -0.212904       -0.833951        0.206706
C           0.921616       -1.683951        0.142846
C           2.149597       -0.885529        0.528817
C           2.500099        0.238420       -0.439438
C           3.784360        0.961267       -0.055334
H          -3.490118       -0.776911       -0.223004
H          -1.676805        0.938507        1.488386
H          -3.153892        1.455669        0.662721
H           0.786311       -2.528850        0.820814
H           1.027562       -2.086319       -0.867946
H           2.989767       -1.583391        0.585010
H           2.013939       -0.478829        1.535034
H           1.683277        0.962390       -0.478018
H           2.594644       -0.173519       -1.447936
H           3.700675        1.400954        0.940486
H           4.630804        0.271865       -0.043231
H           4.015188        1.763354       -0.756876
N          -1.359700        1.661624       -0.425011
H          -0.535655        1.067073       -0.545217
H          -1.833847        1.685682       -1.323701
C          -0.975870        3.018700        0.009948
H          -0.438824        2.941630        0.950914
H          -0.339735        3.474060       -0.742882
H          -1.876198        3.610619        0.145950
```

---

### Compound_26_HEI_8_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.320403 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.105274 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
  1.      28.9606 cm-1
  2.      48.7535 cm-1
  3.      75.6011 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.429704       -0.983449        0.145047
C           1.200946       -0.632996        1.227593
C           2.589295       -0.183592        0.961195
O           0.788719       -0.885258       -1.065113
O          -0.823065       -1.473954        0.435078
C          -1.802568       -1.401233       -0.593270
C          -2.349808        0.004353       -0.777282
C          -3.019312        0.572075        0.468389
C          -3.550858        1.983281        0.255697
H           0.810759       -0.643969        2.232210
H           3.246461       -0.957338        0.551006
H           3.073485        0.243499        1.836689
H          -1.390253       -1.774317       -1.530419
H          -2.597046       -2.076520       -0.271855
H          -3.068388       -0.020398       -1.602249
H          -1.535528        0.662307       -1.092667
H          -2.302967        0.569960        1.292650
H          -3.838018       -0.088469        0.768685
H          -2.743359        2.665983       -0.016971
H          -4.289158        2.006882       -0.548574
H          -4.026013        2.371516        1.157276
N           2.571714        0.875630       -0.118597
H           1.954477        0.430470       -0.833787
H           2.079168        1.689884        0.236778
C           3.884645        1.250386       -0.670045
H           3.750407        2.011244       -1.433110
H           4.514121        1.632541        0.129044
H           4.342354        0.368062       -1.108188
```

---

### Compound_26_HEI_9_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -520.319871 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -520.104983 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 78)

```
1.      28.0513 cm-1
2.      48.3215 cm-1
3.      79.1605 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.437764       -0.248010        0.383458
C          -1.259829        0.535595        1.160758
C          -2.517463        1.023135        0.546202
O          -0.694869       -0.616034       -0.799206
O           0.720014       -0.678149        0.988429
C           1.643372       -1.418944        0.202569
C           2.566878       -0.527998       -0.611439
C           3.423362        0.407188        0.233806
C           4.340775        1.283212       -0.609102
H          -1.035374        0.749094        2.193216
H          -2.376477        1.725146       -0.282198
H          -3.192713        1.480067        1.266328
H           2.222992       -2.001205        0.921365
H           1.107822       -2.107160       -0.450464
H           1.966949        0.052842       -1.316480
H           3.214772       -1.176287       -1.209728
H           4.021073       -0.186395        0.931902
H           2.772857        1.037770        0.843439
H           5.020144        0.674723       -1.209676
H           3.762334        1.906439       -1.294206
H           4.945351        1.943786        0.013390
N          -3.248336       -0.136418       -0.096766
H          -2.483083       -0.585925       -0.643667
H          -3.518209       -0.789814        0.632597
C          -4.402016        0.221528       -0.939408
H          -4.841388       -0.682096       -1.351238
H          -5.135376        0.750042       -0.336318
H          -4.058367        0.863124       -1.745759
```

---

### Compound_20_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -270.569658 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.478966 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
1.      90.0999 cm-1
2.     171.3832 cm-1
3.     218.6749 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.591607        0.169284       -0.000008
O           2.104705       -0.925523       -0.000027
C           0.134433        0.410745        0.000006
H           2.215649        1.081677        0.000002
C          -0.256274        1.684158        0.000028
H          -1.298285        1.973423        0.000039
H           0.474133        2.484391        0.000035
C          -0.764986       -0.790456       -0.000007
H          -0.507667       -1.404093       -0.867295
H          -0.507657       -1.404119        0.867259
C          -2.254292       -0.487362        0.000006
H          -2.826332       -1.414330       -0.000004
H          -2.545203        0.084496        0.882347
H          -2.545213        0.084523       -0.882314
```

---

### Compound_20_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -270.564848 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -270.474832 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 36)

```
  1.      70.0305 cm-1
  2.     108.9158 cm-1
  3.     233.3242 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.417981       -0.615235       -0.000009
O           2.509259       -0.097701       -0.000015
C           0.118617        0.111345       -0.000000
H           1.332011       -1.717976       -0.000011
C           0.126335        1.440901        0.000004
H          -0.784611        2.023325        0.000010
H           1.065371        1.978849        0.000000
C          -1.104921       -0.763315        0.000004
H          -1.050262       -1.426339       -0.869196
H          -1.050253       -1.426343        0.869201
```

```
C          -2.433707       -0.027584        0.000013
H          -2.536548        0.605827       -0.882231
H          -3.259074       -0.738233        0.000015
H          -2.536539        0.605823        0.882261
```

---

### Compound_20_HEI_1_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.435436 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.278694 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      28.7303 cm-1
  2.      61.0277 cm-1
  3.      90.5881 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.315499       -1.338246       -0.118263
O          -2.533504       -1.369151       -0.448801
C          -0.588064       -0.281743        0.391907
H          -0.730601       -2.279346       -0.228993
C           0.834651       -0.491853        0.696311
H           1.182491        0.035738        1.586547
H           1.093376       -1.546850        0.786398
C           3.216384       -0.171046       -0.155223
H           3.403872       -1.231884       -0.018489
H           3.478249        0.370864        0.748508
H           3.791462        0.204995       -0.995579
N           1.774120        0.021869       -0.418448
H           1.497969       -0.450275       -1.276267
H           1.576120        1.007311       -0.570565
C          -1.227808        1.053056        0.670475
H          -2.290770        0.884386        0.858718
H          -0.813414        1.479233        1.591131
C          -1.105676        2.098612       -0.445171
H          -0.069666        2.406646       -0.608171
H          -1.485363        1.703069       -1.388290
H          -1.668457        3.003568       -0.205623
```

---

### Compound_20_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.435955 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.278761 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      47.4570 cm-1
2.      71.4832 cm-1
3.      91.8589 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.188154       -1.396308       -0.222103
O           2.348221       -1.713746        0.166106
C           0.519647       -0.202442       -0.054744
H           0.607234       -2.164018       -0.781575
C          -0.829889       -0.054887       -0.620410
H          -1.023923        0.917359       -1.078614
H          -1.073026       -0.834939       -1.341098
C          -3.306426        0.039388       -0.039033
H          -3.376756        1.040959       -0.452265
H          -4.006584       -0.075865        0.782410
H          -3.511594       -0.695104       -0.811933
N          -1.928117       -0.170734        0.454252
H          -1.834300       -1.090402        0.878709
H          -1.715864        0.496039        1.192399
C           1.150151        0.978696        0.635489
H           0.435747        1.477475        1.302185
H           1.952275        0.612354        1.278650
C           1.721217        2.026512       -0.324761
H           2.501287        1.585885       -0.947692
H           0.946876        2.415838       -0.989372
H           2.152555        2.873768        0.212947
```

---

### Compound_20_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.435955 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.278761 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      47.4579 cm-1
2.      71.4832 cm-1
3.      91.8597 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.188155       -1.396308       -0.222103
O           2.348222       -1.713745        0.166106
C           0.519648       -0.202442       -0.054743
H           0.607235       -2.164019       -0.781574
C          -0.829888       -0.054888       -0.620410
H          -1.023922        0.917358       -1.078615
H          -1.073026       -0.834940       -1.341097
C          -3.306426        0.039386       -0.039033
H          -3.511594       -0.695109       -0.811931
H          -3.376757        1.040955       -0.452269
H          -4.006584       -0.075863        0.782410
N          -1.928117       -0.170733        0.454253
H          -1.834299       -1.090401        0.878711
H          -1.715865        0.496042        1.192398
C           1.150151        0.978696        0.635489
H           0.435748        1.477474        1.302186
H           1.952276        0.612355        1.278648
C           1.721214        2.026514       -0.324761
H           2.501283        1.585889       -0.947694
H           0.946872        2.415840       -0.989370
H           2.152552        2.873770        0.212947
```

---

### Compound_20_HEI_4_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.434636 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.276308 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      53.7146 cm-1
2.      71.3719 cm-1
3.     127.8318 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.059066       -1.401985        0.111066
O          -2.107261       -1.692016       -0.531186
C          -0.372151       -0.206324        0.150378
H          -0.608130       -2.203238        0.740625
C           0.817928       -0.111263        1.012909
H           0.989916        0.888168        1.414928
H           0.800225       -0.820330        1.840181
C           2.472099        0.422623       -0.855310
H           2.524766        1.448821       -0.503494
H           1.687062        0.319207       -1.596952
H           3.426487        0.120197       -1.275082
N           2.144553       -0.452400        0.290508
H           2.906728       -0.435531        0.964737
H           2.062719       -1.412273       -0.036210
C          -0.889876        1.022901       -0.552687
H          -0.071615        1.615760       -0.972355
H          -1.502853        0.706426       -1.399287
C          -1.726978        1.936488        0.348484
H          -2.078162        2.820964       -0.188133
H          -2.597984        1.401752        0.730699
H          -1.144676        2.278356        1.207235
```

---

### Compound_20_HEI_5_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.434636 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.276309 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      53.7042 cm-1
2.      71.3618 cm-1
3.     127.8095 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.059073       -1.401986        0.111076
O          -2.107267       -1.692033       -0.531169
C          -0.372162       -0.206321        0.150369
H          -0.608132       -2.203226        0.740648
C           0.817915       -0.111244        1.012903
H           0.989904        0.888196        1.414898
H           0.800207       -0.820291        1.840192
C           2.472113        0.422594       -0.855311
H           2.524807        1.448795       -0.503510
H           1.687075        0.319187       -1.596954
H           3.426495        0.120136       -1.275076
N           2.144542       -0.452405        0.290518
H           2.906711       -0.435535        0.964754
H           2.062700       -1.412283       -0.036184
C          -0.889894        1.022895       -0.552706
H          -0.071642        1.615728       -0.972430
H          -1.502916        0.706409       -1.399268
C          -1.726935        1.936523        0.348479
H          -2.597936        1.401817        0.730748
H          -1.144589        2.278403        1.207195
H          -2.078125        2.820993       -0.188146
```

---

### Compound_20_HEI_6_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.458329 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.301027 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      62.9026 cm-1
  2.      96.8921 cm-1
  3.     119.0152 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.512831        1.592174       -0.020459
O           0.689975        2.186732       -0.215812
C          -0.701992        0.315122        0.314867
```

```
H          -1.345691        2.271854       -0.163546
C           0.465865       -0.609711        0.558283
H           0.139830       -1.656004        0.499601
H           0.836756       -0.464871        1.579165
C           2.774688       -1.119053       -0.019500
H           3.158827       -0.800321        0.950049
H           3.545789       -0.938821       -0.766653
H           2.580745       -2.197608        0.029118
N           1.586231       -0.346223       -0.346859
H           1.294091       -0.561478       -1.291653
H           1.342897        1.450657       -0.266864
C          -2.085956       -0.244399        0.496668
H          -2.140134       -0.767876        1.456760
H          -2.803995        0.576071        0.553568
C          -2.505553       -1.205854       -0.616382
H          -3.493624       -1.624292       -0.420319
H          -2.538250       -0.688931       -1.576479
H          -1.805988       -2.038350       -0.709098
```

---

### Compound_20_HEI_7_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.458484 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.301045 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
1.      79.5480 cm-1
2.      93.1886 cm-1
3.     120.3019 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.461944        1.588990        0.021043
O          -0.714568        2.150174       -0.351215
C           0.686269        0.285497        0.196011
H           1.245882        2.322909        0.171877
C          -0.390721       -0.744377       -0.044971
H          -0.153517       -1.664680        0.506489
H          -0.407707       -1.023118       -1.104137
C          -2.787685       -1.159462       -0.112882
H          -2.652383       -2.172839        0.284469
H          -2.816667       -1.223493       -1.201037
```

```
H          -3.747533       -0.777727        0.231024
N          -1.726796       -0.248829        0.290528
H          -1.773900       -0.102028        1.290781
H          -1.383046        1.429140       -0.284492
C           2.048531       -0.220522        0.580953
H           2.703489        0.626438        0.794368
H           1.972889       -0.797897        1.508323
C           2.690526       -1.100389       -0.493105
H           3.669817       -1.456478       -0.171392
H           2.075343       -1.975377       -0.710154
H           2.818256       -0.542864       -1.422388
```

---

### Compound_20_HEI_8_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -366.458329 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -366.301026 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 57)

```
  1.      62.8978 cm-1
  2.      96.8797 cm-1
  3.     119.0238 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.512777        1.592153       -0.020417
O           0.690036        2.186681       -0.215779
C          -0.701977        0.315081        0.314815
H          -1.345625        2.271865       -0.163423
C           0.465847       -0.609814        0.558160
H           0.139817       -1.656096        0.499272
H           0.836658       -0.465145        1.579095
C           2.774723       -1.119050       -0.019472
H           2.580760       -2.197604        0.029052
H           3.158808       -0.800395        0.950123
H           3.545867       -0.938772       -0.766568
N           1.586294       -0.346182       -0.346840
H           1.294248       -0.561317       -1.291690
H           1.342941        1.450563       -0.266852
C          -2.085963       -0.244362        0.496689
H          -2.140109       -0.767868        1.456767
H          -2.803942        0.576155        0.553669
```

```
C          -2.505727       -1.205739       -0.616360
H          -3.493747       -1.624226       -0.420149
H          -2.538617       -0.688735       -1.576407
H          -1.806158       -2.038210       -0.709275
```

---

### Compound_28_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.773824 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.600226 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      39.2307 cm-1
  2.      52.4531 cm-1
  3.      99.3067 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.703586        0.316899       -0.000056
C          -2.734826       -0.748680        0.000094
C          -4.026429       -0.456054        0.000050
O          -1.925104        1.504990       -0.000222
O          -0.480580       -0.206738        0.000016
C           0.624054        0.706603       -0.000112
C           1.931015       -0.078141        0.000021
C           2.026401       -0.949074       -1.254405
H          -4.362853        0.572956       -0.000098
H          -4.777543       -1.233809        0.000161
H           0.553317        1.341532       -0.885205
H           0.553299        1.341804        0.884785
H           1.958838       -0.340188       -2.158260
H           2.980763       -1.477632       -1.274165
H           1.228564       -1.691290       -1.282605
C           2.026377       -0.948690        1.254715
H           1.958792       -0.339528        2.158383
H           1.228542       -1.690901        1.283126
H           2.980740       -1.477239        1.274657
C           3.065314        0.950159       -0.000124
H           4.031038        0.443062       -0.000038
H           3.020392        1.588434       -0.884661
H           3.020375        1.588700        0.884220
H          -2.378718       -1.770052        0.000241
```

### Compound_28_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.773249 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.598819 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      50.8791 cm-1
2.      51.6436 cm-1
3.      70.3217 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.544581       -0.224593       -0.273890
C          -2.685304        0.690458       -0.026002
C          -3.848763        0.235379        0.413716
O          -1.569298       -1.421920       -0.118933
O          -0.481654        0.461827       -0.696974
C           0.743720       -0.237974       -0.957024
C           1.799497        0.054721        0.109731
C           1.323327       -0.432842        1.479205
H          -3.997249       -0.820376        0.601720
H          -4.678957        0.903486        0.596698
H           0.540704       -1.305589       -1.016784
H           1.081175        0.119541       -1.929722
H           1.104432       -1.501569        1.461638
H           2.094752       -0.254621        2.229959
H           0.422822        0.094509        1.798097
C           2.095201        1.554786        0.163383
H           2.443173        1.919784       -0.805061
H           1.207006        2.122143        0.442625
H           2.872808        1.760043        0.900898
C           3.062731       -0.707098       -0.299030
H           3.860080       -0.527932        0.423480
H           2.879845       -1.782575       -0.339355
H           3.418676       -0.384521       -1.279455
H          -2.516626        1.741410       -0.218017
```

### Compound_28_3

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.77339 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.599782 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      33.8430 cm-1
2.      49.7828 cm-1
3.      98.9524 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.786479        0.662293       -0.000118
C          -2.958369       -0.243777        0.000007
C          -2.878463       -1.566556        0.000218
O          -1.887714        1.868284       -0.000314
O          -0.624758        0.020655        0.000004
C           0.568541        0.812739       -0.000110
C           1.781852       -0.110235        0.000033
C           1.779085       -0.986687        1.254354
H          -1.923930       -2.075685        0.000315
H          -3.772114       -2.175886        0.000300
H           0.566568        1.451359       -0.885383
H           0.566561        1.451624        0.884972
H           0.904219       -1.636619        1.280419
H           2.669491       -1.616997        1.275390
H           1.777103       -0.374515        2.158511
C           3.022852        0.786043       -0.000097
H           3.048726        1.425408       -0.884602
H           3.048723        1.425668        0.884220
H           3.926606        0.175301       -0.000005
C           1.779094       -0.987063       -1.254025
H           2.669500       -1.617380       -1.274866
H           0.904228       -1.637002       -1.279905
H           1.777121       -0.375161       -2.158365
H          -3.911703        0.267825       -0.000090
```

---

### Compound_28_4

| Datum | Value |
|---|---|

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.772675 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.59844 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      35.5567 cm-1
2.      62.2215 cm-1
3.      68.5826 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.590875       -0.645672       -0.129868
C          -2.851632        0.063766        0.190891
C          -3.020032        1.373960        0.085176
O          -1.445889       -1.831331        0.059237
O          -0.658830        0.156046       -0.639290
C           0.642863       -0.373163       -0.925866
C           1.685754        0.136330        0.069250
C           1.749321        1.664442        0.029541
H          -2.225370        2.020364       -0.262084
H          -3.962964        1.834210        0.347850
H           0.597970       -1.460631       -0.918254
H           0.881624       -0.030023       -1.932410
H           0.796346        2.105966        0.322700
H           2.515888        2.028786        0.715362
H           1.996120        2.019778       -0.972995
C           1.345295       -0.334944        1.484206
H           0.389097        0.070662        1.818863
H           1.290394       -1.423591        1.533512
H           2.110540        0.000089        2.186100
C           3.032567       -0.449974       -0.360881
H           3.822152       -0.110952        0.311072
H           3.014456       -1.541230       -0.335974
H           3.294901       -0.136226       -1.373176
H          -3.642957       -0.583398        0.545171
```

---

### Compound_28_5

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.765922 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.592817 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.       9.9065 cm-1
2.      58.0913 cm-1
3.      94.6671 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.750784       -0.500260       -0.000015
C          -2.381279        0.847143       -0.000049
C          -3.701289        0.968078        0.000015
O          -2.387423       -1.527448        0.000015
O          -0.420182       -0.586521       -0.000020
C           0.437277        0.562953       -0.000035
C           1.891472        0.100771        0.000009
C           2.756267        1.364222       -0.000013
H          -4.341202        0.095437        0.000094
H          -4.170983        1.942031       -0.000010
H           0.239190        1.162561       -0.890697
H           0.239154        1.162613        0.890583
H           2.565355        1.974934        0.884488
H           3.812847        1.093808        0.000017
H           2.565391        1.974878       -0.884561
C           2.184268       -0.724040        1.254748
H           1.978064       -0.147048        2.158541
H           1.579337       -1.630169        1.282404
H           3.234927       -1.017402        1.274124
C           2.184320       -0.724119       -1.254667
H           3.234980       -1.017481       -1.273980
H           1.579391       -1.630250       -1.282291
H           1.978153       -0.147184       -2.158504
H          -1.755270        1.726542       -0.000126
```

---

### Compound_28_6

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.764387 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.59101 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.       3.9382 cm-1
  2.      59.3341 cm-1
  3.      78.5898 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.640364       -0.596018       -0.076760
C           1.988069        0.850543       -0.100639
C           3.249297        1.234376        0.035734
O           2.425363       -1.447801        0.268126
O           0.418373       -0.989852       -0.440375
C          -0.611684       -0.141050       -0.963958
C          -1.719813        0.125769        0.056225
C          -2.315860       -1.199968        0.534237
H           4.043924        0.509621        0.154748
H           3.514989        2.282511        0.028951
H          -0.195912        0.788725       -1.347759
H          -1.019500       -0.693227       -1.810666
H          -1.572184       -1.802636        1.055777
H          -3.142692       -1.013708        1.221202
H          -2.698762       -1.782161       -0.306249
C          -1.187030        0.915894        1.252545
H          -0.389004        0.377791        1.767018
H          -0.804604        1.891478        0.947262
H          -1.987551        1.084458        1.974092
C          -2.793413        0.945433       -0.664423
H          -3.616937        1.165024        0.016084
H          -2.392073        1.894800       -1.024214
H          -3.199210        0.400519       -1.518832
H           1.210044        1.588156       -0.217180
```

---

### Compound_28_HEI_1_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.640883 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.400365 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      24.5634 cm-1
2.      34.5367 cm-1
3.      78.5084 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.771762        0.211761       -0.271285
C          -1.639178        1.248252       -0.009363
C          -3.084451        0.997289       -0.222660
O          -1.117245       -0.953113       -0.624596
O           0.560705        0.489538       -0.104593
C           1.468012       -0.593473       -0.204879
C           2.886226       -0.101606        0.080293
C           3.818837       -1.308720       -0.046176
H          -3.366935        0.819143       -1.265469
H          -3.715471        1.792455        0.168358
H           1.196270       -1.375528        0.510324
H           1.421846       -1.030369       -1.206423
H           3.775681       -1.737148       -1.049681
H           4.851134       -1.013457        0.148869
H           3.551980       -2.090024        0.668560
C           2.975534        0.466467        1.498163
H           2.319141        1.328180        1.618486
H           2.689262       -0.285348        2.236996
H           3.996911        0.783142        1.718005
C           3.292199        0.966225       -0.937556
H           4.320029        1.289142       -0.761094
H           3.231537        0.575894       -1.955890
H           2.644891        1.840432       -0.869613
N          -3.479388       -0.288541        0.472886
H          -2.727525       -0.935879        0.151160
H          -3.358384       -0.163267        1.473579
C          -4.824996       -0.800809        0.163235
H          -4.993163       -1.723409        0.710816
H          -5.566032       -0.059206        0.448957
H          -4.887804       -0.990969       -0.904403
H          -1.297863        2.192288        0.383143
```

---

### Compound_28_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.638645 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.397324 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      30.9153 cm-1
  2.      61.7710 cm-1
  3.      87.8490 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.951843        1.734059       -0.045734
C           2.252689        1.342506        0.231909
C           2.566659       -0.037716        0.636918
O           0.504978        2.848347       -0.353287
O           0.063481        0.648496        0.022474
C          -1.318802        0.928390       -0.090526
C          -2.123559       -0.364380        0.039398
C          -1.782641       -1.328147       -1.099149
H           1.972281       -0.416145        1.471841
H           3.619978       -0.174167        0.872336
H          -1.617410        1.628973        0.694650
H          -1.527518        1.401588       -1.053598
H          -2.419830       -2.213000       -1.051461
H          -1.931645       -0.855483       -2.071898
H          -0.748755       -1.670011       -1.042755
C          -3.603663        0.016598       -0.050034
H          -3.882305        0.703117        0.751853
H          -3.829740        0.498225       -1.003601
H          -4.230953       -0.872154        0.034750
C          -1.846290       -1.031865        1.387781
H          -2.083415       -0.356497        2.212544
H          -2.456368       -1.930016        1.500637
H          -0.798597       -1.320275        1.476505
N           2.252579       -1.035297       -0.482655
H           2.814879       -0.789833       -1.292879
H           1.280564       -0.829655       -0.726478
C           2.419575       -2.458759       -0.131435
H           2.144964       -3.076629       -0.980948
H           3.457063       -2.634152        0.137836
H           1.775991       -2.683923        0.714128
H           3.050226        2.058243        0.106851
```

---

### Compound_28_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.641393 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.399966 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      30.5732 cm-1
  2.      48.8591 cm-1
  3.      60.8518 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.599570       -0.789138       -0.439568
C          -1.510646       -1.354167        0.421766
C          -2.916401       -0.894687        0.321854
O          -0.862314        0.120818       -1.276530
O           0.684941       -1.277115       -0.346497
C           1.743458       -0.515313       -0.902659
C           2.498731        0.310990        0.145499
C           3.645309        1.022734       -0.575572
H          -3.412492       -1.145834       -0.621076
H          -3.538912       -1.251497        1.139382
H           2.429697       -1.234587       -1.356182
H           1.355774        0.137086       -1.684774
H           4.222219        1.626581        0.127114
H           4.326015        0.305125       -1.038784
H           3.267745        1.685269       -1.357338
C           3.063820       -0.607119        1.230390
H           3.736006       -1.352912        0.800051
H           3.627508       -0.029238        1.965543
H           2.263514       -1.132302        1.752313
C           1.568080        1.346948        0.779299
H           1.165862        2.024894        0.024908
H           0.728275        0.865519        1.283345
H           2.109498        1.940800        1.518568
N          -2.948216        0.619151        0.345539
H          -2.217764        0.851797       -0.361176
H          -2.601185        0.932677        1.247277
C          -4.245511        1.242044        0.032130
H          -4.143063        2.322556        0.066990
H          -4.547170        0.933479       -0.964800
H          -4.985312        0.915301        0.757866
H          -1.213331       -2.052149        1.187381
```

### Compound_28_HEI_4_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.640721 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.399195 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      33.4970 cm-1
  2.      46.7922 cm-1
  3.      61.5407 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.635651        0.301612       -0.252697
C          -1.543675        1.292931        0.040082
C          -2.870073        0.875034        0.554733
O          -0.862461       -0.938125       -0.155040
O           0.581964        0.738242       -0.724662
C           1.611112       -0.208737       -0.951518
C           2.711404       -0.146887        0.114292
C           3.339875        1.247483        0.140264
H          -2.845799        0.401674        1.541772
H          -3.588211        1.691509        0.588671
H           1.185738       -1.210905       -0.991167
H           2.042485        0.028042       -1.927954
H           2.598757        2.005248        0.395828
H           4.141400        1.292842        0.880302
H           3.764847        1.502050       -0.833340
C           3.772415       -1.181980       -0.264846
H           3.350417       -2.188992       -0.285367
H           4.194859       -0.971178       -1.249785
H           4.589587       -1.174467        0.458606
C           2.134176       -0.480007        1.490799
H           2.917642       -0.444033        2.250442
H           1.357420        0.232425        1.773247
H           1.695063       -1.478828        1.499355
N          -3.441487       -0.204151       -0.339241
H          -2.627198       -0.848651       -0.431757
H          -3.613638        0.195104       -1.257296
C          -4.639544       -0.892602        0.170592
H          -4.391385       -1.370235        1.114121
H          -5.432892       -0.166011        0.323559
H          -4.956296       -1.642426       -0.548167
H          -1.328641        2.333869       -0.138980
```

---

### Compound_28_HEI_5_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.638212 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.397002 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      37.8968 cm-1
2.      44.5854 cm-1
3.      53.5152 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.660323        1.671040       -0.051269
C          -2.029208        1.525548        0.104936
C          -2.740606        0.318707       -0.348952
O           0.067308        2.628746        0.241114
O          -0.079985        0.510571       -0.610273
C           1.312571        0.506041       -0.869196
C           2.078609       -0.471427        0.028685
C           1.873821       -0.107413        1.499383
H          -2.557069        0.038714       -1.388633
H          -3.815351        0.388815       -0.195160
H           1.444998        0.216997       -1.915679
H           1.700993        1.514425       -0.730883
H           2.427554       -0.793524        2.143034
H           2.219946        0.907316        1.700984
H           0.819856       -0.162058        1.777215
C           3.560966       -0.349197       -0.332085
H           3.926815        0.663485       -0.151701
H           4.158849       -1.035812        0.269592
H           3.731570       -0.589414       -1.383773
C           1.618292       -1.908536       -0.222901
H           0.570122       -2.052006        0.041895
H           1.738850       -2.180622       -1.273391
H           2.202790       -2.608036        0.377577
N          -2.284465       -0.920079        0.424973
H          -2.460603       -0.756928        1.412625
H          -1.268594       -0.919809        0.304872
C          -2.870399       -2.201028       -0.015695
H          -2.469459       -3.008861        0.589026
H          -3.949422       -2.150111        0.096947
```

```
H          -2.614667       -2.357367       -1.059615
H          -2.576849        2.308405        0.606102
```

---

### Compound_28_HEI_6_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.636815 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.396631 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      26.6962 cm-1
  2.      35.2829 cm-1
  3.      65.6519 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.820795        0.197205       -0.488673
C          -1.766861        1.029137        0.102313
C          -3.161857        0.990937       -0.324416
O          -1.000420       -0.666166       -1.365483
O           0.457649        0.408109       -0.004876
C           1.488495       -0.399936       -0.536779
C           2.813028       -0.064716        0.148324
C           3.179583        1.401329       -0.090636
H          -3.286604        0.580010       -1.325713
H          -3.664449        1.955402       -0.262972
H           1.253411       -1.457615       -0.385547
H           1.578888       -0.234017       -1.614685
H           4.146028        1.631382        0.362253
H           3.248629        1.615562       -1.159499
H           2.434127        2.068343        0.341993
C           3.885083       -0.965783       -0.469448
H           3.976038       -0.790910       -1.543551
H           4.856921       -0.768875       -0.013640
H           3.649511       -2.021015       -0.316016
C           2.717274       -0.341415        1.650005
H           1.957611        0.285368        2.116799
H           2.458489       -1.386040        1.836970
H           3.673042       -0.138611        2.137230
N          -4.058519        0.074240        0.559643
H          -3.957212        0.394351        1.519083
H          -5.035553        0.204133        0.307959
```

```
C          -3.705560       -1.358423        0.481260
H          -3.892962       -1.702981       -0.531011
H          -2.649460       -1.454742        0.711885
H          -4.308473       -1.917816        1.190239
H          -1.456513        1.752833        0.841888
```

---

### Compound_28_HEI_8_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.637501 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.396027 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      38.0189 cm-1
2.      45.8502 cm-1
3.      64.4398 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.680018       -0.926038       -0.340120
C           1.715432       -1.065089        0.575679
C           3.098075       -0.799258        0.186896
O           0.749306       -0.545493       -1.520662
O          -0.551079       -1.296855        0.190666
C          -1.722793       -0.925015       -0.508521
C          -2.421740        0.290717        0.113846
C          -2.820194       -0.015080        1.558599
H           3.262791       -0.888663       -0.886267
H           3.826585       -1.411603        0.716972
H          -1.477923       -0.720688       -1.550911
H          -2.396765       -1.785181       -0.470758
H          -3.333219        0.839433        2.004698
H          -3.493535       -0.874075        1.604140
H          -1.942451       -0.239166        2.165516
C          -3.674725        0.574749       -0.716594
H          -4.348953       -0.284618       -0.719191
H          -4.220315        1.427194       -0.307810
H          -3.416310        0.805780       -1.752196
C          -1.494834        1.507218        0.081912
H          -0.588404        1.322284        0.661041
H          -1.199227        1.747972       -0.940359
H          -1.995397        2.378879        0.508436
```

```
N           3.557388        0.650798        0.508423
H           3.381176        0.805776        1.497667
H           4.562176        0.730835        0.371511
C           2.859474        1.686490       -0.282111
H           3.117902        1.550616       -1.327704
H           1.791453        1.547539       -0.148267
H           3.168238        2.669608        0.060337
H           1.502369       -1.410896        1.576640
```

---

### Compound_7_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -247.326498 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -247.273254 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      86.6330 cm-1
2.     280.5262 cm-1
3.     315.9393 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.561413       -0.122571        0.026523
O           1.461095       -0.936461       -0.144043
C          -0.847581       -0.584019        0.183204
C          -1.925906        0.115723       -0.137876
H          -2.914465       -0.311386       -0.035966
H          -1.871440        1.123793       -0.530170
H          -0.932653       -1.606144        0.530461
N           0.786042        1.204447        0.066090
H           0.072776        1.858668        0.327251
H           1.727171        1.540829       -0.032961
```

---

### Compound_7_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -247.328577 |

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -247.275187 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 24)

```
1.      92.2107 cm-1
2.     286.3442 cm-1
3.     304.0799 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.481716        0.123838        0.000031
O          -0.526834        1.346845       -0.000055
C           0.800631       -0.640187       -0.000013
C           1.970598       -0.021149       -0.000160
H           2.900223       -0.573461       -0.000194
H           2.020810        1.060419       -0.000250
H           0.743802       -1.722285        0.000077
N          -1.591956       -0.639273        0.000182
H          -2.494373       -0.198350        0.000182
H          -1.549181       -1.641187        0.000203
```

---

### Compound_7_HEI_1_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -343.183903 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.063084 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      73.0250 cm-1
2.     113.6287 cm-1
3.     146.9944 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.557846       -0.033604       -0.001549
O           2.714442       -0.103867       -0.482830
C           0.656644       -1.077937        0.173733
C          -0.743048       -0.838241        0.564529
H          -1.315924       -1.759403        0.646152
H          -0.894499       -0.274305        1.489584
H           0.939533       -2.064383       -0.163742
C          -2.853227        0.408774       -0.142584
H          -3.448955       -0.488971       -0.005748
H          -3.266660        1.012413       -0.944755
H          -2.832712        0.982046        0.779680
N          -1.472270        0.015739       -0.484568
H          -0.874736        0.839936       -0.606520
H          -1.445685       -0.490220       -1.365416
N           1.080183        1.276784        0.332664
H           1.841879        1.937655        0.302288
H           0.617544        1.334553        1.229670
```

---

### Compound_7_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -343.191867 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.071722 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
  1.      94.8537 cm-1
  2.     135.6881 cm-1
  3.     155.8232 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.365799       -0.103766        0.056406
O          -0.825165       -1.237015        0.323574
C          -0.659226        1.079034        0.010944
C           0.788163        1.035744        0.338661
H           1.313434        1.952135        0.077000
H           1.008296        0.806841        1.387110
H          -1.113842        2.006866       -0.301403
C           2.801595       -0.452046       -0.008720
H           2.793189       -0.739451        1.039008
H           3.449529        0.409817       -0.146900
```

```
H           3.156200       -1.282309       -0.612484
N           1.430676       -0.104969       -0.414241
H           0.737140       -0.875656       -0.217004
H           1.384108        0.096984       -1.408202
N          -2.729272       -0.129223       -0.274058
H          -3.223957        0.730385       -0.098304
H          -3.201002       -0.923952        0.126943
```

---

### Compound_7_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -343.183512 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.06239 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      73.0201 cm-1
2.     111.4786 cm-1
3.     153.5766 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.393552       -0.168608        0.026143
O           2.361473       -0.824566       -0.429262
C           0.367588       -0.643399        0.836418
C          -0.824562        0.165355        1.134898
H          -1.536780       -0.362487        1.765340
H          -0.636012        1.139551        1.593685
H           0.351225       -1.698352        1.067977
C          -2.225160       -0.609121       -0.833470
H          -1.452157       -1.352303       -1.003854
H          -2.648624       -0.280002       -1.777413
H          -3.003378       -1.018564       -0.195641
N          -1.606048        0.540294       -0.145936
H          -0.907363        0.978720       -0.753466
H          -2.310210        1.242300        0.064294
N           1.289046        1.195824       -0.397643
H           1.056642        1.845603        0.340831
H           2.145380        1.483888       -0.846530
```

---

### Compound_7_HEI_4_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -343.186017 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -343.06577 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 45)

```
1.      70.7317 cm-1
2.      99.0636 cm-1
3.     111.8208 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.317890        0.054041        0.092152
O           1.178548        1.074407        0.814805
C           0.379350       -0.965982       -0.078798
C          -0.892992       -0.944565        0.633631
H          -1.272368       -1.934063        0.886695
H          -0.861891       -0.325185        1.529406
H           0.608865       -1.814947       -0.709645
C          -1.897353        1.115641       -0.468331
H          -1.943282        1.651497        0.474745
H          -2.688329        1.449829       -1.133009
H          -0.922198        1.258450       -0.922760
N          -2.062498       -0.326486       -0.192761
H          -2.944721       -0.488451        0.287211
H          -2.106904       -0.835573       -1.071536
N           2.519329       -0.044020       -0.640268
H           2.790689       -0.979070       -0.898863
H           3.272563        0.460991       -0.201405
```

---

### Compound_24_10

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775086 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.600898 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      32.3717 cm-1
2.      51.3325 cm-1
3.      66.7520 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.979185       -0.303209       -0.352802
C           2.281099        0.291989        0.076521
C           3.404610       -0.684069        0.248829
C           2.398672        1.597096        0.296572
O           0.822558       -1.493867       -0.493462
O           0.027207        0.603911       -0.561618
C          -1.292689        0.165675       -0.913787
C          -2.260596        0.382695        0.239063
C          -3.673674        0.051613       -0.232666
C          -1.878073       -0.438271        1.465789
H           4.312556       -0.171365        0.559693
H           3.152857       -1.436831        0.996694
H           3.603344       -1.216215       -0.682246
H           1.565355        2.272056        0.167594
H           3.342268        2.020158        0.616321
H          -1.580358        0.767133       -1.775108
H          -1.260712       -0.883430       -1.204853
H          -2.223516        1.443041        0.503834
H          -3.959817        0.655982       -1.094686
H          -3.750262       -1.000655       -0.516334
H          -4.395366        0.235680        0.563212
H          -1.903726       -1.506250        1.238389
H          -0.876786       -0.190965        1.820118
H          -2.575158       -0.249812        2.282893
```

---

### Compound_24_1

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775595 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.601433 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      36.8487 cm-1
2.      57.0040 cm-1
3.      58.5869 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.989141       -0.563842        0.125278
C          -2.320682        0.087576       -0.083729
C          -2.487416        1.527096        0.300268
C          -3.290829       -0.652948       -0.607656
O          -0.724080       -1.705810       -0.168963
O          -0.118813        0.274061        0.686031
C           1.218862       -0.195602        0.907077
C           2.093976       -0.036216       -0.327647
C           3.482619       -0.590745       -0.024132
C           2.161655        1.417245       -0.784102
H          -3.499258        1.862810        0.081449
H          -2.293114        1.674391        1.363001
H          -1.784527        2.160252       -0.242302
H          -3.119451       -1.687932       -0.869629
H          -4.275234       -0.240325       -0.784617
H           1.595164        0.419747        1.724094
H           1.183302       -1.235554        1.228172
H           1.649844       -0.635598       -1.126106
H           3.438836       -1.640397        0.269853
H           4.125560       -0.512033       -0.900891
H           3.954456       -0.030912        0.787003
H           2.773934        1.508349       -1.681880
H           1.171193        1.812542       -1.009386
H           2.608177        2.043268       -0.007454
```

---

## Compound_24_2

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775615 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.601647 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      30.0859 cm-1
2.      52.4384 cm-1
3.      61.8037 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.979399       -0.435006       -0.172931
C           2.293401        0.249472        0.017912
C           3.390446       -0.611507        0.565231
C           2.441219        1.538127       -0.270402
O           0.783916       -1.581658        0.158981
O           0.056029        0.335020       -0.743819
C          -1.260090       -0.210157       -0.912391
C          -2.111391       -0.059441        0.339929
C          -3.475718       -0.694971        0.089584
C          -2.244632        1.401879        0.755117
H           4.310475       -0.039765        0.667714
H           3.116897       -1.014044        1.541184
H           3.578075       -1.464242       -0.088406
H           1.624772        2.130066       -0.657576
H           3.392429        2.032269       -0.120024
H          -1.689704        0.359585       -1.736253
H          -1.179197       -1.255943       -1.205216
H          -1.616726       -0.609780        1.143975
H          -3.383606       -1.749723       -0.173412
H          -4.100534       -0.622156        0.979861
H          -3.996016       -0.186547       -0.725764
H          -2.838580        1.488716        1.665557
H          -1.271090        1.854749        0.942488
H          -2.742571        1.979546       -0.027724
```

---

## Compound_24_3

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775711 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.601999 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
1.      27.1420 cm-1
2.      56.8344 cm-1
3.      58.3733 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.150959       -0.651664       -0.000013
C          -2.192047        0.424010        0.000003
C          -1.744902        1.855130        0.000024
C          -3.465715        0.047980       -0.000003
O          -1.377435       -1.839430       -0.000030
O           0.075847       -0.142740       -0.000006
C           1.176832       -1.062192       -0.000019
C           2.469234       -0.266187        0.000001
C           2.612893        0.579423       -1.262530
C           2.612884        0.579375        1.262564
H          -2.605437        2.521370        0.000032
H          -1.133337        2.073969        0.876031
H          -1.133336        2.073995       -0.875977
H          -3.735227       -0.999237       -0.000018
H          -4.264113        0.778190        0.000008
H           1.103062       -1.695933        0.884802
H           1.103069       -1.695900       -0.884864
H           3.263208       -1.018500       -0.000011
H           1.839775        1.348245       -1.304634
H           3.582488        1.077858       -1.280690
H           2.530497       -0.033941       -2.161212
H           1.839764        1.348195        1.304692
H           2.530482       -0.034023        2.161223
H           3.582479        1.077810        1.280750
```

---

### Compound_24_4

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775949 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.602342 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      31.1110 cm-1
  2.      54.3762 cm-1
  3.      61.4006 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.186489       -0.633106        0.053632
C          -2.381743        0.261539       -0.054023
C          -2.167716        1.716043       -0.348031
```

```
C          -3.578179       -0.288176        0.119847
O          -1.223056       -1.814716        0.307117
O          -0.055590        0.031343       -0.164193
C           1.170431       -0.706688       -0.078793
C           2.326094        0.249612       -0.303398
C           2.369775        1.339687        0.762551
C           3.629106       -0.543969       -0.339513
H          -3.121195        2.239229       -0.387422
H          -1.544785        2.182123        0.416162
H          -1.655706        1.851662       -1.301172
H          -3.678689       -1.344081        0.330105
H          -4.480614        0.305200        0.055604
H           1.234693       -1.173823        0.906571
H           1.157375       -1.496346       -0.831191
H           2.179773        0.719217       -1.280008
H           2.515547        0.900320        1.752581
H           3.196411        2.025736        0.575114
H           1.446522        1.918103        0.780927
H           3.803864       -1.045188        0.615433
H           3.614292       -1.303400       -1.122510
H           4.474003        0.118579       -0.527219
```

---

## Compound_24_5

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.77566 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.602167 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      24.9478 cm-1
  2.      52.9197 cm-1
  3.      62.2700 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.102924       -0.547216       -0.000074
C          -2.149286        0.518955        0.000027
C          -3.564727        0.028647       -0.000031
C          -1.812883        1.804451        0.000158
O          -1.365214       -1.728480       -0.000182
O           0.137872       -0.076055       -0.000031
C           1.207944       -1.030644       -0.000113
```

```
C           2.525404       -0.276728        0.000004
C           2.696539        0.564023       -1.262327
C           2.696479        0.563734        1.262535
H          -4.259553        0.865944        0.000051
H          -3.761086       -0.590361       -0.876277
H          -3.761095       -0.590540        0.876086
H          -0.779524        2.120056        0.000197
H          -2.573334        2.574725        0.000233
H           1.114964       -1.662088        0.884647
H           1.115006       -1.661888       -0.885020
H           3.294588       -1.054389       -0.000067
H           1.949468        1.358243       -1.303817
H           3.682176        1.029932       -1.280861
H           2.593221       -0.045892       -2.161191
H           1.949403        1.357942        1.304173
H           2.593122       -0.046388        2.161254
H           3.682114        1.029642        1.281221
```

---

### Compound_24_6

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.775938 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.602439 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      30.6921 cm-1
  2.      53.7933 cm-1
  3.      58.2948 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.154123       -0.511308        0.038996
C           2.344353        0.382107       -0.089073
C           3.670392       -0.284016        0.115915
C           2.201229        1.675303       -0.358879
O           1.238245       -1.684040        0.324513
O          -0.002205        0.102290       -0.188403
C          -1.196792       -0.680100       -0.066133
C          -2.391021        0.222707       -0.310069
C          -3.662225       -0.621663       -0.308095
C          -2.468688        1.344293        0.720688
H           4.480359        0.434329        0.007448
```

```
H           3.729804       -0.733159        1.107935
H           3.816133       -1.088762       -0.605709
H           1.226948        2.121007       -0.497976
H           3.065671        2.320892       -0.445669
H          -1.160717       -1.493090       -0.792590
H          -1.235048       -1.116766        0.934565
H          -2.271420        0.665703       -1.302623
H          -3.809698       -1.097282        0.664382
H          -4.533881        0.000961       -0.509685
H          -3.623882       -1.405504       -1.065825
H          -2.588857        0.931854        1.725634
H          -1.568820        1.958669        0.711884
H          -3.323139        1.991207        0.519260
```

---

### Compound_24_7

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.77485 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.600493 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      31.9331 cm-1
  2.      54.2306 cm-1
  3.      68.7368 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.951602       -0.546598       -0.304455
C           2.126005        0.278480        0.123639
C           2.004971        1.772521        0.098151
C           3.220516       -0.365679        0.512340
O           0.917233       -1.754312       -0.291749
O          -0.056843        0.225216       -0.705687
C          -1.300353       -0.383059       -1.090535
C          -2.368588       -0.141378       -0.033549
C          -2.028563       -0.827628        1.286238
C          -2.639564        1.347239        0.165542
H           2.926203        2.233206        0.449607
H           1.797549        2.132037       -0.910084
H           1.182606        2.108550        0.730712
H           3.257616       -1.446253        0.514438
H           4.101066        0.173638        0.835562
```

```
H          -1.575321        0.092797       -2.030808
H          -1.142511       -1.446344       -1.256557
H          -3.273605       -0.604679       -0.437683
H          -1.858829       -1.895735        1.147677
H          -1.128480       -0.396114        1.729628
H          -2.840722       -0.700077        2.002450
H          -1.757748        1.850960        0.565228
H          -2.908725        1.830695       -0.774861
H          -3.458377        1.496696        0.869957
```

---

### Compound_24_8

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -463.774839 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -463.600606 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 66)

```
  1.      29.0922 cm-1
  2.      53.8756 cm-1
  3.      59.6772 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.926165       -0.422242       -0.327412
C          -2.077509        0.436843        0.085090
C          -3.334804       -0.299415        0.433383
C          -1.953633        1.758155        0.151479
O          -0.965021       -1.630009       -0.283597
O           0.127066        0.276385       -0.744009
C           1.340324       -0.415113       -1.080648
C           2.400573       -0.201667       -0.009677
C           2.755633        1.274323        0.146781
C           1.995086       -0.822092        1.324212
H          -4.120612        0.397765        0.716783
H          -3.682527       -0.895759       -0.411096
H          -3.163261       -0.989835        1.259907
H          -1.026955        2.253578       -0.099252
H          -2.785197        2.376046        0.465060
H           1.124215       -1.472480       -1.216265
H           1.661600        0.011840       -2.029721
H           3.284170       -0.730715       -0.379174
H           1.897071        1.842376        0.509108
```

```
H           3.566816        1.399496        0.864654
H           3.072967        1.708640       -0.802555
H           1.115903       -0.321593        1.735986
H           1.761712       -1.881714        1.216137
H           2.800706       -0.721407        2.052015
```

---

### Compound_24_HEI_10_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.636056 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.395342 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      32.4878 cm-1
  2.      46.0363 cm-1
  3.      66.6482 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.181897        0.264228        0.772500
C           0.960092        1.154186        0.081131
C           0.469102        2.427907       -0.542416
C           2.406009        0.802008       -0.028025
O           0.586388       -0.850286        1.245096
O          -1.136625        0.620738        0.965928
C          -2.094823       -0.413126        1.134400
C          -2.770608       -0.797882       -0.179776
C          -3.480578        0.394322       -0.814358
C          -1.791206       -1.440292       -1.159138
H           0.837141        2.542098       -1.567612
H          -0.619361        2.441635       -0.581936
H           0.782286        3.327767        0.001464
H           2.957207        0.848520        0.917223
H           2.930134        1.423440       -0.753003
H          -1.622337       -1.282817        1.590063
H          -2.840656       -0.018371        1.827129
H          -3.526469       -1.544203        0.087248
H          -4.200352        0.840042       -0.125189
H          -2.759290        1.164679       -1.092844
H          -4.016666        0.093487       -1.715745
H          -2.305805       -1.754037       -2.068783
H          -1.009796       -0.731653       -1.442627
```

```
H          -1.307068       -2.313640       -0.720652
N           2.541440       -0.633194       -0.463878
H           2.179216       -0.721995       -1.408272
H           1.848513       -1.097392        0.184741
C           3.891635       -1.208662       -0.360630
H           4.581799       -0.628382       -0.967701
H           4.203903       -1.178485        0.679523
H           3.870304       -2.238075       -0.706202
```

---

### Compound_24_HEI_11_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.635969 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.39664 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      28.4991 cm-1
  2.      31.6924 cm-1
  3.      76.4184 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.432191       -0.032102       -0.376172
C          -1.340263        0.989176       -0.262423
C          -0.992281        2.444546       -0.142483
C          -2.776619        0.591698       -0.333166
O          -0.724859       -1.273448       -0.437951
O           0.894992        0.324477       -0.411413
C           1.849036       -0.700521       -0.200407
C           3.234774       -0.076519       -0.168512
C           3.376109        0.924526        0.973523
C           4.286797       -1.177205       -0.069981
H           0.063394        2.571300        0.094347
H          -1.185208        3.014236       -1.060347
H          -1.567445        2.933056        0.651279
H          -3.100820        0.234599       -1.316961
H          -3.444367        1.398569       -0.033602
H           1.648754       -1.213513        0.746951
H           1.787512       -1.445461       -0.997136
H           3.377389        0.453616       -1.115034
H           2.636736        1.720937        0.895793
H           3.237005        0.425594        1.936466
```

```
H           4.368610        1.377681        0.972043
H           5.291573       -0.753411       -0.074340
H           4.168517       -1.742997        0.857611
H           4.212109       -1.877724       -0.903280
N          -3.023544       -0.577446        0.582454
H          -2.206225       -1.197035        0.330858
H          -2.889411       -0.272072        1.541424
C          -4.320786       -1.253253        0.421877
H          -4.392728       -2.066582        1.137962
H          -5.124475       -0.540566        0.588258
H          -4.384645       -1.648415       -0.588090
```

---

### Compound_24_HEI_12_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.633071 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.393152 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      25.6484 cm-1
  2.      50.9529 cm-1
  3.      56.9421 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.268263        1.191150       -0.287958
C          -1.481343        1.048026        0.355204
C          -2.339127        2.238770        0.682648
C          -1.969532       -0.304949        0.699057
O           0.349123        2.219165       -0.619708
O           0.283072       -0.064841       -0.645315
C           1.668910       -0.110184       -0.925823
C           2.526562       -0.143017        0.334726
C           2.180630       -1.337297        1.216542
C           4.001647       -0.146581       -0.052759
H          -1.899102        3.143869        0.264294
H          -3.352233        2.151117        0.273180
H          -2.453604        2.404854        1.760740
H          -1.258949       -0.923482        1.250697
H          -2.903698       -0.273282        1.258066
H           1.823619       -1.026320       -1.501453
H           1.948668        0.741882       -1.546464
```

```
H           2.317190        0.774600        0.891916
H           1.126879       -1.329904        1.495444
H           2.383898       -2.274395        0.690960
H           2.774039       -1.331139        2.132073
H           4.637326       -0.142322        0.833461
H           4.246501       -1.040052       -0.633195
H           4.257496        0.726265       -0.655803
N          -2.258308       -1.137268       -0.549518
H          -1.375423       -1.112848       -1.067048
H          -2.943572       -0.640773       -1.112124
C          -2.688113       -2.526761       -0.298807
H          -1.910333       -3.031787        0.266635
H          -3.610520       -2.511323        0.274399
H          -2.845820       -3.033608       -1.245943
```

---

### Compound_24_HEI_13_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630708 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.391271 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      31.3367 cm-1
  2.      35.4112 cm-1
  3.      65.3509 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.442556       -0.194258       -0.465422
C          -1.444256        0.754601       -0.287596
C          -1.233390        2.058843        0.437811
C          -2.781007        0.438876       -0.783803
O          -0.523116       -1.302802       -1.034180
O           0.778066        0.190137        0.065589
C           1.877253       -0.670804       -0.153906
C           3.118067       -0.048700        0.466964
C           4.287073       -1.023067        0.357394
C           3.457383        1.292099       -0.176101
H          -0.209441        2.417377        0.331323
H          -1.892946        2.834862        0.035239
H          -1.434421        2.012945        1.517120
H          -2.777326       -0.356894       -1.525483
```

```
H          -3.320898        1.305679       -1.170285
H           1.683877       -1.651582        0.288848
H           2.034215       -0.822763       -1.227298
H           2.906415        0.118497        1.527455
H           4.063838       -1.972241        0.847333
H           4.519701       -1.231274       -0.690063
H           5.182894       -0.607067        0.819805
H           4.337057        1.736548        0.292099
H           3.674789        1.159840       -1.239531
H           2.629953        1.995062       -0.085584
N          -3.746892       -0.092361        0.324892
H          -4.691901       -0.150567       -0.045929
H          -3.770005        0.603263        1.065595
C          -3.342718       -1.396831        0.887022
H          -3.411002       -2.144424        0.102795
H          -2.313816       -1.310558        1.222491
H          -3.997435       -1.653419        1.714360
```

---

### Compound_24_HEI_14_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630155 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.390559 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      27.1606 cm-1
  2.      40.4115 cm-1
  3.      69.0219 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.391259       -0.275304       -0.603457
C           1.297464        0.753906       -0.366262
C           0.931132        2.035472        0.337291
C           2.688807        0.542766       -0.753944
O           0.604222       -1.380615       -1.143672
O          -0.892399        0.016944       -0.176488
C          -1.896644       -0.945725       -0.429757
C          -3.223835       -0.422989        0.101846
C          -3.190526       -0.222269        1.614597
C          -3.661301        0.849712       -0.618492
H           1.553826        2.863056       -0.018696
```

```
H          -0.107977        2.311250        0.156941
H           1.057386        2.001816        1.428460
H           2.806574       -0.258011       -1.480536
H           3.187971        1.445965       -1.111048
H          -1.972644       -1.138463       -1.503619
H          -1.642834       -1.891800        0.056538
H          -3.954579       -1.207064       -0.120186
H          -2.894618       -1.139044        2.127956
H          -2.479691        0.560038        1.884618
H          -4.172615        0.071905        1.987917
H          -4.649098        1.166485       -0.280360
H          -2.961017        1.663320       -0.423314
H          -3.707063        0.695790       -1.698210
N           3.607492        0.101863        0.434293
H           3.547161        0.822207        1.148943
H           4.575941        0.082794        0.124968
C           3.236747       -1.203101        1.017576
H           2.185541       -1.160501        1.285556
H           3.391894       -1.971466        0.266651
H           3.850204       -1.396760        1.892276
```

---

### Compound_24_HEI_15_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630989 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.390573 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      31.8999 cm-1
  2.      42.9333 cm-1
  3.      59.3892 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.341650       -0.495642       -0.771888
C           1.522990       -0.895055       -0.158962
C           1.583673       -1.922500        0.942599
C           2.755488       -0.213827       -0.547926
O           0.187784        0.376165       -1.651847
O          -0.771542       -1.202564       -0.328855
C          -2.041988       -0.691777       -0.681731
C          -2.484840        0.466794        0.207293
```

```
C          -3.839988        0.983283       -0.264514
C          -2.525903        0.062799        1.676786
H           0.827109       -2.697147        0.818306
H           2.558345       -2.421102        0.949286
H           1.440934       -1.508915        1.950492
H           2.674217        0.284843       -1.510952
H           3.637543       -0.856700       -0.535539
H          -2.047242       -0.379865       -1.726740
H          -2.735985       -1.528516       -0.564999
H          -1.747552        1.264692        0.084825
H          -3.802615        1.307434       -1.305998
H          -4.601289        0.202883       -0.182388
H          -4.166898        1.829972        0.340500
H          -2.807691        0.908949        2.305642
H          -3.259966       -0.731977        1.836206
H          -1.555719       -0.302776        2.013204
N           3.161692        0.935495        0.430879
H           4.075824        1.295375        0.168546
H           3.266881        0.526652        1.355532
C           2.180222        2.038240        0.488995
H           2.139553        2.513348       -0.486062
H           1.211675        1.609149        0.727114
H           2.483269        2.752540        1.248573
```

---

### Compound_24_HEI_16_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630281 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.389833 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      30.3656 cm-1
2.      46.2244 cm-1
3.      68.3277 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.496852       -1.197751       -0.111672
C          -1.764872       -0.644900       -0.248600
C          -2.949127       -1.317328        0.393269
C          -1.991019        0.611767       -0.958703
O          -0.196518       -2.258733        0.465721
```

```
O           0.512345       -0.448732       -0.720818
C           1.825970       -0.974400       -0.754318
C           2.810592       -0.066041       -0.024980
C           2.882461        1.318816       -0.661305
C           2.492755        0.021378        1.464158
H          -3.222689       -0.905828        1.375276
H          -3.841852       -1.231724       -0.236022
H          -2.755523       -2.379073        0.547239
H          -1.158039        0.910572       -1.588259
H          -2.914455        0.620001       -1.542413
H           1.829390       -1.968148       -0.309003
H           2.117506       -1.060620       -1.805808
H           3.789834       -0.542632       -0.138838
H           3.138478        1.254120       -1.720482
H           1.922155        1.829959       -0.579627
H           3.634234        1.937055       -0.168310
H           3.217790        0.651747        1.981245
H           1.502541        0.453144        1.619192
H           2.504832       -0.964808        1.930115
N          -2.196524        1.833123       -0.003065
H          -2.990278        1.621782        0.595833
H          -2.458217        2.648725       -0.550774
C          -1.018765        2.139248        0.832083
H          -0.743338        1.231583        1.360574
H          -0.205214        2.444499        0.181640
H          -1.264951        2.932771        1.531056
```

---

### Compound_24_HEI_18_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630432 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.390177 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      29.8943 cm-1
2.      52.5960 cm-1
3.      58.2814 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.256452       -0.477903        0.856226
C          -1.261990       -1.003398        0.054172
```

```
C          -0.992143       -1.912272       -1.118599
C          -2.636378       -0.589035        0.325639
O          -0.370202        0.324999        1.803840
O           1.005548       -0.965762        0.529650
C           2.139710       -0.290637        1.041148
C           2.809903        0.570467       -0.027356
C           3.342174       -0.275534       -1.180387
C           1.872449        1.662108       -0.535530
H          -0.197596       -2.629709       -0.909136
H          -1.888217       -2.488457       -1.368910
H          -0.696739       -1.383838       -2.035039
H          -2.765456       -0.194981        1.331270
H          -3.377032       -1.367476        0.133980
H           1.846097        0.320827        1.893705
H           2.837047       -1.058631        1.385121
H           3.660933        1.049745        0.467851
H           4.040452       -1.035263       -0.824133
H           2.522569       -0.783718       -1.691716
H           3.862005        0.344708       -1.912398
H           2.382216        2.310717       -1.249517
H           1.012790        1.218050       -1.042583
H           1.497375        2.278219        0.282408
N          -3.127752        0.576938       -0.593046
H          -4.120612        0.734622       -0.439559
H          -3.030280        0.267267       -1.556424
C          -2.379967        1.836727       -0.403033
H          -2.565002        2.197914        0.603620
H          -1.323523        1.617626       -0.522624
H          -2.709353        2.566783       -1.136195
```

---

### Compound_24_HEI_19_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.630098 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.389612 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      37.1947 cm-1
2.      43.3156 cm-1
3.      65.6130 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.244830       -0.391652       -0.015621
C           1.107584        0.661959        0.261978
C           0.880261        2.069292       -0.226280
C           2.318656        0.370251        1.025265
O           0.347193       -1.582739        0.341097
O          -0.838784       -0.010637       -0.800180
C          -1.956513       -0.876196       -0.877901
C          -3.116927       -0.377116       -0.020051
C          -2.758132       -0.376623        1.463122
C          -3.595513        0.999650       -0.471558
H          -0.182562        2.305869       -0.287333
H           1.336617        2.791942        0.458172
H           1.301180        2.276617       -1.219643
H           2.255792       -0.570744        1.567162
H           2.612160        1.172354        1.705181
H          -2.260892       -0.901190       -1.927296
H          -1.662619       -1.880769       -0.575380
H          -3.931762       -1.091829       -0.176868
H          -2.455748       -1.369413        1.798239
H          -1.929703        0.308472        1.656559
H          -3.607493       -0.054735        2.067792
H          -4.457888        1.324396        0.112818
H          -2.803409        1.739781       -0.343824
H          -3.883516        0.992796       -1.524592
N           3.591518        0.201717        0.133753
H           4.413824        0.122504        0.726865
H           3.703761        1.058160       -0.402091
C           3.519438       -0.950195       -0.788258
H           3.497326       -1.861661       -0.198981
H           2.600722       -0.860474       -1.359804
H           4.384203       -0.943304       -1.444757
```

---

### Compound_24_HEI_1_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.632685 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.392618 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      37.1596 cm-1
2.      45.5928 cm-1
3.      50.0455 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.929832       -1.277280       -0.100790
C          -1.967967       -0.426925        0.231341
C          -3.402820       -0.864573        0.136453
C          -1.661238        0.957217        0.649284
O          -0.945847       -2.475474       -0.436726
O           0.314283       -0.612096       -0.067670
C           1.483091       -1.400305       -0.185310
C           2.703247       -0.517563        0.036366
C           2.838657        0.561072       -1.035042
C           2.719276        0.089164        1.436711
H          -3.918904       -0.859801        1.104137
H          -3.995740       -0.231115       -0.534156
H          -3.457565       -1.882102       -0.249903
H          -0.921737        1.042965        1.448081
H          -2.554007        1.506352        0.944766
H           1.462949       -2.203594        0.555533
H           1.527602       -1.863226       -1.174734
H           3.562763       -1.188708       -0.054348
H           2.790514        0.134958       -2.038325
H           2.047260        1.307619       -0.946009
H           3.789145        1.086684       -0.934876
H           3.640190        0.649029        1.605477
H           1.880318        0.774348        1.569652
H           2.647444       -0.684091        2.203464
N          -1.033789        1.761740       -0.491058
H          -1.690052        1.782519       -1.266388
H          -0.242976        1.181688       -0.785386
C          -0.588199        3.123978       -0.139304
H          -1.445720        3.698679        0.198252
H           0.144803        3.052245        0.659259
H          -0.142553        3.595216       -1.010174
```

---

### Compound_24_HEI_2_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.632507 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.392602 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      31.9253 cm-1
  2.      55.7686 cm-1
```

```
   3.      61.7422 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.757847       -1.322679        0.066342
C           1.990783       -0.741962       -0.163610
C           3.268096       -1.480343        0.126158
C           2.061010        0.642972       -0.675270
O           0.470709       -2.473154        0.443763
O          -0.298840       -0.407844       -0.141044
C          -1.614499       -0.927451       -0.147816
C          -2.603361        0.219305       -0.286329
C          -4.004797       -0.343009       -0.507583
C          -2.576870        1.142351        0.927868
H           3.849670       -1.711866       -0.774767
H           3.935480       -0.917985        0.789497
H           3.049301       -2.428475        0.617199
H           1.465171        0.836194       -1.569632
H           3.085488        0.956835       -0.870031
H          -1.729545       -1.625978       -0.982087
H          -1.808987       -1.481661        0.774582
H          -2.319067        0.796643       -1.171143
H          -4.316197       -0.951113        0.345434
H          -4.730895        0.462139       -0.624162
H          -4.047265       -0.968542       -1.400393
H          -3.280540        1.966546        0.803916
H          -2.857214        0.593274        1.830284
H          -1.590045        1.573649        1.094550
N           1.503210        1.645430        0.335489
H           2.032074        1.555878        1.198570
H           0.561866        1.292860        0.528028
C           1.462568        3.049415       -0.117929
H           1.037453        3.670419        0.664647
H           2.474004        3.373960       -0.344644
H           0.847168        3.105601       -1.011005
```

---

### Compound_24_HEI_3_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.635969 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.39664 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      28.4999 cm-1
  2.      31.6928 cm-1
  3.      76.4185 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.432191       -0.032101       -0.376172
C          -1.340262        0.989177       -0.262423
C          -0.992280        2.444546       -0.142482
C          -2.776619        0.591699       -0.333165
O          -0.724860       -1.273448       -0.437951
O           0.894992        0.324477       -0.411414
C           1.849035       -0.700522       -0.200406
C           3.234774       -0.076521       -0.168513
C           3.376110        0.924529        0.973519
C           4.286796       -1.177207       -0.069978
H           0.063396        2.571300        0.094345
H          -1.185210        3.014237       -1.060344
H          -1.567442        2.933055        0.651283
H          -3.100821        0.234602       -1.316960
H          -3.444366        1.398569       -0.033598
H           1.648754       -1.213511        0.746953
H           1.787511       -1.445463       -0.997133
H           3.377389        0.453611       -1.115037
H           2.636737        1.720940        0.895785
H           3.237004        0.425600        1.936463
H           4.368611        1.377683        0.972038
H           5.291572       -0.753414       -0.074339
H           4.168516       -1.742995        0.857616
H           4.212107       -1.877729       -0.903274
N          -3.023543       -0.577447        0.582454
H          -2.889410       -0.272074        1.541424
H          -2.206224       -1.197036        0.330856
C          -4.320786       -1.253253        0.421876
H          -4.384645       -1.648414       -0.588091
H          -4.392727       -2.066583        1.137960
H          -5.124474       -0.540566        0.588258
```

---

### Compound_24_HEI_4_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.633071 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.393152 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      25.6484 cm-1
2.      50.9524 cm-1
3.      56.9421 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.268263        1.191150       -0.287957
C          -1.481343        1.048026        0.355204
C          -2.339127        2.238770        0.682647
C          -1.969532       -0.304949        0.699057
O           0.349123        2.219165       -0.619708
O           0.283072       -0.064841       -0.645314
C           1.668910       -0.110184       -0.925823
C           2.526563       -0.143017        0.334726
C           2.180631       -1.337297        1.216542
C           4.001647       -0.146580       -0.052760
H          -3.352234        2.151117        0.273180
H          -2.453603        2.404854        1.760740
H          -1.899102        3.143869        0.264293
H          -1.258949       -0.923482        1.250697
H          -2.903698       -0.273282        1.258066
H           1.823619       -1.026320       -1.501453
H           1.948668        0.741883       -1.546463
H           2.317190        0.774600        0.891916
H           1.126879       -1.329905        1.495444
H           2.383899       -2.274395        0.690959
H           2.774040       -1.331140        2.132073
H           4.637327       -0.142322        0.833460
H           4.246501       -1.040051       -0.633196
H           4.257496        0.726265       -0.655803
N          -2.258309       -1.137268       -0.549518
H          -1.375423       -1.112848       -1.067048
H          -2.943572       -0.640774       -1.112124
C          -2.688113       -2.526761       -0.298807
H          -2.845821       -3.033608       -1.245943
H          -3.610520       -2.511323        0.274400
H          -1.910334       -3.031787        0.266635
```

---

### Compound_24_HEI_5_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.635858 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.396386 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      28.3158 cm-1
  2.      38.7714 cm-1
  3.      77.9370 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.426118        0.032668        0.169947
C           1.358101        1.020308       -0.024747
C           1.054428        2.422723       -0.466123
C           2.768079        0.651396        0.293176
O           0.690250       -1.169098        0.509143
O          -0.889325        0.375984       -0.037708
C          -1.835163       -0.676561       -0.091675
C          -3.216208       -0.082940       -0.317269
C          -4.227211       -1.209207       -0.511478
C          -3.628864        0.834099        0.829465
H           1.142920        3.160923        0.341027
H           1.732170        2.751400       -1.261235
H           0.038981        2.495960       -0.853125
H           2.965008        0.482435        1.357653
H           3.480395        1.393462       -0.065600
H          -1.582943       -1.364261       -0.904342
H          -1.822244       -1.249544        0.840128
H          -3.175628        0.507362       -1.237610
H          -3.956856       -1.849021       -1.353054
H          -4.284874       -1.834960        0.382739
H          -5.223075       -0.806736       -0.699755
H          -4.613378        1.266697        0.645184
H          -3.679473        0.272758        1.766359
H          -2.917802        1.648722        0.961892
N           3.104774       -0.665205       -0.356112
H           2.258396       -1.234895       -0.088774
H           3.082594       -0.543990       -1.363951
C           4.367378       -1.288294        0.071639
H           4.314323       -1.485705        1.138607
H           4.507125       -2.221206       -0.466691
H           5.193603       -0.613209       -0.135765
```

---

### Compound_24_HEI_6_reopt

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.632051 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.391386 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
  1.      39.8164 cm-1
  2.      55.5942 cm-1
  3.      66.5077 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -0.588604       -1.288199       -0.259785
C          -1.834284       -0.720068       -0.076956
C          -2.976016       -1.514443        0.493998
C          -2.058257        0.693953       -0.446897
O          -0.210102       -2.455973       -0.066313
O           0.359166       -0.330490       -0.710768
C           1.679978       -0.761455       -0.990582
C           2.697522       -0.149399       -0.032654
C           2.775606        1.369511       -0.159848
C           2.437862       -0.573962        1.409246
H          -3.778244       -1.704612       -0.229925
H          -2.620979       -2.485328        0.839034
H          -3.443564       -1.015733        1.350741
H          -1.756791        0.960180       -1.462156
H          -3.095689        0.994268       -0.307163
H           1.715966       -1.847944       -0.928483
H           1.909853       -0.457908       -2.015640
H           3.665363       -0.557811       -0.341009
H           2.935673        1.674552       -1.195206
H           1.860161        1.849045        0.192259
H           3.594705        1.766362        0.441438
H           3.191011       -0.156215        2.078837
H           1.459650       -0.222968        1.745748
H           2.453084       -1.659562        1.509982
N          -1.226661        1.635666        0.421011
H          -0.274442        1.274426        0.311450
H          -1.487194        1.489996        1.392214
C          -1.298188        3.064836        0.059949
H          -0.955558        3.179242       -0.964324
H          -2.328313        3.398241        0.144112
H          -0.664299        3.639168        0.728841
```

### Compound_24_HEI_8_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.632874 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.391991 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      38.9543 cm-1
2.      54.8980 cm-1
3.      69.8762 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.493006       -1.261469       -0.276831
C           1.804641       -0.881882       -0.070556
C           2.803315       -1.831445        0.530640
C           2.251668        0.472092       -0.467840
O          -0.068254       -2.347498       -0.052555
O          -0.278330       -0.194196       -0.809216
C          -1.679501       -0.355210       -0.928924
C          -2.427641        0.498214        0.089135
C          -3.924991        0.447558       -0.197113
C          -2.123967        0.064543        1.519305
H           3.561313       -2.177433       -0.183518
H           3.348741       -1.383715        1.368897
H           2.295420       -2.717551        0.910991
H           2.039898        0.747778       -1.503371
H           3.315511        0.618399       -0.286915
H          -1.952895       -0.047627       -1.941254
H          -1.935792       -1.407896       -0.803012
H          -2.089536        1.532190       -0.039324
H          -4.150267        0.792226       -1.207707
H          -4.301320       -0.573637       -0.097715
H          -4.476413        1.074884        0.504107
H          -2.602642        0.732146        2.237152
H          -2.494719       -0.947181        1.698171
H          -1.051941        0.064147        1.721549
N           1.536024        1.553731        0.335179
H           1.709261        1.382428        1.321861
H           0.544656        1.356638        0.168605
C           1.870955        2.944796       -0.026461
H           1.631794        3.097561       -1.074746
H           1.291835        3.626638        0.588790
H           2.932683        3.104251        0.137220
```

---

### Compound_24_HEI_9_

| Datum | Value |
|---|---|
| WB97XD/def2tzvpp-IEFPCM Energy | -559.632912 |
| WB97XD/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -559.392241 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 87)

```
1.      41.4119 cm-1
2.      48.3834 cm-1
3.      68.6323 cm-1
```

### WB97XD/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           0.277053       -1.267678       -0.425896
C           1.419693       -0.987225        0.295469
C           2.399220       -2.068099        0.659810
C           1.683317        0.400675        0.734493
O          -0.176714       -2.356396       -0.819395
O          -0.409364       -0.080387       -0.790430
C          -1.787777       -0.163195       -1.105761
C          -2.661328        0.306949        0.054163
C          -2.488770       -0.585548        1.279900
C          -2.399721        1.770552        0.396785
H           2.404166       -2.308238        1.730417
H           2.157443       -2.988494        0.128116
H           3.428990       -1.801568        0.396830
H           0.858490        0.876104        1.270374
H           2.579007        0.471400        1.349989
H          -1.951535        0.476457       -1.976014
H          -2.029746       -1.189979       -1.379548
H          -3.694777        0.217147       -0.296336
H          -2.713841       -1.627152        1.046925
H          -1.460275       -0.539017        1.645102
H          -3.147167       -0.265967        2.088991
H          -3.071690        2.112960        1.185107
H          -1.375629        1.904667        0.750500
H          -2.542598        2.413714       -0.473537
N           1.914198        1.334039       -0.451275
H           1.066650        1.219294       -1.015238
H           2.684931        0.963746       -1.000583
C           2.143058        2.751779       -0.111311
H           1.282432        3.120058        0.439506
```

```
H           3.034400        2.825749        0.504880
H           2.271517        3.325857       -1.023866
```

---

### embelin_shortened_1_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -610.857107 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -610.740679 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
  1.      44.6140 cm-1
  2.      91.8153 cm-1
  3.     102.4651 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -2.076914        0.231563        0.177551
C          -1.524579       -0.990989        0.058013
C          -0.040743       -1.197875       -0.177934
C           0.834756       -0.054311       -0.289537
C           0.262192        1.164051       -0.157460
C          -1.216256        1.376625        0.075697
O           0.955360        2.295422       -0.223813
O          -2.213645       -2.118216        0.133736
C           2.305447       -0.261720       -0.502240
C           3.061940       -0.478720        0.814674
O           0.328704       -2.365706       -0.263209
O          -1.590716        2.543395        0.164467
H          -3.133265        0.378837        0.345725
H           0.304979        3.017155       -0.107818
H          -1.564947       -2.841824        0.014482
H           2.714723        0.603354       -1.022612
H           2.445308       -1.128333       -1.148355
H           4.123621       -0.636461        0.623891
H           2.958197        0.387413        1.468627
H           2.678716       -1.351061        1.344025
```

---

### embelin_shortened_2_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -610.857108 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -610.740678 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      44.6961 cm-1
2.      91.8014 cm-1
3.     102.4839 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.077087        0.229694        0.177586
C           1.523601       -0.992324        0.057984
C           0.039590       -1.197763       -0.177964
C          -0.834824       -0.053347       -0.289403
C          -0.261121        1.164465       -0.157400
C           1.217523        1.375592        0.075782
O          -0.953198        2.296516       -0.223866
O           2.211617       -2.120222        0.133609
C          -2.305670       -0.259557       -0.502150
C          -3.062203       -0.476854        0.814678
O          -0.331018       -2.365211       -0.263409
O           1.593135        2.541987        0.164587
H           3.133575        0.375972        0.345765
H          -0.302144        3.017621       -0.107830
H           1.562241       -2.843211        0.014334
H          -2.446153       -1.125689       -1.148787
H          -2.714361        0.606094       -1.022026
H          -4.123908       -0.634375        0.623844
H          -2.679124       -1.349448        1.343732
H          -2.958320        0.389033        1.468915
```

---

### embelin_shortened_3_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -610.849718 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -610.733663 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      51.6526 cm-1
2.      75.6654 cm-1
3.      96.5221 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.035133        0.316062        0.168066
C           1.559786       -0.939232        0.048930
C           0.086626       -1.223454       -0.183143
C          -0.834423       -0.097159       -0.288812
C          -0.331586        1.147818       -0.157862
C           1.125873        1.426986        0.071173
O          -1.086463        2.245863       -0.221118
O           2.292389       -2.048042        0.117066
C          -2.294442       -0.372540       -0.496084
C          -3.034112       -0.626163        0.824116
O          -0.279155       -2.384045       -0.274796
O           1.460718        2.605489        0.163759
H           3.082547        0.526988        0.334717
H          -0.476179        3.000078       -0.107150
H           3.223973       -1.834984        0.261261
H          -2.397339       -1.244150       -1.141884
H          -2.746003        0.474181       -1.011713
H          -4.088647       -0.831484        0.638439
H          -2.608796       -1.481253        1.349296
H          -2.966589        0.242592        1.479434
```

---

### embelin_shortened_4_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -610.849006 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -610.732864 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
1.      59.6980 cm-1
2.      82.5784 cm-1
3.      91.0941 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.069749        0.258358        0.173705
C           1.539924       -0.969477        0.051339
C           0.066839       -1.183429       -0.181238
C          -0.816012       -0.039627       -0.283981
C          -0.268195        1.192807       -0.153064
C           1.211165        1.419785        0.079265
O          -0.948932        2.339122       -0.211851
O           2.246454       -2.091938        0.122635
C          -2.283248       -0.291819       -0.487521
C          -3.026325       -0.551104        0.829486
O          -0.307361       -2.349000       -0.273267
O           1.631222        2.562331        0.180261
H           3.124340        0.419135        0.342081
H          -1.886336        2.174125       -0.375179
H           1.609497       -2.823529        0.002039
H          -2.394133       -1.155535       -1.142272
H          -2.747003        0.543969       -1.016907
H          -4.082747       -0.740202        0.640150
H          -2.610219       -1.419405        1.339204
H          -2.947829        0.304359        1.500716
```

---

### embelin_shortened_4_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -610.849006 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -610.732859 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 54)

```
  1.      59.9508 cm-1
  2.      82.8788 cm-1
  3.      91.2568 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           2.070017        0.256147        0.173777
C           1.538786       -0.971068        0.051281
C           0.065443       -1.183318       -0.181291
C          -0.816126       -0.038500       -0.283883
```

```
C          -0.266861        1.193294       -0.152958
C           1.212772        1.418554        0.079393
O          -0.946194        2.340422       -0.211815
O           2.244076       -2.094361        0.122425
C          -2.283642       -0.289089       -0.487398
C          -3.026772       -0.549130        0.829439
O          -0.310096       -2.348442       -0.273464
O           1.634134        2.560617        0.180400
H           3.124788        0.415701        0.342172
H          -1.883743        2.176577       -0.375411
H           1.606292       -2.825217        0.001746
H          -2.395433       -1.152024       -1.143027
H          -2.746740        0.547687       -1.015785
H          -4.083377       -0.737094        0.640010
H          -2.611381       -1.418364        1.338141
H          -2.947461        0.305509        1.501621
```

---

### embelin_shortened_HEI_10_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.736035 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.555044 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      31.2180 cm-1
  2.      60.3678 cm-1
  3.      87.5235 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.413343        0.172411       -0.316375
C           0.747928       -1.122366       -0.133574
C          -0.614661       -1.277558       -0.219572
C          -1.450879       -0.062259       -0.289295
C          -0.905872        1.190294       -0.325976
C           0.501087        1.396748       -0.231775
O          -1.688558        2.314856       -0.312264
O           1.529664       -2.259257       -0.235275
C          -2.933610       -0.243658       -0.270592
C          -3.458355       -0.384298        1.167948
O          -1.137866       -2.453840       -0.281097
O           1.006668        2.512568       -0.045955
```

```
H           1.884879        0.225865       -1.305643
H          -1.084860        3.069330       -0.247568
H           0.857329       -2.962706       -0.323488
H          -3.169161       -1.152538       -0.822751
H          -3.419543        0.600803       -0.756275
H          -4.537510       -0.539135        1.164270
H          -2.990955       -1.235190        1.661940
H          -3.243844        0.512413        1.749564
C           3.849784       -0.193448        0.324307
N           2.544448        0.443975        0.661641
H           3.705702       -1.266066        0.275622
H           4.566951        0.067333        1.095717
H           4.174614        0.191275       -0.637102
H           2.634563        1.468088        0.692771
H           2.238853        0.142893        1.587602
```

---

### embelin_shortened_HEI_13_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.770017 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.594633 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      38.6967 cm-1
  2.      49.9248 cm-1
  3.      57.2466 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.504191        0.655735       -1.152155
C          -0.701645        1.594288       -0.617726
C           0.631145        1.250736        0.015277
C           1.030896       -0.145688        0.075731
C           0.201644       -1.069232       -0.454781
C          -1.093866       -0.725953       -1.127545
O           0.480511       -2.373181       -0.464968
O          -0.966624        2.903438       -0.585081
C           2.343653       -0.498182        0.712510
C           3.518484       -0.409346       -0.269552
O           1.322377        2.157699        0.459540
O          -1.704928       -1.639717       -1.675982
H          -2.449991        0.897864       -1.617560
```

```
H          -0.269043       -2.799147       -0.924935
H          -1.822555        3.085767       -0.993789
H           2.282024       -1.507557        1.118336
H           2.518942        0.180248        1.547380
H           4.456135       -0.660269        0.227591
H           3.380032       -1.099178       -1.102626
H           3.608610        0.598145       -0.675756
C          -1.472067       -0.099670        2.489281
N          -1.965573       -1.121104        1.571119
H          -0.391535       -0.198386        2.590002
H          -1.911591       -0.139313        3.492049
H          -1.676764        0.887411        2.073684
H          -2.967868       -1.049485        1.450913
H          -1.772414       -2.050411        1.922573
```

---

### embelin_shortened_HEI_1_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.737125 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.555916 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      53.0982 cm-1
  2.      67.9285 cm-1
  3.      76.8080 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.509024       -0.053578       -0.620393
C          -0.784901        1.200648       -0.409671
C           0.580132        1.285003       -0.335250
C           1.342282        0.016978       -0.320293
C           0.731263       -1.203150       -0.408628
C          -0.687390       -1.331062       -0.461502
O           1.444192       -2.370872       -0.322622
O          -1.524520        2.362457       -0.519251
C           2.823470        0.107757       -0.148598
C           3.207883        0.188788        1.338418
O           1.177385        2.427750       -0.305781
O          -1.273417       -2.416829       -0.354321
H          -1.928524       -0.095658       -1.633027
H           0.794334       -3.088938       -0.330244
```

```
H          -0.839104        3.055447       -0.493560
H           3.166661        1.010469       -0.652051
H           3.305344       -0.756551       -0.602745
H           4.289654        0.271668        1.445830
H           2.749237        1.060270        1.803972
H           2.878642       -0.701549        1.874323
C          -2.434040        0.011988        1.737487
N          -2.716884       -0.218696        0.290801
H          -3.345726       -0.176739        2.294622
H          -1.653187       -0.673393        2.049207
H          -2.108789        1.037697        1.863042
H          -3.041452       -1.180764        0.151565
H          -3.456070        0.408634       -0.020173
```

---

### embelin_shortened_HEI_2_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.736934 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.555957 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      48.8686 cm-1
  2.      64.9313 cm-1
  3.      81.8544 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.399412       -0.042627       -0.720788
C          -0.750516        1.205483       -0.316705
C           0.556506        1.283627        0.086410
C           1.293887        0.013819        0.262747
C           0.728197       -1.202369       -0.005492
C          -0.638020       -1.325176       -0.391167
O           1.410724       -2.372730        0.202152
O          -1.439582        2.372183       -0.586079
C           2.711625        0.095117        0.727721
C           3.685406        0.177248       -0.460151
O           1.128960        2.423641        0.276329
O          -1.232481       -2.410604       -0.444051
H          -1.555823       -0.065473       -1.806389
H           0.777693       -3.089702        0.049667
H          -0.779164        3.061185       -0.386009
```

```
H           2.951894       -0.780211        1.330510
H           2.820339        0.988411        1.339580
H           4.712957        0.248301       -0.102551
H           3.603710       -0.707195       -1.091936
H           3.473102        1.055339       -1.069041
C          -2.884990        0.022586        1.330978
N          -2.792628       -0.226573       -0.137502
H          -3.896376       -0.207744        1.649565
H          -2.647610        1.062894        1.517832
H          -2.174955       -0.624119        1.835335
H          -3.446660        0.377208       -0.631500
H          -3.047780       -1.199040       -0.340680
```

---

### embelin_shortened_HEI_5_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.736035 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.555044 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      31.2165 cm-1
  2.      60.3668 cm-1
  3.      87.5278 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.413351        0.172399       -0.316351
C           0.747907       -1.122364       -0.133560
C          -0.614685       -1.277524       -0.219573
C          -1.450875       -0.062208       -0.289314
C          -0.905841        1.190334       -0.325964
C           0.501122        1.396755       -0.231739
O          -1.688502        2.314914       -0.312252
O           1.529615       -2.259275       -0.235259
C          -2.933610       -0.243589       -0.270672
C          -3.458399       -0.384381        1.167837
O          -1.137917       -2.453794       -0.281099
O           1.006726        2.512561       -0.045890
H           1.884887        0.225852       -1.305620
H          -1.084788        3.069373       -0.247533
H           0.857262       -2.962706       -0.323485
H          -3.169156       -1.152409       -0.822936
```

```
H          -3.419517        0.600929       -0.756280
H          -4.537556       -0.539200        1.164111
H          -2.991025       -1.235334        1.661746
H          -3.243891        0.512264        1.749559
C           3.849781       -0.193529        0.324337
N           2.544458        0.443923        0.661668
H           4.566951        0.067237        1.095749
H           4.174620        0.191190       -0.637072
H           3.705675       -1.266144        0.275648
H           2.634599        1.468034        0.692812
H           2.238849        0.142843        1.587625
```

---

### embelin_shortened_HEI_7_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.737125 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.555916 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      53.1302 cm-1
  2.      67.8790 cm-1
  3.      76.8649 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C           1.509060        0.053841       -0.620469
C           0.785180       -1.200539       -0.409899
C          -0.579820       -1.285188       -0.335269
C          -1.342210       -0.017298       -0.320379
C          -0.731449        1.202962       -0.408679
C           0.687181        1.331171       -0.461579
O          -1.444639        2.370512       -0.322649
O           1.525089       -2.362179       -0.519259
C          -2.823390       -0.108317       -0.148709
C          -3.207780       -0.188757        1.338351
O          -1.176831       -2.428068       -0.305509
O           1.272971        2.417051       -0.354429
H           1.928760        0.096091       -1.633009
H          -0.794949        3.088732       -0.330289
H           0.839879       -3.055339       -0.493259
H          -3.166410       -1.011287       -0.651779
H          -3.305400        0.755733       -0.603199
```

```
H          -4.289550       -0.271607        1.445811
H          -2.749110       -1.060027        1.804281
H          -2.878540        0.701803        1.873891
C           2.433600       -0.011629        1.737641
N           2.716700        0.219070        0.291001
H           3.345200        0.177070        2.294931
H           2.108320       -1.037339        1.863121
H           1.652710        0.673771        2.049231
H           3.455970       -0.408240       -0.019819
H           3.041271        1.181150        0.151821
```

---

### embelin_shortened_HEI_9_

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -706.736004 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -706.554431 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 75)

```
  1.      48.4751 cm-1
  2.      73.1894 cm-1
  3.      91.5558 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
C          -1.374349       -0.152885       -0.349558
C          -0.756282        1.127467        0.012591
C           0.595903        1.272346        0.210182
C           1.425897        0.052801        0.268146
C           0.901083       -1.190707        0.052908
C          -0.496793       -1.388163       -0.141679
O           1.669211       -2.320814        0.149160
O          -1.497825        2.275118       -0.206023
C           2.886026        0.217925        0.539531
C           3.682992        0.375722       -0.766336
O           1.125195        2.444395        0.295490
O          -1.029506       -2.506286       -0.109786
H          -1.646321       -0.162408       -1.412386
H           1.062357       -3.072647        0.082001
H          -0.819782        2.974434       -0.131236
H           3.257965       -0.647656        1.087107
H           3.022658        1.108915        1.149209
H           4.742769        0.511438       -0.549007
```

```
H           3.573642       -0.505949       -1.397857
H           3.332869        1.243774       -1.323520
C          -3.887656        0.214887       -0.164925
N          -2.672410       -0.455074        0.381115
H          -4.740335       -0.081120        0.437486
H          -4.021578       -0.108771       -1.191890
H          -3.736488        1.286806       -0.121987
H          -2.770752       -1.478219        0.347267
H          -2.547665       -0.198737        1.361119
```

---

### warfarin_1_reopt2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1035.087311 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1034.824974 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 111)

```
  1.      30.4050 cm-1
  2.      35.2168 cm-1
  3.      43.6410 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O          -0.635780       -0.739401        2.101780
C           0.233100       -0.545810        1.276430
C           0.081460        0.196470        0.048600
C          -1.319180        0.613099       -0.366070
C          -1.840720        1.811719        0.423880
C          -1.164431        3.114629        0.081870
C          -1.461221        4.280199        0.975720
O          -0.422501        3.235739       -0.882620
C          -2.258230       -0.587101       -0.385720
C          -1.978569       -1.621611       -1.280730
C          -2.795909       -2.741091       -1.360040
C          -3.915939       -2.845021       -0.540560
C          -4.203989       -1.820742        0.352720
C          -3.379900       -0.701801        0.430170
C           1.187560        0.484750       -0.703710
O           1.160060        1.289070       -1.771320
O           1.473750       -1.087910        1.560140
C           2.553950       -0.898810        0.753970
C           2.470650       -0.095190       -0.384830
```

```
C           3.622400        0.098350       -1.159500
C           4.810650       -0.511319       -0.804580
C           4.869751       -1.317849        0.335570
C           3.745751       -1.512580        1.120670
H           0.444450        1.957580       -1.650660
H          -1.251750        0.933119       -1.406230
H          -1.777320        1.648139        1.500310
H          -2.902320        1.976239        0.212720
H          -1.137631        5.209829        0.516040
H          -2.521781        4.322609        1.223200
H          -0.921391        4.136539        1.915240
H          -1.108829       -1.547491       -1.921420
H          -4.556179       -3.714762       -0.598990
H          -5.069469       -1.891362        0.997990
H          -3.615610        0.071129        1.146390
H          -2.561249       -3.529501       -2.062670
H           3.561780        0.726720       -2.035150
H           5.695270       -0.362879       -1.407190
H           5.800491       -1.792529        0.613230
H           3.774191       -2.125110        2.010170
```

---

### warfarin_2_reopt2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1035.081516 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1034.819287 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 111)

```
1.      17.5570 cm-1
2.      27.0571 cm-1
3.      39.0814 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O           0.348850       -0.866419        2.461611
C          -0.411840       -0.554970        1.567301
C          -0.064440        0.274180        0.424231
C           1.429590        0.555631        0.355191
C           1.930710        1.742121       -0.505869
C           1.369659        3.065801       -0.054169
C           2.127029        3.838301        0.974621
O           0.314329        3.478001       -0.519759
```

```
C           2.170620       -0.694809       -0.102669
C           1.768860       -1.389549       -1.242169
C           2.477041       -2.503409       -1.677409
C           3.596451       -2.938369       -0.975009
C           4.002451       -2.250838        0.163531
C           3.292310       -1.135849        0.594661
C          -1.039810        0.592690       -0.482239
O          -0.869880        1.390880       -1.546629
O          -1.693890       -1.045050        1.669641
C          -2.644590       -0.794970        0.728991
C          -2.369260        0.030990       -0.359989
C          -3.391400        0.276770       -1.287659
C          -4.636430       -0.300271       -1.124349
C          -4.886330       -1.127961       -0.026229
C          -3.893670       -1.377031        0.906501
H          -0.360331        2.207680       -1.296479
H           1.748080        0.747851        1.378611
H           1.687400        1.584671       -1.553959
H           3.015080        1.758841       -0.410989
H           1.551919        4.689091        1.327921
H           2.397219        3.186921        1.807481
H           3.065469        4.182541        0.532851
H           0.896050       -1.063159       -1.791879
H           4.145421       -3.807648       -1.310659
H           4.868371       -2.584428        0.719501
H           3.607430       -0.606179        1.484431
H           2.153061       -3.032849       -2.563349
H          -3.185200        0.921320       -2.128089
H          -5.418630       -0.109171       -1.845119
H          -5.861440       -1.576841        0.101561
H          -4.066879       -2.008681        1.765701
```

---

### warfarin_3_reopt2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1035.087036 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1034.824135 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 111)

```
1.      30.9651 cm-1
2.      37.7553 cm-1
3.      45.9163 cm-1
```

## B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O           0.766550       -1.361090        2.796610
C           1.138480       -0.862830        1.750250
C           0.279400       -0.452150        0.663270
C          -1.210050       -0.559810        0.944810
C          -1.826149       -1.900291        0.512250
C          -2.087689       -2.144511       -0.950080
C          -2.832449       -3.400911       -1.289730
O          -1.741570       -1.370441       -1.830130
C          -2.010300        0.684979        0.573160
C          -3.329650        0.618499        0.128890
C          -4.061110        1.774759       -0.126100
C          -3.486401        3.024299        0.063200
C          -2.173661        3.105349        0.517250
C          -1.448770        1.949230        0.769980
C           0.842370        0.036940       -0.487020
O           0.149410        0.376020       -1.568260
O           2.500080       -0.684640        1.620180
C           3.057440       -0.124980        0.511960
C           2.270210        0.246570       -0.577960
C           2.896800        0.801160       -1.702390
C           4.266580        0.982621       -1.718260
C           5.035200        0.605251       -0.613400
C           4.436440        0.048201        0.503950
H          -0.706320       -0.126860       -1.600330
H          -1.254690       -0.610050        2.034080
H          -2.768599       -2.071651        1.038590
H          -1.175479       -2.710290        0.852540
H          -2.423999       -4.252341       -0.745560
H          -3.871739       -3.289111       -0.971270
H          -2.803469       -3.583471       -2.360100
H          -3.811670       -0.335421       -0.024390
H          -4.052441        3.923449       -0.138420
H          -1.712021        4.070969        0.674830
H          -0.429390        2.029910        1.121730
H          -5.081730        1.692569       -0.475060
H           2.290830        1.083390       -2.549840
H           4.744420        1.414201       -2.586120
H           6.106980        0.745821       -0.627880
H           5.013400       -0.254169        1.365860
```

---

## warfarin_4_reopt2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1035.07928 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1034.818163 |

| Datum | Value |
|---|---|
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 111)

```
  1.      20.7849 cm-1
  2.      28.9668 cm-1
  3.      36.6725 cm-1
```

## B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O          -0.115999       -1.352461        2.128040
C          -0.821400       -0.918891        1.239170
C          -0.376220       -0.418451       -0.041360
C           1.098250       -0.452160       -0.407800
C           1.821471       -1.736180        0.018100
C           3.080821       -2.003309       -0.780650
C           4.041802       -2.988768       -0.173440
O           3.299371       -1.466909       -1.848860
C           1.828919        0.799690        0.057180
C           2.399359        1.664781       -0.874400
C           3.058218        2.820561       -0.466860
C           3.158628        3.123581        0.885190
C           2.597848        2.262411        1.824090
C           1.938869        1.110400        1.414410
C          -1.296980        0.132758       -0.890330
O          -0.989991        0.692048       -2.070110
O          -2.177600       -0.910962        1.505970
C          -3.095500       -0.397503        0.644890
C          -2.703420        0.153787       -0.575000
C          -3.685641        0.683967       -1.423620
C          -5.015561        0.651286       -1.051340
C          -5.386440        0.090685        0.174540
C          -4.431060       -0.434784        1.027540
H          -0.038841        0.680549       -2.226390
H           1.164120       -0.463870       -1.497910
H           1.175152       -2.605960       -0.137430
H           2.056731       -1.735130        1.078850
H           4.793532       -3.290088       -0.898150
H           4.532181       -2.515028        0.680710
H           3.512172       -3.861349        0.210630
H           2.346819        1.426341       -1.928910
H           3.670677        4.020552        1.206120
H           2.673348        2.489241        2.879230
H           1.503699        0.448580        2.149440
H           3.494717        3.478641       -1.206110
H          -3.387371        1.113687       -2.367670
H          -5.769971        1.059675       -1.708310
```

```
H          -6.427800        0.066545        0.463590
H          -4.697190       -0.869284        1.980120
```

---

### warfarin_5_reopt2

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1035.080857 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1034.819159 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 111)

```
  1.      24.5341 cm-1
  2.      37.5294 cm-1
  3.      49.2981 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O           0.094370        2.114610        1.472870
C           0.677650        1.251430        0.846620
C           0.100580        0.331240       -0.102040
C          -1.365680        0.380340       -0.507650
C          -2.153830        1.633050       -0.109610
C          -1.595160        2.926190       -0.657910
C          -2.088931        4.186820       -0.004170
O          -0.816720        2.941980       -1.591660
C          -2.121800       -0.857130       -0.042840
C          -1.978420       -1.343200        1.257290
C          -2.694760       -2.455461        1.677940
C          -3.562120       -3.103211        0.802070
C          -3.710000       -2.628771       -0.494950
C          -2.994450       -1.510351       -0.912710
C           0.900610       -0.631380       -0.656700
O           0.447390       -1.567800       -1.503430
O           2.037790        1.165820        1.088230
C           2.837330        0.234810        0.505660
C           2.310940       -0.707380       -0.378060
C           3.170680       -1.660340       -0.942690
C           4.515530       -1.653289       -0.627640
C           5.022920       -0.697579        0.258160
C           4.189020        0.248231        0.829540
H          -0.519200       -1.588860       -1.522920
H          -1.369480        0.371800       -1.601130
H          -2.273290        1.712720        0.967100
```

```
H          -3.162560        1.534479       -0.524480
H          -1.762111        5.061680       -0.560230
H          -3.177341        4.175589        0.073700
H          -1.694461        4.227710        1.012470
H          -1.299830       -0.851330        1.941310
H          -4.114719       -3.973201        1.129300
H          -4.378310       -3.126901       -1.184050
H          -3.117970       -1.139491       -1.922940
H          -2.574150       -2.820641        2.688860
H           2.766460       -2.393560       -1.623870
H           5.176360       -2.387719       -1.065240
H           6.075760       -0.695139        0.503340
H           4.561540        0.991881        1.518910
```

---

### warfarin_HEI_1_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1130.974464 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1130.647522 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 132)

```
  1.      26.6748 cm-1
  2.      37.3721 cm-1
  3.      40.3352 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O          -0.411360        0.061590        2.538040
C           0.324020       -0.012691        1.545550
C          -0.009260        0.122479        0.206070
C          -1.446840        0.386600       -0.203450
C          -2.086770        1.562610        0.549120
C          -1.626859        2.923070        0.103530
C          -2.059279        4.083880        0.953830
O          -0.943329        3.100840       -0.894090
C          -2.359470       -0.838660       -0.171340
C          -3.584530       -0.788110       -0.843490
C          -4.442511       -1.879559       -0.861150
C          -4.090871       -3.053379       -0.200010
C          -2.874661       -3.118480        0.467880
C          -2.016551       -2.021290        0.478630
C           0.983110        0.030239       -0.863030
```

```
O           0.504640       -0.593301       -2.055790
O           1.680120       -0.280971        1.886210
C           2.579290       -0.627831        0.935400
C           2.298400       -0.527491       -0.424350
C           3.268940       -0.926282       -1.346550
C           4.499849       -1.398482       -0.924290
C           4.773129       -1.479782        0.442230
C           3.818400       -1.101662        1.370010
H           0.035629       -1.391681       -1.789230
H          -1.427610        0.685250       -1.252890
H          -1.918810        1.464880        1.622190
H          -3.173880        1.565510        0.419770
H          -1.927159        5.022030        0.421320
H          -3.092599        3.969960        1.280220
H          -1.439479        4.094430        1.854200
H          -3.865710        0.115970       -1.370150
H          -4.755521       -3.906709       -0.211570
H          -2.587581       -4.026020        0.982780
H          -1.070851       -2.085780        0.994860
H          -5.381311       -1.817469       -1.395630
H           3.043560       -0.866661       -2.402240
H           5.242569       -1.702212       -1.648270
H           5.731629       -1.847242        0.782580
H           4.007620       -1.169152        2.432150
C           2.099080        2.364739       -0.660030
H           3.115760        1.989209       -0.642690
H           1.683970        2.372419        0.343690
H           2.074481        3.367779       -1.073840
N           1.257140        1.481589       -1.494550
H           1.653530        1.363969       -2.424500
H           0.331530        1.925629       -1.583210
```

---

### warfarin_HEI_2_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1130.97106 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1130.644732 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 132)

```
1.      18.9230 cm-1
2.      29.1516 cm-1
3.      39.5714 cm-1
```

## B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

| | | | |
|---|---|---|---|
| O | 0.435319 | 0.274910 | -2.634639 |
| C | -0.304930 | 0.158139 | -1.648769 |
| C | 0.019390 | 0.179579 | -0.301799 |
| C | 1.450029 | 0.390310 | 0.166521 |
| C | 2.200799 | 1.504170 | -0.576039 |
| C | 1.726548 | 2.899360 | -0.276029 |
| C | 2.274828 | 3.991160 | -1.150239 |
| O | 0.944618 | 3.156300 | 0.627821 |
| C | 2.294450 | -0.878850 | 0.197011 |
| C | 3.298430 | -1.008159 | 1.159051 |
| C | 4.098971 | -2.142949 | 1.214641 |
| C | 3.909391 | -3.173289 | 0.299131 |
| C | 2.912651 | -3.056019 | -0.663499 |
| C | 2.110211 | -1.920160 | -0.711309 |
| C | -0.999010 | 0.080919 | 0.747571 |
| O | -0.555260 | -0.558581 | 1.933371 |
| O | -1.672920 | -0.019361 | -2.011849 |
| C | -2.582470 | -0.440672 | -1.101299 |
| C | -2.310060 | -0.455382 | 0.265561 |
| C | -3.272750 | -0.966802 | 1.139151 |
| C | -4.494810 | -1.416893 | 0.666771 |
| C | -4.766120 | -1.364113 | -0.700579 |
| C | -3.813430 | -0.886012 | -1.584299 |
| H | -0.041930 | -1.327681 | 1.663301 |
| H | 1.395829 | 0.717730 | 1.205931 |
| H | 2.162219 | 1.344980 | -1.653169 |
| H | 3.261869 | 1.489601 | -0.304689 |
| H | 2.086847 | 4.967620 | -0.711739 |
| H | 3.340378 | 3.850711 | -1.330779 |
| H | 1.777108 | 3.932380 | -2.121599 |
| H | 3.448290 | -0.212249 | 1.878821 |
| H | 4.528152 | -4.059629 | 0.339511 |
| H | 2.755661 | -3.852679 | -1.378929 |
| H | 1.337070 | -1.837070 | -1.460369 |
| H | 4.864381 | -2.225578 | 1.975001 |
| H | -3.044010 | -1.023342 | 2.193081 |
| H | -5.230650 | -1.808833 | 1.354551 |
| H | -5.717520 | -1.712463 | -1.078939 |
| H | -3.995250 | -0.862263 | -2.649639 |
| C | -1.897771 | 1.737938 | 2.651961 |
| H | -2.889031 | 1.297368 | 2.645361 |
| H | -1.971852 | 2.801178 | 2.865891 |
| H | -1.275431 | 1.249689 | 3.391491 |
| N | -1.273521 | 1.568219 | 1.317551 |
| H | -0.365341 | 2.059139 | 1.265721 |
| H | -1.852271 | 2.014058 | 0.609701 |

### warfarin_HEI_7_reopt

| Datum | Value |
|---|---|
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Energy | -1130.974461 |
| B3LYP-D3(BJ)/def2tzvpp-IEFPCM Free Energy (Quasiharmonic) | -1130.647691 |
| Number of Imaginary Frequencies | 0 |

**Frequencies** (Top 3 out of 132)

```
1.      22.7487 cm-1
2.      34.1300 cm-1
3.      38.5422 cm-1
```

### B3LYP-D3(BJ)/def2tzvpp-IEFPCM Molecular Geometry in Cartesian Coordinates

```
O          -0.453700        0.324680        2.524429
C           0.277510        0.128420        1.544919
C          -0.038960        0.158380        0.194179
C          -1.466070        0.432900       -0.272981
C          -2.123680        1.645160        0.393829
C          -1.593450        2.977280       -0.062681
C          -2.024620        4.175300        0.734469
O          -0.856660        3.102080       -1.029711
C          -2.355631       -0.798240       -0.192831
C          -2.704341       -1.377429        1.031059
C          -3.508961       -2.508949        1.075169
C          -3.982021       -3.086369       -0.100771
C          -3.643771       -2.518379       -1.322481
C          -2.839631       -1.382369       -1.363631
C           0.968399       -0.028210       -0.848691
O           0.495649       -0.702820       -2.014351
O           1.620139       -0.162700        1.920879
C           2.518139       -0.610420        1.012629
C           2.258679       -0.596790       -0.354761
C           3.226279       -1.093010       -1.231581
C           4.433529       -1.577300       -0.757581
C           4.685479       -1.572300        0.615409
C           3.732879       -1.096240        1.499359
H          -0.016671       -1.462760       -1.716711
H          -1.407250        0.672400       -1.334161
H          -2.043720        1.588040        1.478969
H          -3.196650        1.664451        0.171889
H          -1.457930        4.183240        1.669239
H          -1.824680        5.094140        0.189609
H          -3.078790        4.109761        1.002839
H          -2.326051       -0.940250        1.943659
```

```
H          -4.607311       -3.968249       -0.062851
H          -4.005171       -2.954919       -2.244301
H          -2.583891       -0.943779       -2.320381
H          -3.768261       -2.944309        2.031579
H           3.017309       -1.100880       -2.292141
H           5.174249       -1.957331       -1.446761
H           5.625279       -1.948861        0.995639
H           3.905289       -1.095360        2.566499
C           2.166460        2.278970       -0.769531
H           1.752650        2.353870        0.231959
H           2.175110        3.259340       -1.235301
H           3.170150        1.871390       -0.731201
N           1.295010        1.381970       -1.557221
H           1.685640        1.202520       -2.479651
H           0.384890        1.851410       -1.668901
```

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