

Electronic Supplementary Information

for

“Node” Facilitated Thermostable Mechanophores for Rapid Self-strengthening in Double Network Materials

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1. Computational Section

1.1. Computational Methods

All the calculations were performed at the DFT level of theory with the B3LYP hybrid functional¹ as implemented in Gaussian 16.² To describe the dispersion properly, an explicit dispersion correction term called GD3,³ was also employed in the DFT calculations. The 6-311G(d,p) basis set⁴ was used for all the atoms involved in this study during both the geometry optimization and the single-point calculation processes. To describe the open-shell singlet species involved in the homolysis process, the unrestricted DFT, as well as the procedure to test and optimize the wavefunction, was used in this work.⁵ To describe the solvation environment, the implicit solvation model, IEF-PCM,⁶ is applied to all the calculations involved in this study and toluene ($\epsilon = 2.3741$) was used as the solvent. All the structures were fully optimized with the consideration of external tensile force when necessary. The external tensile force F_τ is properly simulated through our extended artificial force induced reaction method (i.e., EX-AFIR).⁷ The EX-AFIR method can provide a series of TSs under different F_τ efficiently. In this study, F_τ was applied to the terminal methyl groups in all cases. For the computation of hydrogenation enthalpies, it was conducted at the level of B3LYP-D3/6-311G(d,p)//B3LYP-D3/6-311G(d,p) in gas phase without any constraints.

The automated explorations of degradation pathways of mechanoradicals generated from camphanediol and pinanediol were done using the single component (SC) algorithm of the EX-AFIR method. During the explorations, the constant tensile force of 3000 pN and 4000 pN was applied between the two terminal methyl groups for camphanediol and pinanediol, respectively, in order to trigger all possible reactions. Such an exploration is denoted as SC/EX-AFIR. The collision energy parameter γ of the AFIR calculations was set as 400 kJ/mol throughout the search. In order to efficiently obtain energy and force of the quality at the B3LYP-D3/Def2-SV(P) level, we adopted a machine learning framework with a Neural Network Potential (NNP), using an iterative scheme based on continual learning and Δ -learning. In this scheme, the SC/EX-AFIR exploration and machine learning of the energy difference ΔE between the GFN0-xTB⁸ and B3LYP-D3/Def2-SV(P) levels are done alternately. Each iteration of the incremental scheme consists of the following three steps. First, n paths are explored by the SC/EX-AFIR method on the PES of GFN0-xTB (E^{xTB}) augmented by the neural network representation of ΔE (ΔE^{NN}), where $\Delta E^{\text{NN}} = 0$ at any configuration in the first iteration. Second, B3LYP-D3/Def2-SV(P) energy and force calculations are done at all local minima and approximate transition states obtained in the first step. Third, ΔE^{NN} is trained using SpookyNet⁹ for all the data (xTB and DFT energy and force) acquired in the second step of the present and previous iterations. In the present applications, for camphanediol, 5 iterations were performed with $n = 1000, 1000, 1000, 1000$ and 1000, while 3 iterations with $n = 300, 1000, 1000$ were performed for pinanediol. Finally, the final exploration was performed by SC/EX-AFIR for 1500 paths on $E^{\text{xTB}} + \Delta E^{\text{NN}}$ using the final ΔE^{NN} . Important paths were extracted from the reaction pathway network obtained by the final SC/EX-AFIR exploration and

recalculated at the UB3LYP-D3/6-311G(d,p)//UB3LYP-D3/6-311G(d,p) level of theory under the stretching force of 1800 pN for camphanediol and 2300 pN for pinanediol. Therefore, the energetics shown in **Scheme 1** are not affected at all by the accuracy of ΔE^{NN} . See ref. 10 for details of how we trained ΔE^{NN} .

References:

1. (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 1372–1377. (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.
2. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
3. (a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154014. (b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465.
4. (a) A. D. McLean, *J. Chem. Phys.* **1980**, *72*, 5639–5648. (b) K. Raghavachari, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.* **1980**, *72*, 650–654.
5. R. Bauernschmitt, R. Ahlrichs, *J. Chem. Phys.* **1996**, *104*, 9047–9052.
6. G. Scalmani, M. J. Frisch, *J. Chem. Phys.* **2010**, *132*, 114110.
7. J. Jiang, K. Kubota, M. Jin, Z. Wang, T. Nakajima, H. Ito, J. P. Gong, S. Maeda, *ChemRxiv* **2022**, DOI: 10.26434/chemrxiv-2022-fr09l.
8. (a) P. Pracht, E. Caldeweyher, S. Ehlert, S. Grimme, *ChemRxiv* **2019**, DOI: 10.26434/chemrxiv.8326202.v1. (b) C. Bannwarth, E. Caldeweyher, S. Ehlert, A. Hansen, P. Pracht, J. Seibert, S. Spicher, S. Grimme, *WIREs Comput. Mol. Sci.* **2021**, *11*, e1493.
9. O. T. Unke, S. Chmiela, M. Gastegger, K. T. Schütt, H. E. Sauceda, K. -R. Müller, *Nat. Commun.* **2021**, *12*, 7273.
10. R. Staub, P. Gantzer, Y. Harabuchi, S. Maeda, A. Varnek, *Molecules* **2023**, *28*, 4477.

1.2. Supporting Computational Results

Mechano-reactivities of *cis*- and *trans*- VA-PNB under forces

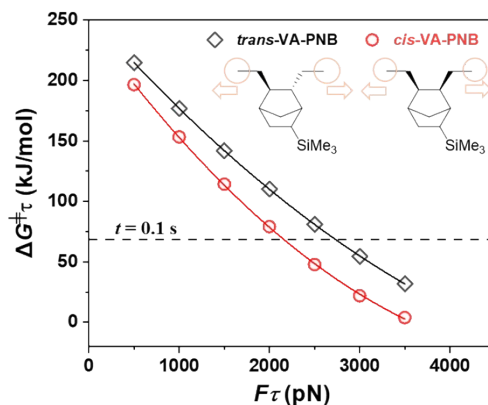


Figure S1. $\Delta G^\ddagger_\tau - F\tau$ graph of *cis*-VA-PNB and *trans*-VA-PNB, suggesting ring strain is not the major reason for the mechanochemical reactivity observed in the sonication reaction.

Distortion of *cis*-pulling and *trans*-pulling based on a tetramethyl norbornane model

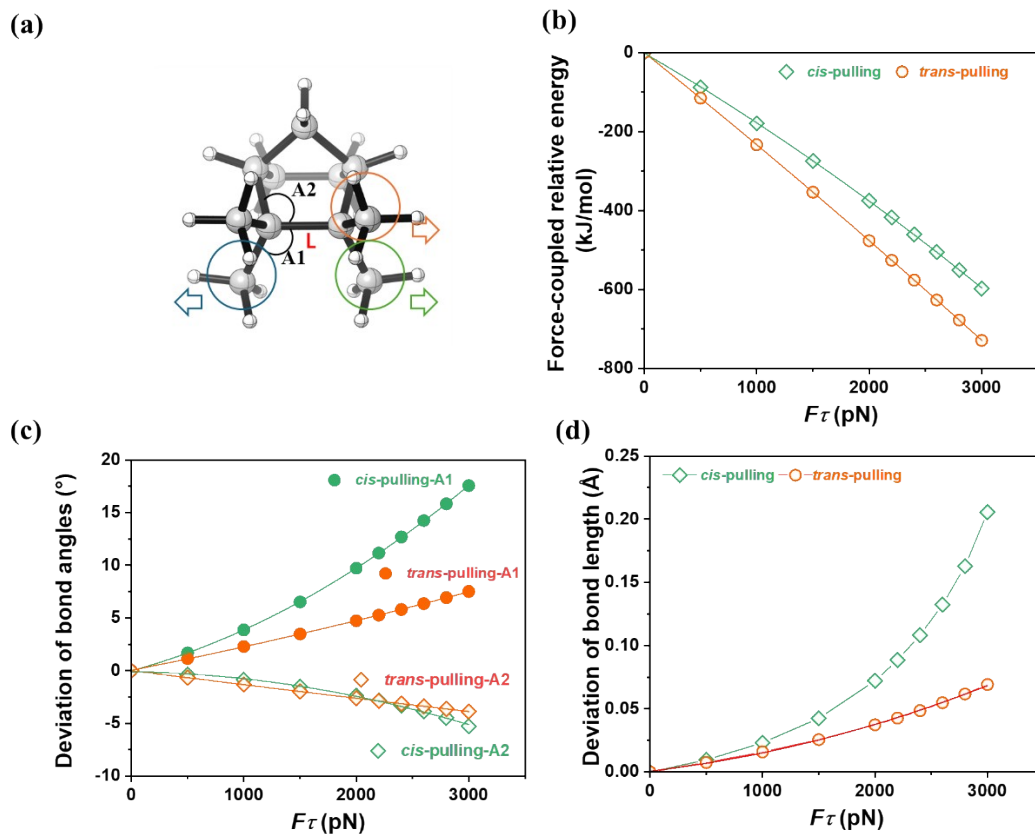


Figure S2. Here we used a model molecule (tetramethyl norbornene, on which repulsive force can be readily added to the specific Me groups to simulate the tensile force) for the illustration of how the pulling direction (a) affects: (b) Energy; (c) bond angles; (d) bond length. Note that the dihedral angle of *cis*-pulling is 0° (i.e., having an ideal node) and it is 120° for the *trans*-pulling.

Computed Hydrogenation Enthalpies of Cyclic Diols

The hydrogenation enthalpies of a series of cyclic diols were computed, suggesting that the ring strain in camphanediol and pinanediol is much smaller than that in cyclobutane-1,2-diol and cyclopropane-1,2-diol. The calculation results therefore indicate that the ring strain does not contribute significantly to the mechanochemical reactivity observed for camphanediol and pinanediol.

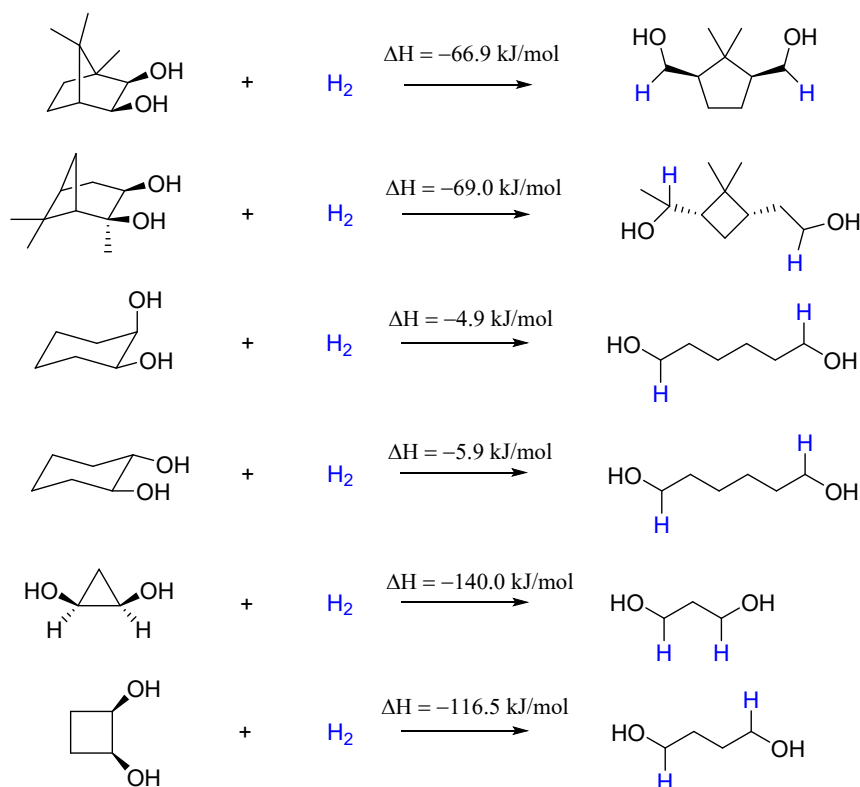
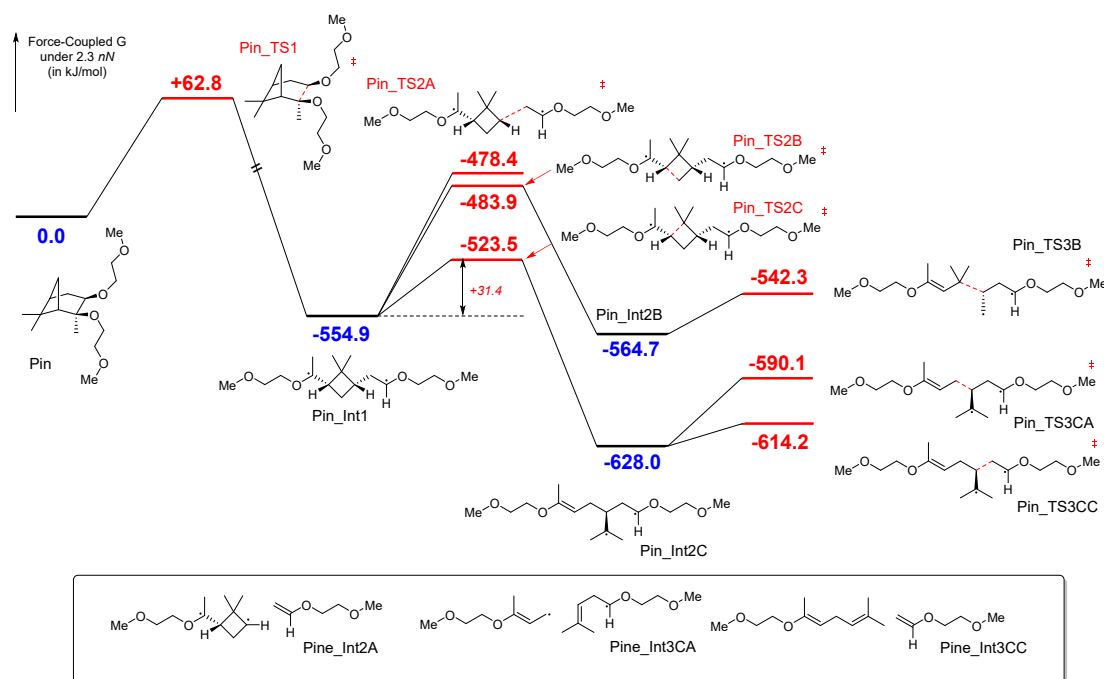


Figure S3. Computed hydrogenation enthalpies of a series of diols, from which we can find that hydrogenation enthalpies of camphanediol and pinanediol are much smaller than those of cyclopropane-1,2-diol and cyclobutane-1,2-diol.

Degradation Pathways of Pinanediol under Tensile Force

Calculations regarding the degradation of pinanediol were also performed with the assistance of the neutral network potential (NNP) developed by Varnek and co-workers. Shown in **Scheme S1** is the SC-AFIR derived pathways under $F_{\tau} = 2300$ pN which have accessible barriers. Pinanediol shows a slightly low reactivity towards the force-triggered homolytic cleavage. Once the six-membered ring is opened, the resultant intermediate **Pin_Int1** has three plausible pathways to follow, and each TS has been successfully located. **Pin_TS2C** was found to have the lowest barrier, which is only +31.4 kJ/mol, since an alkene and a tertiary carbon radical are generated upon the opening of the cyclobutane ring. **Pin_Int3C**, as the product connecting to **TS3C**, is actually a 1,4-diradical. Therefore, the following C-C cleavage through **TS3CC** is almost barrierless (i.e., 13.8 kJ/mol), given the fact that two stable alkenes can be generated. Based on the computational studies illustrated above, pinanediol, though has a relatively low F_{act} , from which the diradical species generated are very short-lived. Therefore, it is very unlikely that these mechanoradicals can be experimentally observed or be further utilized.



Scheme S1. Mechanodegradation of pinanediol under $F_{\tau} = 2300$ pN, from which we can see the resultant intermediate **Pin_Int1** undergoes a rapid decomposition (via **Pin_TS2C** and **Pin_TS3CC**) leading to two alkene molecules.

Further Stretching of Intermediate Cam_Int2C

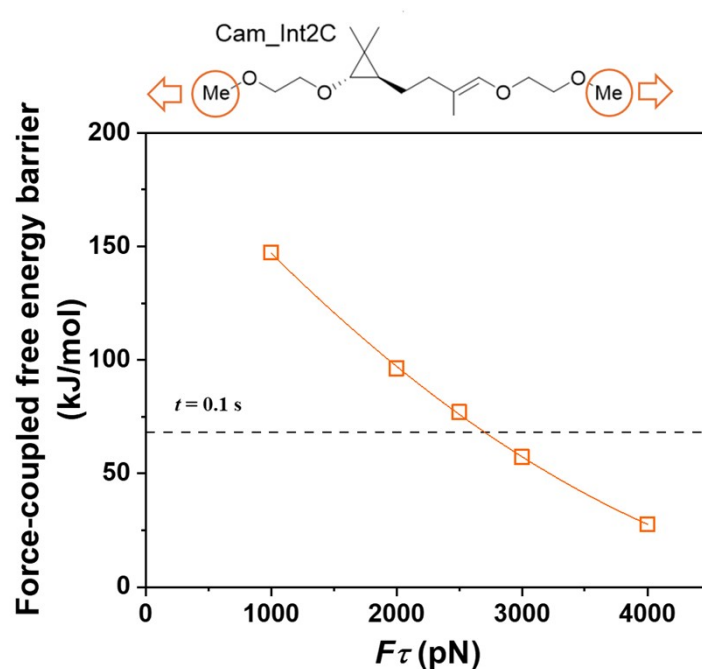


Figure S4. $\Delta G^\ddagger_\tau - F_\tau$ graph for the ring-opening reaction of **Cam_Int2C** via **TS3C**, which generates a 1,3-diradical that cannot further decompose at $F_{\text{act}} = 2700$ pN.

Stability of Two Different Cyclic Diradicals

Two different cyclic diradical species were generated from the stretching experiments of camphanediol and pinanediol, respectively. Once generated, both cyclic diradical can undergo a ring-opening reaction via a transition state called **TS2C**. However, the reactivity of these two species is completely different, with **Pin_Int1** being much more reactive than **Cam_Int1**. Shown in **Figure S4** is how the barrier of ring-opening reaction evolves with an increasing force level. The high reactivity of **Pin_Int1** can be owed to the ring-strain of the four-membered ring. In addition, **Pin_TS2C** will lead to a 1,4-diradical species, which will immediately turn into two alkene molecules via the C2–C3 bond cleavage process.

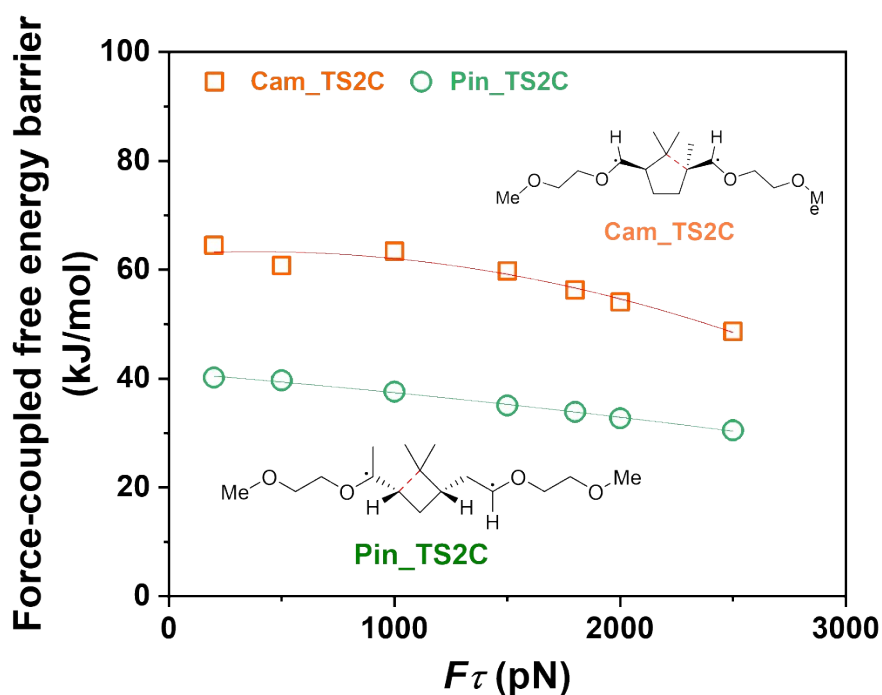


Figure S5. Stability of two cyclic mechanoradicals generated from the stretching experiments of camphanediol and pinanediol, respectively. From which we can figure out that the mechanoradical generated from camphanediol is relatively long-lived, and its stability is not significantly affected by the external tensile force.

Tables of All $\Delta G^\ddagger_\tau - F_\tau$ Data

Table S1. $\Delta G^\ddagger_\tau - F_\tau$ Data of Figure S1

F_τ (in pN)	$\Delta G^\ddagger_\tau$ (cis-VA-PNB) (in kJ/mol)	$\Delta G^\ddagger_\tau$ (trans-VA-PNB) (in kJ/mol)
3500	3.8	31.9
3000	21.9	54.5
2500	47.7	81.0
2000	79.1	110.2
1500	114.2	141.9
1000	153.3	176.9
500	196.5	214.7

Table S2. $\Delta G^\ddagger_\tau - F_\tau$ Data of Figure 3a

F_τ (in pN)	$\Delta G^\ddagger_\tau$ (Cam) (in kJ/mol)	$\Delta G^\ddagger_\tau$ (Pin) (in kJ/mol)	$\Delta G^\ddagger_\tau$ (cis-Cy) (in kJ/mol)	$\Delta G^\ddagger_\tau$ (trans-Cy) (in kJ/mol)
4000	—	—	22.1	65.7
3500	0.2	9.8	42.1	89.7
3000	9.0	26.5	68.1	114.3
2500	28.5	52.3	93.7	140.0
2000	58.4	83.2	126.2	163.9
1500	97.6	129.4	161.6	198.6
1000	139.0	168.0	199.5	234.5
800	156.8	—	—	—
600	173.0	—	—	—
500	—	204.6	244.8	266.5
400	196.0	—	—	—
200	223.9	226.3	—	—

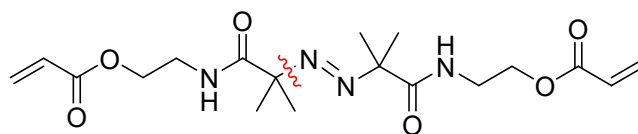
Table S3. $\Delta G^\ddagger_\tau - F_\tau$ Data of Figure S4

F_τ (in pN)	$\Delta G^\ddagger_\tau$ (Cam_TS3C) (in kJ/mol)
4000	27.6
3000	57.3
2500	77.0
2000	96.3
1000	147.3

Table S4. $\Delta G^\ddagger_\tau - F_\tau$ Data of Figure S5

F_τ (in pN)	$\Delta G^\ddagger_\tau$ (Cam_TS2C) (in kJ/mol)	$\Delta G^\ddagger_\tau$ (Pin_TS2C) (in kJ/mol)
2500	48.2	30.5
2000	53.7	32.7
1800	56.1	33.9
1500	59.7	35.1
1000	63.5	37.6
500	60.8	39.7
200	64.4	40.2

Table S5. $\Delta G^\ddagger_\tau - F_\tau$ Data of Azoalkane (shown in Figure 3a as reference)



F_τ (in pN)	$\Delta G^\ddagger_\tau$ (Azoalkane) (in kJ/mol)
4000	5.7
3000	18.8
2500	41.2
2000	55.1
1800	63.7
1500	70.0
1000	85.9
800	88.9
600	95.9
400	96.5
200	100.4

2. Experimental Section

2.1. Experiment Materials and Methods

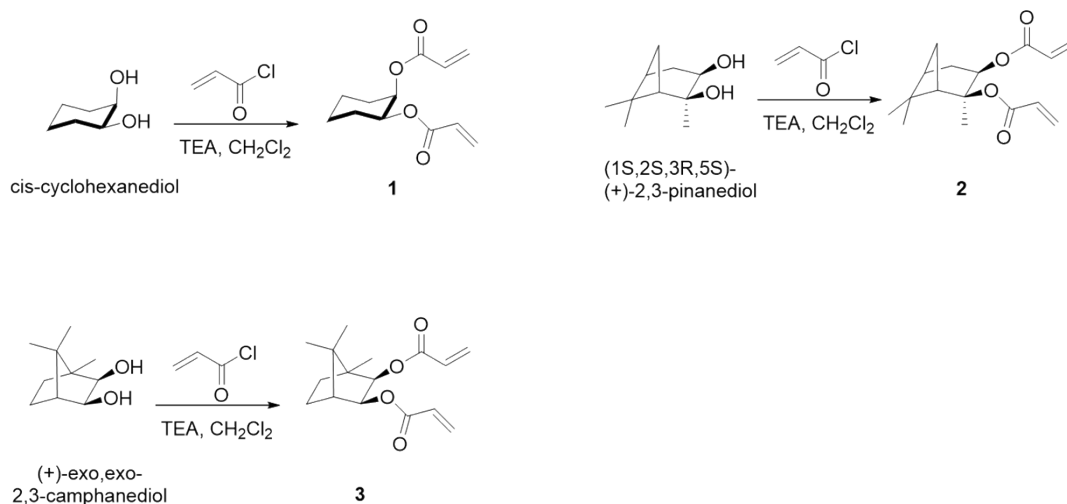
Materials

Cis-1,2-cyclohexanediol, (1S,2S,3R,5S)-(+)-2,3-pinenediol, acryloyl chloride are purchased from Tokyo Chemical Industry. ($\pm$)-exo,exo-2,3-camphanediol is purchased from Sigma-Aldrich. Triethylamine is purchased from Wako Pure Chemical Corporation. 2-Acrylamido-2-methylpropanesulfonic acid (AMPS) was provided by Toagosei. Acrylamide (AAm) was purchased from Junsei Chemical. *N*, *N'*-methylenebis (acrylamide) (MBA), 2,2'-azobis(2,4-dimethyl) valeronitrile (ABVN), *N,N*-dimethylformamide (DMF), 2,2'-azobis[2-(2-imidazolin-2-yl)propane] dihydrochloride (VA-044) were purchased from Wako Pure Chemical Industry.

General Process for the Synthesis of Diacrylate Linkers

Diacrylate linkers were synthesized by the treatment of diol with acryloyl chloride. To a 250 ml three-necked round-bottomed flask equipped with a magnetic stirrer and purged with Argon gas, diol (1 equiv.) and triethylamine (TEA, 8 equiv.) were added sequentially to CH_2Cl_2 (5 ml/mmol diol). The resulting solution was cooled in an ice

bath. After that, a solution of acryloyl chloride (6 equiv.) in CH_2Cl_2 (1 ml/mmol) was added dropwise into the solution. The reaction mixture was stirred overnight, and it was allowed to warm slowly to room temperature. After the reaction was completed, the solution was poured onto saturated NaHCO_3 to quench the reaction and CH_2Cl_2 to extract the organic compound. The layers were separated, and the aqueous layer was extracted with CH_2Cl_2 twice. The combined organics were washed with saturated NaHCO_3 and pure water, and then dried over Na_2SO_4 . After removal of solvent by evaporation, the crude product was then purified by silica gel chromatography (10% ~ 20% EtOAc / Hexane gradient eluent) to give the product.



Compound 1: ^1H NMR (400 MHz, CDCl_3): δ 6.35 (dd, $J = 17.3, 1.5$ Hz, 2H), 6.08 (dd, $J = 17.3, 10.6$ Hz, 2H), 5.79 (dd, $J = 10.5, 1.5$ Hz, 2H), 5.15 – 5.07 (m, 2H), 1.95 – 1.81 (m, 2H), 1.74 – 1.57 (m, 4H), 1.52 – 1.38 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.44, 130.78, 128.72, 71.29, 27.79, 21.76. FTMS-ESI (m/z): $[\text{M} + \text{Na}]^+$ calculated for $\text{C}_{12}\text{H}_{16}\text{O}_4\text{Na}$, 247.0946; observed 247.0941.

Compound 2: ^1H NMR (400 MHz, CDCl_3): δ 6.41 (dd, $J = 17.3, 1.5$ Hz, 1H), 6.28 (dd, $J = 17.3, 1.7$ Hz, 1H), 6.14 (dd, $J = 17.3, 10.4$ Hz, 1H), 6.01 (dd, $J = 17.2, 10.3$ Hz, 1H), 5.83 (dd, $J = 10.4, 1.5$ Hz, 1H), 5.72 (dd, $J = 10.4, 1.7$ Hz, 1H), 5.39 (dd, $J = 9.4, 6.0$ Hz, 1H), 2.82 (t, $J = 5.8$ Hz, 1H), 2.53 – 2.41 (m, 1H), 2.27 – 2.16 (m, 1H), 2.04 – 1.94 (m, 1H), 1.82 – 1.75 (m, 1H), 1.69 (s, 3H), 1.39 (d, $J = 10.5$ Hz, 1H), 1.29 (s, 3H), 1.04 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.77, 164.69, 130.85, 130.27, 129.76, 128.74, 85.39, 71.31, 52.06, 40.11, 38.70, 34.54, 28.20, 27.92, 25.51, 24.10. FTMS-ESI (m/z): $[\text{M} + \text{Na}]^+$ calculated for $\text{C}_{16}\text{H}_{22}\text{O}_4\text{Na}$, 301.1416; observed 301.1410.

Compound 3: ^1H NMR (400 MHz, CDCl_3): δ 6.38 – 6.15 (m, 2H), 6.10 – 5.87 (m, 2H), 5.83 – 5.64 (m, 2H), 4.89 (s, 2H), 1.89 (d, $J = 4.9$ Hz, 1H), 1.82 – 1.67 (m, 1H), 1.65 – 1.48 (m, 1H), 1.30 – 1.16 (m, 2H), 1.14 (s, 3H), 0.85 (s, 3H), 0.83 (s, 3H). ^{13}C NMR

(100 MHz, CDCl₃) δ 165.14, 165.04, 130.74, 130.66, 128.58, 128.45, 79.87, 77.31, 49.67, 48.90, 47.58, 32.96, 23.93, 21.01, 20.53, 11.06. FTMS-ESI (m/z): [M + Na]⁺ calculated for C₁₆H₂₂O₄Na, 301.1416; observed 301.1410.

Gel Preparation

DN gels were prepared by the conventional two-step sequential polymerization as shown in Figure S5. The precursor N,N-dimethylformamide solution containing AMPS (1 mol/L, monomer), ABVN (0.01 mol/L, initiator) and different diacrylate crosslinkers (16 mol% in relative to monomer) was injected into the mold with two parallel glass plates and 0.5-mm silicone spacers. Then the mold was kept at 44°C for 10 hours to form PAMPS single network (SN) hydrogel. The resulting PAMPS SN hydrogel was then immersed into aqueous solution containing AAM (2 mol/L, monomer), MBA (0.0002 mol/L, crosslinker), VA-044 (0.001 mol/L, initiator) for 1 day until equilibrium was reached. The equilibrated PAMPS SN hydrogel was sandwiched by two glass substrates and then kept at 44°C for 10 hours to form DN hydrogels. The as-prepared DN gel was then swelled in a large amount of water to remove the residual and to reach the equilibrium state.

Mechanical Test

Uniaxial tensile tests in air were performed using a commercial tensile tester (Instron 5965, Instron Co.). The gels, with a thickness of 1.7 mm, were cut into dumbbell-shaped specimens using a metal cutter. Two gauge dimensions were used: one with a gauge length of 17 mm and a gauge width of 4 mm, and another with a gauge length of 12 mm and a gauge width of 2 mm. These specimens were then stretched in air at a crosshead velocity of 100 mm/min, corresponding to a strain rate of approximately 0.1 s⁻¹.

Uniaxial tensile tests in glove box were performed using a commercial tensile tester (RTC-1150A, Orientec Co.).

Evaluation of Mechanoradicals by Fenton-related Chemical Reaction

The mechanoradical concentration was estimated by the Fenton color reaction as reported in our previous work. DN gels were cut into dumbbell-shaped strips (17 mm gauge length and 4 mm width). The cut gels were immersed in a large amount of aqueous solution of 250 μ M (NH₄)₂Fe^{II}(SO₄)₂, 250 μ M XO and 20 mM H₂SO₄ for 1 day. Then gels were stretched in air to a preset strain at a velocity of 100 mm/min and then immediately recovered to the initial position. After 30 mins, when no further color change was observed, the gels were cut with scissors to obtain the gel in the necked region. The gel sample was then placed in a quartz cuvette and UV-Vis absorption

spectroscopy (UV-1800, Shimadzu Co.) was performed.

To quantify the Fe^{3+} concentration, a calibration experiment was done by immersing DN gels in a large amount of aqueous solution of 0 - 200 μM $\text{NH}_4\text{Fe}^{\text{III}}(\text{SO}_4)_2$ (as a Fe^{3+} source), 250 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$, 250 μM XO and 20 mM H_2SO_4 to get the calibration curve of normalized absorbance (measured absorbance divided by the gel thickness) at 580 nm as a function of Fe^{3+} concentration (Figure S6). Here, we also assume the concentration of $\text{NH}_4\text{Fe}^{\text{III}}(\text{SO}_4)_2$, $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$ and XO in the equilibrated gel was the same as that in the solution. By comparing the normalized absorbance at 580 nm of DN gels after stretching with the calibration curve, we can evaluate the Fe^{3+} concentration, which is assumed to be equal to the mechanoradical concentration.

Application of Mechanoradicals for Fast Mechanoresponsive Strengthening of DN gels

Various DN gels with different crosslinkers were immersed in an aqueous solution containing 2.0 M NIPAm and 0.15 M MBA for one day. After immersion, the samples were cut into dumbbell-shaped strips with a gauge length of 12 mm and a width of 2 mm. The strips were then placed in an argon glove box for 2 hours to remove oxygen. Following this, the gels underwent a cyclic tensile test with a preset strain of 6 at a velocity of 300 mm/min. After a 3-minute waiting period, the gels were subjected to a second cyclic tensile test under the same conditions.

Evaluation of Thermal and UV Stability of Diols

15 mg of diols were dissolved in ~ 0.5 ml of d_6 -DMSO. The solution was then either heated at 80°C or exposed to UV light (3.9 Mw/cm^2) for 10 hours. After the treatment, NMR was used to analyze if any reaction has occurred.

2.2. Supporting Experiment Results (Figs. S5-S7, Scheme 2)

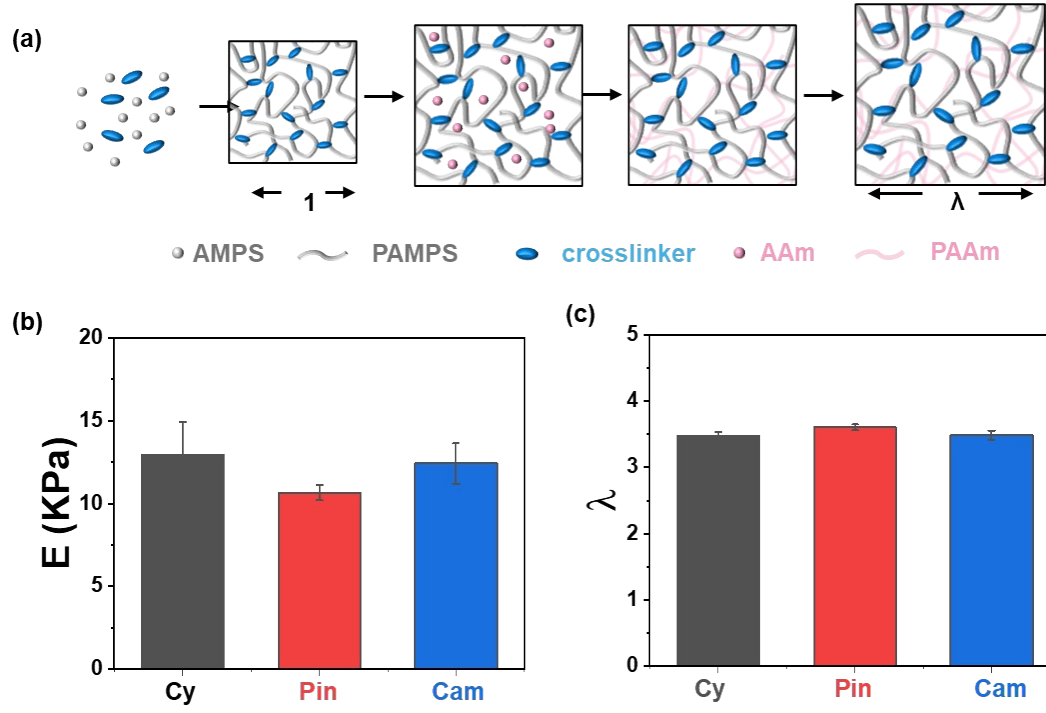


Figure S6. (a) Illustration of preparation of DN gels with different crosslinkers. (b) Modulus, E , of as-prepared single network PAMPS hydrogels. (c) Length swelling ratio, λ , of PAMPS network in equilibrated DN gels.

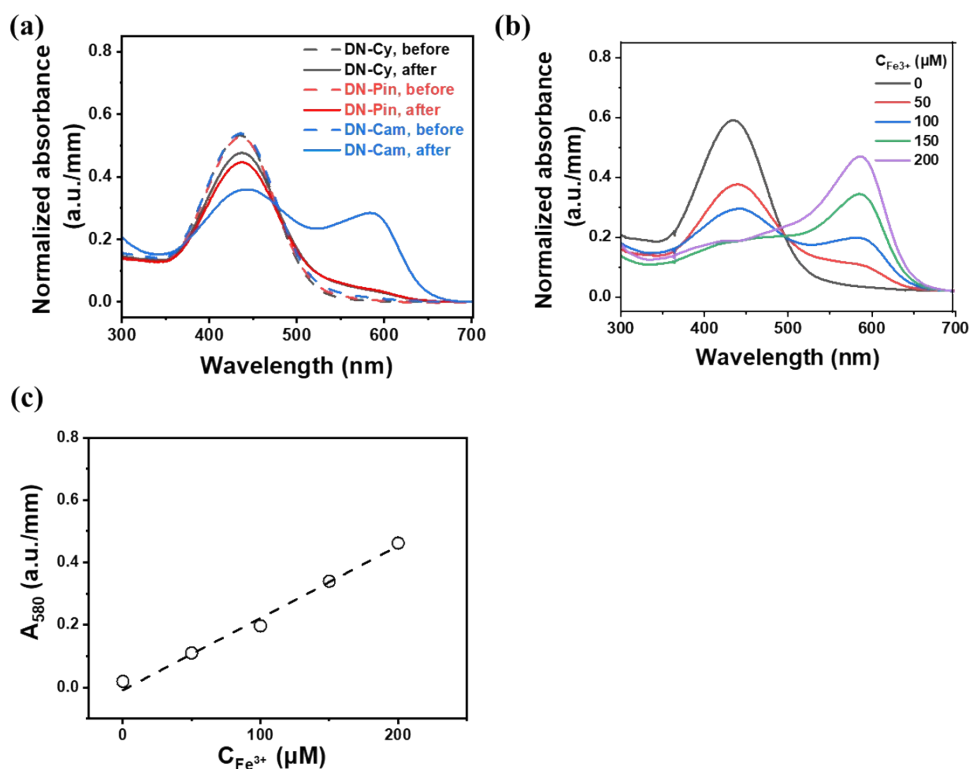


Figure S7. (a) UV spectrums of DN-Cy, DN-Pin, and DN-Cam gels fed with 250 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$ and 250 μM xylenol orange (XO) before and after stretching. (b) UV spectra of equilibrated DN gels after immersion into a large amount of aqueous solution of 0 - 200 μM $\text{NH}_4\text{Fe}^{\text{III}}(\text{SO}_4)_2$ (as a Fe^{3+} source), 250 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$, 250 μM XO and 20 mM H_2SO_4 . (c) The calibration curve of the normalized absorbance at 580 nm (A_{580}) as a function of the Fe^{3+} concentration ($C_{\text{Fe}^{3+}}$).

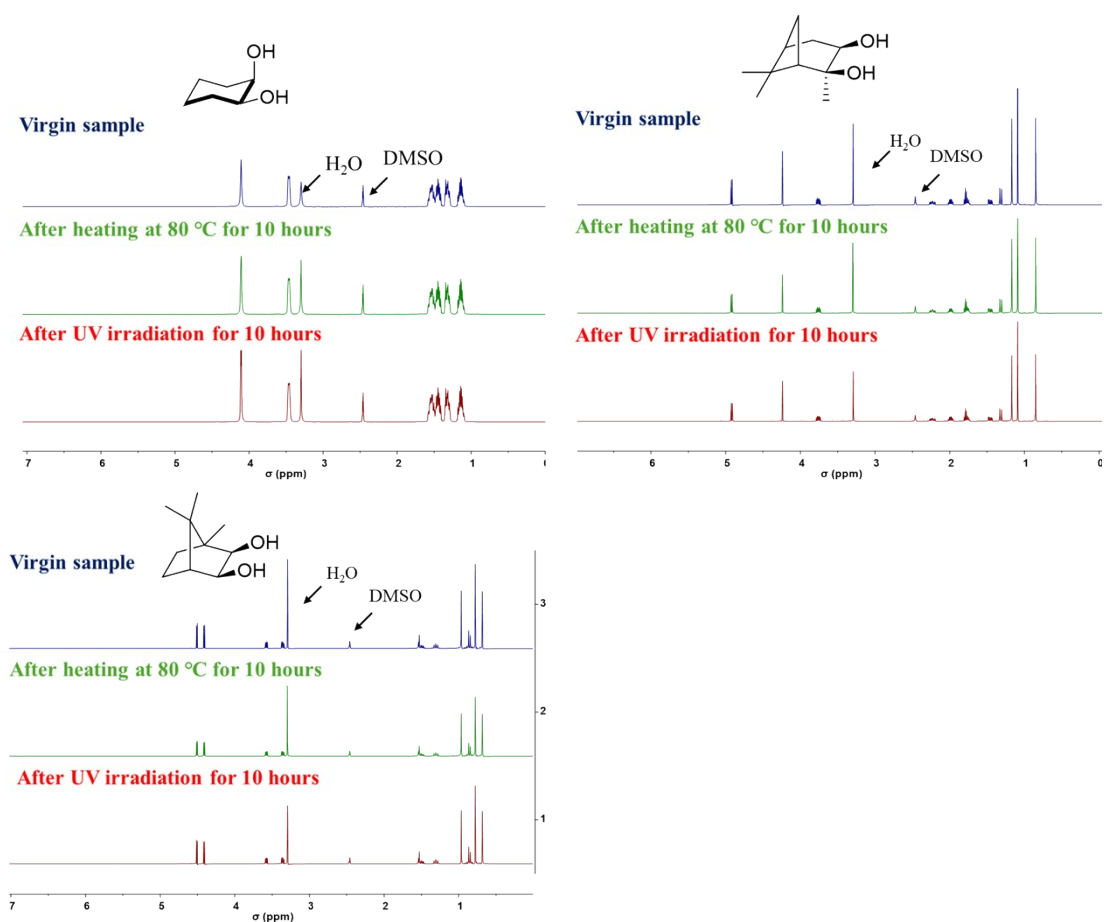
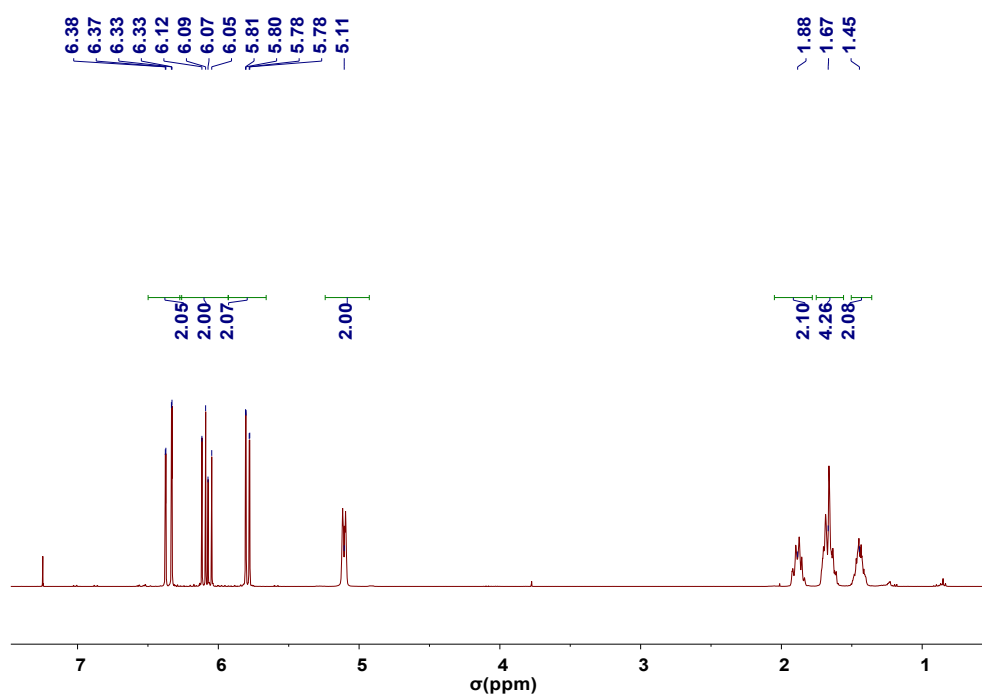
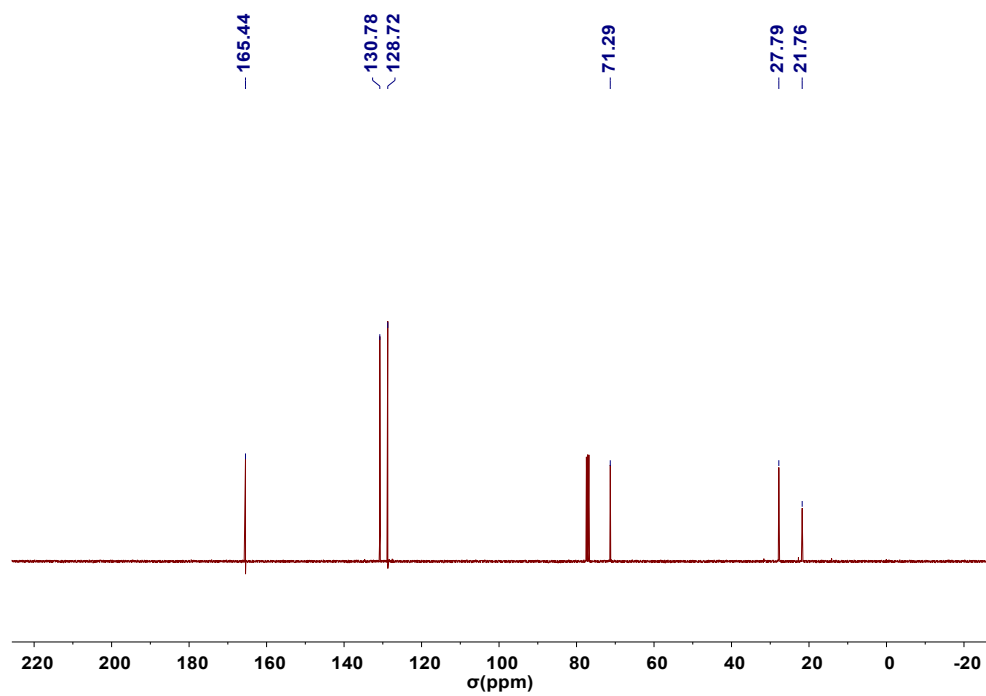


Figure S8. NMR spectra of three diols before and after thermal and UV treatment. After heating or UV irradiation, NMR of three diols remains unchanged.

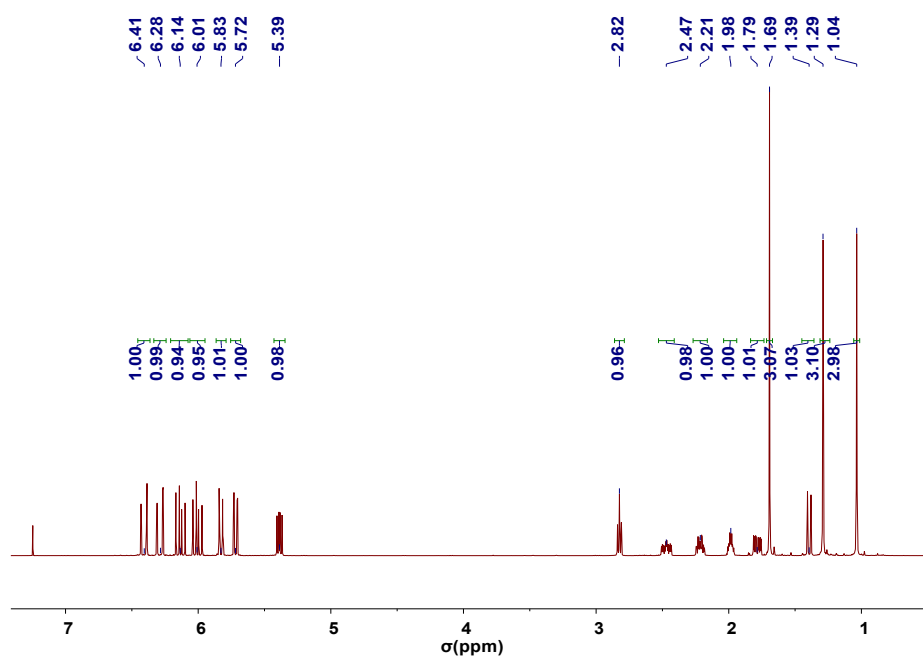
2.3. NMR Spectra



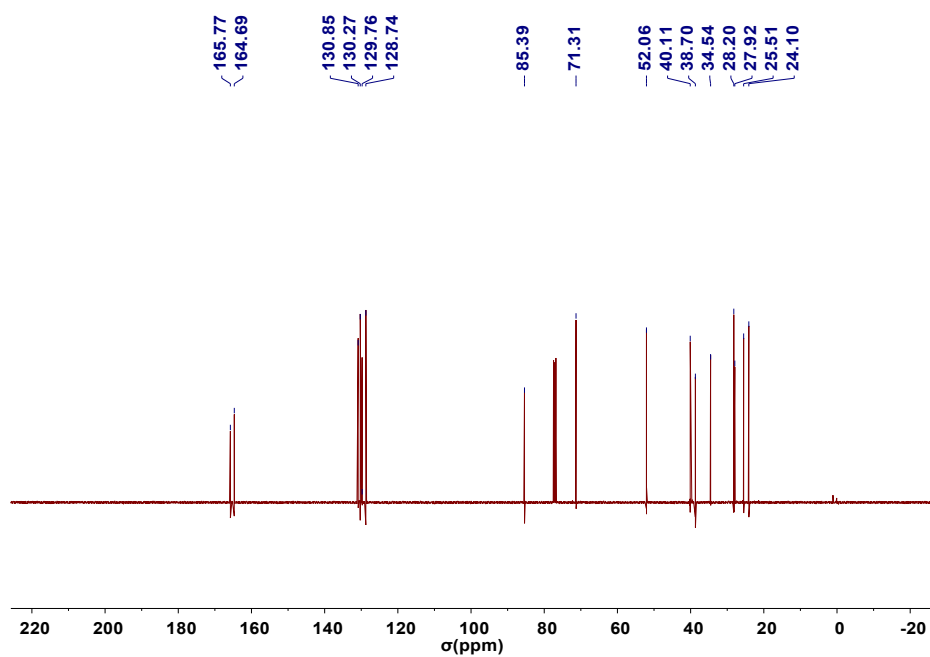
¹H NMR of compound **1**



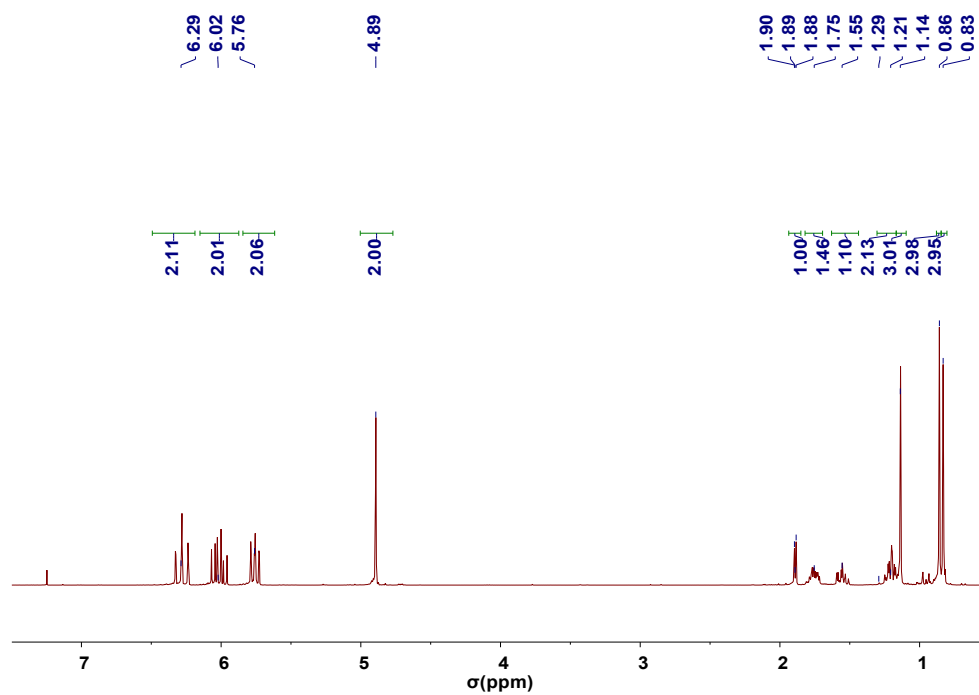
¹³C NMR of compound **1**



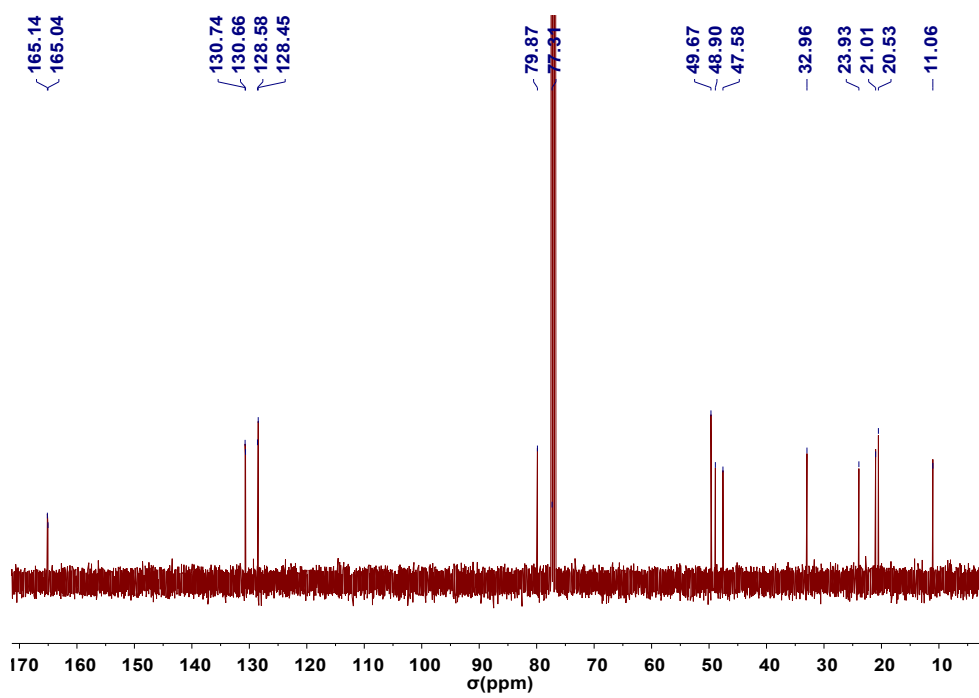
¹H NMR of compound **2**



¹³C NMR of compound **2**



¹H NMR of compound **3**



¹³C NMR of compound **3**

Cartesian Coordinates of Optimized Structures

(E_F : Electronic Energy on the FMPES at $F = F_\tau$ pN; G_F : Gibbs Free Energy at $F = F_\tau$ pN, 298.15 K and 1 atm)

cisVAPNB_TS-F3500

($E_F = -840.62520779$ a.u.; $G_F = -840.28835867$ a.u.)

0 1

C	2.127266544069	0.088711514564	-5.321031576641
C	3.161680866472	0.565836335188	-4.252049699899
C	1.697319120388	-0.777681512228	-3.083898159789
C	1.239310127482	-0.937895968043	-4.547005976103
H	1.515570067732	0.945370082690	-5.627055908275
H	0.170834635117	-0.748241287459	-4.675469676274
H	1.422407838442	-1.967866882133	-4.874742717338
C	3.216705876631	-0.611000203104	-3.258880460433
H	3.727629422068	-0.348707746788	-2.329152414556
H	3.686317111293	-1.504680698557	-3.682093573747
C	2.667634841721	1.767909488835	-3.455813644856
H	1.918346122229	2.354615123842	-3.987086717525
C	1.162833587499	0.512059874021	-2.458004403291
H	0.363122452904	0.958608239893	-3.049910171299
H	4.146363174649	0.783497643665	-4.678890417133
H	1.438855556756	-1.642959715288	-2.466078341015
C	3.841433213702	2.712082633857	-2.990125126474
H	3.430978609846	3.488649118023	-2.337876880140
H	4.536051731283	2.131183580691	-2.373773002296
C	0.657393064501	0.313613067103	-0.980120025200

H	1.489216302040	-0.059761225590	-0.372781214228
H	0.387889104887	1.289243828958	-0.564463935635
C	4.775009581602	3.494721287249	-4.103229522847
H	5.490869140102	4.105166036266	-3.550895354251
H	5.316211601305	2.785316878939	-4.731382072698
H	4.164374391600	4.138961403561	-4.739314732012
C	-0.615886466401	-0.686230565380	-0.663588385315
H	-0.394520085771	-1.711270183676	-0.965595756287
H	-0.789173845526	-0.656966431861	0.413184911292
H	-1.514043605297	-0.347326890452	-1.184289632047
Si	2.901615243446	-0.575207541489	-6.918469428515
C	4.117067793965	-1.971809432202	-6.538029013702
H	3.626903666217	-2.799881933770	-6.017498458499
H	4.550106914490	-2.369548306251	-7.461148623082
H	4.939691823855	-1.620721355959	-5.908124689796
C	3.818711210902	0.830979788941	-7.786141845080
H	4.615538183112	1.234534731049	-7.154096330876
H	4.274841694047	0.490837050474	-8.720995123578
H	3.137007403216	1.653015336950	-8.026110367328
C	1.528675738980	-1.226590137945	-8.040552704770
H	1.935301033832	-1.619461117236	-8.977572705154
H	0.971402426704	-2.032956897069	-7.554058548954
H	0.817212759876	-0.433384969573	-8.290917872917

cisVAPNB_P-F3500

($E_F = -840.84782002$ a.u.; $G_F = -840.52107887$ a.u.)

0 1

C	2.189857255169	0.483266945730	-4.925869785244
C	3.155804520085	1.153445152356	-3.876247854764
C	1.418323669275	-0.195990591010	-2.586218434269
C	1.261068994217	-0.495702553376	-4.127221115189
H	1.560434413153	1.295853156122	-5.312665325579
H	0.222548997110	-0.356861630505	-4.438591868337
H	1.499902473144	-1.546753601621	-4.315436930634
C	2.163385024475	1.209450191319	-2.621428991410
H	1.435233054735	2.012552799512	-2.785742665106
H	2.686477929846	1.419809012902	-1.685197052083
C	3.858923991891	2.436187466025	-4.407722302792
H	3.216977089032	3.298549769850	-4.576767613337
C	0.108526867231	-0.405887154496	-1.770291410676
H	-0.608213888641	0.413516040186	-1.782819645071
H	3.940698178512	0.431263976837	-3.615183176735
H	2.150802019612	-0.916514063780	-2.199727529752
C	5.374979305087	2.576771568167	-4.729151221731
H	5.898660605020	2.662058604138	-3.763230941618
H	5.717101705354	1.612350231699	-5.127638659611
C	-0.383485754493	-1.809174155028	-1.306399617534
H	-0.471317766544	-2.428876392183	-2.214241286107
H	0.445243432369	-2.271910772658	-0.752305019739
C	6.049142138524	3.723903409350	-5.674702150203
H	7.126258813780	3.552316526115	-5.671361982735
H	5.678342893450	3.662809243960	-6.699955618160

H	5.845004817214	4.723513500811	-5.285327708363
C	-1.733085040278	-2.123317194723	-0.447115167457
H	-2.626793692307	-1.793029587440	-0.981027578454
H	-1.781377224631	-3.203807373673	-0.305544757639
H	-1.704517710574	-1.634876607252	0.529215918364
Si	2.999658590154	-0.335005805442	-6.438841943941
C	4.375052642994	-1.494189886718	-5.859323811036
H	4.000079934634	-2.219760010044	-5.130681340657
H	4.796171260037	-2.053891563470	-6.700046853332
H	5.190219682625	-0.938676535144	-5.386597857291
C	3.700035310919	0.954689463507	-7.627148751629
H	4.498149302748	1.541527968208	-7.169365272109
H	4.104703897051	0.472400139783	-8.522928959759
H	2.918014917898	1.650110022685	-7.947350492722
C	1.687630834438	-1.332381476552	-7.366228628653
H	2.112590980110	-1.790009304111	-8.265152447238
H	1.273448837904	-2.132891988450	-6.747105924272
H	0.858241901804	-0.690731537606	-7.680310839061

cisVAPNB_R-F3500

($E_F = -840.62838971$ a.u.; $G_F = -840.28979007$ a.u.)

0 1

C	2.116845506219	0.059541295413	-5.352661739672
C	3.134360234130	0.565338009285	-4.281481115871
C	1.746002970187	-0.775508683535	-3.109492984522
C	1.255304118487	-0.976588732525	-4.554828803448

H	1.484944188320	0.900102280358	-5.664605462156
H	0.181919497126	-0.801696576925	-4.663018135413
H	1.447304735650	-2.007825591882	-4.874020295302
C	3.258943712142	-0.630970895399	-3.322894583854
H	3.803538058891	-0.384228926753	-2.407475889867
H	3.714161500634	-1.515454809185	-3.775354932092
C	2.503753613283	1.651452227426	-3.374238972318
H	1.874896905929	2.316369001598	-3.973244118704
C	1.300435281355	0.620017895183	-2.580688987966
H	0.405037219028	0.930776138266	-3.127781538820
H	4.078806935817	0.901454743396	-4.711548231133
H	1.453572808783	-1.586424640261	-2.440622243105
C	3.654844991098	2.581725649634	-2.785379371079
H	3.199080518966	3.326282434585	-2.125002176707
H	4.316619725106	1.980875980692	-2.152408401633
C	0.825202742981	0.504228999704	-1.070043906450
H	1.664015751844	0.154192228264	-0.457837703733
H	0.572074535871	1.502661551815	-0.698957764444
C	4.626437246661	3.407083661538	-3.820960768827
H	5.265918650403	4.058363743640	-3.223183583653
H	5.253973849300	2.730659139694	-4.402558428990
H	4.034290453086	4.018019329335	-4.506537948615
C	-0.451259793040	-0.463913988812	-0.715179101290
H	-0.235372035864	-1.507466476663	-0.948894301752
H	-0.649530330343	-0.371727685397	0.353767245604
H	-1.338152862804	-0.152810348963	-1.272395907106

Si	2.895031353332	-0.600018260924	-6.949602007651
C	4.141178025674	-1.972660153151	-6.581980707614
H	3.674615290548	-2.808717956462	-6.052755562801
H	4.567882493230	-2.364052591976	-7.510797930475
H	4.966081934446	-1.604275784569	-5.965231488693
C	3.778325873034	0.818783288447	-7.831851866080
H	4.573896150084	1.238623542219	-7.208868527652
H	4.231682813438	0.483063068438	-8.769650612087
H	3.079928721310	1.627494774725	-8.068655067921
C	1.523734630010	-1.281276734942	-8.056185118853
H	1.928391714027	-1.672014865906	-8.994932138252
H	0.985436600385	-2.094656200369	-7.560242521632
H	0.795986713932	-0.502254787976	-8.303816120260

cisVAPNB_TS-F3000

($E_F = -840.53661626$ a.u.; $G_F = -840.19998312$ a.u.)

0 1

C	2.130022190758	0.098617668217	-5.307901632880
C	3.171047638638	0.569902772875	-4.242458190161
C	1.675634425824	-0.779704638346	-3.072027309877
C	1.236796079367	-0.928122827675	-4.543184923505
H	1.522182049028	0.958987819681	-5.610440449097
H	0.169627754267	-0.739735780328	-4.683148141254
H	1.423983209227	-1.956908162223	-4.871922999074
C	3.197843720079	-0.593365691578	-3.228138396482
H	3.690884400597	-0.318179872780	-2.293060450431

H	3.678918326378	-1.490595340876	-3.633282301811
C	2.732643076439	1.815885107006	-3.503815016305
H	1.945732521577	2.380185340004	-4.000909328196
C	1.093636475268	0.459998651506	-2.416729271703
H	0.328569624484	0.953637689043	-3.014414201927
H	4.169841625879	0.732775967277	-4.665936444677
H	1.440245265361	-1.667936167336	-2.475234042808
C	3.896872831194	2.744386036575	-3.048129923154
H	3.494756120477	3.523414317385	-2.393412771120
H	4.596651557690	2.162359128301	-2.438193394971
C	0.613599320170	0.258714408962	-0.950610538941
H	1.449176840599	-0.125143276552	-0.354653403837
H	0.353268995596	1.232200826637	-0.523988545591
C	4.800312911928	3.506628418356	-4.173726633328
H	5.541614041063	4.113121984469	-3.650638513232
H	5.314566914399	2.789305993539	-4.816042453650
H	4.180129728317	4.155012328411	-4.796528493365
C	-0.650138872716	-0.729785107853	-0.651714875221
H	-0.436109345820	-1.749103018552	-0.978692968897
H	-0.826029776447	-0.729176885020	0.425425913546
H	-1.548606790560	-0.376471913351	-1.162595961828
Si	2.904801127247	-0.562969019253	-6.906271068468
C	4.113910006522	-1.963570672029	-6.521045440344
H	3.617976600192	-2.790663349337	-6.004551754919
H	4.551364780585	-2.361596336990	-7.441897029706
H	4.933692696638	-1.616109976854	-5.885512366094

C	3.828176384998	0.842545313628	-7.767706228959
H	4.621941160026	1.244694980699	-7.131133854455
H	4.288642389766	0.502852550655	-8.700545003471
H	3.148672701473	1.665484044838	-8.010241790281
C	1.533981856379	-1.208601330051	-8.033902846913
H	1.942464749281	-1.599025931787	-8.971119766601
H	0.974292427582	-2.015613721023	-7.551535088205
H	0.824486236207	-0.413570285562	-8.283562396368

cisVAPNB_P-F3000

($E_F = -840.72167371$ a.u.; $G_F = -840.39413000$ a.u.)

0 1

C	2.173472439021	0.509732895006	-4.962869387480
C	3.138999202612	1.179578367552	-3.910918739309
C	1.442897455011	-0.184148001108	-2.625629031008
C	1.198493972271	-0.421186961182	-4.161396862470
H	1.578892857652	1.327446624867	-5.390206555856
H	0.162853012571	-0.181379030320	-4.416747184921
H	1.333939528938	-1.481808434327	-4.392879244136
C	2.176014364014	1.216200359876	-2.643438372667
H	1.440713247260	2.018464709088	-2.779489920211
H	2.717440252056	1.413208557114	-1.714645934297
C	3.801246749966	2.473290299559	-4.431219836684
H	3.134480062340	3.313647516438	-4.616082168551
C	0.185110762112	-0.415203643987	-1.758785267187
H	-0.525865609456	0.406763584352	-1.695235427813

H	3.940752704114	0.470103965554	-3.666687858385
H	2.193987803087	-0.920296197873	-2.308508615778
C	5.310247567561	2.677196893679	-4.679886957698
H	5.778320324253	2.877710569814	-3.701393449943
H	5.733914939087	1.710066553207	-4.981032357853
C	-0.285319103903	-1.829267799096	-1.348998552372
H	-0.422413550261	-2.406013845011	-2.279431122344
H	0.562992373620	-2.325258944776	-0.855835169195
C	5.917637460319	3.787892966021	-5.679389770602
H	7.005766726415	3.722593181351	-5.632290628492
H	5.593749547557	3.614525734053	-6.707954564942
H	5.610899799155	4.793297136180	-5.381693441757
C	-1.586608971950	-2.134835661674	-0.451215101213
H	-2.493965017226	-1.759614707503	-0.930532211140
H	-1.669785744052	-3.216856504340	-0.337744635050
H	-1.501486787959	-1.680234564275	0.538529370475
Si	2.995164028076	-0.382821921899	-6.424732854682
C	4.198230513354	-1.680286403068	-5.760237416423
H	3.699544977304	-2.366924958311	-5.069168355748
H	4.620602327503	-2.276661118731	-6.574737142256
H	5.029521763752	-1.213234860649	-5.223961667572
C	3.913533013852	0.820003079243	-7.554040873727
H	4.771600127804	1.273392729422	-7.054666867565
H	4.277870522596	0.302434048201	-8.447453258317
H	3.254037961702	1.629281890357	-7.881724891094
C	1.647695245075	-1.235809672961	-7.440683302836

H	2.078978799796	-1.751294554411	-8.304545554652
H	1.101542536703	-1.975214447749	-6.848308320477
H	0.921901150674	-0.507496956212	-7.816232366596

cisVAPNB_R-F3000

($E_F = -840.54788301$ a.u.; $G_F = -840.20833049$ a.u.)

C	2.118423115186	0.062231494258	-5.368712806837
C	3.126020413645	0.565459205439	-4.287680171343
C	1.732127074334	-0.773590927175	-3.127058068361
C	1.243377407815	-0.966314515114	-4.574288053605
H	1.494232746622	0.905265402934	-5.689744255718
H	0.172257307628	-0.779204280998	-4.684581185942
H	1.424510067234	-1.998969344028	-4.895069173798
C	3.246733094429	-0.637156062454	-3.336124391330
H	3.791226214814	-0.399112724507	-2.418360099647
H	3.698575000439	-1.520898808697	-3.792759608991
C	2.465738554430	1.632625367199	-3.373784780610
H	1.858122452456	2.308317531673	-3.984022181435
C	1.305898509918	0.631905283172	-2.602194072583
H	0.384505727567	0.926459307633	-3.115589328190
H	4.069838057387	0.914725160091	-4.707491926918
H	1.428654715164	-1.582108716827	-2.460792241909
C	3.580076939947	2.549767063960	-2.729096853700
H	3.098700885740	3.271618085513	-2.061073767403
H	4.234923740073	1.942003552449	-2.095083860360
C	0.903818572068	0.550060027147	-1.080265079447

H	1.762619529664	0.196652807811	-0.497800980015
H	0.680719064264	1.557651379827	-0.713630670677
C	4.535729601989	3.392140338216	-3.732376208034
H	5.160362927170	4.056455247236	-3.132511504156
H	5.183223337930	2.734932777497	-4.314475810000
H	3.938907604935	3.995136980119	-4.421721418097
C	-0.359556725554	-0.388148680406	-0.694025202613
H	-0.164173936430	-1.436503504035	-0.925071229021
H	-0.544049060304	-0.293199236809	0.377559742163
H	-1.254287213057	-0.071767960149	-1.236487362897
Si	2.905209954606	-0.606556616815	-6.957730407781
C	4.131901355674	-1.994572689722	-6.582399190881
H	3.652213333395	-2.823764660188	-6.054115028744
H	4.557044971580	-2.392712885590	-7.509084109706
H	4.959215101357	-1.636396503058	-5.962913276182
C	3.812547070204	0.802011438472	-7.831947848224
H	4.610139276616	1.209741069717	-7.203547794354
H	4.266857939254	0.461875808248	-8.767692112233
H	3.126624876639	1.620587207144	-8.071298509775
C	1.535224898643	-1.271175929533	-8.076076817192
H	1.943108388585	-1.667115380044	-9.011236454613
H	0.982716063942	-2.077779977780	-7.584685863201
H	0.819238928165	-0.483344994734	-8.330034149471

cisVAPNB_TS-F2500

($E_F = -840.44717461$ a.u.; $G_F = -840.11095188$ a.u.)

0 1

C	2.130342235671	0.101011849029	-5.303953607466
C	3.174667847639	0.571927981944	-4.241329067002
C	1.664048271833	-0.783711816688	-3.068523369937
C	1.237467594587	-0.928629831126	-4.543904907599
H	1.521856942313	0.961796961301	-5.603711165251
H	0.170484907853	-0.744882380066	-4.691130246119
H	1.430911964672	-1.956295014236	-4.872318860481
C	3.187136388965	-0.581398182217	-3.212819118631
H	3.668744037950	-0.296202066873	-2.275001057433
H	3.677625751519	-1.479911975814	-3.605080648704
C	2.764545057603	1.840372429519	-3.535630725021
H	1.961055375012	2.396678327545	-4.013340474183
C	1.053139408265	0.428790900867	-2.401918433642
H	0.304476862348	0.945220268055	-3.000015964744
H	4.179468621468	0.705562427308	-4.663589496306
H	1.442816159744	-1.683684208764	-2.482525709665
C	3.917514108297	2.751599674321	-3.064821701474
H	3.516319973618	3.526128228698	-2.403862761442
H	4.616106100901	2.162480692639	-2.459866126587
C	0.603519154252	0.240298036598	-0.939087739749
H	1.444327768069	-0.149761664837	-0.354132680083
H	0.355600276073	1.216178033617	-0.510033975047
C	4.799515083227	3.504187753231	-4.188604294871
H	5.556603010083	4.108331493225	-3.684723557389
H	5.298005680917	2.785613267771	-4.842569924851

H	4.173316418823	4.156599922920	-4.801652972055
C	-0.652567449850	-0.731906398747	-0.649283103884
H	-0.447973267769	-1.748828718704	-0.990754228489
H	-0.833434565972	-0.749459191953	0.427392857768
H	-1.549965548747	-0.367481014776	-1.154913373142
Si	2.905785171529	-0.557865550696	-6.903126921247
C	4.113866732312	-1.958622308751	-6.515067115481
H	3.616117059965	-2.786148903859	-6.001015433771
H	4.554899385432	-2.355985417928	-7.434482269998
H	4.931158196820	-1.611584838840	-5.876079683527
C	3.830391131262	0.848283870870	-7.762013120194
H	4.622654517635	1.250452476195	-7.123584323996
H	4.292859642346	0.509128814049	-8.694069801977
H	3.151098302016	1.671111437439	-8.005520714397
C	1.536783757032	-1.203115628683	-8.033111893634
H	1.946737358650	-1.593133398329	-8.969858544972
H	0.976413475079	-2.010368624287	-7.551943527730
H	0.827637076502	-0.408015668266	-8.283550514147

cisVAPNB_P-F2500

($E_F = -840.59720961$ a.u.; $G_F = -840.26903833$ a.u.)

0 1

C	2.165580183221	0.507797334661	-4.976829272948
C	3.126445827340	1.177002084553	-3.920776444602
C	1.451522512666	-0.180769878285	-2.641909070478
C	1.185714868938	-0.413311296140	-4.173890181066

H	1.577385784005	1.325141795302	-5.413308370785
H	0.150488186458	-0.158312128667	-4.416130177217
H	1.303935158483	-1.475131764191	-4.409032331949
C	2.173631903763	1.215388405444	-2.656408670470
H	1.435136163245	2.015495560202	-2.789301125785
H	2.717964388372	1.413472826853	-1.729478174655
C	3.775989511310	2.469725504708	-4.425570136777
H	3.108369542686	3.308514576802	-4.614258056784
C	0.213381039074	-0.407258536371	-1.766119483815
H	-0.494972896971	0.415179936935	-1.683325534477
H	3.931089658511	0.469801651492	-3.678879374465
H	2.206971332094	-0.918496023078	-2.337806559062
C	5.278088488095	2.676785085526	-4.645474661787
H	5.734321174058	2.892019646979	-3.663926069761
H	5.715724036882	1.711989836302	-4.934575309473
C	-0.249437732836	-1.818170576234	-1.377765023391
H	-0.406713986610	-2.382585152697	-2.313133960384
H	0.601439174912	-2.328216869205	-0.903041834455
C	5.848441725586	3.781286838527	-5.645738097107
H	6.938918647418	3.754765099564	-5.607775671095
H	5.525384228824	3.590247240785	-6.671700150084
H	5.512997412710	4.780999608020	-5.358548785408
C	-1.530586448125	-2.089687131802	-0.471439366381
H	-2.434772281089	-1.688119432952	-0.936050230884
H	-1.649650131180	-3.167968493791	-0.351435094413
H	-1.420123182990	-1.636667186849	0.516910858987

Si	2.997498375942	-0.395878065474	-6.425399324863
C	4.177155320989	-1.705157720074	-5.742407455505
H	3.662283494242	-2.385071113484	-5.056612835464
H	4.603686910175	-2.307586622693	-6.550262195552
H	5.006457259548	-1.245891721774	-5.196401856098
C	3.946846731740	0.795811637037	-7.540633263172
H	4.803745682939	1.236538594570	-7.027871730764
H	4.317403385929	0.274831052205	-8.429463588189
H	3.303306120088	1.614548354943	-7.876325126366
C	1.655045216143	-1.235479884637	-7.458764734935
H	2.092527908068	-1.760178737900	-8.313909454541
H	1.090654700439	-1.965339209515	-6.871596558620
H	0.944341478741	-0.499560191572	-7.848061212034

cisVAPNB_R-F2500

($E_F = -840.46961471$ a.u.; $G_F = -840.12912793$ a.u.)

0 1

C	2.120762735026	0.065802691244	-5.387385811859
C	3.117788245237	0.563792489373	-4.294964597498
C	1.712511899410	-0.772987293035	-3.148035395074
C	1.227560559230	-0.952439872218	-4.598562121015
H	1.507648456149	0.912990254527	-5.718879787871
H	0.159755002907	-0.748939690468	-4.712050700226
H	1.394108324697	-1.986571996313	-4.922223069273
C	3.229398083250	-0.645316922534	-3.349940254196
H	3.771728796738	-0.416766097557	-2.428529543891

H	3.677967489139	-1.528702490595	-3.809968216798
C	2.432503706921	1.617147304615	-3.380464121585
H	1.839811588510	2.299048568532	-3.999330128714
C	1.304024318681	0.637195599022	-2.620276968463
H	0.359993756631	0.923384525995	-3.097006591279
H	4.063742468492	0.921252397235	-4.702460532249
H	1.397526376696	-1.582060023117	-2.488160554226
C	3.509456073094	2.523266889012	-2.685479997124
H	3.002720948756	3.219681742188	-2.008786933520
H	4.160836415709	1.909084150658	-2.053717387049
C	0.981688503350	0.584452659601	-1.088614462783
H	1.862447263366	0.226642961955	-0.542306796003
H	0.790270376962	1.600160261211	-0.725762649911
C	4.447505596301	3.387798235196	-3.656789094130
H	5.063880414772	4.055421497727	-3.051380913299
H	5.107161717074	2.751943814517	-4.249231930302
H	3.844652132151	3.992442490875	-4.340040950754
C	-0.265867917566	-0.325565537198	-0.660462677990
H	-0.093465498608	-1.377877254408	-0.892610413395
H	-0.423562459757	-0.229473210477	0.415690882369
H	-1.173570445931	-0.001891569401	-1.177232577328
Si	2.916873350817	-0.614803035882	-6.966959121741
C	4.117113501604	-2.023220267646	-6.582186285903
H	3.619887961529	-2.843259659964	-6.055834313874
H	4.540274539695	-2.429820391345	-7.506124916595
H	4.947254578923	-1.679089770012	-5.958577248826

C	3.855728901420	0.779878744303	-7.830040824337
H	4.655274651861	1.171782279268	-7.194103387974
H	4.311678257628	0.433960921026	-8.762863217241
H	3.186419144815	1.611061721156	-8.072936002389
C	1.548253974979	-1.256700157361	-8.100246695507
H	1.959541102287	-1.658840129402	-9.031255638528
H	0.977680519210	-2.054518701680	-7.615158262987
H	0.847729138715	-0.457363889418	-8.361254992425

cisVAPNB_TS-F2000

($E_F = -840.35810044$ a.u.; $G_F = -840.02194448$ a.u.)

0 1

C	2.129311445020	0.099182855734	-5.306103861533
C	3.175137811186	0.571255373029	-4.245209059342
C	1.654484217490	-0.789395322350	-3.070849669775
C	1.237628369818	-0.933550444044	-4.549034866179
H	1.519190698703	0.959436033728	-5.603869625170
H	0.170656736744	-0.754562865639	-4.702129440737
H	1.437106624157	-1.960259852216	-4.876693916285
C	3.177519269953	-0.573540433516	-3.205553086267
H	3.650410937934	-0.280327574905	-2.265800868224
H	3.676112631675	-1.472545215938	-3.587051669879
C	2.781196141623	1.854005259409	-3.562022135758
H	1.969363292159	2.407697731328	-4.027737585517
C	1.023509772339	0.406339118941	-2.399533372488
H	0.283356798129	0.936321161010	-2.995733281891

H	4.183082515294	0.686612015435	-4.666965245480
H	1.441842971608	-1.696540076365	-2.491823507271
C	3.920624414333	2.747447723232	-3.062641164293
H	3.515375442536	3.513336710779	-2.393762156832
H	4.614615996787	2.148467863902	-2.461700616894
C	0.610638464219	0.239419968799	-0.935191344093
H	1.458793850300	-0.154541891970	-0.363188355640
H	0.378261256170	1.220334022705	-0.508407636516
C	4.787565014127	3.497850045506	-4.176330993742
H	5.554299632598	4.100345462224	-3.684191212333
H	5.277367513295	2.782353336302	-4.840672475168
H	4.157700673716	4.154498516813	-4.781569922512
C	-0.638750436564	-0.714115356851	-0.644201259133
H	-0.445802527590	-1.730877083046	-0.993843963938
H	-0.821657106789	-0.742356887664	0.432393311840
H	-1.536003107964	-0.340881710801	-1.144286252806
Si	2.906391414895	-0.556917920443	-6.905489150898
C	4.115579716371	-1.956036164949	-6.514725719759
H	3.617380250629	-2.784708687484	-6.002961942833
H	4.560655918683	-2.352098948503	-7.432736130746
H	4.929925800901	-1.608068884649	-5.872470812891
C	3.830419398639	0.850825131599	-7.762286303147
H	4.620323853463	1.254497680079	-7.121896053835
H	4.295783383883	0.512518737450	-8.693197021137
H	3.150163370114	1.672353919904	-8.007421525897
C	1.540101249719	-1.203934754523	-8.037702931550

H	1.952068829335	-1.593398882811	-8.973793549264
H	0.980004786900	-2.011929446303	-7.557467685226
H	0.830338689418	-0.409748220229	-8.289276237527

cisVAPNB_R-F2000

($E_F = -840.39338548$ a.u.; $G_F = -840.05209056$ a.u.)

0 1

C	2.122648082342	0.068048587828	-5.407042143059
C	3.109706663593	0.560361884994	-4.303703296053
C	1.691307758519	-0.773842461546	-3.170058861452
C	1.210986312292	-0.939482791475	-4.624217013120
H	1.521047819186	0.919572856791	-5.748527122018
H	0.146870046728	-0.719274918369	-4.741275901019
H	1.362732649983	-1.974819071895	-4.950986800026
C	3.210597238425	-0.654904222749	-3.364535846589
H	3.750610781543	-0.435916460830	-2.439546153749
H	3.655736157971	-1.538171056548	-3.827655609521
C	2.402712516596	1.602846713471	-3.391771223252
H	1.823088156830	2.290157144853	-4.017586287822
C	1.298638784348	0.638952450169	-2.638702659349
H	0.335225600259	0.919945500499	-3.079074678528
H	4.058789192405	0.923388150402	-4.698822873156
H	1.365084712473	-1.583925521414	-2.517050436082
C	3.442425311839	2.496268154370	-2.646992009568
H	2.910065725269	3.163724781267	-1.960514676481
H	4.090821226633	1.873918907800	-2.019928909023

C	1.056888049015	0.615758847421	-1.100393980873
H	1.958800771633	0.254109960526	-0.592223616113
H	0.897968561177	1.639868580472	-0.745038948462
C	4.364595994014	3.387574952806	-3.581714585604
H	4.976115172704	4.050053347191	-2.965146864025
H	5.032407613385	2.775887780934	-4.190677471556
H	3.756845333478	4.002247604740	-4.252065483004
C	-0.172871525370	-0.265332018786	-0.623310299059
H	-0.026075390291	-1.321424037250	-0.856876890217
H	-0.295404009324	-0.167647579481	0.457655391449
H	-1.095540686878	0.067184501004	-1.107616951828
Si	2.927661774428	-0.624103244139	-6.977311901612
C	4.104455748296	-2.049544122876	-6.582954521546
H	3.591831653009	-2.861497992671	-6.058830176361
H	4.526923605679	-2.463438790874	-7.503985433911
H	4.936017093570	-1.717227570835	-5.954875871391
C	3.894107033808	0.757786199616	-7.830365851038
H	4.693370729223	1.137461558956	-7.186693334781
H	4.353625619271	0.406076373326	-8.759259328569
H	3.239152324416	1.598758368126	-8.078607181589
C	1.561544993408	-1.246970640626	-8.124251162767
H	1.976433664081	-1.654551499304	-9.051284967735
H	0.975467542159	-2.037064865753	-7.645016773799
H	0.874512040672	-0.438164742243	-8.391849790399

cisVAPNB_P-F2000

($E_F = -840.47430989$ a.u.; $G_F = -840.14447886$ a.u.)

0 1

C	2.152460428764	0.513179751713	-5.003306994116
C	3.113619598704	1.178862439666	-3.945062144703
C	1.464397167996	-0.179715709119	-2.671918700664
C	1.154065646369	-0.382746515412	-4.197645079131
H	1.581885192918	1.332273333448	-5.458732453260
H	0.124351219685	-0.081755883404	-4.409238862848
H	1.222966938595	-1.444809560368	-4.450354585223
C	2.180380771694	1.210343877248	-2.675561966940
H	1.439691934035	2.011221189696	-2.791801798105
H	2.735899224317	1.399479209753	-1.753373143880
C	3.742493545132	2.475486345242	-4.433704062691
H	3.066180424825	3.305946991494	-4.628621996048
C	0.257232411953	-0.408280418239	-1.772467116624
H	-0.446380769519	0.414129101140	-1.656606292386
H	3.925361869861	0.476343818699	-3.713254407995
H	2.225369092756	-0.925731767727	-2.402461504220
C	5.236455694311	2.707608977231	-4.611668613433
H	5.664025696111	2.969916486046	-3.628129283369
H	5.708582752761	1.747940715718	-4.860807472973
C	-0.193705145413	-1.817281835432	-1.401855815065
H	-0.377651372915	-2.369721641499	-2.339899049230
H	0.663193965769	-2.339744964456	-0.951503863548
C	5.763617989380	3.792502413479	-5.633176881940
H	6.854061807667	3.826386830440	-5.589872812658

H	5.459937756376	3.551991679511	-6.654810856956
H	5.376402982353	4.784342485063	-5.385156293230
C	-1.447891961188	-2.057328796897	-0.476156494678
H	-2.351968751479	-1.631677621129	-0.919821786279
H	-1.598839979413	-3.130857036601	-0.346912236345
H	-1.304890621925	-1.605098154122	0.508714480770
Si	2.995459504177	-0.420770946714	-6.425190422700
C	4.098156921587	-1.775574189037	-5.703235998180
H	3.530823430398	-2.441712677437	-5.045958985362
H	4.538500368016	-2.386927070389	-6.496830811100
H	4.918386160383	-1.349335060875	-5.117941388159
C	4.032650321003	0.734958554506	-7.498998636863
H	4.890786785170	1.132182916451	-6.953355514239
H	4.409759473048	0.204871552925	-8.379601479663
H	3.438626939635	1.584889075834	-7.847899084856
C	1.657075625583	-1.205284485287	-7.505488412642
H	2.101589251449	-1.755813094151	-8.340514254346
H	1.037807386248	-1.904169064330	-6.936054030749
H	0.996357016593	-0.440204600621	-7.925373551931

cisVAPNB_TS-F1500

($E_F = -840.26931535$ a.u.; $G_F = -839.93348166$ a.u.)

0 1

C	2.127254066616	0.095500460106	-5.307796729935
C	3.175415990593	0.569396475651	-4.249453471528
C	1.642027575604	-0.797203943257	-3.072849638066

C	1.238769438266	-0.942528688491	-4.554655942193
H	1.513849899953	0.954659288847	-5.601716446031
H	0.171648349122	-0.771992567569	-4.716176310368
H	1.448460095042	-1.967785609996	-4.880377624979
C	3.164671311130	-0.563500805138	-3.194806758106
H	3.625771621046	-0.259135103787	-2.252791244599
H	3.673936930087	-1.463044580904	-3.561483840515
C	2.803485797351	1.870403332485	-3.595603490830
H	1.981585153613	2.421118031399	-4.045911054705
C	0.984767333929	0.377979765243	-2.398091896250
H	0.257022915610	0.924347111879	-2.993976149581
H	4.186967009857	0.661039193062	-4.670315693551
H	1.440380048564	-1.712233609390	-2.501199703369
C	3.930227154129	2.743663814718	-3.065199253718
H	3.520894129476	3.500858874015	-2.388585619833
H	4.617414821047	2.132997244558	-2.467894106897
C	0.611073314696	0.236315499279	-0.931566825966
H	1.467366452563	-0.160312383678	-0.373381102039
H	0.395304583001	1.223374803886	-0.509798234219
C	4.787505912100	3.493002082120	-4.166229796359
H	5.563440096515	4.091174005019	-3.682212440539
H	5.268782189494	2.780680390044	-4.840634211346
H	4.156932067807	4.156232504140	-4.763898833311
C	-0.632069209414	-0.698290712181	-0.632040358694
H	-0.452020626388	-1.715746451430	-0.987407137988
H	-0.812831011384	-0.733553919509	0.445191966396

H	-1.530573503730	-0.317364966118	-1.124464437647
Si	2.906102930417	-0.554599214321	-6.908599857180
C	4.120768608866	-1.948600438940	-6.516194921836
H	3.624667277317	-2.780453941680	-6.007553614898
H	4.571384696806	-2.341130994232	-7.432997364548
H	4.930878612280	-1.597688657046	-5.870173957573
C	3.824748075728	0.858070628652	-7.762948793926
H	4.610421962400	1.266084952693	-7.120105686790
H	4.294685749823	0.522464567295	-8.692529047483
H	3.140599094014	1.675802508751	-8.009925885029
C	1.543911707199	-1.207108321109	-8.042553920636
H	1.958582699736	-1.593908199434	-8.978555093748
H	0.987216291704	-2.018131810582	-7.563465829129
H	0.830648363376	-0.416088572335	-8.294199939023

cisVAPNB_R-F1500

($E_F = -840.31908329$ a.u.; $G_F = -839.97699563$ a.u.)

0 1

C	2.123545697035	0.068336797986	-5.424372649159
C	3.102660163721	0.557574988288	-4.312934496689
C	1.674792411973	-0.776002552498	-3.189071929403
C	1.198773798995	-0.931893200528	-4.646156118429
H	1.529836339699	0.922403537519	-5.773355136432
H	0.137458751428	-0.700057700491	-4.766301749819
H	1.340443738999	-1.967826000487	-4.975244498306
C	3.195960315991	-0.662476083015	-3.378225430856

H	3.734738148440	-0.451210775477	-2.450889474596
H	3.638648161585	-1.545257788687	-3.844234119721
C	2.377297121313	1.590934140229	-3.404604959297
H	1.809811159282	2.284305261610	-4.035200153252
C	1.292068738193	0.638491122771	-2.657492110267
H	0.313644009574	0.913842244911	-3.067713811628
H	4.053964266753	0.925502832436	-4.698403174507
H	1.340596896724	-1.586569845580	-2.540691633314
C	3.381948917309	2.468859775260	-2.611254209783
H	2.825438041902	3.108033827867	-1.917007915844
H	4.025255470482	1.836754856244	-1.988719195871
C	1.120170436095	0.646119630341	-1.116895469421
H	2.039433538933	0.284366683437	-0.640943153019
H	0.987076201845	1.678133576258	-0.774054100541
C	4.292947345575	3.386563274671	-3.505063334203
H	4.900365783401	4.038698425082	-2.872957522805
H	4.967807465871	2.799641764986	-4.130955034563
H	3.683595005380	4.015767150049	-4.160764606637
C	-0.090633032816	-0.207770551802	-0.593163578724
H	0.032634523119	-1.267643847536	-0.824496158593
H	-0.179408549665	-0.106046060742	0.491101845234
H	-1.026553552651	0.131612207329	-1.046950175951
Si	2.935337436059	-0.632224928227	-6.987616545662
C	4.096765257336	-2.068193792167	-6.586031686959
H	3.574169728576	-2.874802064677	-6.063490383508
H	4.519264187436	-2.486938718049	-7.504867784558

H	4.928745831761	-1.743151736717	-5.954730479844
C	3.919653518440	0.740719229839	-7.834523551488
H	4.718317956613	1.113057973977	-7.185836021005
H	4.381795458142	0.384600162027	-8.760430451142
H	3.274043599347	1.587616282093	-8.087026212053
C	1.571501747811	-1.243591944923	-8.143504631579
H	1.988996507700	-1.655084820155	-9.067633454727
H	0.975500964217	-2.028473190740	-7.667938379070
H	0.893188628668	-0.429038539052	-8.415868865329

cisVAPNB_P-F1500

($E_F = -840.35298938$ a.u.; $G_F = -840.02396995$ a.u.)

0 1

C	2.134205767367	0.533579625143	-5.047332309151
C	3.100518959037	1.190769815313	-3.986654352592
C	1.479206788460	-0.183705772658	-2.727600693076
C	1.094403256340	-0.309988544338	-4.240600445374
H	1.601877728240	1.355551457493	-5.540938603334
H	0.086243255977	0.085719892001	-4.393531222509
H	1.061004229256	-1.363485560635	-4.533172134880
C	2.201312703779	1.194334055362	-2.700409711144
H	1.462777125238	2.002372528736	-2.773730634110
H	2.780655562866	1.351743168380	-1.786964067834
C	3.691835017617	2.502582069106	-4.450140880785
H	2.992934136997	3.312444916842	-4.653341770929
C	0.319039856665	-0.426006100182	-1.787894214588

H	-0.373133483655	0.395986573048	-1.615016528602
H	3.928548797303	0.499110829419	-3.781318519672
H	2.241885459570	-0.950217414226	-2.528104245880
C	5.172015397827	2.795945050370	-4.563935028152
H	5.539565872468	3.147851288393	-3.583692497641
H	5.706525683663	1.852213813087	-4.732359109758
C	-0.117356737451	-1.835710736700	-1.439628144381
H	-0.338858421148	-2.369821208096	-2.380389628586
H	0.749109979639	-2.373438463825	-1.026524748801
C	5.652518245898	3.838717521036	-5.631861565996
H	6.735289142718	3.965072858779	-5.563541981466
H	5.402745056395	3.506893011416	-6.642583339583
H	5.182294698877	4.812095794466	-5.466628749147
C	-1.334013678717	-2.050639168644	-0.481430983179
H	-2.241479955179	-1.598700102851	-0.891595024113
H	-1.514234789491	-3.119193659615	-0.345955927219
H	-1.146971924846	-1.605145144203	0.499425609922
Si	2.992783247232	-0.460840761958	-6.416443085320
C	3.937469174595	-1.899007387078	-5.633654821268
H	3.276586178114	-2.526464973398	-5.027925170969
H	4.388030758457	-2.535092504912	-6.401691847181
H	4.742531998401	-1.539994726006	-4.985727015508
C	4.188837778045	0.618520791848	-7.400696160563
H	5.028157456734	0.951862334585	-6.786378291806
H	4.595290021828	0.065065380161	-8.253331706925
H	3.686321150468	1.510140038933	-7.786977660259

C	1.673369886317	-1.138944223790	-7.587590941547
H	2.126035302866	-1.731128233213	-8.389023277562
H	0.961188819534	-1.780001823118	-7.059918930302
H	1.108298760745	-0.325070428478	-8.052774958387

cisVAPNB_TS-F1000

($E_F = -840.18052539$ a.u.; $G_F = -839.84543400$ a.u.)

0 1

C	2.125387198889	0.084186094899	-5.304547986836
C	3.177131465646	0.565125114317	-4.251731557433
C	1.629012776392	-0.811223723891	-3.069543293458
C	1.249799399527	-0.967473891979	-4.556464916297
H	1.501064700239	0.938738067175	-5.588496658792
H	0.181663604406	-0.819971128589	-4.733312739894
H	1.485224805801	-1.989333704027	-4.875137330052
C	3.149561830775	-0.545888600811	-3.171172175384
H	3.589831783994	-0.219070102374	-2.226715038711
H	3.678432538192	-1.445170567561	-3.510811579172
C	2.836671547096	1.892851924470	-3.644153081222
H	2.000911464034	2.437849276013	-4.074008828143
C	0.928497335611	0.336057571703	-2.399343488291
H	0.220779411085	0.900390397082	-3.001508927106
H	4.192827444401	0.622505095809	-4.671006906363
H	1.445461382973	-1.734117060137	-2.503055475610
C	3.950821548480	2.743725290667	-3.080134887510
H	3.536460844238	3.494548877239	-2.399019418837

H	4.626489349851	2.120305083613	-2.482543961376
C	0.595037169388	0.230795220852	-0.930250140818
H	1.460948203871	-0.161546224334	-0.383613326563
H	0.393604190674	1.226897635019	-0.522238338948
C	4.807923279487	3.488973857585	-4.165166974913
H	5.592183870379	4.080152847172	-3.684780333166
H	5.281836729774	2.777420911045	-4.846123084564
H	4.182418497822	4.160543041898	-4.759183251138
C	-0.639533979477	-0.686204394848	-0.610536577673
H	-0.470106780625	-1.706919126970	-0.962835753389
H	-0.814833250506	-0.718798956377	0.468226474650
H	-1.541464394792	-0.304394828119	-1.096409200696
Si	2.903453177305	-0.549069518611	-6.912116728333
C	4.127049835515	-1.937378779590	-6.527060217844
H	3.635122950649	-2.776937968442	-6.027096244626
H	4.584425278589	-2.319283894129	-7.444982996675
H	4.931860842936	-1.585708984251	-5.874806728341
C	3.812067361739	0.874779231427	-7.758369921587
H	4.594462223698	1.284623980434	-7.112710798699
H	4.284641621265	0.547968251693	-8.689740483709
H	3.122138024675	1.689024879764	-8.000687564235
C	1.544124090470	-1.203976058541	-8.048084093956
H	1.959895217658	-1.582898285212	-8.986813788063
H	0.993322368791	-2.021196946178	-7.572709734727
H	0.825469015036	-0.416137862193	-8.294332240063

cisVAPNB_R-F1000

($E_F = -840.24651443$ a.u.; $G_F = -839.90384164$ a.u.)

0 1

C	2.122599388008	0.066399514172	-5.438677874831
C	3.096016358073	0.554768047081	-4.321932506577
C	1.662662876233	-0.779796466694	-3.204269353501
C	1.190140524925	-0.930029374724	-4.663489548547
H	1.533113230922	0.921454506028	-5.792450967203
H	0.130529396378	-0.691728210036	-4.786099505455
H	1.326497033785	-1.966147768969	-4.993978405628
C	3.185115505345	-0.668718859592	-3.390380546995
H	3.723766171053	-0.463178499063	-2.461892798151
H	3.626228433351	-1.550726360621	-3.859047467693
C	2.355986054101	1.580601653256	-3.417250621300
H	1.799284203864	2.280300855178	-4.050635709298
C	1.284970624995	0.635966047999	-2.675121939749
H	0.295304798669	0.905268799082	-3.061903262693
H	4.048468441506	0.927232834828	-4.700530524874
H	1.323599153597	-1.590421574937	-2.558381604989
C	3.330290680306	2.441982682115	-2.580778511141
H	2.753700915715	3.057142941426	-1.881643827676
H	3.967551725266	1.800162251296	-1.962163062433
C	1.170027194579	0.673587874702	-1.135287639979
H	2.102898636051	0.314696128298	-0.684655528877
H	1.054995273159	1.712218087666	-0.806976532374
C	4.233195984650	3.381988193330	-3.434583794367

H	4.837981623297	4.021191536152	-2.786333917201
H	4.913428047639	2.818356282346	-4.076557657573
H	3.624259965580	4.027385243187	-4.075189807058
C	-0.021684559723	-0.155696069576	-0.570648766444
H	0.081571616007	-1.219308792094	-0.796159492236
H	-0.081198329979	-0.047744054088	0.515374237568
H	-0.968560006579	0.187951840022	-0.998392112795
Si	2.939739302611	-0.638334159569	-6.997393802216
C	4.094868406453	-2.078070543601	-6.591141201399
H	3.567867105033	-2.882847303349	-6.070184193746
H	4.518955675880	-2.498423883548	-7.508518898617
H	4.925905571069	-1.755626029614	-5.957269623677
C	3.932054215029	0.731026507981	-7.840718552126
H	4.729317881649	1.100846264467	-7.188850451167
H	4.396825584213	0.372986402255	-8.764564827728
H	3.290371023787	1.580017645908	-8.096210668107
C	1.578696654107	-1.245781118214	-8.158678621718
H	1.998789651412	-1.658978665596	-9.080865551696
H	0.978206002723	-2.028594695808	-7.685344304828
H	0.904128089226	-0.429188257488	-8.434238491151

cisVAPNB_P-F1000

($E_F = -840.23314106$ a.u.; $G_F = -839.90404154$ a.u.)

0 1

C	2.123094541887	0.535061534111	-5.078052810685
C	3.093619991789	1.177685783093	-4.013288429455

C	1.486284412327	-0.197176359525	-2.766950719624
C	1.071063625500	-0.291236296116	-4.273008372072
H	1.605900192659	1.361987002489	-5.579016332527
H	0.072649957420	0.137072346119	-4.400691174916
H	1.001131666245	-1.338434538006	-4.581304777525
C	2.214025647712	1.169580378411	-2.721603702532
H	1.479825101279	1.983354457981	-2.772501328389
H	2.805229134998	1.307706138092	-1.812667606190
C	3.668328188219	2.496533939305	-4.446776818679
H	2.962879740244	3.300482192279	-4.651035436379
C	0.348575342209	-0.429630701508	-1.812748845268
H	-0.337739523750	0.394698717963	-1.628349187932
H	3.926478554570	0.487061519180	-3.824623098518
H	2.243444336193	-0.975756426592	-2.594641634518
C	5.138827446308	2.812263359441	-4.513492326753
H	5.473872637721	3.194302685289	-3.532731260036
H	5.699128126504	1.878977063232	-4.652885680593
C	-0.080695321180	-1.829906520807	-1.452950813532
H	-0.321383762013	-2.374206950174	-2.383339563029
H	0.786275629522	-2.369770713597	-1.043331210636
C	5.590384458449	3.839966370042	-5.591738437807
H	6.666567701314	4.015391303231	-5.521042290448
H	5.363496153692	3.475611317237	-6.596742019161
H	5.079732112859	4.797626058649	-5.455493164608
C	-1.278570195616	-1.991366585935	-0.480314650031
H	-2.180311268093	-1.526524862498	-0.889312401212

H	-1.489172539025	-3.049391358034	-0.308411859067
H	-1.066792634608	-1.522929652806	0.484955238925
Si	2.986848599184	-0.472179191066	-6.433782458964
C	3.876951393878	-1.939338964101	-5.640643390899
H	3.185736190925	-2.559337769663	-5.061725494696
H	4.335669022619	-2.576193854235	-6.403223342358
H	4.670758821736	-1.605623378697	-4.965863819429
C	4.234883354968	0.587840115117	-7.373397912912
H	5.056892289401	0.905326293159	-6.727575441483
H	4.662828057819	0.030024288059	-8.212516036162
H	3.761791838710	1.488993702127	-7.774370825317
C	1.680629934959	-1.108932250801	-7.641943662658
H	2.136681824229	-1.710485412243	-8.434396501226
H	0.938353323490	-1.732241399375	-7.134727367456
H	1.149657976202	-0.278166039059	-8.117236636749

cisVAPNB_TS-F500

($E_F = -840.09104935$ a.u.; $G_F = -839.75739529$ a.u.)

0 1

C	2.126836165269	0.044371964162	-5.275017958634
C	3.186903342682	0.546505261096	-4.237661051258
C	1.617115188524	-0.845628642109	-3.040309909752
C	1.299528822034	-1.048312440071	-4.535619216329
H	1.465708804172	0.882331514120	-5.523101751783
H	0.230736997589	-0.975314282900	-4.751260762523
H	1.614580838963	-2.056827801668	-4.826986812799

C	3.128224323935	-0.508725653358	-3.097297960935
H	3.516573924815	-0.122811067738	-2.152463173120
H	3.702960154924	-1.403992450601	-3.367005279342
C	2.907422243850	1.924028178991	-3.728393200748
H	2.049966956040	2.457543515789	-4.126937448026
C	0.824846170580	0.256910522656	-2.409522416081
H	0.158245760025	0.835575808255	-3.043013919997
H	4.207364504487	0.536335366935	-4.651714108134
H	1.469052732397	-1.771188110572	-2.466168354516
C	4.013988401335	2.749440550976	-3.137268265312
H	3.597792852075	3.511208640386	-2.468844128211
H	4.664221725996	2.115647602152	-2.522091094965
C	0.519751896325	0.225151107996	-0.940386446953
H	1.396189462830	-0.135787597335	-0.388360518814
H	0.316370216823	1.238339890466	-0.576733863242
C	4.893226411167	3.461927746740	-4.209067083764
H	5.687176122850	4.044007585182	-3.732199254989
H	5.358857864510	2.733302833361	-4.878197651962
H	4.288756847797	4.138981494748	-4.818666628155
C	-0.696476397987	-0.680437110294	-0.579799084823
H	-0.521567007657	-1.712075923385	-0.897050715405
H	-0.871182551931	-0.679647876055	0.500168883247
H	-1.604231741159	-0.324763561952	-1.074899518268
Si	2.891692570785	-0.526981441945	-6.911300975461
C	4.146963078522	-1.900096246853	-6.575934082835
H	3.674284159891	-2.767269336667	-6.105385259994

H	4.611848260104	-2.239818561274	-7.506556126260
H	4.944722083224	-1.553914581153	-5.912118823734
C	3.760634688294	0.938038088285	-7.728172568996
H	4.539229697703	1.348138823578	-7.078131006560
H	4.231753628055	0.646531801051	-8.671933141783
H	3.050680731642	1.742895466811	-7.942496273742
C	1.531476007024	-1.180273484703	-8.047114074445
H	1.942159679810	-1.525090927782	-9.001161934830
H	1.004885533457	-2.021628731478	-7.586374644577
H	0.792804824175	-0.401865891136	-8.262582689759

cisVAPNB_R-F500

($E_F = -840.17547689$ a.u.; $G_F = -839.83225324$ a.u.)

0 1

C	2.119628114703	0.062295223190	-5.449458943348
C	3.088650278244	0.552781565862	-4.329813993805
C	1.656609310158	-0.787608836613	-3.215331173155
C	1.185661341756	-0.934805179944	-4.675765703551
H	1.529936467462	0.916262136038	-5.805566336140
H	0.126405652398	-0.695245658977	-4.799064729711
H	1.321279421745	-1.970462493850	-5.007781307780
C	3.179478746267	-0.673514140324	-3.401298880460
H	3.719039044167	-0.471495452531	-2.472786830352
H	3.621211130064	-1.553319787095	-3.873277210521
C	2.335193806924	1.570098073639	-3.427339758720
H	1.785069554495	2.274520460045	-4.061265535158

C	1.278294482741	0.627809378851	-2.688314646395
H	0.278969587348	0.889140990299	-3.055239395010
H	4.040379517275	0.931915847862	-4.703995346811
H	1.317272602584	-1.599343025309	-2.570815409625
C	3.282530132734	2.417725074894	-2.555046484467
H	2.689298703797	3.009110514425	-1.850211701554
H	3.918663458292	1.768660693199	-1.943268989309
C	1.211260219708	0.691641093602	-1.150824879158
H	2.155828694950	0.338304114181	-0.721269106539
H	1.106812804878	1.735040877254	-0.836037855139
C	4.172240982415	3.381484522169	-3.372307794210
H	4.775096446546	4.007890292401	-2.709358540833
H	4.856645359172	2.843701876476	-4.032506410040
H	3.559958800451	4.041935633209	-3.994538368440
C	0.040018965271	-0.117711959639	-0.550444782834
H	0.127394637339	-1.184524890049	-0.769339928082
H	0.007027006090	-0.003643050974	0.536427180551
H	-0.916955983154	0.227664124394	-0.954294272404
Si	2.941216833117	-0.641814308126	-7.006226840417
C	4.097120596929	-2.080558673076	-6.598778804823
H	3.570252940733	-2.886110703701	-6.078896767405
H	4.522748121680	-2.500066764652	-7.515833582300
H	4.927067196052	-1.757577857610	-5.963772359723
C	3.933635090072	0.728808580958	-7.847265934232
H	4.729473173259	1.099028337196	-7.193896260014
H	4.400267928224	0.371525540272	-8.770466757056

H	3.291627427431	1.577313475230	-8.103512807658
C	1.582959200073	-1.250346540937	-8.170186955336
H	2.005234367281	-1.662955963159	-9.091638111612
H	0.982327228411	-2.033851304626	-7.698188179419
H	0.908115215103	-0.434377249773	-8.446879184880

cisVAPNB_P-F500

($E_F = -840.11484851$ a.u.; $G_F = -839.78553423$ a.u.)

0 1

C	2.070645453494	0.555071846260	-5.187452568239
C	3.062057274648	1.114017084849	-4.097319337958
C	1.414016887495	-0.267158510915	-2.921611629158
C	0.968795175975	-0.230158980142	-4.413972123153
H	1.609076364641	1.417865127804	-5.681599464904
H	0.007870956411	0.287953359396	-4.486963824339
H	0.801353658264	-1.245475555905	-4.785128452705
C	2.203747553369	1.064213287065	-2.797354209665
H	1.502547913995	1.907150644433	-2.785701037370
H	2.810795106286	1.117829673427	-1.889919594861
C	3.647452271893	2.443648480928	-4.438124576685
H	2.949805712189	3.253561230998	-4.646263360750
C	0.293237155079	-0.469871425337	-1.957946238555
H	-0.488780021119	0.287474332513	-1.935160328702
H	3.884341212218	0.400172702149	-3.953868909800
H	2.136827671109	-1.085257356820	-2.804260052259
C	5.107846029520	2.774651212128	-4.382396209977

H	5.365245331714	3.173887797468	-3.385369323794
H	5.693464465101	1.851755511570	-4.478020414130
C	0.233392588267	-1.580467306776	-0.952952662697
H	0.799821767064	-2.441011574199	-1.331886421034
H	0.759441923275	-1.279418775864	-0.029234278551
C	5.585244068008	3.797518529602	-5.440002624098
H	6.649183853168	4.015997137604	-5.316298466016
H	5.427213249803	3.413001001833	-6.450802398763
H	5.034240063254	4.738137639634	-5.347693328993
C	-1.190990504767	-2.036277559007	-0.562785487409
H	-1.731487593395	-2.414950232242	-1.434652704445
H	-1.153320058099	-2.828637358761	0.189258874908
H	-1.766768920029	-1.203776208212	-0.147480671282
Si	2.923723421244	-0.462670579787	-6.540889567477
C	3.651037312729	-2.028382426927	-5.769830173611
H	2.878755426170	-2.621743249831	-5.271158909686
H	4.114428248974	-2.660357528241	-6.533637110736
H	4.418355886294	-1.788330989556	-5.027962640716
C	4.305573370376	0.541554127295	-7.344931808393
H	5.084664529935	0.794033285330	-6.621042987574
H	4.772676549003	-0.018895164026	-8.160953719305
H	3.921007986666	1.479318053960	-7.756483515729
C	1.648265093755	-0.943047267460	-7.849161867229
H	2.100138905301	-1.553689428575	-8.637021966554
H	0.827527351910	-1.518263223874	-7.410272240947
H	1.217753574880	-0.054206205762	-8.320868327890

transVAPNB_TS-F3500

($E_F = -840.63341093$ a.u.; $G_F = -840.29655712$ a.u.)

0 1

C	2.053015792263	-0.041472096172	-5.567086882517
C	2.950640173645	0.658190352006	-4.499214022221
C	1.561370717772	-0.755337234920	-3.251805609431
C	1.149742231124	-0.998303071642	-4.719555178207
H	1.428330537198	0.703855825476	-6.067222715324
H	0.084870534462	-0.810819971703	-4.880116572864
H	1.322619022230	-2.050444773676	-4.971777119042
C	3.059973294910	-0.397511079963	-3.391117932074
H	3.493167492964	0.000819011356	-2.469822004081
H	3.649937599951	-1.263630292946	-3.703058901360
C	2.297275951626	1.893736257887	-3.922278312464
H	2.856474986872	2.296753760246	-3.077700526020
C	0.854415427198	0.415848014919	-2.615595062071
H	-0.098368615284	0.678452796263	-3.070593630183
H	3.942715586701	0.929411534978	-4.890160857231
H	1.421526423171	-1.656802332834	-2.642930102495
C	0.792184535775	0.372004622259	-1.049842182439
H	1.817653471802	0.331755717297	-0.666130881195
H	0.372636360467	1.317478640791	-0.693762325879
C	1.871842431927	3.021924247410	-4.927604075242
H	1.038834682517	2.659855213578	-5.538357177635
H	1.467252898463	3.849830929822	-4.338210251305

C	2.921324326614	3.710381555445	-6.004152299139
H	3.764604170127	4.172807018581	-5.487178350583
H	3.296998115429	2.968583073770	-6.709590183814
H	2.362328215447	4.476116612518	-6.543726362348
C	-0.019375979295	-0.815845805913	-0.232258655695
H	-1.078587038793	-0.817984689637	-0.496815988080
H	0.405148682012	-1.798299621523	-0.445340516329
H	0.089262145670	-0.597997528377	0.831070332750
Si	2.984379793832	-0.905824656252	-6.976137440011
C	4.201053104563	-2.194425294149	-6.318086257277
H	3.700793273356	-2.936761849987	-5.689075953251
H	4.677052188178	-2.728289676738	-7.146691547971
H	4.992740240836	-1.729320717380	-5.723566349972
C	3.933650452784	0.375052099425	-7.990757283464
H	4.669413926525	0.905293754527	-7.378800188336
H	4.470563915169	-0.100762725180	-8.817299490515
H	3.255043344351	1.119146190736	-8.418996586971
C	1.715357569576	-1.762625578789	-8.083765717620
H	2.202067063467	-2.271346327385	-8.921604519561
H	1.143012681563	-2.510488354752	-7.526672680351
H	1.005020075760	-1.040092428819	-8.497887997452

transVAPNB_P-F3500

($E_F = -840.84621719$ a.u.; $G_F = -840.51788396$ a.u.)

0 1

C	1.711592843439	0.469420580825	-5.395451558639
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C	2.667760176335	1.518375206410	-4.658017449290
C	1.657048723469	-0.083817067979	-2.944295467545
C	0.873426534672	-0.251402290004	-4.279793130755
H	1.028343621210	1.021703806053	-6.049588628856
H	-0.104396862601	0.229160818750	-4.168624520546
H	0.677740476368	-1.305168832866	-4.499089541226
C	2.151631049493	1.414067442578	-3.149610607236
H	1.300736711700	2.090985015803	-3.007608772158
H	2.928054574764	1.704016282981	-2.437846333353
C	2.759064362546	2.916784654144	-5.343593172742
H	1.937604595877	3.601681132905	-5.137875623733
C	0.866823039806	-0.534486081334	-1.681770565542
H	0.130224805006	0.162556358954	-1.286799542995
H	3.686106575875	1.106964273797	-4.659056088461
H	2.549126151233	-0.720227405108	-3.007487215135
C	0.822154444258	-2.015350091732	-1.200979043323
H	0.456377716549	-2.612907864629	-2.052287128700
H	1.864378670171	-2.343413921193	-1.080482293355
C	3.674706641412	3.222808201360	-6.565829700636
H	4.666751184760	2.811986095556	-6.335704546601
H	3.311903060178	2.589545683984	-7.388363938906
C	3.935075639949	4.674765918282	-7.261821253251
H	3.002613454530	5.110042111260	-7.627918808071
H	4.402203489449	5.375400508900	-6.566448535079
H	4.605262863219	4.506932897818	-8.105934449083
C	0.017611103505	-2.585589189891	0.097084279954

H	0.380326084006	-2.128874073623	1.020347073365
H	-1.055215874213	-2.400735519166	0.009440896148
H	0.191916938311	-3.661577333599	0.137653240763
Si	2.590522485337	-0.836657948485	-6.470195913113
C	3.581376288526	-1.998853631819	-5.354333881378
H	2.939804996639	-2.515174227598	-4.634954195185
H	4.089157599001	-2.760236007381	-5.954607598077
H	4.346862262295	-1.456424496081	-4.791386262994
C	3.774204274641	-0.109669985801	-7.748726683692
H	4.579424810472	0.465525802774	-7.286079368740
H	4.231562029512	-0.925083511444	-8.318754868121
H	3.257737150410	0.541418524398	-8.459408823849
C	1.273333872790	-1.830076259812	-7.394405572968
H	1.735358097349	-2.608203347042	-8.010087554218
H	0.574473855362	-2.318711133279	-6.709806954718
H	0.691796613501	-1.182462395690	-8.058156363725

transVAPNB_R-F3500

($E_F = -840.64935795$ a.u.; $G_F = -840.30872135$ a.u.)

0 1

C	2.092921271957	-0.042936922749	-5.596376780670
C	2.939759420596	0.561966956119	-4.435541747293
C	1.456735120752	-0.747151980665	-3.342354303599
C	1.077037054525	-0.953546832980	-4.823525917851
H	1.549150112976	0.750573401220	-6.116243120124
H	0.037657069487	-0.678649108062	-5.023006849123

H	1.182400128752	-2.011735875833	-5.088130575956
C	2.988529562546	-0.601011390918	-3.430981160547
H	3.456178208100	-0.326551032933	-2.482041891986
H	3.482108689512	-1.495380419853	-3.815282552756
C	2.106549951488	1.634537816267	-3.677517377457
H	2.756500627213	2.096206275115	-2.924717787224
C	1.016825982968	0.649606184391	-2.839244127594
H	0.001361572771	0.876763563726	-3.181279587014
H	3.910445328618	0.953389417300	-4.749328509105
H	1.097528892440	-1.555587347817	-2.704430815873
C	1.015619403658	0.675240233810	-1.235737470259
H	2.060004032179	0.681253103863	-0.905437288886
H	0.605347464193	1.641977766073	-0.924862185049
C	1.597447010559	2.799680302432	-4.647974683891
H	0.709512882135	2.435510485631	-5.174937775228
H	1.239788427825	3.617844279077	-4.014298198625
C	2.550729698241	3.483718293283	-5.788885949549
H	3.431015759031	3.949444791830	-5.339739106432
H	2.881206964165	2.747367331361	-6.522285980097
H	1.959054637162	4.250966611484	-6.290336905768
C	0.269487927933	-0.460838324351	-0.321534196843
H	-0.789109049342	-0.546585976692	-0.578209143598
H	0.741909301813	-1.437428567420	-0.438067082908
H	0.358668397818	-0.146624044825	0.719523989479
Si	3.055091841138	-0.905634467666	-6.985471881808
C	4.148914080415	-2.311811409171	-6.353707695706

H	3.570971910466	-3.054314845107	-5.795653956004
H	4.625142201047	-2.826086057038	-7.194588902622
H	4.942220727587	-1.940809708486	-5.698544992411
C	4.141317114761	0.363973550166	-7.869117978726
H	4.844420203341	0.837098405128	-7.177101284066
H	4.724805173541	-0.106045511437	-8.666883408509
H	3.535650276913	1.154702350844	-8.322180528339
C	1.796059643386	-1.611807188738	-8.205267526709
H	2.292509691108	-2.106620883041	-9.045701151190
H	1.146907214120	-2.347729114694	-7.721184922210
H	1.157784253469	-0.821050649917	-8.611679509717

transVAPNB_TS-F3000

($E_F = -840.54255008$ a.u.; $G_F = -840.20598992$ a.u.)

0 1

C	2.048432281517	-0.042904171302	-5.562830111072
C	2.952401080177	0.665395650934	-4.505369445285
C	1.571943869340	-0.759138607317	-3.242267169369
C	1.158630138235	-1.006530942934	-4.708891398881
H	1.413940884498	0.697165293882	-6.058371725624
H	0.091343275523	-0.830463532893	-4.866135561835
H	1.341125888258	-2.057159268004	-4.960463355050
C	3.065274941649	-0.379136310375	-3.386397505373
H	3.493707044407	0.030960545720	-2.468092835536
H	3.665456576848	-1.241224953519	-3.690853472408
C	2.318288653882	1.915446663029	-3.945939862350

H	2.862681863670	2.313688817753	-3.089879815166
C	0.840555917784	0.388590706090	-2.597126876341
H	-0.103951010914	0.661282792864	-3.062507140352
H	3.946783051498	0.920273634544	-4.903589120329
H	1.454616394620	-1.667016415235	-2.637081186390
C	0.787961981415	0.365572688235	-1.045013618630
H	1.813863692392	0.321338401704	-0.662000972425
H	0.373657669347	1.315605444618	-0.694228465260
C	1.877949623113	3.028632371918	-4.938446563180
H	1.053182396249	2.657536923310	-5.555603769461
H	1.460645916574	3.851799285283	-4.350864398418
C	2.934916228340	3.703628820935	-5.983757311805
H	3.770805153986	4.164329382684	-5.452578647389
H	3.324804531996	2.958930958219	-6.678918592247
H	2.398260629710	4.471802591654	-6.543085036447
C	-0.028108095755	-0.809030713880	-0.255496609927
H	-1.085231048488	-0.801926613878	-0.529764860664
H	0.388253892217	-1.793535958394	-0.476987367660
H	0.066919064391	-0.613453739756	0.813923289792
Si	2.975415152895	-0.904465052409	-6.976497577306
C	4.201600567546	-2.184134459385	-6.319221736012
H	3.707846142849	-2.927118350255	-5.686002714872
H	4.678144734411	-2.717957146174	-7.147470077023
H	4.992232942878	-1.712278020534	-5.728748140687
C	3.913400650113	0.377975368999	-7.999207815677
H	4.656663427453	0.906253683351	-7.394778396549

H	4.440414013464	-0.096763478510	-8.832697838443
H	3.230713911853	1.123558127558	-8.418048252862
C	1.705271427432	-1.770661929983	-8.075173215911
H	2.190209853158	-2.278811869262	-8.914375133414
H	1.139998653071	-2.520126841643	-7.513235133755
H	0.988937841330	-1.053018657094	-8.487200819681

transVAPNB_P-F3000

($E_F = -840.71602844$ a.u.; $G_F = -840.38820955$ a.u.)

0 1

C	1.794497352371	0.434743041601	-5.404554503083
C	2.711670252268	1.429132349540	-4.603479701903
C	1.612860544874	-0.119429269172	-2.954042319552
C	0.918129104560	-0.321761331279	-4.337294069967
H	1.131975093311	1.006705074540	-6.062723222231
H	-0.081906753288	0.121441699205	-4.289282885901
H	0.776956997407	-1.382760684652	-4.563370179154
C	2.092079093851	1.374307924400	-3.140073222142
H	1.225799695707	2.043150347662	-3.078145421341
H	2.812429576918	1.686901911196	-2.379788839332
C	3.037925301998	2.812858493713	-5.227169026991
H	3.461201622117	3.526138700413	-4.521785028406
C	0.760116905390	-0.540788352273	-1.738242542243
H	-0.046628889099	0.127738592941	-1.443628066787
H	3.698346845220	0.946759488702	-4.481648826609
H	2.516163926217	-0.743847821778	-2.949579504030

C	0.778928167960	-1.976410331466	-1.166608353152
H	0.518807170854	-2.658060185955	-1.993866154659
H	1.826790080073	-2.224521556070	-0.943645199340
C	2.871358043007	3.308270180109	-6.677376455375
H	2.810431777162	2.442992869209	-7.341877377289
H	1.875343989445	3.777334358512	-6.746520317997
C	3.877055625661	4.366082250200	-7.372446554798
H	3.929165060266	5.293904547079	-6.797920169309
H	4.884025845704	3.952136928102	-7.461825509522
H	3.492715099544	4.588413747444	-8.369286087744
C	-0.090548221448	-2.467303801847	0.096339671187
H	0.170450558799	-1.908789776463	0.998256073065
H	-1.160503839074	-2.348332440202	-0.090263965844
H	0.123151476921	-3.524586020118	0.260673193144
Si	2.759170117768	-0.810963618212	-6.474291633960
C	3.668499537475	-2.018630242603	-5.336763091038
H	2.978207684166	-2.556877326784	-4.681379580321
H	4.213328849388	-2.760586333510	-5.928757006577
H	4.396130770328	-1.501907106347	-4.703988011492
C	4.043385241758	0.030244216298	-7.576448324572
H	4.670799070446	0.721671100861	-7.006745239409
H	4.697914354518	-0.722401304376	-8.027473791030
H	3.577575140171	0.592351402389	-8.390507933345
C	1.542212657749	-1.768680925369	-7.556691221757
H	2.060395370139	-2.515931224174	-8.165696557318
H	0.794991518738	-2.291347565445	-6.952258611085

H	1.010004738182	-1.095332616751	-8.235909511352
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transVAPNB_R-F3000

($E_F = -840.56819503$ a.u.; $G_F = -840.22676368$ a.u.)

0 1

C	2.090768144744	-0.051975396784	-5.595002110826
C	2.941304922554	0.557019042004	-4.439010948317
C	1.467728006620	-0.753071586001	-3.337338464513
C	1.084325582912	-0.968346347299	-4.816247188305
H	1.539007262349	0.738615686251	-6.111168815126
H	0.042222827654	-0.702392410044	-5.013601906193
H	1.197667681316	-2.026514618322	-5.077591253949
C	2.998740354620	-0.604829394813	-3.432981354245
H	3.470805951481	-0.327741842850	-2.486976497026
H	3.492193196660	-1.498765650809	-3.818459021443
C	2.104218868181	1.621538612080	-3.671730452820
H	2.758419456318	2.083983752233	-2.922460761881
C	1.028757938987	0.650879607627	-2.848427417968
H	0.012023738765	0.871186957054	-3.192585944278
H	3.908557023957	0.952937694786	-4.756965556995
H	1.110456212326	-1.557168207373	-2.693233884518
C	1.032657584377	0.710049798193	-1.258625147992
H	2.076804713875	0.707551140150	-0.926659729115
H	0.635228139272	1.687771040259	-0.964636719263
C	1.574454570217	2.778843246897	-4.618662690884
H	0.694077915170	2.406765342060	-5.153289091504

H	1.201847188779	3.585249328883	-3.978045077786
C	2.532801317272	3.461547279800	-5.726429438804
H	3.409817430901	3.919312534852	-5.261748752900
H	2.873854386580	2.730683394699	-6.460974753833
H	1.960232349346	4.237885453508	-6.236844823785
C	0.270795928181	-0.399535081176	-0.361763171531
H	-0.784111314332	-0.478966687244	-0.637113750411
H	0.733688855387	-1.382427327418	-0.464882414380
H	0.338635459399	-0.089730950708	0.682636985370
Si	3.050785408899	-0.906700710169	-6.990181637668
C	4.158419629351	-2.304926600544	-6.365013566090
H	3.588558042147	-3.053207792975	-5.806351772977
H	4.636124436022	-2.813772697506	-7.208349124178
H	4.950739662760	-1.928472345358	-5.711762902534
C	4.122140777421	0.373075483862	-7.877236090918
H	4.830702271182	0.844450636859	-7.189601551219
H	4.698923310530	-0.088799305012	-8.684562132852
H	3.508075492812	1.164379633819	-8.317874512348
C	1.790367922869	-1.620870964779	-8.203802803665
H	2.285655803957	-2.112802397714	-9.046602422747
H	1.148149050759	-2.360670300383	-7.716365819311
H	1.145230478359	-0.834136874679	-8.607172733218

transVAPNB_TS-F2500

($E_F = -840.45223840$ a.u.; $G_F = -840.11555874$ a.u.)

0 1

C	2.045011231266	-0.046424852074	-5.558707295335
C	2.955284152148	0.666903128866	-4.509088863525
C	1.579509792995	-0.765805531194	-3.234961570217
C	1.167161161427	-1.017647618736	-4.701115600991
H	1.401927329506	0.690229227105	-6.048161281123
H	0.097878847623	-0.853528276883	-4.857287939120
H	1.360618699984	-2.066416901678	-4.952016422385
C	3.068543357811	-0.369529167598	-3.381680999307
H	3.493210019667	0.048697318838	-2.465351715884
H	3.676081440462	-1.228779537551	-3.680291262545
C	2.337565693928	1.928641231021	-3.962319056327
H	2.866200032684	2.320499017410	-3.093766610792
C	0.828854823042	0.365039770888	-2.585536873122
H	-0.107061743082	0.649035556158	-3.061020589447
H	3.951446009619	0.907449173216	-4.913221553730
H	1.477585214918	-1.677570061527	-2.632112065145
C	0.785604572457	0.366961941826	-1.045275627972
H	1.811842711141	0.318760156236	-0.662911851490
H	0.377647941843	1.323130095710	-0.703089347096
C	1.882711512553	3.030575121829	-4.941059958999
H	1.063658920133	2.653335465646	-5.562602894584
H	1.456642523265	3.849178397982	-4.353075149311
C	2.946038746888	3.692403048867	-5.958846576477
H	3.776825703330	4.148764529683	-5.415381094208
H	3.345818205924	2.944905362427	-6.645702727083
H	2.431580264668	4.464691426164	-6.533989413056

C	-0.036622691993	-0.791821550868	-0.277662161001
H	-1.091334185249	-0.775878139690	-0.562008882557
H	0.371459523331	-1.779202804953	-0.503164933322
H	0.044484115442	-0.613157288431	0.796316366034
Si	2.967794300020	-0.902392678916	-6.978496539682
C	4.207261582572	-2.170770938478	-6.324253646975
H	3.722048627722	-2.917683702677	-5.689053171501
H	4.686791690359	-2.700869117318	-7.153159749741
H	4.994855521102	-1.690928269381	-5.736104302932
C	3.890750692526	0.384433043799	-8.009314105659
H	4.640287123270	0.912610910934	-7.412644555881
H	4.408766605234	-0.087636555504	-8.849909560789
H	3.201959043805	1.129786474741	-8.418419389147
C	1.697500029937	-1.780000288575	-8.067821178397
H	2.181182687063	-2.286139652382	-8.908957999608
H	1.141120501803	-2.532530165917	-7.501115958084
H	0.973469471789	-1.068406178469	-8.476932248761

transVAPNB_P-F2500

($E_F = -840.59186379$ a.u.; $G_F = -840.26331745$ a.u.)

0 1

C	1.802103672030	0.415912876036	-5.404269960251
C	2.715511831536	1.401045790574	-4.592009538302
C	1.612036445288	-0.128257581664	-2.958393519836
C	0.929174698257	-0.349896903441	-4.344241910703
H	1.137741248636	0.994220816197	-6.054874606004

H	-0.078384165213	0.076778519558	-4.306261509176
H	0.807847051797	-1.414615360736	-4.564111037005
C	2.081749278319	1.360025725070	-3.141813861122
H	1.212037080835	2.025893123243	-3.095783792377
H	2.791327771868	1.680378898262	-2.374586530358
C	3.050610357586	2.772451575577	-5.207394115774
H	3.536311935599	3.463254476168	-4.519942924852
C	0.756133598658	-0.533320688335	-1.753737053717
H	-0.059143980757	0.130571414703	-1.472549603510
H	3.697173482399	0.911721324131	-4.456032441473
H	2.518178139949	-0.749064976586	-2.940992104630
C	0.781794838677	-1.956913885353	-1.181210923497
H	0.524826740521	-2.648411426883	-2.001933965641
H	1.828690979603	-2.202694976476	-0.949959589123
C	2.810917650263	3.290250223900	-6.627708449925
H	2.663990400154	2.441429199564	-7.300487262225
H	1.840999986771	3.816616899894	-6.631923731515
C	3.842368046582	4.289381676494	-7.331518127459
H	3.983451220067	5.192771010806	-6.732799548510
H	4.815069413233	3.812722687101	-7.475012633773
H	3.440698570458	4.574082686294	-8.305828757523
C	-0.095300555229	-2.400579063703	0.071676132813
H	0.162929576939	-1.820307125682	0.960993345230
H	-1.162148069206	-2.270805926457	-0.127340803307
H	0.095969665072	-3.455869845388	0.274137330289
Si	2.777320773331	-0.806102498329	-6.490075465142

C	3.695597589143	-2.019929352616	-5.366527544770
H	3.008761126221	-2.567921077559	-4.715476334593
H	4.243903954736	-2.753521301671	-5.965667195291
H	4.420805954979	-1.505212707946	-4.729391193173
C	4.052456672891	0.073337321344	-7.572768966594
H	4.663272291889	0.765851652076	-6.986462247380
H	4.722980453201	-0.658318867396	-8.034524068201
H	3.580462425467	0.643265720010	-8.377786246907
C	1.571707976232	-1.759961147558	-7.588100006275
H	2.097346023374	-2.494056136422	-8.206614054767
H	0.828710377043	-2.297591874744	-6.991528919112
H	1.033999465945	-1.082268545652	-8.258598376582

transVAPNB_R-F2500

($E_F = -840.48847611$ a.u.; $G_F = -840.14641945$ a.u.)

0 1

C	2.088753741356	-0.062912058034	-5.593379253139
C	2.943868310928	0.551389725404	-4.443678570688
C	1.482326949861	-0.761332144894	-3.331122490885
C	1.094320947961	-0.986581223388	-4.807382635367
H	1.527401129339	0.724354499350	-6.104647761303
H	0.048896109391	-0.731689886723	-5.001657152336
H	1.217490995746	-2.044469790277	-5.065360309975
C	3.012174430507	-0.608356541884	-3.435309830564
H	3.488949680844	-0.327112934866	-2.492864896331
H	3.506577564860	-1.501439449602	-3.821618028222

C	2.103823303238	1.607998651887	-3.667546197361
H	2.761965317612	2.070833210116	-2.921427153279
C	1.041229978640	0.648394126329	-2.856555652516
H	0.023447056648	0.860694470746	-3.203816141041
H	3.907163988431	0.951916242739	-4.767201908553
H	1.129491058409	-1.561673295072	-2.680177829028
C	1.047775844822	0.740946761390	-1.280033280991
H	2.090660139240	0.723731354824	-0.943836841361
H	0.668073358770	1.731302204918	-1.004327670270
C	1.554155405185	2.759288299057	-4.590616008502
H	0.682200187729	2.380865654666	-5.134920571039
H	1.166580434940	3.552276770298	-3.941760179776
C	2.518597636588	3.444804823309	-5.664885596727
H	3.392796591177	3.891146987662	-5.183064639066
H	2.868286898192	2.721733022575	-6.403551863820
H	1.965311098858	4.232860473102	-6.179396715762
C	0.261672568097	-0.338406362488	-0.399847540794
H	-0.789635006789	-0.402889940009	-0.693986847841
H	0.707238208472	-1.330689604843	-0.490657477634
H	0.311017622999	-0.033011468880	0.647277180472
Si	3.045906831310	-0.908140131570	-6.995902646748
C	4.169758128011	-2.296812876091	-6.378590214424
H	3.609594478223	-3.051847752933	-5.819193321818
H	4.649110362683	-2.799200891341	-7.224852005260
H	4.960888689503	-1.913862264940	-5.727663962569
C	4.099777802505	0.383293789396	-7.886954650961

H	4.813935370996	0.853659282542	-7.204421842744
H	4.669394340532	-0.069431185197	-8.704470318373
H	3.476012524873	1.174428376473	-8.314142287364
C	1.784063289906	-1.631723968616	-8.202354433740
H	2.278091363899	-2.119865096584	-9.048087152060
H	1.150249218506	-2.376345169035	-7.711252271797
H	1.130715175940	-0.849810487238	-8.601865743972

transVAPNB_TS-F2000

($E_F = -840.36231289$ a.u.; $G_F = -840.02562786$ a.u.)

0 1

C	2.040731622917	-0.050285973321	-5.553435339033
C	2.958149541622	0.670165254368	-4.513620735103
C	1.589147763656	-0.773724495674	-3.225922211757
C	1.178430395742	-1.031506668171	-4.691498379023
H	1.386631854837	0.681559555966	-6.035450987153
H	0.106670680839	-0.882983068797	-4.846377895268
H	1.386214520711	-2.077744628140	-4.941560843075
C	3.072334039496	-0.355437583869	-3.375280481380
H	3.491013647084	0.073969079657	-2.461386081254
H	3.690258207276	-1.210435227667	-3.665656402679
C	2.359937543372	1.946172790741	-3.983638997229
H	2.869450396300	2.332352177635	-3.101578095553
C	0.813957031627	0.335133891004	-2.571194435191
H	-0.112015674252	0.631719258190	-3.057695866023
H	3.956040658552	0.893516949080	-4.924904834233

H	1.507300359991	-1.689882932296	-2.625730209658
C	0.781084833318	0.362397272306	-1.042173234577
H	1.807769147041	0.308229726710	-0.661137611378
H	0.381103656421	1.325148778523	-0.708375054022
C	1.890591493881	3.035646216436	-4.951466275714
H	1.080296079331	2.649977813114	-5.579792588733
H	1.452439014320	3.849223576190	-4.365034957467
C	2.962251830494	3.687727214681	-5.940625907805
H	3.783672242328	4.143660250084	-5.382075508782
H	3.376957824798	2.937389130140	-6.615966800871
H	2.468971736632	4.460756565676	-6.533959850367
C	-0.049285093852	-0.780467172297	-0.294051304197
H	-1.101960251172	-0.751873072138	-0.586087409669
H	0.347463622810	-1.771352983742	-0.526219761802
H	0.021386568572	-0.619455312221	0.783913004761
Si	2.958573865360	-0.899804347779	-6.980225441856
C	4.209509943692	-2.158288807650	-6.328754154506
H	3.731584087660	-2.908598469010	-5.692043683154
H	4.692019725194	-2.685042210332	-7.158031348873
H	4.994050587915	-1.671455018716	-5.742215580699
C	3.868116297078	0.390920380834	-8.017992537338
H	4.625113902697	0.916963882555	-7.428915216657
H	4.375792824200	-0.078488832822	-8.866393382922
H	3.174449571800	1.137727893494	-8.416101413831
C	1.687716205019	-1.786928849399	-8.061066924513
H	2.169965502496	-2.292334925385	-8.903467919490

H	1.138265335202	-2.541148707066	-7.489861980460
H	0.957808661932	-1.080207250344	-8.468221718738

transVAPNB_P-F2000

($E_F = -840.46931877$ a.u.; $G_F = -840.14007743$ a.u.)

0 1

C	1.810910694508	0.398979760990	-5.405138543033
C	2.722120959214	1.375854189465	-4.583048645455
C	1.615709311361	-0.138191147882	-2.964665602658
C	0.940592778762	-0.373611931822	-4.351353388307
H	1.145288571065	0.983040327879	-6.049060033384
H	-0.072166778370	0.041018270700	-4.320187307117
H	0.833594452626	-1.440816160133	-4.566397746224
C	2.080015820013	1.344081953763	-3.143674159336
H	1.209005060172	2.009080892023	-3.107841200463
H	2.782585756296	1.667871716193	-2.371407375247
C	3.054791879439	2.741059897224	-5.186176253611
H	3.573167341018	3.419654802591	-4.510506789276
C	0.757379012562	-0.527144744440	-1.769756947427
H	-0.062129337676	0.135529588828	-1.498262255817
H	3.700982411938	0.882670160205	-4.440130061236
H	2.522569054891	-0.758135053051	-2.937509055834
C	0.783168093834	-1.941022822256	-1.198964691190
H	0.522383770188	-2.639220290147	-2.013371276001
H	1.828136517988	-2.190995834574	-0.962595957358
C	2.766727201283	3.272050215380	-6.582520133388

H	2.573703357784	2.435920162861	-7.259724311401
H	1.814153145515	3.828801847367	-6.549175710859
C	3.813672538781	4.233963618917	-7.280827656998
H	4.004991541465	5.117207783079	-6.665587466696
H	4.763635172890	3.721018651537	-7.450962988362
H	3.414197103448	4.561158581232	-8.243065315128
C	-0.100630251632	-2.336193898215	0.045969518753
H	0.161330326068	-1.737539382067	0.922342086643
H	-1.163796838403	-2.189609239811	-0.162878246286
H	0.063138102786	-3.389262927768	0.283001456002
Si	2.790760547859	-0.805487287324	-6.505026768974
C	3.721018038430	-2.022228924237	-5.394779005734
H	3.039747904642	-2.577021967104	-4.743528525252
H	4.269519412509	-2.749954416255	-6.000835666890
H	4.447002918843	-1.508119942361	-4.758063242791
C	4.053193166299	0.101208060226	-7.579796946052
H	4.657359795141	0.791922081897	-6.984493603270
H	4.730623357714	-0.615207829796	-8.055044301571
H	3.571710753888	0.678546002142	-8.373879325116
C	1.589738195644	-1.757894981820	-7.609111903125
H	2.119189163000	-2.481351200169	-8.236833530947
H	0.853258034693	-2.307603210766	-7.015428763795
H	1.044187081391	-1.077837812313	-8.270821743293

transVAPNB_R-F2000

($E_F = -840.41011198$ a.u.; $G_F = -840.06758921$ a.u.)

0 1

C	2.086503938910	-0.075889364775	-5.590943144015
C	2.947696638810	0.544666929463	-4.449275107339
C	1.500673044801	-0.771608898994	-3.323094312905
C	1.107104610002	-1.008540679470	-4.796125905270
H	1.513660220903	0.707721175888	-6.095535294534
H	0.057730746389	-0.767293364227	-4.986344034344
H	1.242384037478	-2.065845980891	-5.050385360467
C	3.028974703744	-0.611961643593	-3.437703789408
H	3.511095902690	-0.325104867165	-2.499629657109
H	3.524944187669	-1.504000384732	-3.824551817967
C	2.106118830873	1.593529623028	-3.664142540614
H	2.768362666027	2.055752402607	-2.920774449671
C	1.055062707552	0.643094329935	-2.863912188455
H	0.036668847274	0.846478361302	-3.215712754927
H	3.906493578194	0.949643341591	-4.780000829770
H	1.154507897870	-1.568135496500	-2.664065757211
C	1.061196950603	0.769528752365	-1.300497715994
H	2.101120358806	0.729036916740	-0.956575702130
H	0.706740985416	1.774880184091	-1.045095111793
C	1.537531903984	2.741034369219	-4.562240764022
H	0.674910320088	2.358227998209	-5.118518108386
H	1.134768339659	3.518451331876	-3.903518861635
C	2.509057197505	3.433674749072	-5.601488877616
H	3.380184515146	3.865700908398	-5.100557172767
H	2.866697354109	2.721109357447	-6.347031469574

H	1.975058962969	4.235628395247	-6.115681300147
C	0.239391590632	-0.272639551516	-0.437560955912
H	-0.808168952455	-0.309663029292	-0.750644870630
H	0.655958958312	-1.278527678694	-0.517971079697
H	0.273920345172	0.027549911878	0.612038806817
Si	3.039361075809	-0.909587861204	-7.002780109559
C	4.185076138714	-2.284425208292	-6.394987909783
H	3.638158044433	-3.048136582747	-5.834249881900
H	4.666745020927	-2.778535005127	-7.244795631459
H	4.974310282665	-1.892116646655	-5.747316873772
C	4.069324052553	0.396093091823	-7.900971642391
H	4.788789691702	0.868721022814	-7.225599628997
H	4.631418559541	-0.046293663261	-8.729264709677
H	3.432360499960	1.184248348033	-8.314057237743
C	1.775816653240	-1.647308641516	-8.198749713858
H	2.268206190240	-2.130579317494	-9.048224418378
H	1.153941041703	-2.398390080612	-7.702243535234
H	1.110984074705	-0.872610615275	-8.593342794163

transVAPNB_TS-F1500

($E_F = -840.27251916$ a.u.; $G_F = -839.93611987$ a.u.)

0 1

C	2.035516827464	-0.054302105757	-5.546726754249
C	2.961296234090	0.673830954087	-4.518091500237
C	1.598148739736	-0.783329613396	-3.215278065427
C	1.190670148307	-1.046953741830	-4.680773203578

H	1.369369846158	0.672454162576	-6.019729739286
H	0.116541362853	-0.916228243414	-4.834979733128
H	1.414916619320	-2.089860187940	-4.930261943173
C	3.074127444671	-0.338427557502	-3.366196552439
H	3.484302797052	0.104076912521	-2.454749936560
H	3.704535808938	-1.188274742930	-3.645806942004
C	2.388488963568	1.968502670290	-4.010790257591
H	2.874824817932	2.348872715952	-3.113603883063
C	0.793452683519	0.297103001039	-2.553053076572
H	-0.119499583024	0.610797287594	-3.052477349584
H	3.961660420152	0.874696547808	-4.936802142473
H	1.540076725407	-1.704617641714	-2.619078085823
C	0.771387960244	0.350532331798	-1.034959499316
H	1.798483373255	0.291165685681	-0.655352920943
H	0.378961978114	1.319808185454	-0.710515329807
C	1.906258499504	3.044598579486	-4.970582549194
H	1.106401762644	2.649680055162	-5.606875123003
H	1.454703883476	3.853265035045	-4.387219149292
C	2.986503820535	3.689618862859	-5.931467897835
H	3.797631103024	4.145719229428	-5.357745860006
H	3.416221669106	2.937598651583	-6.595776451254
H	2.513329874727	4.463124715603	-6.541197741231
C	-0.066390093759	-0.776472521953	-0.302262631949
H	-1.117012645168	-0.736990839456	-0.601186215037
H	0.320310122405	-1.770502990081	-0.539044185381
H	-0.005609292494	-0.629681215993	0.778845217517

Si	2.947658598459	-0.896328174844	-6.981570211360
C	4.211609822053	-2.143546942257	-6.333682594241
H	3.741997794850	-2.899004823402	-5.696938209074
H	4.698613911039	-2.664810376506	-7.163754429885
H	4.991730361382	-1.649242010226	-5.747469465000
C	3.841985145076	0.398929123982	-8.026719506463
H	4.607501629744	0.922252478364	-7.446366419595
H	4.337509335459	-0.067236397649	-8.884041698780
H	3.143051819201	1.147562648263	-8.411870435260
C	1.676512575829	-1.794029594754	-8.053122339646
H	2.157190273207	-2.298414838676	-8.897021389962
H	1.134943482615	-2.550206660312	-7.477091033911
H	0.940045184264	-1.092817493435	-8.457889122170

transVAPNB_R-F1500

($E_F = -840.33306422$ a.u.; $G_F = -839.99015163$ a.u.)

0 1

C	2.084075762259	-0.091558086620	-5.587676708755
C	2.953081131198	0.536500108407	-4.456165200214
C	1.523731636621	-0.784419479033	-3.313165186658
C	1.123420316715	-1.035153803589	-4.782186348783
H	1.497429928967	0.687746460431	-6.083609590798
H	0.069441390490	-0.810598684463	-4.967090164177
H	1.273503065391	-2.091440962659	-5.032357628126
C	3.050005056448	-0.615962773822	-3.440550438485
H	3.538282489943	-0.321874479069	-2.507846934607

H	3.548205898089	-1.506695154070	-3.827726456854
C	2.111458544634	1.577382186963	-3.661255121856
H	2.778210727157	2.037760736393	-2.920278951332
C	1.071207221390	0.634558463864	-2.870819231965
H	0.052735811602	0.828005781573	-3.228870016676
H	3.906593072442	0.945961215716	-4.795992777610
H	1.186683829018	-1.576745325670	-2.644393279433
C	1.073539202437	0.795663031982	-1.320555930312
H	2.107638284273	0.721354799977	-0.964347456192
H	0.754287190040	1.818423859554	-1.087720024690
C	1.523862659932	2.723360167773	-4.532106824105
H	0.672382364408	2.337627094924	-5.103521535910
H	1.104026761206	3.481401369715	-3.861270034506
C	2.502606315926	3.429869124692	-5.532870687723
H	3.368567311868	3.846777124445	-5.009915773587
H	2.870560979623	2.731836130109	-6.287639416897
H	1.986377911479	4.246552307917	-6.042772810203
C	0.202415873153	-0.199201131184	-0.477170436848
H	-0.840100962593	-0.192829243516	-0.809782418405
H	0.574793053849	-1.223054388039	-0.550257186283
H	0.225930348209	0.093917325676	0.575097988618
Si	3.030843549428	-0.911472164099	-7.011071472519
C	4.203653278925	-2.268258891389	-6.414805416231
H	3.673521777553	-3.042164479978	-5.851916890572
H	4.687856863280	-2.752522670727	-7.268816434339
H	4.990431432944	-1.863873078937	-5.771555495166

C	4.030608367624	0.410851653545	-7.918950424375
H	4.755540085489	0.888090085972	-7.252700107668
H	4.584139991650	-0.019838080406	-8.759072434591
H	3.377450875836	1.193847488836	-8.316371506485
C	1.765424598482	-1.667821905544	-8.193242054806
H	2.255685527371	-2.144731473335	-9.047532663151
H	1.159493936190	-2.427244942705	-7.689749900128
H	1.085600064840	-0.902922578115	-8.581349929863

transVAPNB_P-F1500

($E_F = -840.34830740$ a.u.; $G_F = -840.01913832$ a.u.)

0 1

C	1.825012768664	0.375477967499	-5.406383826865
C	2.731685005239	1.343886621750	-4.572352746676
C	1.618361496778	-0.155178898099	-2.970559838082
C	0.959363088031	-0.409628698245	-4.361121757749
H	1.155782083975	0.965834778003	-6.040508676197
H	-0.061572181823	-0.015047678009	-4.341717062285
H	0.875743483233	-1.479964899044	-4.570672780870
C	2.075435510134	1.322103495472	-3.146044457239
H	1.201872189424	1.984563255632	-3.125177246680
H	2.767104062891	1.651816405012	-2.366462431804
C	3.064705392878	2.703812136160	-5.161769378413
H	3.620217669692	3.365557311612	-4.499033187489
C	0.750251740516	-0.524923722631	-1.789119096442
H	-0.077651640569	0.135534330376	-1.538602005793

H	3.706748343700	0.846756169604	-4.418600826551
H	2.526738240292	-0.772314636731	-2.925883383620
C	0.775548093325	-1.924999720996	-1.207811629746
H	0.516667883450	-2.637230544617	-2.011036128998
H	1.817307134808	-2.175000226595	-0.957367981626
C	2.721526076466	3.257705641180	-6.527406785492
H	2.470768903983	2.440159294419	-7.208409648593
H	1.793998776751	3.850938885355	-6.446253982348
C	3.784476195135	4.176856525078	-7.229084806104
H	4.036847521762	5.034317207118	-6.599091610815
H	4.703768418105	3.622609059895	-7.435255355280
H	3.383352406259	4.550325760132	-8.174090430162
C	-0.121957710289	-2.263498007719	0.026830780579
H	0.138141919922	-1.639138540109	0.885892242948
H	-1.179698574179	-2.103904396998	-0.200415388366
H	0.014286233048	-3.310055478104	0.307409007125
Si	2.810901451168	-0.803853829258	-6.526461417172
C	3.765186078281	-2.019263849311	-5.435630825510
H	3.096158308229	-2.582301184709	-4.778645337240
H	4.311630655025	-2.739950860583	-6.051839636736
H	4.494965104297	-1.502687126254	-4.805311728991
C	4.049400522063	0.138833575654	-7.597629729748
H	4.647712978465	0.827920818430	-6.994547342987
H	4.733404958315	-0.557220867159	-8.093155852794
H	3.550694382947	0.724021054045	-8.375229033865
C	1.614529764080	-1.759979190524	-7.632225285200

H	2.148870622949	-2.467675412353	-8.273612757335
H	0.891618023573	-2.327840494447	-7.038928851620
H	1.053105804152	-1.079906256383	-8.280501980305

transVAPNB_TS-F1000

($E_F = -840.18242944$ a.u.; $G_F = -839.84686569$ a.u.)

0 1

C	2.024777070281	-0.065637988457	-5.531248527656
C	2.964254441155	0.677381483194	-4.522755548958
C	1.613706166737	-0.798208377225	-3.192927551856
C	1.215214273503	-1.079806033683	-4.657310157008
H	1.334855836985	0.651195267214	-5.984630007590
H	0.137309823366	-0.986805413450	-4.812351184439
H	1.474769296499	-2.115629085335	-4.901830755127
C	3.076500267959	-0.309083563704	-3.346505228569
H	3.470381715324	0.158342703049	-2.440377371886
H	3.728694771865	-1.149684396504	-3.605061365314
C	2.429378723300	2.001083831325	-4.056137154131
H	2.881711090900	2.378707231369	-3.140634584517
C	0.762524664404	0.240157261300	-2.526531188987
H	-0.130447436269	0.574517589433	-3.047199951498
H	3.966800163060	0.843689572739	-4.953513644259
H	1.592948775941	-1.722203532398	-2.597211347714
C	0.744280851491	0.323904550813	-1.019502859506
H	1.770123641104	0.260453779831	-0.636620845424
H	0.357654792610	1.300269880787	-0.708692858542

C	1.947200149263	3.059519448840	-5.020290104506
H	1.175099243496	2.649188332074	-5.680861746272
H	1.464639129944	3.860801149612	-4.451225807202
C	3.050598632298	3.706675185721	-5.930984936814
H	3.833177201860	4.171983521530	-5.325483046180
H	3.516586325074	2.956173747227	-6.572425159807
H	2.603915468625	4.474812885605	-6.567832039834
C	-0.104044800786	-0.786140681800	-0.301589753388
H	-1.151474110730	-0.735528530233	-0.610592806419
H	0.273033625930	-1.783718854866	-0.540578493009
H	-0.056064641083	-0.651163380567	0.782257028487
Si	2.925100334272	-0.889858960535	-6.983521081805
C	4.216136482794	-2.115653914785	-6.348073511319
H	3.764181518876	-2.884643962479	-5.714769129031
H	4.712180712922	-2.621524795478	-7.182272507192
H	4.987067451411	-1.608647632812	-5.760397674810
C	3.787135216089	0.418063112719	-8.039872543676
H	4.568649897905	0.935409835822	-7.475817098450
H	4.258565864911	-0.038317409517	-8.915876349436
H	3.077127738938	1.170363614327	-8.396577891222
C	1.653419626411	-1.806640624775	-8.037910752723
H	2.130607964974	-2.307346066140	-8.885970800965
H	1.128015720793	-2.567770176375	-7.453475040087
H	0.903668120524	-1.115769482865	-8.436092978627

transVAPNB_P-F1000

($E_F = -840.22886855$ a.u.; $G_F = -839.89911672$ a.u.)

0 1

C	1.844218364515	0.306068535220	-5.446526293296
C	2.776624447077	1.191136341648	-4.558326525046
C	1.554174484334	-0.279296720371	-3.029772206447
C	0.964487747494	-0.520090603642	-4.448472447710
H	1.184882729983	0.959658256380	-6.026840270134
H	-0.068686176072	-0.159059944771	-4.467011698881
H	0.921481545886	-1.589502334337	-4.673886882894
C	2.053972780868	1.191938425484	-3.167604765964
H	1.197700115722	1.875877098492	-3.188771745558
H	2.714186051604	1.497357965287	-2.351688058727
C	3.212964902368	2.530666287786	-5.095283588739
H	3.913967156749	3.074352566993	-4.463962743858
C	0.612032584863	-0.609552214399	-1.910248960969
H	-0.344828360026	-0.090541562538	-1.889785541951
H	3.707182893842	0.628894026648	-4.368086592804
H	2.449261116535	-0.906934335763	-2.924734300880
C	0.960152180651	-1.513045506798	-0.756096852855
H	1.685522867402	-2.262225897857	-1.099822906132
H	1.502230984172	-0.932031935900	0.011473725055
C	2.748276156874	3.242107702360	-6.337977991913
H	2.328674781799	2.524707639869	-7.048870498786
H	1.910707027708	3.915692852048	-6.085311246370
C	3.827832698229	4.096021625516	-7.069387308791
H	4.250793285084	4.849260886084	-6.398475092429

H	4.644548213174	3.464466309716	-7.428121145846
H	3.386872053154	4.611453160321	-7.926215031761
C	-0.217184663682	-2.241298839610	-0.046921671344
H	-0.938516954516	-1.522570622214	0.352727631265
H	-0.746311988411	-2.898164937860	-0.742624208355
H	0.155805955918	-2.845723986489	0.783348316970
Si	2.785073718447	-0.803300257110	-6.669481622270
C	3.777277028105	-2.081731778874	-5.691112302043
H	3.132864915337	-2.672517180677	-5.033644453435
H	4.287266532589	-2.774327299828	-6.367769488227
H	4.540543375904	-1.604398361319	-5.069593225616
C	3.976132755197	0.213884935907	-7.724726207799
H	4.623019842527	0.832643743246	-7.096177195653
H	4.613783329327	-0.439608634002	-8.328181004339
H	3.440942287772	0.880342762473	-8.406949520821
C	1.544782201519	-1.689401554515	-7.785093481074
H	2.052107031086	-2.353962312217	-8.491285916946
H	0.845787237522	-2.294737334482	-7.200288686572
H	0.958433091285	-0.970273324519	-8.365626927393

transVAPNB_R-F1000

($E_F = -840.25735855$ a.u.; $G_F = -839.91424893$ a.u.)

0 1

C	2.080035716855	-0.111699318954	-5.583212932118
C	2.960173787644	0.526285502130	-4.465953895725
C	1.554627489338	-0.800912864314	-3.300037918708

C	1.144528554855	-1.068994138262	-4.763365186280
H	1.475572687054	0.661816429557	-6.067409331005
H	0.084900037813	-0.865702457126	-4.940081969473
H	1.313195604266	-2.123588271370	-5.008887554042
C	3.077980953694	-0.620451274913	-3.445160784986
H	3.574436330830	-0.316658200862	-2.519820866525
H	3.579110326372	-1.509430330241	-3.832826084662
C	2.120948057958	1.558394362753	-3.658857856622
H	2.793670532359	2.015288170639	-2.920593997743
C	1.092229462204	0.621587645949	-2.876683041171
H	0.074147547461	0.803311124582	-3.242749526138
H	3.906640880132	0.940690164060	-4.818764232287
H	1.230849380433	-1.588121108414	-2.618521959947
C	1.087549977559	0.819186439617	-1.339943828888
H	2.110941702580	0.697186327737	-0.965800129604
H	0.817880908841	1.861720752553	-1.132267345781
C	1.511812492343	2.705306148017	-4.497493200347
H	0.674679258311	2.317658168754	-5.088602200925
H	1.070583106378	3.436694824169	-3.810673988929
C	2.495862284592	3.437530082180	-5.453131532124
H	3.352466939945	3.840336012607	-4.903774707648
H	2.879927536776	2.761284709733	-6.220239288776
H	1.993282687976	4.268947337517	-5.953535078489
C	0.150591561662	-0.112505032901	-0.520145614957
H	-0.883397997707	-0.040221050897	-0.871875471268
H	0.456933345812	-1.158410894769	-0.592093737220

H	0.168736813661	0.169208377594	0.535705259037
Si	3.016816635848	-0.914948930388	-7.022017577808
C	4.223958352083	-2.247902074522	-6.441147665605
H	3.715873719905	-3.033261899222	-5.873802705551
H	4.709423486176	-2.721034269455	-7.300641786049
H	5.008501355592	-1.827715180209	-5.805303114032
C	3.976722560888	0.426975795097	-7.943931720728
H	4.708710065193	0.911203668008	-7.290535204698
H	4.518315867385	0.009988218775	-8.798598140664
H	3.303119920981	1.202376298717	-8.321726827118
C	1.748070971962	-1.696102435945	-8.184220233087
H	2.234164344533	-2.164513945740	-9.045570689449
H	1.164543872519	-2.466386244748	-7.670846646588
H	1.047892625183	-0.944735948248	-8.562442638308

transVAPNB_TS-F500

($E_F = -840.09107784$ a.u.; $G_F = -839.75788261$ a.u.)

0 1

C	2.015094823460	-0.155598662728	-5.436085381058
C	2.993476627645	0.640629222072	-4.493478376692
C	1.686960055798	-0.850568062349	-3.084035776022
C	1.371917522151	-1.256115497618	-4.536146229076
H	1.224742974708	0.520548320023	-5.774098271441
H	0.298636735079	-1.357583301397	-4.716593504033
H	1.817219866007	-2.238696160358	-4.728482575882
C	3.108127833283	-0.247294552191	-3.237126152466

H	3.436783092200	0.310390819034	-2.356431072456
H	3.826641071256	-1.056461438932	-3.409271068334
C	2.519022526123	2.023767749434	-4.161095638421
H	2.862556259012	2.433738355478	-3.213419122351
C	0.710672685019	0.128488891640	-2.509753033401
H	-0.120863734254	0.457803766593	-3.125648990589
H	3.994251676234	0.726860531318	-4.952890055299
H	1.734857619720	-1.733928577328	-2.430561643978
C	0.601925440854	0.305914736169	-1.023924550098
H	1.602997750057	0.282100326227	-0.575424766335
H	0.180077532445	1.290246010093	-0.792995196777
C	2.138972077437	3.024837960134	-5.214293015044
H	1.555388515412	2.543647652641	-6.006580303478
H	1.487823729346	3.787324272148	-4.771728108015
C	3.348174230228	3.748356862290	-5.879178712348
H	3.933221980180	4.294435136606	-5.133958049851
H	4.010083360067	3.032430939912	-6.370886643195
H	2.999472689360	4.461666637795	-6.631484743839
C	-0.270448222314	-0.779738999526	-0.323864257372
H	-1.294753928434	-0.759817187460	-0.705761875046
H	0.135615849473	-1.779530214485	-0.499544660876
H	-0.302832462383	-0.609232198326	0.756200040367
Si	2.826145253499	-0.860305251965	-6.997381740081
C	4.263361212089	-1.987659181084	-6.509732777329
H	3.924505871192	-2.832490335394	-5.903116771483
H	4.758423177417	-2.393783146996	-7.397261649579

H	5.013969459565	-1.440907265238	-5.930970581616
C	3.480901983542	0.540391032042	-8.082368078727
H	4.302485624501	1.070670980535	-7.593044019030
H	3.857741950530	0.152689694450	-9.033934770777
H	2.697481015355	1.271283204041	-8.304732799678
C	1.539412403567	-1.854019563624	-7.959561064304
H	1.973610894930	-2.296207281810	-8.861586028938
H	1.132567961065	-2.667240400539	-7.350982943959
H	0.703538822499	-1.218134700771	-8.268061398375

transVAPNB_R-F500

($E_F = -840.18312030$ a.u.; $G_F = -839.83966797$ a.u.)

0 1

C	2.067164242607	-0.143509888152	-5.573763654433
C	2.968424240486	0.516989943043	-4.486667618008
C	1.616024361240	-0.825260931588	-3.273675367204
C	1.180515493820	-1.122122828998	-4.724033150760
H	1.429878299807	0.616507694243	-6.037610451788
H	0.111411256289	-0.954003664422	-4.878870559201
H	1.377832327700	-2.173129959333	-4.963670173577
C	3.132026375808	-0.618410738636	-3.458061734233
H	3.645567369992	-0.295858396595	-2.548397706067
H	3.639553438658	-1.502326485382	-3.849247412546
C	2.135487519964	1.535116222591	-3.658255149190
H	2.820022624360	1.992503065823	-2.930649514102
C	1.133682308137	0.597322541290	-2.871406102336

H	0.112283274693	0.756561061253	-3.239448844835
H	3.898548154966	0.942892229555	-4.867862909955
H	1.322792925085	-1.605901226040	-2.570540372734
C	1.129189443273	0.837821620695	-1.349338371267
H	2.137815814363	0.659862527821	-0.957320334931
H	0.921377723190	1.899847064547	-1.170077945659
C	1.484633806508	2.679580720398	-4.452740113766
H	0.665006283794	2.284265552727	-5.063092372955
H	1.015402585740	3.369392433331	-3.741520274197
C	2.455980232259	3.462161251986	-5.360623928499
H	3.298347320575	3.859904190000	-4.785684938527
H	2.863952103773	2.822188617914	-6.147101964779
H	1.949340148741	4.303540827824	-5.840647360037
C	0.120664267193	-0.013603128750	-0.550572114744
H	-0.899773540091	0.143754590725	-0.914369904240
H	0.340807829964	-1.080977271427	-0.629947072521
H	0.143719221334	0.252061883533	0.509693231083
Si	2.979709063931	-0.924035173007	-7.039818790742
C	4.244653337280	-2.215085338152	-6.488598882335
H	3.776804200735	-3.014724759477	-5.906786166839
H	4.723964432392	-2.674800102741	-7.358721518390
H	5.030234214421	-1.767203816633	-5.873258375919
C	3.867576238958	0.444705492764	-7.993745364255
H	4.611845531665	0.945583846010	-7.367284466465
H	4.385761808434	0.045525628873	-8.871088923618
H	3.159337619005	1.203610755286	-8.340541404615

C	1.700812394177	-1.750156041695	-8.158897406157
H	2.174248617728	-2.206109448758	-9.033879851214
H	1.159488023844	-2.536864144971	-7.624618396630
H	0.964730411754	-1.023598232418	-8.516869649643

transVAPNB_P-F500

($E_F = -840.11170128$ a.u.; $G_F = -839.78118002$ a.u.)

0 1

C	1.895471520401	0.223337957081	-5.467105524373
C	2.868871851829	1.024826472334	-4.547999420662
C	1.523166028911	-0.355347749792	-3.060505945288
C	0.995273837620	-0.612445762085	-4.498941001339
H	1.253993400239	0.936274413117	-5.995320766096
H	-0.044279407129	-0.277484820532	-4.566269448663
H	0.987207256689	-1.684594344411	-4.715152096177
C	2.098246344653	1.086470962443	-3.189459141127
H	1.280050162538	1.812774820984	-3.254092999444
H	2.740300881553	1.366222219359	-2.350359855989
C	3.403572894071	2.329359891325	-5.052063922495
H	4.224922452012	2.754309999634	-4.477927106897
C	0.519987338907	-0.586925616853	-1.983832963798
H	-0.459119703237	-0.124992447752	-2.103111034586
H	3.745428341683	0.393365997384	-4.331134994105
H	2.382907843781	-1.016658992934	-2.886819819370
C	0.828668823937	-1.240218763819	-0.670230819101
H	1.716357368572	-1.874997768146	-0.781504372716

H	1.113242874853	-0.473764656402	0.072202835143
C	2.833901835952	3.193282966699	-6.136482573877
H	2.289202994100	2.582462351441	-6.862824791827
H	2.078784173367	3.880703787629	-5.716104291448
C	3.890849499499	4.040350074605	-6.884030453771
H	4.438841380764	4.683582480788	-6.189129853448
H	4.615190082346	3.396615167211	-7.389577230495
H	3.416933317966	4.679210819869	-7.633864047474
C	-0.326164779782	-2.075442843533	-0.068092635332
H	-1.216059997231	-1.457501458810	0.084219857272
H	-0.599894122418	-2.898308880472	-0.733970476376
H	-0.037620687206	-2.496026083400	0.898809687028
Si	2.765266404128	-0.837399296317	-6.779574314842
C	3.796679415348	-2.162623762209	-5.910867082692
H	3.183293209138	-2.770831205170	-5.239505762573
H	4.258130089223	-2.835110112923	-6.640549458493
H	4.600073618494	-1.716685648582	-5.317243285471
C	3.900024637055	0.226670483109	-7.849578713172
H	4.612108038872	0.778883970421	-7.229726906079
H	4.467454372380	-0.391183708214	-8.552487732367
H	3.330712324713	0.957802950020	-8.430805520256
C	1.461058544032	-1.666578892368	-7.865965857186
H	1.925617337584	-2.300404206210	-8.627654500903
H	0.790612349152	-2.294909894247	-7.272072453431
H	0.848961564725	-0.919660794566	-8.381212796348

Cam_TS1-F3500

($E_F = -929.94992891$ a.u.; $G_F = -929.56046475$ a.u.)

0 1

C	-1.822153526586	1.024127495599	-2.610955382130
C	-1.199171812584	2.323666140222	-1.991367338219
C	-1.975812923301	2.135437820212	-0.175663528773
C	-2.517658523680	0.734876950933	-0.447632267995
C	-1.373689633913	-0.296108656584	-0.613329397866
C	-0.957308391500	-0.156565621389	-2.100474551518
H	-0.185602794946	2.137817567580	-1.630346564944
H	-1.035318953506	2.157239293707	0.379285188679
H	-3.223526676726	0.456707101565	0.338303545183
H	-0.550262802348	-0.091046396399	0.075218588303
H	-1.728185043299	-1.303992828392	-0.389347450633
H	-1.181423444574	-1.063653923726	-2.666274523602
H	0.109259409205	0.040607824085	-2.231803849728
C	-3.171842100026	0.801859025314	-1.852039958148
C	-3.904911255555	-0.502418991362	-2.208327639568
H	-4.288447702834	-0.467754455420	-3.231517987139
H	-3.285558453419	-1.395194389674	-2.115645469352
H	-4.765032190207	-0.628224914933	-1.543802370731
C	-4.163181425222	1.960541526357	-2.040486158126
H	-4.550634446206	1.954802725024	-3.063580914582
H	-5.010631315284	1.851038589359	-1.358691095322
H	-3.714861211128	2.935503659266	-1.854164697925
O	-1.120499471930	3.407820765178	-2.947418998591

O	-2.974248467580	2.873870204238	0.602073379160
C	-1.940390123504	1.058601420337	-4.131259737663
H	-0.957343230699	1.083101360252	-4.606449594101
H	-2.446356863922	0.156636788904	-4.484146713982
H	-2.500050139287	1.930005192052	-4.470097195150
C	0.143199547593	3.476271973277	-3.741038208192
H	0.651972910247	2.510324932581	-3.700274334974
H	0.787141769018	4.223657252348	-3.270164501532
C	-0.005541831246	3.862108116225	-5.280051536511
H	-0.666711362093	3.142078518049	-5.774799743418
H	-0.455880859420	4.859017364216	-5.361238218971
C	-2.959684122104	2.543465082364	2.054218976452
H	-2.345625890980	3.292541697734	2.562487017687
H	-2.495853021764	1.564758762698	2.204964376961
C	-4.373055425216	2.496347490980	2.783594262475
H	-4.873576800069	3.466307384392	2.674244469579
H	-4.997571180018	1.728637728713	2.308688405818
O	1.318371620862	3.844844915585	-5.894574309572
C	1.535967605376	4.162497886020	-7.338694432125
H	0.998265968203	3.455601039974	-7.979163521120
H	1.221315649747	5.186499820547	-7.565107272030
H	2.609882538129	4.057111780024	-7.476290923761
O	-4.156138471811	2.183787109066	4.192676887471
C	-5.273989283578	2.069684875252	5.177311334754
H	-5.820523174950	3.014868759472	5.259800294145
H	-5.960694216076	1.263867828816	4.897722694557

H	-4.778641972400	1.835726601679	6.117126879210
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Cam-F3500

($E_F = -929.95033850$ a.u.; $G_F = -929.56055311$ a.u.)

0 1

C	-1.856188723878	1.002742275394	-2.601119112226
C	-1.220880653807	2.279769894042	-1.921748001820
C	-1.905623309765	2.125849387389	-0.249708022841
C	-2.485142124511	0.717227635094	-0.435798428944
C	-1.359492381095	-0.328753802998	-0.632020615700
C	-0.990671862987	-0.193234263736	-2.134344493504
H	-0.190810939345	2.056602378034	-1.633862378465
H	-0.988867268585	2.139439568622	0.344796180622
H	-3.151177244274	0.472936728380	0.393677609656
H	-0.511974747416	-0.129057254042	0.028616040790
H	-1.715876832689	-1.332410186766	-0.393264995668
H	-1.247020391407	-1.094780477210	-2.695292488232
H	0.073425392712	-0.009244463257	-2.301107972270
C	-3.187729232308	0.774883927281	-1.816859072684
C	-3.929815894469	-0.529681091464	-2.150422038589
H	-4.314463249965	-0.508496902604	-3.173786037151
H	-3.317906705874	-1.425842327519	-2.044203982025
H	-4.790086478606	-0.638510517498	-1.482959131803
C	-4.183605223601	1.932880470238	-1.993438538533
H	-4.609522563469	1.899930624808	-3.000728153056
H	-5.004178468128	1.844333954451	-1.277011117687

H	-3.730496296434	2.913219385791	-1.852621758886
O	-1.138313840635	3.408251490032	-2.842322193710
O	-2.900764936641	2.918506591355	0.494139160848
C	-1.998015513073	1.090560611948	-4.114380673674
H	-1.023822100664	1.105043995824	-4.608032155924
H	-2.534598244109	0.214191601460	-4.487043801470
H	-2.541148830926	1.986794516936	-4.413448615713
C	0.109487005903	3.453662268397	-3.658848276157
H	0.582702314388	2.468963611263	-3.658696266161
H	0.791228503996	4.159243277845	-3.176093494099
C	-0.038490273133	3.892824362698	-5.183331282447
H	-0.736923089216	3.219899607032	-5.692923894098
H	-0.441270385114	4.911959983230	-5.231316641678
C	-2.907459210075	2.652844768805	1.956513244124
H	-2.432735026219	3.508079646164	2.445308350476
H	-2.309528231916	1.763906853875	2.175694421305
C	-4.325673655992	2.438208118534	2.649924974625
H	-4.962514224358	3.309258548213	2.452026682725
H	-4.810137836708	1.550901861851	2.221724943190
O	1.278684949699	3.831257179422	-5.810708033187
C	1.502873858443	4.185837473981	-7.244903286714
H	0.927451423821	3.527876243608	-7.904460017686
H	1.237549780439	5.230949959597	-7.435219928834
H	2.569483981831	4.032835902128	-7.394138198080
O	-4.116890846479	2.266972130843	4.084378446213
C	-5.239334551105	2.058681788969	5.047990632174

H	-5.923346646410	2.913677749382	5.042364182648
H	-5.787891254064	1.139584332703	4.816814699498
H	-4.748363670457	1.973242342920	6.014943485833

Cam_Int1-F3500

($E_F = -930.19722043$ a.u.; $G_F = -929.81668258$ a.u.)

0 1

C	-1.473137592157	1.774175419490	-2.576446993270
C	-0.879673868771	2.715608822960	-3.673021566664
C	-3.308106029862	1.956925378027	1.002858858517
C	-2.647312550180	1.450802212650	-0.302211225196
C	-1.137388867688	1.048455059740	-0.159331110312
C	-0.406816133155	1.359627116243	-1.503614452514
H	-0.413664063771	3.647700537213	-3.360344159751
H	-2.906307165126	2.849999467234	1.478471052933
H	-3.213717573687	0.563845861363	-0.601185116788
H	-0.680219386012	1.619664387673	0.652697058129
H	-1.053230187334	-0.005014416486	0.116455359703
H	0.179293617934	0.508626347190	-1.859698171380
H	0.297642049123	2.182034422786	-1.358080295792
C	-2.607833632315	2.432686474634	-1.587922224699
C	-3.983974877238	2.528417299441	-2.248197730600
H	-3.931683158107	3.123542337196	-3.165236443687
H	-4.384480810131	1.544948873579	-2.502391395433
H	-4.694290134767	3.007735137190	-1.568123916526
C	-2.169934932611	3.843246791499	-1.155091445906

H	-2.120873901260	4.512435217998	-2.017497726090
H	-2.895051132529	4.265049997417	-0.454676794950
H	-1.192297734430	3.848026668314	-0.666608310831
O	-0.383983971358	2.211240180501	-4.892405810429
O	-3.954475786847	1.075282397575	1.892103318137
C	-2.011820382889	0.511356016409	-3.272604690221
H	-1.201970339855	0.018609564551	-3.814379728517
H	-2.419775126671	-0.200415146224	-2.551645450687
H	-2.790654837168	0.753762000891	-3.997688441847
C	0.273110055747	3.165171263620	-5.817112627870
H	1.127126384484	3.617433162842	-5.303243494318
H	-0.441809779893	3.953560968215	-6.068384685685
C	0.794237599252	2.513300454600	-7.168384891708
H	1.512975151152	1.719403728785	-6.929000191938
H	-0.054633967709	2.063772957137	-7.698651456172
C	-4.431635290578	1.638973614345	3.179039297201
H	-5.131858372578	2.450824980727	2.963421798204
H	-3.572832886643	2.051619397261	3.717615302358
C	-5.156949261438	0.594922965990	4.130598884487
H	-6.028720124408	0.180262780865	3.609203208754
H	-4.464917508478	-0.226234745264	4.356029351838
O	1.420933403669	3.547219083497	-7.981729297723
C	2.011169732836	3.260336241868	-9.324835376771
H	2.829585707695	2.537463790909	-9.245155977130
H	1.247526399386	2.887270798207	-10.014979433910
H	2.387936379982	4.223586875472	-9.661423267625

O	-5.563512733734	1.276184460526	5.353112225801
C	-6.281726447457	0.574083534335	6.460191788711
H	-7.242743471881	0.180165605504	6.113869331174
H	-5.670253118580	-0.236455462379	6.869890489547
H	-6.437020637005	1.347296181480	7.209315837864

Cam_TS1-F3000

($E_F = -929.78387267$ a.u.; $G_F = -929.39490480$ a.u.)

0 1

C	-1.787140257251	1.031932398354	-2.621702779311
C	-1.161045123019	2.351238965685	-2.095697255632
C	-2.059428732484	2.120686108674	-0.070572115027
C	-2.567536016740	0.746272736185	-0.455234922316
C	-1.411767451889	-0.276557805179	-0.585253490835
C	-0.933439640479	-0.132474519753	-2.050385698803
H	-0.172105332730	2.214768874623	-1.656228788187
H	-1.089874673457	2.148480316085	0.430671205989
H	-3.322604415260	0.432722835306	0.271948229213
H	-0.618198361496	-0.074799427723	0.138141631769
H	-1.772637022596	-1.286819777718	-0.382491761258
H	-1.119546139047	-1.045350575534	-2.620590918786
H	0.135725753454	0.075702957101	-2.134554994558
C	-3.159731375284	0.831437794788	-1.889167385536
C	-3.891320184572	-0.467554410230	-2.272192441919
H	-4.268206293712	-0.416170118236	-3.296899094011
H	-3.270745914514	-1.360869509831	-2.190502579914

H	-4.755517233475	-0.604918897146	-1.615516528694
C	-4.136617150260	1.997154158635	-2.097281800314
H	-4.478107317676	2.019960618866	-3.136368423706
H	-5.015300014997	1.873683660414	-1.458243579918
H	-3.687816864193	2.961639573350	-1.863986206441
O	-1.106030934532	3.380685626418	-3.075915159659
O	-3.041208572214	2.813100010501	0.725708582140
C	-1.877386401668	0.992515793119	-4.147829316371
H	-0.884215776506	1.037671651250	-4.600428864344
H	-2.339654963344	0.057409151277	-4.471688979342
H	-2.461348863547	1.826272407545	-4.536704111991
C	0.172149390610	3.524217408713	-3.817660102563
H	0.751916981083	2.602248566229	-3.727215052371
H	0.740610133486	4.337498855102	-3.358903044921
C	0.014205646917	3.836562840715	-5.358704551216
H	-0.575973233402	3.044626881674	-5.834193454102
H	-0.518420338179	4.787673357182	-5.485748142671
C	-3.005660711207	2.435159021373	2.158045554738
H	-2.288531343222	3.084049138278	2.670489408897
H	-2.660750879914	1.401637765918	2.255871821623
C	-4.388049524527	2.526781350857	2.910875367120
H	-4.764448070301	3.557028702854	2.874888299346
H	-5.115965463469	1.875079096594	2.409757260620
O	1.340233407028	3.907083648393	-5.944495713283
C	1.522750213642	4.171655407460	-7.388550273925
H	1.051830595707	3.389026528831	-7.994027818531

H	1.112186216818	5.149419933064	-7.664346057929
H	2.600715553671	4.162741354767	-7.537602870651
O	-4.174853623848	2.102741542098	4.282905203879
C	-5.284180658081	2.066164189290	5.259711605171
H	-5.712734987888	3.063806072836	5.406926118256
H	-6.068438604560	1.371145560229	4.939152254267
H	-4.827998943997	1.715140373029	6.183287648448

Cam-F3000

($E_F = -929.78942143$ a.u.; $G_F = -929.39834475$ a.u.)

0 1

C	-1.856660201833	0.947443898013	-2.584926295314
C	-1.215381442169	2.209984416961	-1.879461193308
C	-1.866510083233	2.071890018886	-0.284831265289
C	-2.516810076455	0.685085017462	-0.432687325541
C	-1.429459955302	-0.402213702781	-0.609095042699
C	-1.026280801237	-0.267930871313	-2.103656481833
H	-0.172770852828	1.980182529762	-1.644947922351
H	-0.966930266992	2.041038164446	0.336531045888
H	-3.189529361354	0.487720225014	0.403246811579
H	-0.588755925273	-0.238553805677	0.070085165457
H	-1.827582889533	-1.393564202685	-0.385584592241
H	-1.288903001340	-1.161898774946	-2.673720544966
H	0.044867340610	-0.105368051222	-2.246515348229
C	-3.205232633877	0.751725671655	-1.821462010965
C	-3.973417074704	-0.534565122511	-2.165190255889

H	-4.339422152276	-0.504230108386	-3.195286483637
H	-3.385739079799	-1.445533763556	-2.049089009833
H	-4.847645896536	-0.622101703469	-1.512790426687
C	-4.170266163950	1.933465115413	-2.015516759673
H	-4.588690944336	1.902072028444	-3.026060268162
H	-4.999328181930	1.870480646002	-1.305847713840
H	-3.695391025021	2.903908265984	-1.880220248534
O	-1.174057822014	3.373684435425	-2.749505142364
O	-2.811747766673	2.950138829668	0.403155867970
C	-1.961036989680	1.044709953889	-4.098938986305
H	-0.974162944472	1.062346144859	-4.567750571922
H	-2.489877638373	0.172218351800	-4.491649441004
H	-2.496631653951	1.943527038531	-4.404054497562
C	0.060897513380	3.480542024893	-3.558380161986
H	0.578258374731	2.518024140434	-3.572130361196
H	0.715564431519	4.209035907113	-3.070968991022
C	-0.111501514419	3.922171723809	-5.066234134781
H	-0.792013982952	3.234703448264	-5.580845524191
H	-0.539791954250	4.931533479438	-5.111489211072
C	-2.846961205345	2.767959601290	1.865730890172
H	-2.530984866263	3.715233848011	2.310491705003
H	-2.127672862258	1.999848256192	2.164688952598
C	-4.235496871626	2.389357225717	2.524932850543
H	-4.988067748870	3.139678690204	2.250396247022
H	-4.573674867915	1.411691089272	2.156418514554
O	1.203558083120	3.894482905801	-5.683969089900

C	1.391147154582	4.252217653361	-7.106216534309
H	0.825511833527	3.578337440307	-7.759575277882
H	1.089385682068	5.288548003880	-7.295118331186
H	2.458644272769	4.135615760938	-7.282809543361
O	-4.042961977145	2.353685454436	3.963821771838
C	-5.155921956883	2.047161532469	4.887257181583
H	-5.959072734327	2.786945808746	4.795577613119
H	-5.555901640623	1.043645607990	4.703075886336
H	-4.713531638897	2.096731682616	5.880324727555

Cam_Int1-F3000

($E_F = -929.99127034$ a.u.; $G_F = -929.60949123$ a.u.)

0 1

C	-1.479451458139	1.779389435354	-2.563294275566
C	-0.906631389372	2.726241531896	-3.649268361066
C	-3.297579237195	1.968947002298	0.984546649733
C	-2.638698416994	1.456160853475	-0.305339933343
C	-1.129102363419	1.056424254778	-0.155720542711
C	-0.402740845557	1.371628001861	-1.498242243316
H	-0.451277282015	3.664063118586	-3.338142154995
H	-2.899390923711	2.863988033852	1.459575512278
H	-3.203016426062	0.565894182731	-0.598755352265
H	-0.675316551897	1.627501434432	0.658269107036
H	-1.044457711897	0.002681457773	0.118683168650
H	0.186843445715	0.524974893359	-1.858591687161
H	0.296670829527	2.198791460286	-1.355482824578

C	-2.609231559124	2.432955562198	-1.583201263681
C	-3.987691173014	2.521431933413	-2.241253597752
H	-3.939232354681	3.114117692918	-3.160017952438
H	-4.385082508318	1.535774247943	-2.491757253274
H	-4.698254448673	2.999993623202	-1.561035721245
C	-2.180584369100	3.848208639978	-1.152935109769
H	-2.140457910683	4.517451981145	-2.015515090372
H	-2.906936305753	4.265034020583	-0.451125488971
H	-1.201422708019	3.861414921702	-0.667578652775
O	-0.401903136551	2.220092945101	-4.856236738161
O	-3.928536695883	1.081706828451	1.868619404788
C	-2.009896097049	0.511662891498	-3.258519255710
H	-1.197042629073	0.024284630252	-3.800320170328
H	-2.411841801362	-0.202456034198	-2.536636684001
H	-2.791086049782	0.747798341166	-3.983072699751
C	0.229696217629	3.181338974776	-5.774174873932
H	1.073662137571	3.657121984517	-5.263871348887
H	-0.500554669648	3.953480064851	-6.033648855302
C	0.759461050537	2.526225023012	-7.104966651232
H	1.494215150694	1.748520602693	-6.858810854408
H	-0.078328265559	2.054373973536	-7.634471798879
C	-4.408591717974	1.648434567085	3.140831873753
H	-5.119675440754	2.450763206731	2.922858924659
H	-3.557168671418	2.075314331658	3.681049633048
C	-5.113416271075	0.599471806216	4.080450559075
H	-5.980863679330	0.171788878162	3.561301433815

H	-4.411853850634	-0.213570414947	4.308392909724
O	1.361694733761	3.566212944558	-7.915532495298
C	1.947914482678	3.259164158013	-9.238506635999
H	2.776503243036	2.548226462172	-9.146055703467
H	1.190314577889	2.857507452368	-9.920555299770
H	2.314341917780	4.215156583219	-9.607170756753
O	-5.522554678239	1.282287263207	5.292257033838
C	-6.225336214953	0.561071043585	6.375729133145
H	-7.178367169259	0.152120123374	6.022192816481
H	-5.603472746352	-0.245924172107	6.778971216434
H	-6.402142132069	1.315008431399	7.140231194241

Cam_TS1-F2500

($E_F = -929.61668918$ a.u.; $G_F = -929.22889556$ a.u.)

0 1

C	-1.768102660351	1.026261026725	-2.631854463160
C	-1.125408508509	2.350390589644	-2.175354806327
C	-2.104511324255	2.096519233059	0.000947143912
C	-2.601261639653	0.749048714426	-0.459160332327
C	-1.447931229152	-0.278682030319	-0.571391693010
C	-0.929559966089	-0.131319432365	-2.020601261552
H	-0.152101007898	2.246017498169	-1.696499630432
H	-1.119000620032	2.124475719110	0.468973958284
H	-3.387204645028	0.418186682592	0.228450354241
H	-0.672166307056	-0.089326189420	0.174111046456
H	-1.821573412048	-1.287681135883	-0.385975867355

H	-1.094214147239	-1.046429027592	-2.593716670373
H	0.141061575764	0.079639465314	-2.073355977018
C	-3.154418762141	0.854378368732	-1.910820462272
C	-3.899126033580	-0.433161245146	-2.310635150338
H	-4.270550599150	-0.367778029430	-3.336381404234
H	-3.287086018633	-1.333200925165	-2.235160049147
H	-4.767652703204	-0.568346270818	-1.659417512599
C	-4.108806158076	2.035462540462	-2.129587713440
H	-4.426400291520	2.075940916871	-3.175694565023
H	-5.003907765276	1.917301705901	-1.512379910137
H	-3.647558979095	2.988233304286	-1.873353908280
O	-1.096216941094	3.347600470677	-3.163565402447
O	-3.071414933703	2.768610319490	0.804490693285
C	-1.845082165576	0.934071421327	-4.159311396357
H	-0.846426795102	0.983322130114	-4.599903927089
H	-2.288168664867	-0.017935445970	-4.458723789139
H	-2.437249011813	1.745808615867	-4.581169107860
C	0.185040068651	3.585254103734	-3.854476818601
H	0.847767396711	2.729525787727	-3.701746153100
H	0.653698151564	4.471807388515	-3.419378731418
C	0.030743364023	3.806263721781	-5.399849234900
H	-0.458551132293	2.933840453802	-5.849085671889
H	-0.599275097772	4.686403110388	-5.583920850810
C	-3.021612274376	2.372405656716	2.222514574650
H	-2.257400891642	2.969185740919	2.731471151410
H	-2.737890249293	1.318160221391	2.298501221027

C	-4.379520662421	2.535655291377	2.982187768128
H	-4.691091297027	3.588421885173	2.977106555245
H	-5.153271743947	1.944588778222	2.473754290216
O	1.350771689722	3.992721022214	-5.954151048157
C	1.508862542439	4.189430826667	-7.398320344049
H	1.133902332977	3.324530604861	-7.958225623704
H	0.989320444014	5.094714123423	-7.733568188130
H	2.580366713109	4.297208166064	-7.556848584374
O	-4.174016431389	2.064334262106	4.332509415529
C	-5.282346380152	2.071587665076	5.290281879901
H	-5.653210357285	3.089375881141	5.460227893723
H	-6.106975692320	1.435520770791	4.946796175978
H	-4.865484296007	1.670963739568	6.212758039512

Cam_Int1-F2500

($E_F = -929.78756119$ a.u.; $G_F = -929.40479269$ a.u.)

0 1

C	-1.483986500494	1.784607492901	-2.551238754895
C	-0.930838539765	2.736851439237	-3.627268807264
C	-3.286749914409	1.980371114879	0.966862215220
C	-2.629295540506	1.461334085041	-0.308880284938
C	-1.119883167021	1.065013047936	-0.152633223269
C	-0.397443487741	1.384560203769	-1.493359224119
H	-0.486208707802	3.680135992778	-3.317293227116
H	-2.891463479823	2.876704537066	1.441942320448
H	-3.191258541959	0.567690722919	-0.596750846733

H	-0.669764699027	1.636121090352	0.663341802528
H	-1.034163762877	0.011025849346	0.120327441821
H	0.196310850675	0.542579280006	-1.857475525955
H	0.296284683021	2.216900668378	-1.353094999113
C	-2.610039325910	2.433108204997	-1.579553131523
C	-3.990594521546	2.513108628812	-2.235753527568
H	-3.946097121439	3.103101049230	-3.156389127494
H	-4.384076157118	1.524931093706	-2.482396605142
H	-4.701935647042	2.990618499637	-1.555727691660
C	-2.191625479478	3.853240950147	-1.152017265475
H	-2.160570080612	4.522312116758	-2.014867315176
H	-2.919583685397	4.264702811728	-0.448997655654
H	-1.211149939782	3.875509075617	-0.669557258578
O	-0.416456933088	2.229377410997	-4.822082265502
O	-3.903744973090	1.087670850323	1.845298304571
C	-2.005540196391	0.511898526467	-3.245544481899
H	-1.189419748517	0.030069310639	-3.787085124491
H	-2.401527658993	-0.204551758060	-2.522791237199
H	-2.788889663762	0.741457593957	-3.969821487581
C	0.191393951274	3.197556724940	-5.733578351133
H	1.025346389882	3.694876102662	-5.226357083164
H	-0.553043461881	3.953994897418	-6.000590810235
C	0.729623931734	2.539117817416	-7.045182040651
H	1.478412617034	1.776528745691	-6.791975185013
H	-0.097593535008	2.046951039177	-7.573763528000
C	-4.387265961364	1.656435287769	3.104159302330

H	-5.108459476000	2.449687368485	2.884151318349
H	-3.543116173474	2.096047303277	3.646515465131
C	-5.073158270334	0.601314236729	4.030973807464
H	-5.935567446501	0.161778112888	3.512346439644
H	-4.362243375264	-0.203797579542	4.260418635767
O	1.310124135137	3.583285363251	-7.854032110756
C	1.893068403675	3.254553229738	-9.157890032767
H	2.729054315561	2.553031999450	-9.052068590702
H	1.140580910321	2.827532842542	-9.831357771493
H	2.252514814961	4.201389529356	-9.557012145068
O	-5.486638505752	1.282781824937	5.233898697130
C	-6.174848195738	0.539672906421	6.293045710052
H	-7.118858699251	0.116258476633	5.930111676839
H	-5.542008729928	-0.263719265572	6.688389012092
H	-6.373451125369	1.272430958576	7.073208488023

Cam-F2500

($E_F = -929.63223347$ a.u.; $G_F = -929.23976291$ a.u.)

0 1

C	-1.824607515276	0.874892560160	-2.564488726035
C	-1.199955639735	2.126486572057	-1.833695704025
C	-1.885110891100	1.992360600415	-0.299908384565
C	-2.638404315922	0.655741005317	-0.463166668638
C	-1.611990005495	-0.495504996514	-0.557876931779
C	-1.072981641453	-0.362716870723	-2.009715983915
H	-0.149032951034	1.914086266660	-1.618822528451

H	-1.021711319906	1.878911947597	0.364761550421
H	-3.372651767862	0.522257927554	0.330859476955
H	-0.826458851849	-0.395679726169	0.195605115669
H	-2.088783926782	-1.463099265379	-0.391732779244
H	-1.302957186328	-1.248255302143	-2.606295005874
H	0.010519624048	-0.225915490067	-2.053080874911
C	-3.229934891237	0.742852870223	-1.893740094907
C	-4.026717398141	-0.508859215484	-2.294372734802
H	-4.339615986481	-0.447704356277	-3.340504693123
H	-3.477910363718	-1.442468113106	-2.168140181843
H	-4.934798577714	-0.575596573453	-1.687232963184
C	-4.130278109730	1.965220918747	-2.140648531296
H	-4.476364105414	1.965198083352	-3.178648251137
H	-5.011235386933	1.923152754062	-1.493801628712
H	-3.629678521983	2.913573632451	-1.955747553635
O	-1.208874298254	3.317081046616	-2.657679736531
O	-2.748230426434	2.977620404915	0.310104951054
C	-1.816248989549	0.948725574715	-4.082289708387
H	-0.797248683648	0.975258360427	-4.477396823212
H	-2.304475345842	0.064756212864	-4.501057151253
H	-2.341863808948	1.834920172945	-4.437304621564
C	0.016333290805	3.520396139611	-3.442017662669
H	0.614151446280	2.605105504637	-3.446355990252
H	0.603832263281	4.303297030215	-2.952512364663
C	-0.182983440821	3.935696142712	-4.942820330162
H	-0.805484446384	3.197541787397	-5.459950763695

H	-0.684505419907	4.910690842560	-5.000089789475
C	-2.814948091869	2.952783332875	1.768808042107
H	-2.844462749973	4.000361162249	2.075508286756
H	-1.900688325235	2.507572679094	2.176736389958
C	-4.048425099064	2.254905254889	2.461527366538
H	-4.978438448231	2.648277484250	2.029423246935
H	-4.025528683043	1.169145216687	2.301702254199
O	1.131221699319	3.999108960485	-5.543918147145
C	1.268344050057	4.331148888250	-6.963992877826
H	0.752649685553	3.596343282727	-7.593958211217
H	0.876257728944	5.332785567562	-7.177088011379
H	2.338333655694	4.302973520153	-7.162960098169
O	-3.968410211571	2.551087622238	3.873539378261
C	-4.976556206639	2.017065347864	4.792626463930
H	-5.977586229793	2.387233323300	4.541066588145
H	-4.980186937532	0.920415740093	4.782923520850
H	-4.685663391238	2.377287457423	5.777939018180

Cam_TS1-F2000

($E_F = -929.45027302$ a.u.; $G_F = -929.06281588$ a.u.)

0 1

C	-1.799579650618	1.000658272109	-2.666252445279
C	-1.108537028115	2.306997079283	-2.245649490031
C	-2.075351839500	2.049742689346	0.017143645732
C	-2.604536547437	0.726839342733	-0.469699112978
C	-1.475979327955	-0.323760910021	-0.613071336156

C	-0.976518176981	-0.175064233891	-2.068649625819
H	-0.123097525505	2.197632764061	-1.794173144041
H	-1.079632090505	2.055401749161	0.464259556966
H	-3.391279554899	0.396564926742	0.218546886048
H	-0.684076013570	-0.158941798195	0.121297367151
H	-1.867794238791	-1.326618912389	-0.431679688639
H	-1.166206167361	-1.083273373421	-2.644901198477
H	0.097428039017	0.014929937656	-2.135257931824
C	-3.174498301320	0.867692078553	-1.913311090770
C	-3.966946493443	-0.392372658083	-2.310791660557
H	-4.361849680866	-0.304079206845	-3.325944730919
H	-3.379120683179	-1.310480960514	-2.260833390473
H	-4.822356212917	-0.510644296605	-1.639290763901
C	-4.093516159525	2.080948305360	-2.102918120441
H	-4.424425789239	2.146238279388	-3.143714587237
H	-4.982884856006	1.983859902639	-1.473933803264
H	-3.596781813097	3.014043797792	-1.840500750488
O	-1.135690538976	3.314614569917	-3.200095933110
O	-3.014533018019	2.743049402366	0.821390652314
C	-1.913145408506	0.897540293515	-4.191591842110
H	-0.921693374784	0.908223689712	-4.650089541133
H	-2.394660789704	-0.040603128948	-4.474351627778
H	-2.484007186198	1.726301287779	-4.610142269222
C	0.110511426677	3.780604283722	-3.804373309752
H	0.954113726040	3.207282547445	-3.409660254656
H	0.243606475641	4.831110742671	-3.535893853408

C	0.098022442630	3.667775537920	-5.360794835312
H	0.028068130035	2.614513726586	-5.658889140205
H	-0.783930683296	4.193022129485	-5.752473661624
C	-2.960676563179	2.352043886585	2.230505021650
H	-2.187732711812	2.938559916424	2.739372934964
H	-2.692948724875	1.293587621551	2.311236460500
C	-4.312608043546	2.539997544985	2.972841977660
H	-4.610130410671	3.597249561299	2.962228516610
H	-5.092892346788	1.958295850814	2.462721472255
O	1.310460561162	4.252642256411	-5.861134708115
C	1.540004736852	4.219676005056	-7.297250522349
H	1.579426731829	3.188084461834	-7.668949536424
H	0.758512980224	4.768872616670	-7.836848367252
H	2.503074486836	4.703296967315	-7.453364121790
O	-4.117443032827	2.071874092582	4.319221531363
C	-5.241693512184	2.095174864362	5.238602243150
H	-5.609475731970	3.117227119725	5.393551995456
H	-6.065191083591	1.466598351233	4.876822659003
H	-4.862021942274	1.696379218457	6.178229387166

Cam_Int1-F2000

($E_F = -929.58595229$ a.u.; $G_F = -929.20247217$ a.u.)

0 1

C	-1.489687581727	1.799620812996	-2.542446204988
C	-0.957017412393	2.760581573137	-3.606857007219
C	-3.274465798592	1.989753175337	0.950086553038

C	-2.619131976099	1.469025366510	-0.314707497890
C	-1.109417779827	1.077123897105	-0.154823193098
C	-0.392409251627	1.405417508478	-1.493656404084
H	-0.523360180422	3.708435963000	-3.295445136079
H	-2.881421519087	2.885462060087	1.428253945686
H	-3.178357954160	0.572511206107	-0.599089561322
H	-0.662539858773	1.646330134573	0.664231619433
H	-1.021248367997	0.022206262002	0.113578485626
H	0.205947149011	0.569678760960	-1.864266429168
H	0.294958677098	2.243112390406	-1.354035878308
C	-2.612178711040	2.439577171262	-1.575913836243
C	-3.995443995470	2.511348787009	-2.228678114289
H	-3.956437426056	3.101183745986	-3.149601916287
H	-4.384148851272	1.520918597988	-2.473778457845
H	-4.707416225734	2.985182131400	-1.546848148012
C	-2.204982776573	3.863626710795	-1.147493665097
H	-2.184596328023	4.534929596960	-2.008696237424
H	-2.934100319017	4.266891688307	-0.441209733033
H	-1.222767154667	3.894526765931	-0.668965422212
O	-0.433289369809	2.255738754059	-4.791596273313
O	-3.877436634548	1.088556116523	1.820127882580
C	-2.002043698767	0.523742674346	-3.239078731223
H	-1.182861737015	0.049582012061	-3.782471733883
H	-2.391006738650	-0.197332615212	-2.517207086414
H	-2.788274574775	0.748311309697	-3.961743406558
C	0.150900077121	3.233084670498	-5.695019391310

H	0.975065454383	3.749488276536	-5.189967860443
H	-0.607383552692	3.974519872067	-5.966574336896
C	0.696516222052	2.574389380169	-6.990442816138
H	1.458227370180	1.825770020867	-6.732242823668
H	-0.120885444472	2.064282348237	-7.518160697904
C	-4.364544365070	1.653877238518	3.069024037510
H	-5.096498043963	2.438111211172	2.850436723392
H	-3.527746528375	2.104310241854	3.614723210894
C	-5.030372858321	0.587363256668	3.979046080266
H	-5.886669169172	0.137380637228	3.458364106327
H	-4.308734699191	-0.209552715646	4.205683867200
O	1.256421392815	3.622992654127	-7.796964629322
C	1.835479577092	3.273981583683	-9.083590404110
H	2.677074501618	2.579991606421	-8.965964570647
H	1.086762569691	2.825112949359	-9.748126907876
H	2.189875058806	4.211000982703	-9.510481310351
O	-5.450094520443	1.259707786547	5.177466783522
C	-6.121560476020	0.487051923237	6.209098972468
H	-7.054995419288	0.049194240457	5.834044235054
H	-5.475134492603	-0.312673165893	6.591634513243
H	-6.342932242640	1.193170072894	7.008004997682

Cam-F2000

($E_F = -929.47876953$ a.u.; $G_F = -929.08504818$ a.u.)

0 1

C	-1.810237173614	0.827807612085	-2.554364235501
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C	-1.189471622765	2.061109963358	-1.799965003383
C	-1.902671424677	1.933631000872	-0.314726951288
C	-2.743603515678	0.648184415488	-0.499891547023
C	-1.778415675664	-0.556011560412	-0.536836606955
C	-1.133699811333	-0.430857686951	-1.946722552724
H	-0.134295554291	1.855226816665	-1.597728356964
H	-1.076102100738	1.753458942403	0.383123754185
H	-3.524447528941	0.568782331578	0.255498783265
H	-1.043147598616	-0.509067649662	0.270517293008
H	-2.316222187733	-1.498665909145	-0.421996549764
H	-1.340601990228	-1.309184957562	-2.561880804476
H	-0.046711839705	-0.321272583945	-1.909936845737
C	-3.254761492388	0.752763958017	-1.959778766926
C	-4.071309023453	-0.469267969321	-2.410413446605
H	-4.342540595786	-0.379313110958	-3.466104430682
H	-3.553207366758	-1.420202817584	-2.284107089255
H	-5.003031417409	-0.521977645377	-1.838742970152
C	-4.103358498926	2.004235252508	-2.242112063452
H	-4.373584011492	2.039235413200	-3.301817571591
H	-5.030730588336	1.963996114033	-1.662747059066
H	-3.598485961935	2.934965438368	-1.994661611512
O	-1.230302346175	3.275140865143	-2.577268879851
O	-2.690451955677	2.997190498529	0.237254209373
C	-1.710606595027	0.886478366373	-4.068891924207
H	-0.669547631345	0.918272460953	-4.402539666433
H	-2.168546167047	-0.003026363514	-4.509568182706

H	-2.220767219223	1.765536913026	-4.461775859460
C	-0.014715744334	3.552268522188	-3.333387006886
H	0.630117983813	2.669225103659	-3.351687363257
H	0.530032926117	4.355114165587	-2.826075182950
C	-0.236936927931	3.978327323235	-4.816681761477
H	-0.823573285430	3.219429496646	-5.345726657812
H	-0.784414835229	4.929457359620	-4.861687851954
C	-2.763266432615	3.053129996849	1.683117011782
H	-2.966461190494	4.099952203867	1.915460343257
H	-1.790176657614	2.792252719962	2.117026131693
C	-3.868086188841	2.214105333854	2.412853129486
H	-4.838928314857	2.390254461234	1.928706629374
H	-3.646387605360	1.139757345109	2.361513739971
O	1.068760867066	4.109640534113	-5.410267114229
C	1.158158622679	4.437425479498	-6.822670702545
H	0.670501482522	3.672372759863	-7.440105578074
H	0.705815052520	5.414221265940	-7.035328109188
H	2.222440630678	4.469422183195	-7.051632189542
O	-3.886481270311	2.649324132508	3.783519704951
C	-4.800463308148	1.997569722410	4.706189363426
H	-5.844015016324	2.134813084794	4.396267774007
H	-4.586298437681	0.924278138369	4.787084087644
H	-4.638503681500	2.477140770639	5.670475962914

Cam_TS1-F1500

($E_F = -929.28538410$ a.u.; $G_F = -928.89760082$ a.u.)

0 1

C	-1.817826213712	0.991956800967	-2.708014913435
C	-1.097829431719	2.284604644643	-2.318316016341
C	-2.057966188073	1.997884533878	0.050418820690
C	-2.583914328983	0.695496910110	-0.483201063346
C	-1.454887107918	-0.349019137748	-0.668464877305
C	-0.993091593251	-0.194208594328	-2.136141554903
H	-0.102545594080	2.184562492864	-1.887457259777
H	-1.052932855820	2.008789410690	0.475416576716
H	-3.364127930776	0.338198056396	0.200452399666
H	-0.643054041984	-0.184820332285	0.044105896242
H	-1.836512811383	-1.354715349501	-0.481005972148
H	-1.206702223567	-1.097059639398	-2.712367291339
H	0.080936723455	-0.015333472514	-2.228881231045
C	-3.175300791924	0.872816683952	-1.916233463443
C	-3.997578573855	-0.368600070028	-2.313632818445
H	-4.411412910465	-0.262189491617	-3.319361377972
H	-3.423414814797	-1.296568738213	-2.285388362875
H	-4.840924202893	-0.480951614454	-1.626113194719
C	-4.076361312780	2.104282133361	-2.066441150234
H	-4.429641311447	2.192449229877	-3.098187279270
H	-4.952404264016	2.013975555763	-1.418208956070
H	-3.555445776244	3.023208971679	-1.800819297970
O	-1.190135530523	3.313921607601	-3.229640633660
O	-2.989560234229	2.690191361097	0.846705012539
C	-1.981166280727	0.893077370913	-4.230979703396

H	-1.005960988981	0.909744717065	-4.722790608181
H	-2.470071053069	-0.044189754117	-4.503073132008
H	-2.567407939059	1.722897037506	-4.625965980880
C	0.009457126353	3.908353112883	-3.787367342281
H	0.893029604042	3.567541822463	-3.239291949155
H	-0.078442247620	4.990499205712	-3.673383072694
C	0.167119212033	3.585885423604	-5.296221660127
H	0.369333388124	2.514995640382	-5.434196768595
H	-0.773544280166	3.824142724447	-5.812165148194
C	-2.925584393889	2.318561090474	2.251589662760
H	-2.140183093859	2.897826893371	2.750718379739
H	-2.677083657867	1.256087973222	2.345612763142
C	-4.269379797354	2.544265461746	2.976814376222
H	-4.547719476450	3.606888973260	2.948744592006
H	-5.058471411894	1.970015837980	2.471047358611
O	1.247718631726	4.370264046642	-5.806758449764
C	1.557179655992	4.207326101521	-7.207999667073
H	1.850027969318	3.173598464163	-7.433825487679
H	0.702453188607	4.483603981538	-7.839011396417
H	2.392678665990	4.875451741404	-7.413487546661
O	-4.087332475719	2.093403659220	4.324666528776
C	-5.230264819039	2.141166478801	5.202039434027
H	-5.595697737612	3.168657525067	5.329267486578
H	-6.049854421323	1.514798161513	4.825609265154
H	-4.890413563645	1.755572548755	6.162681986981

Cam-F1500

($E_F = -929.32878687$ a.u.; $G_F = -928.93475824$ a.u.)

0 1

C	-1.905812273574	0.800365679167	-2.619634570981
C	-1.228113931543	2.009221939878	-1.875822189473
C	-1.841029921827	1.864127503426	-0.372435991944
C	-2.713957560179	0.595162900803	-0.512668857272
C	-1.760846253242	-0.614677249305	-0.626791549596
C	-1.203092525643	-0.471949535191	-2.072301712225
H	-0.153581713417	1.815281726269	-1.787331003171
H	-0.993466879164	1.674946733192	0.298755314546
H	-3.446627106665	0.509112597462	0.288299029755
H	-0.976047190265	-0.583420920465	0.133392302651
H	-2.295868377170	-1.556085775165	-0.491810407703
H	-1.452595066219	-1.338953541290	-2.687684830530
H	-0.115006110661	-0.369057968365	-2.100594813947
C	-3.312809302650	0.720143168537	-1.938310792541
C	-4.155721709237	-0.499205692782	-2.349310717833
H	-4.504821259450	-0.393524117486	-3.380300295194
H	-3.628787221708	-1.450783849356	-2.276921636741
H	-5.042919371159	-0.563812099685	-1.711813235470
C	-4.182586962225	1.969257448288	-2.161017547551
H	-4.505529615715	2.012657394544	-3.205768911012
H	-5.080336292828	1.913379476011	-1.537445973310
H	-3.672892113726	2.899746130476	-1.927700950105
O	-1.382116077550	3.258722528133	-2.549859879610

O	-2.571373154064	2.970011505310	0.161068753489
C	-1.895354258743	0.882073266190	-4.134630524626
H	-0.879694213878	0.792193059448	-4.527943613201
H	-2.479822709495	0.061678392234	-4.559562641253
H	-2.316702676070	1.824603668256	-4.484902643473
C	-0.221962579078	3.851811965379	-3.167722689786
H	0.692873520642	3.514795686783	-2.666677041993
H	-0.313078904167	4.929218198258	-3.012180264209
C	-0.076828508504	3.619253825169	-4.698304558242
H	0.180282587768	2.574847314621	-4.910618959624
H	-1.033745333956	3.843083270179	-5.190698142495
C	-2.626202431501	3.062504895415	1.596717670387
H	-2.807566051571	4.117409591199	1.811208252026
H	-1.656215921501	2.790121768686	2.031979798177
C	-3.742903729679	2.259157295638	2.326333638753
H	-4.705302760364	2.434460183787	1.824391188694
H	-3.534950080885	1.180978967499	2.304733631832
O	0.958402915262	4.484494039737	-5.177678844094
C	1.287739390950	4.371817879472	-6.578331102045
H	1.642515877833	3.362261307579	-6.824867081494
H	0.423575066826	4.610969404286	-7.211863786072
H	2.084065808494	5.092041712862	-6.762944715774
O	-3.773303985970	2.725058567567	3.680330213484
C	-4.701853661207	2.078396712455	4.574910135032
H	-5.738181354552	2.205098991740	4.235342446874
H	-4.485369643285	1.005944165247	4.668846095691

H	-4.575700515429	2.560475542413	5.543717741774
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Cam_Int1-F1500

($E_F = -929.38634125$ a.u.; $G_F = -929.00240061$ a.u.)

0 1

C	-1.503899880917	1.805616759888	-2.539989446161
C	-0.976830341708	2.772741329318	-3.588367629279
C	-3.252694627764	1.997200448966	0.937654279188
C	-2.614797504957	1.472419090634	-0.323966172407
C	-1.111758694014	1.055233803680	-0.170281723301
C	-0.399522578248	1.388673387876	-1.507847431562
H	-0.535538866365	3.714848614208	-3.270461295099
H	-2.841256950251	2.879323251078	1.425576179708
H	-3.189597466693	0.586095102361	-0.609203495948
H	-0.653795210635	1.607874445387	0.653966171170
H	-1.039941563782	-0.004058939744	0.085321892259
H	0.186007493351	0.550795425662	-1.893527814445
H	0.297855402518	2.217575303608	-1.365349952106
C	-2.606955597246	2.451235595023	-1.568822070382
C	-3.994201954435	2.545707251870	-2.211394534540
H	-3.953805893176	3.141839617235	-3.128132882009
H	-4.397634837679	1.562313513429	-2.460894827955
H	-4.694854012023	3.023669283324	-1.520862715934
C	-2.182133565063	3.867968350113	-1.130482973500
H	-2.163138524585	4.547638576133	-1.984907240418
H	-2.901724107604	4.271349338250	-0.414814164514

H	-1.195756899081	3.885178527970	-0.659794044188
O	-0.456105378799	2.268326495181	-4.767828302183
O	-3.858140300066	1.092351901499	1.793092261084
C	-2.034493769505	0.541989809483	-3.246440612348
H	-1.223832874477	0.064088938560	-3.798977374416
H	-2.427294835177	-0.181784773926	-2.529433032471
H	-2.822224980487	0.782448477776	-3.962262746157
C	0.119069812905	3.248967789929	-5.660837993505
H	0.943419801655	3.767779206796	-5.157741693878
H	-0.641057610745	3.989253829579	-5.931613729889
C	0.657345398532	2.585223611732	-6.944737970127
H	1.419476836026	1.836764014452	-6.685788655964
H	-0.160682035024	2.072941309934	-7.470117205993
C	-4.332746002770	1.651502584349	3.040328905622
H	-5.059054860201	2.444700787594	2.833888323371
H	-3.491724214002	2.088303556382	3.591371001729
C	-4.998825207920	0.577163883418	3.923612744936
H	-5.859748666247	0.141456168297	3.397667356907
H	-4.282487429470	-0.229223338107	4.134890686333
O	1.212891464810	3.630013144597	-7.748979949949
C	1.778837028757	3.252975203617	-9.021240397739
H	2.613987533047	2.551735576411	-8.894982845765
H	1.024028510595	2.796956451232	-9.674992643651
H	2.143196652999	4.174094037700	-9.474436736492
O	-5.407760281526	1.232998705155	5.127976537367
C	-6.075068064118	0.430970999874	6.124014305695

H	-7.007583590532	0.003102617084	5.733513613829
H	-5.429632641959	-0.382369074749	6.480491443203
H	-6.302024552398	1.103415361578	6.950426957224

Cam_TS1-F1000

($E_F = -929.12165882$ a.u.; $G_F = -928.73480771$ a.u.)

0 1

C	-1.817704561741	0.975147392682	-2.753863071649
C	-1.074999625479	2.256908222285	-2.405473670831
C	-2.051287202282	1.921252740332	0.108619576699
C	-2.557521279455	0.648881576970	-0.500305495348
C	-1.418569242247	-0.378611724335	-0.724007044328
C	-0.991425301749	-0.217667249013	-2.201461610304
H	-0.068420714637	2.176097029101	-1.999099505388
H	-1.039009984840	1.949556924738	0.513073828060
H	-3.336745950722	0.251645446135	0.163709382113
H	-0.590559623864	-0.205290866206	-0.032384553606
H	-1.780157346310	-1.390275839655	-0.529016468455
H	-1.224882147074	-1.116798716444	-2.775793061545
H	0.081863025136	-0.047576428781	-2.317309142558
C	-3.158990049871	0.870961620244	-1.926389184229
C	-4.011892549873	-0.348295071965	-2.329553889016
H	-4.437755311538	-0.221079315162	-3.327666112964
H	-3.453506648200	-1.286693362648	-2.320797875945
H	-4.847180363197	-0.454583184823	-1.631389048678
C	-4.036633651064	2.122568907567	-2.035833922874

H	-4.405107801584	2.241082298925	-3.059167059280
H	-4.902658225179	2.037668348326	-1.373690783084
H	-3.489866169292	3.023285203549	-1.759984695197
O	-1.250453207870	3.314887449170	-3.260839312831
O	-2.987811167630	2.601824713748	0.888265286902
C	-2.024838131337	0.872029947015	-4.273764208308
H	-1.063569821547	0.897656210702	-4.792581624321
H	-2.514438281133	-0.068089134228	-4.533823271866
H	-2.627982569694	1.698331340148	-4.650822949043
C	-0.097773654734	3.999971605641	-3.790554639039
H	0.780764866752	3.819862358749	-3.162924409064
H	-0.324348172558	5.067305173942	-3.777161100939
C	0.189011494418	3.572731831919	-5.243123897679
H	0.506475627838	2.520304945033	-5.272181631659
H	-0.734801380147	3.664599087635	-5.831686251165
C	-2.904029850992	2.279125327716	2.296229015439
H	-2.110420714909	2.868977305423	2.770231692220
H	-2.664537243857	1.217767498876	2.423864717149
C	-4.241357952773	2.545971885385	2.999062779662
H	-4.507470837406	3.610359873818	2.931028532649
H	-5.033844620758	1.963948267728	2.507063396753
O	1.211026907328	4.422002628393	-5.754716144512
C	1.570668746799	4.191529626027	-7.124159705555
H	1.959744478269	3.174868786171	-7.270334645372
H	0.712911566769	4.343030767517	-7.793000416247
H	2.349605504661	4.913981311984	-7.366272350486

O	-4.073551067968	2.141220841183	4.357308735652
C	-5.239388954092	2.218724140946	5.185436319921
H	-5.611799099580	3.249410421593	5.261411137105
H	-6.046113127061	1.578270863956	4.803248017445
H	-4.940882128790	1.870519164310	6.174076248044

Cam_Int1-F1000

($E_F = -929.18866883$ a.u.; $G_F = -928.80461945$ a.u.)

0 1

C	-1.513514528988	1.793151485933	-2.546314771907
C	-0.970322362258	2.758825300759	-3.575439771785
C	-3.210166148668	2.005217621574	0.925162718051
C	-2.605779076801	1.471069720855	-0.339516202607
C	-1.120268601813	0.993135268538	-0.200076583962
C	-0.410088853451	1.319892998042	-1.538009522183
H	-0.496953772755	3.681716921253	-3.247588350985
H	-2.758193670186	2.858294126398	1.428736849777
H	-3.217235351690	0.611107285209	-0.628986384763
H	-0.635668149949	1.515019226662	0.628980881859
H	-1.088893767782	-0.071934331310	0.038999843016
H	0.138646463400	0.467605896834	-1.945343024505
H	0.319011086009	2.120410230812	-1.391925079019
C	-2.577500784343	2.464942112463	-1.562495602809
C	-3.967434707950	2.619239853184	-2.188625725945
H	-3.914320408146	3.225016835100	-3.098311625312
H	-4.410142867211	1.654861354741	-2.445568725712

H	-4.642090396626	3.114150020317	-1.484386192391
C	-2.099143337612	3.860118612429	-1.107937935003
H	-2.068328545973	4.552708926213	-1.951402235395
H	-2.796022407789	4.275945262878	-0.377287546862
H	-1.107006133545	3.836840744338	-0.649670425593
O	-0.467665997887	2.246676628725	-4.752934506325
O	-3.838614341418	1.104554167709	1.759464234310
C	-2.096172793519	0.560825275115	-3.268158036540
H	-1.308530801640	0.062954406047	-3.835810243344
H	-2.508803016192	-0.159894204600	-2.559344747298
H	-2.880817105326	0.841687029543	-3.972507945927
C	0.126282767563	3.217258751063	-5.632916839430
H	0.969258763125	3.708698612114	-5.132500225260
H	-0.612768321901	3.981742797649	-5.895770486269
C	0.629667377021	2.536413178824	-6.910904824341
H	1.366745532525	1.761230027849	-6.656487401546
H	-0.208532166033	2.052257370441	-7.431906432463
C	-4.286489391149	1.655128109642	3.011883052215
H	-4.988934904466	2.475078824692	2.827107178995
H	-3.431187524232	2.052636231249	3.571259191794
C	-4.976418616474	0.577791745300	3.856256337010
H	-5.849974605702	0.181573189375	3.319287487965
H	-4.282699327749	-0.254905612617	4.041223681371
O	1.213785980384	3.559562447773	-7.713184000958
C	1.745352156952	3.138039278278	-8.975234776959
H	2.549010306269	2.400587902096	-8.845780817812

H	0.964761557598	2.703697323607	-9.614302827621
H	2.148383479433	4.029827193474	-9.454472279055
O	-5.362475614665	1.208136393970	5.075307147174
C	-6.042376597850	0.376886498688	6.023648855523
H	-6.981469913051	-0.016500706796	5.611661645857
H	-5.413887879577	-0.465912097450	6.341750719538
H	-6.262826855385	1.007008869800	6.884895957937

Cam-F1000

($E_F = -929.18259484$ a.u.; $G_F = -928.78773634$ a.u.)

0 1

C	-1.940303159443	0.761735964549	-2.638732774057
C	-1.257074869623	1.961290326067	-1.892837639396
C	-1.848843114279	1.819659815935	-0.401230678210
C	-2.748520302882	0.566135204037	-0.528811011102
C	-1.806273282064	-0.652869743245	-0.642441136321
C	-1.244225458263	-0.513191037728	-2.087785236979
H	-0.177174107189	1.784473734663	-1.839846604960
H	-1.009739710645	1.620035435281	0.278079252261
H	-3.480444573733	0.491121240041	0.273951868308
H	-1.022012604033	-0.630419318516	0.118606421543
H	-2.350123205726	-1.589423355748	-0.509853958426
H	-1.494511314324	-1.379885732708	-2.703101805063
H	-0.155622053593	-0.414199588149	-2.112319777097
C	-3.348283261361	0.688278507277	-1.955389776386
C	-4.192002117721	-0.531610330597	-2.365077441410

H	-4.543621006264	-0.423546761141	-3.394993291552
H	-3.665409302959	-1.483541580890	-2.296535380350
H	-5.077604201444	-0.597429791701	-1.725497239961
C	-4.222166653521	1.934588323014	-2.178225187976
H	-4.540454098151	1.980676801847	-3.224346198650
H	-5.123237672094	1.869461418933	-1.560003838208
H	-3.718265357457	2.865541695936	-1.937529056181
O	-1.464169220057	3.219843063280	-2.524117279107
O	-2.540203988910	2.964974926539	0.085647163912
C	-1.925467015776	0.849977174565	-4.153392559299
H	-0.907693595359	0.770433158770	-4.544446736920
H	-2.504070146899	0.029174357783	-4.585620998295
H	-2.351152207455	1.792646939248	-4.498446529444
C	-0.324806144130	3.898165396963	-3.066734439841
H	0.581859557201	3.651155316869	-2.501562299152
H	-0.515724491318	4.966727646019	-2.944381103794
C	-0.082437327041	3.630187502021	-4.567777977542
H	0.239500591674	2.593143564989	-4.728931966532
H	-1.021854797727	3.783486285096	-5.117975915703
C	-2.571575929274	3.124664090114	1.507590071668
H	-2.801355437498	4.178116348386	1.678768159834
H	-1.583132788526	2.918203696151	1.939260552649
C	-3.634557296399	2.296757171160	2.267594182963
H	-4.606403109403	2.400087322837	1.762829323232
H	-3.369277590956	1.230618303517	2.285229421762
O	0.924375469608	4.534263401390	-5.017488906610

C	1.278588830793	4.407816863155	-6.400874979779
H	1.679125584208	3.409034271238	-6.622490304645
H	0.415373254883	4.595449750180	-7.053761631621
H	2.047171783190	5.155523952735	-6.595739170682
O	-3.686801813288	2.809975963551	3.597551661194
C	-4.586703713338	2.135482138616	4.485529431560
H	-5.623034783614	2.192868607372	4.125879046255
H	-4.312529659420	1.078619710419	4.608120949800
H	-4.511008364846	2.640975830310	5.448055383896

Cam_TS1-F800

($E_F = -929.05840319$ a.u.; $G_F = -928.67120573$ a.u.)

0 1

C	-1.821943025863	0.929812769732	-2.709530378270
C	-1.003253548659	2.161137178321	-2.372757722874
C	-2.253549539404	1.890357324745	0.192099588114
C	-2.814688370353	0.700568815141	-0.518105863550
C	-1.761671980698	-0.430122912158	-0.630940306719
C	-1.150273646160	-0.303548939441	-2.045894486320
H	0.001554813872	2.030453441142	-1.975201993587
H	-1.312811793400	1.806852569893	0.733124849838
H	-3.700763785938	0.373400679127	0.043165631313
H	-1.006398166080	-0.349828630144	0.154689499132
H	-2.242263829904	-1.401791805064	-0.500259933030
H	-1.362490141431	-1.194776112034	-2.640746686279
H	-0.062434216721	-0.199639364857	-2.025817774789

C	-3.234229141721	0.978827938680	-2.001489538653
C	-4.167277272320	-0.149954885500	-2.485341409047
H	-4.493465552841	0.021195873578	-3.513791272659
H	-3.702639901158	-1.137706346223	-2.442036330988
H	-5.064330631163	-0.177724441580	-1.860026879803
C	-3.963356172543	2.313486859860	-2.188057418722
H	-4.202715075807	2.472959013276	-3.243574975466
H	-4.901293902270	2.314303469515	-1.625392198063
H	-3.361267597607	3.152371987050	-1.843176229846
O	-1.146803457709	3.238212062729	-3.216195152739
O	-3.181636777601	2.730059481575	0.768332609702
C	-1.909338519570	0.766213405114	-4.239226436043
H	-0.906473962842	0.696772510143	-4.668943970809
H	-2.445897698735	-0.145740070513	-4.506863112170
H	-2.411198303668	1.617491782232	-4.700433679953
C	0.023934038436	3.895129803714	-3.729648702903
H	0.909812809686	3.624743216437	-3.145985284355
H	-0.136838712939	4.971490734801	-3.641029693835
C	0.238731828476	3.545386340673	-5.210795153971
H	0.479052058502	2.477691925097	-5.316279846390
H	-0.692302193416	3.738637513092	-5.762903529988
C	-3.071314553105	3.025151243602	2.170689333890
H	-3.335245618183	4.076020089791	2.303810452362
H	-2.045019250044	2.875118543326	2.522008184929
C	-4.040474188381	2.158873570023	2.990253416564
H	-5.056434934346	2.282078440416	2.588426019412

H	-3.765874634055	1.096915489344	2.898565238487
O	1.302149331356	4.353746048612	-5.700117634078
C	1.598974518839	4.178082700722	-7.088428080935
H	1.907887801751	3.146306449368	-7.305421815235
H	0.733459981108	4.427528781747	-7.717296812294
H	2.420282213355	4.855484886911	-7.321595138639
O	-3.968232773949	2.590718042877	4.344110901484
C	-4.887684441531	1.952157045324	5.233955244059
H	-5.928155378825	2.129932646372	4.929555439425
H	-4.713762411369	0.868367742043	5.282048344393
H	-4.722247810108	2.386103283673	6.219966602240

Cam_Int1-F800

($E_F = -929.11014652$ a.u.; $G_F = -928.72608852$ a.u.)

0 1

C	-1.524807480740	1.808952852885	-2.540412250944
C	-0.969760821707	2.756361350777	-3.575503997082
C	-3.204920125327	2.081718540673	0.923184078927
C	-2.613018127746	1.526241435738	-0.334631178990
C	-1.137172821024	1.021324504774	-0.191833864976
C	-0.425403604994	1.322437017427	-1.534069103862
H	-0.484203123711	3.676245420524	-3.257252077791
H	-2.734066736658	2.925493101550	1.425186126295
H	-3.241104839948	0.675540800804	-0.615588124547
H	-0.641384958756	1.541714666863	0.631536592829
H	-1.125916349407	-0.041855686372	0.057202457588

H	0.104233093339	0.456195447823	-1.937137597385
H	0.320031334886	2.109550004017	-1.397890731805
C	-2.570658435697	2.509259437557	-1.562221939945
C	-3.959599292648	2.685454377257	-2.185214656715
H	-3.897718643558	3.282254846280	-3.100235257514
H	-4.422071840324	1.727817273513	-2.432338510757
H	-4.621892411061	3.199479225526	-1.482969098625
C	-2.065030918951	3.898843280026	-1.119376828038
H	-2.026031541309	4.585474486359	-1.967305543814
H	-2.751017545402	4.331795428426	-0.388435881043
H	-1.071341585529	3.860880241758	-0.665487597990
O	-0.468752027733	2.220005084087	-4.740436443826
O	-3.851393265023	1.195916482606	1.756154504066
C	-2.132838780269	0.582109984826	-3.251230648608
H	-1.356326861096	0.065298973603	-3.817071723396
H	-2.556877893966	-0.125415265889	-2.535932649724
H	-2.914079144365	0.872354795115	-3.955563709688
C	0.138262223912	3.169565732578	-5.629961807273
H	0.986173264452	3.658497513764	-5.135174959272
H	-0.590076591304	3.939020771670	-5.908218448199
C	0.633480666093	2.457170023901	-6.889595368943
H	1.358977775743	1.676785992811	-6.617824728153
H	-0.210265539664	1.974037192135	-7.402780930185
C	-4.289777562110	1.757310404736	3.003887049885
H	-4.975605270877	2.591026749780	2.817644635118
H	-3.428653762098	2.137445523376	3.566641388077

C	-5.000636890843	0.690916287493	3.838393843645
H	-5.879408383940	0.313086764857	3.296424748540
H	-4.322975018853	-0.155517736218	4.021385845456
O	1.232544459471	3.454707518379	-7.709184114526
C	1.755732328075	2.989912565297	-8.955347400567
H	2.546081810776	2.241785166804	-8.805142091714
H	0.968071144126	2.551047428410	-9.582909265832
H	2.175414002011	3.859158868610	-9.461280669404
O	-5.378427676979	1.321908426478	5.057245720522
C	-6.074530416349	0.490917346072	5.988468194998
H	-7.016994779571	0.116326023653	5.566227002999
H	-5.461031270813	-0.365843776950	6.299186105736
H	-6.291946764403	1.110955036395	6.857929286021

Cam-F800

($E_F = -929.12507898$ a.u.; $G_F = -928.73091641$ a.u.)

0 1

C	-1.996123749111	0.765136894369	-2.650966951203
C	-1.276330255512	1.942345466148	-1.907904574203
C	-1.855247235674	1.817692952710	-0.416772129795
C	-2.794726650684	0.592018650452	-0.534492019778
C	-1.886133675438	-0.652184293927	-0.654906912371
C	-1.330587999738	-0.527954829793	-2.104696700947
H	-0.199377495722	1.744312442558	-1.873849810906
H	-1.021145725631	1.595143139298	0.261690831422
H	-3.522241027187	0.537152110246	0.273952718110

H	-1.095870666019	-0.651068124147	0.100244263217
H	-2.454001325009	-1.573711386061	-0.518137135578
H	-1.607745330679	-1.387838158901	-2.717950310047
H	-0.239896806701	-0.457865994484	-2.136374867993
C	-3.401355974131	0.727873642865	-1.957488551734
C	-4.276779636708	-0.471771575218	-2.361177469261
H	-4.631434382240	-0.355374828999	-3.389156713474
H	-3.773317575784	-1.436261250037	-2.295402211453
H	-5.160049179718	-0.515809711965	-1.716532772440
C	-4.248657446561	1.993534519175	-2.174602043329
H	-4.572716477022	2.046953802902	-3.218612835969
H	-5.147100812185	1.947162574470	-1.550783549022
H	-3.722828606523	2.912718344174	-1.936611320373
O	-1.474662265423	3.207477819150	-2.524574243656
O	-2.500321300343	2.994564235936	0.053256184045
C	-1.986348751165	0.859768411087	-4.165436408338
H	-0.971742260079	0.763366761457	-4.561294602687
H	-2.582923304037	0.052972113263	-4.599651604771
H	-2.394351656031	1.812961884332	-4.503234180162
C	-0.325124437378	3.895064963277	-3.022846378924
H	0.560279004826	3.672582668758	-2.415171454482
H	-0.537309110800	4.962267645202	-2.927823871105
C	-0.023669628167	3.596902552501	-4.503049818746
H	0.300971429643	2.554951435140	-4.628997033127
H	-0.940741342147	3.738783481067	-5.092666321721
C	-2.515008979996	3.181241427320	1.469074037995

H	-2.717729959227	4.242706228309	1.624618376312
H	-1.529282646995	2.957091470840	1.898620699884
C	-3.592850547279	2.390237133843	2.239139691905
H	-4.562812568519	2.510076503517	1.734085966391
H	-3.352954570481	1.318203868174	2.269004667229
O	0.999772574923	4.489133700588	-4.930969751251
C	1.379476044664	4.343271652819	-6.301917226843
H	1.775464532711	3.338366160638	-6.504289535268
H	0.531049857330	4.529752863943	-6.974565917035
H	2.158547667284	5.081251421261	-6.493002223714
O	-3.631042436624	2.919911847652	3.560803668828
C	-4.550865271337	2.273894611448	4.443817844823
H	-5.583232502211	2.353579242802	4.076445756070
H	-4.303801083577	1.211060585812	4.574117976242
H	-4.471803789112	2.781135590241	5.405326831933

Cam_TS1-F600

($E_F = -928.99354045$ a.u.; $G_F = -928.60751483$ a.u.)

0 1

C	-1.834652763254	0.935297598912	-2.758804335002
C	-0.987058195125	2.150724979483	-2.452439973942
C	-2.294968034703	1.851938756882	0.246828060085
C	-2.790611642993	0.679538040469	-0.531861408819
C	-1.690165274011	-0.405521059247	-0.674261905389
C	-1.159615162468	-0.307426113437	-2.122897648617
H	0.029124411619	2.017385757975	-2.086603722896

H	-1.360972605740	1.797658703836	0.801396554167
H	-3.667406949365	0.288092937489	0.003632339723
H	-0.895038805227	-0.255779077690	0.060211512749
H	-2.108955333903	-1.394742162182	-0.478344361813
H	-1.433558593184	-1.196763769936	-2.694900327646
H	-0.069775636310	-0.237005584246	-2.167891219231
C	-3.226233273398	0.992642970265	-2.007837924007
C	-4.183515343145	-0.119889178410	-2.483843614096
H	-4.515157204843	0.052914055881	-3.510081649289
H	-3.735044424893	-1.115400548329	-2.438193519612
H	-5.075615582204	-0.130024367224	-1.851113851847
C	-3.943792345980	2.337323733278	-2.160867065579
H	-4.209374948730	2.510467677163	-3.207921711765
H	-4.864940272748	2.344668515117	-1.571833116247
H	-3.321403001155	3.164643570376	-1.824566202726
O	-1.175767346645	3.252506292590	-3.250546427059
O	-3.263146995479	2.658520572396	0.795673560460
C	-1.971107857797	0.780406358622	-4.287438206367
H	-0.981990432666	0.714634521275	-4.748566837932
H	-2.516216388369	-0.129068980476	-4.545721448771
H	-2.486371274138	1.635692892830	-4.726289739073
C	-0.026573760475	3.947807839498	-3.752359384584
H	0.844424499036	3.778930208670	-3.110355928914
H	-0.264228599471	5.012984045887	-3.742694480841
C	0.282250048804	3.518477510524	-5.191576979194
H	0.584112904472	2.460889419293	-5.214377791005

H	-0.627938848966	3.622985146864	-5.799566350759
C	-3.148880651302	3.028530439212	2.176610108979
H	-3.477411129204	4.065634536966	2.265748545343
H	-2.110367447338	2.960218299578	2.517309305078
C	-4.049411529763	2.138333770230	3.040443179085
H	-5.075738183897	2.181829861133	2.648188901940
H	-3.709241615273	1.092874864119	2.983505653106
O	1.322826310539	4.353340948138	-5.679228919752
C	1.668471633525	4.124647633366	-7.044753940679
H	2.029543881434	3.098756345606	-7.201773268850
H	0.812108008144	4.302355299633	-7.709761100216
H	2.465542969411	4.826208124715	-7.290896034629
O	-3.989527581790	2.624046371668	4.374154198556
C	-4.864206920306	1.960146866122	5.284992172608
H	-5.914663221913	2.065802232969	4.980586209373
H	-4.626237725686	0.890259256607	5.364291360555
H	-4.723735280153	2.430812077836	6.258094647680

Cam-F600

($E_F = -929.06817690$ a.u.; $G_F = -928.67341716$ a.u.)

0 1

C	-2.031341422664	0.750574194466	-2.675828101817
C	-1.307674581571	1.926134004226	-1.938831176991
C	-1.859169599210	1.797712278514	-0.444130921344
C	-2.799935864725	0.571009255346	-0.547793076505
C	-1.886925455765	-0.668957704225	-0.683461333453

C	-1.352452520947	-0.540409968535	-2.141326489698
H	-0.227980781945	1.741140487396	-1.931288813812
H	-1.018594003142	1.577343712784	0.227058938363
H	-3.515265461475	0.511689200537	0.271277108897
H	-1.085673975861	-0.665420695022	0.060017127388
H	-2.448436398218	-1.593271377597	-0.539799659792
H	-1.634172255810	-1.400710695419	-2.751832890432
H	-0.262625863827	-0.465239771966	-2.187943395939
C	-3.427243632873	0.703951690360	-1.962745425767
C	-4.299124223900	-0.501665065124	-2.356932483082
H	-4.666056894148	-0.386416237964	-3.380752103101
H	-3.788830023330	-1.462941955740	-2.298052812531
H	-5.174699212185	-0.552183334542	-1.702358304473
C	-4.288706723145	1.962434552354	-2.165601766151
H	-4.626082174796	2.016235710722	-3.205382200814
H	-5.179238423582	1.904719526041	-1.531340092299
H	-3.768481546942	2.885273463336	-1.930463195082
O	-1.541259645139	3.190840676468	-2.540198205280
O	-2.491003978727	2.984064392339	0.015707319264
C	-2.038692006463	0.856062102538	-4.189864410981
H	-1.026321733497	0.780229926634	-4.596373762996
H	-2.627077191025	0.043767431948	-4.625086593752
H	-2.464003788727	1.806136355874	-4.515173978538
C	-0.403993837550	3.928377174696	-2.982336206120
H	0.454251856864	3.770407773014	-2.317957609503
H	-0.678275322040	4.984092846266	-2.929924488833

C	-0.008794002667	3.600141845434	-4.429469612337
H	0.352741051006	2.564385196024	-4.504046804697
H	-0.895026293444	3.694252517216	-5.073287344265
C	-2.484619543413	3.194045521921	1.425394220977
H	-2.684834064671	4.257792887649	1.568730183251
H	-1.494023148004	2.974794754510	1.846576586641
C	-3.553791944586	2.412669787279	2.209182960731
H	-4.527066297610	2.527413094952	1.709091923259
H	-3.313831918709	1.340776260138	2.247148423360
O	1.007628078274	4.511072462259	-4.825995909914
C	1.435383374005	4.352578480938	-6.177630245040
H	1.859806357539	3.353631562916	-6.350872339960
H	0.606138812636	4.508762057216	-6.881500351964
H	2.204421708514	5.103999342258	-6.357473633211
O	-3.583458474662	2.954182335144	3.524025969069
C	-4.504709680620	2.314379491159	4.404558975540
H	-5.536171044059	2.394319663038	4.034147343450
H	-4.260756000445	1.251133841451	4.538947191253
H	-4.429194570906	2.822902656196	5.365842426237

Cam_Int1-F600

($E_F = -929.03196324$ a.u.; $G_F = -928.64781319$ a.u.)

0 1

C	-1.576647695422	1.811194683486	-2.563282847205
C	-0.941303781640	2.745985151985	-3.558363193134
C	-3.123198488603	2.074740957940	0.952014523382

C	-2.627925817467	1.530714077732	-0.348379455084
C	-1.219066440055	0.851958696400	-0.276397992293
C	-0.515670285309	1.135975355281	-1.626216739143
H	-0.353455668020	3.590690102508	-3.206164053433
H	-2.541191187022	2.815629792031	1.497974682856
H	-3.357446408011	0.776405345275	-0.658005795991
H	-0.643942293552	1.271313157932	0.553034129552
H	-1.325276902546	-0.216276686914	-0.076225311505
H	-0.113293558596	0.234488411136	-2.093689691321
H	0.327497158524	1.814845538754	-1.478126850380
C	-2.500430489204	2.572856700482	-1.515979431508
C	-3.873895319870	2.952755208320	-2.079718308866
H	-3.764128643833	3.591009906011	-2.961600872105
H	-4.457365907003	2.074689950492	-2.363526785387
H	-4.448159263094	3.500588396316	-1.327330628798
C	-1.817501082395	3.862233395822	-1.011126468415
H	-1.724449366489	4.593500643847	-1.816420886086
H	-2.422565758994	4.324226645236	-0.228395631486
H	-0.821150067769	3.678551206264	-0.600763134769
O	-0.515305596906	2.212063386078	-4.751486048307
O	-3.866190097430	1.223197133368	1.735193044866
C	-2.347965116147	0.710466192734	-3.321444952075
H	-1.655513573204	0.141167433995	-3.943203109109
H	-2.832816783793	0.015396774841	-2.633125600631
H	-3.108883229588	1.133388475442	-3.979414515810
C	0.181045335960	3.128544535520	-5.605227251846

H	1.085208054859	3.496895472761	-5.105339039776
H	-0.459763754235	3.986309623517	-5.837019518828
C	0.572572047859	2.418493999973	-6.898108433784
H	1.206599956366	1.549056117377	-6.670905348014
H	-0.328342490068	2.056867185177	-7.414426522933
C	-4.219888597509	1.749537169481	3.021313506646
H	-4.803281441577	2.669285727278	2.902789567541
H	-3.314473051174	1.985752176388	3.593528101384
C	-5.042897211306	0.717923968454	3.787512704437
H	-5.962933590108	0.483500842478	3.232870865477
H	-4.467164530346	-0.212264443154	3.900360540901
O	1.270451377643	3.372849089622	-7.686831845511
C	1.710797034511	2.893663197577	-8.955440170299
H	2.407976726337	2.051260127345	-8.847305382704
H	0.865297098573	2.573519839900	-9.579891943295
H	2.223396283253	3.722149297521	-9.444172764881
O	-5.336639378310	1.298774244026	5.051188158427
C	-6.114375736079	0.479920616105	5.921311540162
H	-7.094302033629	0.244865421903	5.483337259242
H	-5.598271234917	-0.461366230387	6.155960302152
H	-6.259936295329	1.047129314579	6.840597408118

Cam_TS1-F400

($E_F = -928.92862315$ a.u.; $G_F = -928.54274974$ a.u.)

0 1

C	-1.866278971849	0.927921664088	-2.833685623414
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C	-0.981060859141	2.117657124927	-2.545173541908
C	-2.361126014234	1.807332399054	0.290918982206
C	-2.745717304737	0.646843649706	-0.559775506653
C	-1.548280984188	-0.330441278803	-0.739615217085
C	-1.193084946105	-0.330340512526	-2.240142566481
H	0.048207061651	1.965313472490	-2.226639734081
H	-1.442805023748	1.804564483886	0.872396962458
H	-3.585171217313	0.146799132759	-0.054575798781
H	-0.695828612303	0.000890288562	-0.141055727356
H	-1.803907748004	-1.332151019266	-0.387815128462
H	-1.594978665649	-1.218028528511	-2.733821565228
H	-0.114502276540	-0.337666805576	-2.419207320994
C	-3.223923402456	0.995921294000	-2.021605848521
C	-4.220055031641	-0.091812066377	-2.475759968286
H	-4.566915212396	0.083090226524	-3.496573706939
H	-3.798612880857	-1.099176045095	-2.428519279841
H	-5.099315173473	-0.073174314683	-1.825552900726
C	-3.924234621898	2.354021043700	-2.132020497910
H	-4.228689226873	2.540922111227	-3.166043231031
H	-4.818358660320	2.372350402365	-1.504067057967
H	-3.274263874831	3.167313930890	-1.814798195309
O	-1.206931779559	3.254699251674	-3.278881636963
O	-3.399628612937	2.537384794886	0.810631764579
C	-2.066644580354	0.800324249222	-4.357880160894
H	-1.097443355027	0.740598879488	-4.860533372801
H	-2.626171074770	-0.102105087940	-4.610362790890

H	-2.595848466350	1.665634036925	-4.759393740675
C	-0.070964665762	3.981083241635	-3.757765589363
H	0.775115229191	3.886251436964	-3.068226617244
H	-0.362451400571	5.031231220137	-3.806761517110
C	0.325979613781	3.501076987132	-5.154904569777
H	0.651149443211	2.450404866983	-5.114031225122
H	-0.550326927134	3.556995051132	-5.816847686823
C	-3.288886721661	3.025666142894	2.151030063232
H	-3.728133726509	4.024663351684	2.174728543046
H	-2.240903660093	3.097924915387	2.460240341332
C	-4.062759854040	2.107822172778	3.098162653510
H	-5.095917931111	2.010064568657	2.734233346416
H	-3.609251108087	1.104522366473	3.100779717398
O	1.372221789904	4.339243670728	-5.617855977953
C	1.778239307385	4.067020706383	-6.955053696980
H	2.159632136634	3.041532901392	-7.059114511202
H	0.948820449399	4.206790848463	-7.662194601165
H	2.575717916971	4.770319729618	-7.195417476015
O	-4.028693456626	2.688519789570	4.391845792872
C	-4.810879089458	1.993065082961	5.356716220691
H	-5.871158883310	1.965808476276	5.068922399293
H	-4.457527925037	0.961437131098	5.494287960314
H	-4.709662538205	2.533176756353	6.298274752948

Cam-F400

($E_F = -929.01194947$ a.u.; $G_F = -928.61742012$ a.u.)

0 1

C	-2.069756228100	0.718872960495	-2.701551314977
C	-1.347079330447	1.895600530713	-1.972375277030
C	-1.883053573004	1.771573952978	-0.477474869930
C	-2.831868020733	0.548950594150	-0.569472820080
C	-1.920753085263	-0.692877173409	-0.702878082303
C	-1.388091025234	-0.568931718106	-2.162269627901
H	-0.265410202954	1.722982250382	-1.981802096656
H	-1.041560338582	1.549660274239	0.191946044236
H	-3.544071798835	0.495701152838	0.252947511863
H	-1.118244666724	-0.688935642395	0.039216999287
H	-2.483575312315	-1.615848502668	-0.556090504313
H	-1.668275791542	-1.432233316696	-2.769139107621
H	-0.298444326761	-0.491569233247	-2.209869957854
C	-3.464087512878	0.673514252119	-1.983804898881
C	-4.333178909551	-0.536139145010	-2.372357957605
H	-4.703264214965	-0.423287948951	-3.395347591260
H	-3.819656070233	-1.495674608018	-2.314015009757
H	-5.206648069477	-0.588715925324	-1.715163687595
C	-4.331982652090	1.927521151908	-2.186809449234
H	-4.666747258513	1.982178015951	-3.227386376871
H	-5.224165280479	1.861874354714	-1.555527125033
H	-3.817798988171	2.852415950034	-1.947436306562
O	-1.610004851762	3.155188241987	-2.569326872899
O	-2.498036004271	2.971231592699	-0.033252309318
C	-2.074101106656	0.824570843855	-4.215740449173

H	-1.058170606274	0.765366575273	-4.617142530171
H	-2.648938734264	0.004730210119	-4.654962956169
H	-2.510148759901	1.769830368968	-4.541045098278
C	-0.484235101886	3.943685513471	-2.937601759013
H	0.339517626585	3.824559405398	-2.223287918023
H	-0.806674139781	4.986486075195	-2.905785955246
C	0.000185619568	3.619185857336	-4.353946993570
H	0.378758874526	2.587168958963	-4.402457859133
H	-0.848676161201	3.696881006684	-5.048640049124
C	-2.463654412281	3.211935314100	1.368357608110
H	-2.669171036803	4.276844587458	1.494968809307
H	-1.463916857852	3.007493936893	1.775596833735
C	-3.512082899170	2.435117036693	2.176365856957
H	-4.493854950075	2.538793376521	1.690427795857
H	-3.265408882303	1.364747147558	2.220656131434
O	1.022986891147	4.542599646796	-4.693436252875
C	1.511206690832	4.389632407755	-6.021411310341
H	1.950935333255	3.394160220819	-6.177014292613
H	0.713356947318	4.539624807123	-6.762286125674
H	2.282004114936	5.146628557021	-6.168271621771
O	-3.524233264763	2.989468467658	3.483891401095
C	-4.439468671173	2.355409481765	4.369571133555
H	-5.472933665010	2.434107340770	4.003916967783
H	-4.196310105818	1.292168577204	4.507061655740
H	-4.360710020367	2.866160833619	5.329577768360

Cam_Int1-F400

($E_F = -928.95123648$ a.u.; $G_F = -928.56778312$ a.u.)

0 1

C	-1.379517911107	1.500170164814	-2.528102564848
C	-0.486460501616	2.243771337860	-3.477937878544
C	-3.171721950858	2.133275526311	0.809395778068
C	-2.633771493179	1.479377494559	-0.418378917439
C	-1.334945459637	0.643487797944	-0.182849186911
C	-0.513240355568	0.730064645102	-1.492506236199
H	0.561110750074	1.976075997742	-3.599123930913
H	-2.602979460644	2.908167742026	1.321367505594
H	-3.416336973441	0.797734088104	-0.767396223218
H	-0.769967588228	1.060229948258	0.654894765760
H	-1.586291638396	-0.383513052597	0.089042430439
H	-0.235066060309	-0.254366134091	-1.876576366098
H	0.418870865441	1.273147159440	-1.314263398104
C	-2.275111775678	2.436195962421	-1.603125055690
C	-3.530884485631	2.972847009135	-2.299887347351
H	-3.259414483865	3.549341554422	-3.187356093169
H	-4.202288516967	2.168485305026	-2.607721181125
H	-4.087091200320	3.621815924363	-1.617359133791
C	-1.443901715209	3.636905340408	-1.108068352354
H	-1.125717534574	4.250533218396	-1.953142907535
H	-2.040379235060	4.266783972517	-0.443461068200
H	-0.546315929267	3.328631133787	-0.566181385181
O	-1.089875670482	2.855178451567	-4.547712862386

O	-3.919295619467	1.319242372321	1.625471028841
C	-2.245059945036	0.496320552318	-3.333660561190
H	-1.592972239125	-0.221816570793	-3.838489155967
H	-2.926894230224	-0.066046108153	-2.690823219765
H	-2.830512504943	1.008908106443	-4.097100055510
C	-0.239013806938	3.600848092953	-5.425767376854
H	0.629052132220	3.987375358978	-4.882782645951
H	-0.825460865170	4.448219282822	-5.784650702523
C	0.220053788337	2.770905179032	-6.624762059501
H	0.828593125646	1.916366533706	-6.291953133631
H	-0.657480666745	2.375014579459	-7.156424763250
C	-4.308045650405	1.900033911407	2.873653184341
H	-4.931593929691	2.784550184388	2.701986417074
H	-3.421621302513	2.206115833580	3.442702495046
C	-5.088103420210	0.864025156045	3.672203007791
H	-5.986715193441	0.560399244018	3.115672284447
H	-4.467046648880	-0.030467723991	3.827395986904
O	0.972759858777	3.645922169841	-7.450454969042
C	1.425426828916	3.065083871106	-8.667672101312
H	2.089822354150	2.209247103224	-8.483538217802
H	0.584246835821	2.729394936923	-9.289995152175
H	1.978867237365	3.837719170496	-9.201581790089
O	-5.429347016381	1.473891500252	4.907356203835
C	-6.167205327747	0.634376305245	5.787359912897
H	-7.123191663499	0.325373485173	5.341958412112
H	-5.597632430681	-0.266229846699	6.056486428421

H	-6.364514656828	1.214576252660	6.688891843705
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Cam_TS1-F200

($E_F = -928.86369367$ a.u.; $G_F = -928.47748199$ a.u.)

0 1

C	-1.890142282754	0.894425976752	-2.905430126653
C	-0.961122658624	2.059792771233	-2.673006219212
C	-2.521317714781	1.746730093744	0.350960701555
C	-2.748601580793	0.624684361260	-0.597502211296
C	-1.452375847275	-0.215428323959	-0.777980923609
C	-1.235068064298	-0.360322281973	-2.291231822229
H	0.084258583469	1.886340804250	-2.425434318883
H	-1.630572844088	1.806656721818	0.970318780256
H	-3.546303684844	0.001161390162	-0.167580928698
H	-0.604650018640	0.315389649485	-0.335361263080
H	-1.521781356860	-1.180896982046	-0.271976657606
H	-1.734955898240	-1.253641649374	-2.673682158048
H	-0.179246697679	-0.450240854500	-2.562427110654
C	-3.225162399672	1.020626283975	-2.059628228307
C	-4.283320252329	-0.006526022747	-2.515066529050
H	-4.643734461551	0.208680824538	-3.523590112692
H	-3.910661114534	-1.033992291156	-2.499022096936
H	-5.145167265620	0.039791892950	-1.843254363507
C	-3.862895460358	2.411829628305	-2.144098375395
H	-4.143555497998	2.637427488306	-3.176965958549
H	-4.762426059699	2.453697009740	-1.525978442930

H	-3.182741029068	3.188785807154	-1.800044237077
O	-1.224315853970	3.212455576386	-3.365661789936
O	-3.650678754425	2.344735074165	0.844622449793
C	-2.129485660518	0.735926229360	-4.421518974905
H	-1.172369147262	0.664207617766	-4.945950816768
H	-2.698623255736	-0.168733306837	-4.643288081352
H	-2.665618430619	1.595925358936	-4.826244118550
C	-0.103699165864	3.985279320900	-3.797607506030
H	0.710984416109	3.940158682709	-3.066135460385
H	-0.442232863729	5.019153307147	-3.875808419256
C	0.380730045017	3.498692359788	-5.160636241592
H	0.713989376116	2.451960451265	-5.087369259727
H	-0.453716451150	3.536336579724	-5.876150542719
C	-3.565970856766	2.989095898426	2.115936022847
H	-4.196066213606	3.879309197095	2.074208800203
H	-2.539239832424	3.300666552867	2.334597220000
C	-4.083032127954	2.047613055662	3.199374285240
H	-5.095720756861	1.713954542271	2.929267741978
H	-3.439309131673	1.156297493916	3.259561838764
O	1.442187356019	4.344017907963	-5.565904405222
C	1.929469009614	4.051025825306	-6.867706982055
H	2.325032650750	3.027263964368	-6.928883502810
H	1.143292464846	4.168741032992	-7.626645348192
H	2.734362651247	4.756420016201	-7.075592986015
O	-4.088178508508	2.759376618490	4.423916765661
C	-4.654902523159	2.025729845215	5.499975190351

H	-5.702596323131	1.761810727893	5.298112313266
H	-4.093055084209	1.102073961038	5.698746406222
H	-4.611906938967	2.664842003386	6.382263916117

Cam_Int1-F200

($E_F = -928.87803746$ a.u.; $G_F = -928.49289924$ a.u.)

0 1

C	-1.332263774510	1.310134031651	-2.501813692475
C	-0.566558065269	2.194718768321	-3.432198309796
C	-2.908386578901	1.467309689882	1.001775103429
C	-2.428102324627	1.005423345367	-0.323694978848
C	-1.069607754409	0.268332255665	-0.245953549575
C	-0.351886749385	0.512114206759	-1.596815714866
H	0.323544962742	2.724275540969	-3.094347505106
H	-2.254312583548	2.002631173594	1.689411857938
H	-3.190656794173	0.320919842844	-0.710145535114
H	-0.473582756663	0.666113096036	0.580490425862
H	-1.217720500622	-0.793276247569	-0.038678351171
H	-0.053068383272	-0.418769291535	-2.083362066382
H	0.564801466263	1.086777131923	-1.438734000519
C	-2.216447159884	2.104617314273	-1.436039753447
C	-3.547795432400	2.616982840069	-1.992085421195
H	-3.376052460431	3.285659995531	-2.839601221744
H	-4.191820037834	1.800731951153	-2.325344074310
H	-4.090606115183	3.162330163658	-1.215855739556
C	-1.432169702680	3.302549405594	-0.868324230842

H	-1.261360164475	4.052346599491	-1.644128687166
H	-2.001031914178	3.778180360041	-0.065545906694
H	-0.460051603967	3.013697685824	-0.460712409110
O	-1.295440816061	2.826262993690	-4.408123358195
O	-4.244097134754	1.769126673069	1.081890335176
C	-2.189918177593	0.332231632797	-3.337889159126
H	-1.533237370407	-0.284420506365	-3.957102240244
H	-2.780435391780	-0.335592125357	-2.707533158879
H	-2.866426962288	0.868719524823	-4.002818461326
C	-0.567252781459	3.688727523214	-5.281617027066
H	0.165577869857	4.280410932409	-4.720041374111
H	-1.296227250176	4.368936398223	-5.723431405876
C	0.135842244275	2.906533369641	-6.387424362315
H	0.870327347033	2.213783124243	-5.950388093930
H	-0.603873433831	2.310508340148	-6.942190931837
C	-4.705457519359	2.275515088329	2.334406712719
H	-5.642689359804	2.794890253910	2.131368223325
H	-3.990772979455	2.996650626021	2.748569492684
C	-4.953334769056	1.154155714901	3.339703963882
H	-5.661971881101	0.429544361638	2.911985168093
H	-4.013638642449	0.623300502816	3.553379058952
O	0.763002624976	3.860220863241	-7.227012277008
C	1.415935897310	3.288566306790	-8.350812127704
H	2.212488271788	2.595683919391	-8.044924859945
H	0.708515452669	2.746828241358	-8.994329410718
H	1.856412554150	4.109330604500	-8.917444829966

O	-5.478564698868	1.760909424324	4.507518144498
C	-5.824573448728	0.833641484190	5.525596210118
H	-6.597416147526	0.130855721468	5.183726072160
H	-4.950428452023	0.257346151325	5.860140152501
H	-6.213480538415	1.409969203650	6.365446818266

Cam-F200

($E_F = -928.95670907$ a.u.; $G_F = -928.56276360$ a.u.)

0 1

C	-2.161375283219	0.619478064568	-2.756064885142
C	-1.433651214442	1.810120370431	-2.067464131177
C	-1.939008624571	1.723823083177	-0.565098499421
C	-2.900149673793	0.506525828165	-0.610903328263
C	-1.994268170264	-0.741468082364	-0.722190102952
C	-1.474136316407	-0.654040242957	-2.189339826678
H	-0.350565772745	1.648776478600	-2.102306831617
H	-1.091133045355	1.511402683127	0.098965567512
H	-3.602473971677	0.479809793778	0.221657639262
H	-1.185003400464	-0.723179293450	0.012286008605
H	-2.559096420407	-1.658498050691	-0.548701882868
H	-1.758208290013	-1.532666022186	-2.771739730608
H	-0.385039247028	-0.576806361415	-2.247698388150
C	-3.548746575459	0.592247521007	-2.021932724199
C	-4.418063853187	-0.628757500954	-2.373349293646
H	-4.797138773109	-0.539211948732	-3.395410917432
H	-3.901501270234	-1.585455800922	-2.298878109060

H	-5.285442624470	-0.669108374864	-1.707313769693
C	-4.424961870568	1.837252057172	-2.242956346363
H	-4.764369965744	1.873218792288	-3.282825296528
H	-5.314303375218	1.774944395277	-1.607220059180
H	-3.915302067416	2.768641159088	-2.020587784623
O	-1.734173039676	3.044204199546	-2.694946873163
O	-2.529792846942	2.947221218453	-0.155409776164
C	-2.168334047357	0.696999074786	-4.272247609282
H	-1.147736904452	0.673602442184	-4.667663620034
H	-2.709555869554	-0.151464386076	-4.699877153056
H	-2.636506433145	1.620834602280	-4.613813381658
C	-0.644237562184	3.936328486121	-2.882414821385
H	0.093530917969	3.851234254844	-2.075938231025
H	-1.049105387998	4.950196856562	-2.858649669708
C	0.020099715174	3.684674125155	-4.234741203456
H	0.422117910376	2.660047522600	-4.274226626692
H	-0.738070734268	3.773993414868	-5.026684363644
C	-2.433676098042	3.253443817633	1.228010712076
H	-2.659437573321	4.317899467098	1.318391736181
H	-1.411432983489	3.089421914504	1.596241232634
C	-3.423317599910	2.483830425670	2.105927896696
H	-4.428999260403	2.554920357657	1.664933349023
H	-3.153554243130	1.419478826852	2.166448589585
O	1.054552996413	4.637537722949	-4.408692434351
C	1.692470446200	4.544240484875	-5.673620438283
H	2.163086377107	3.560812158111	-5.816580987827

H	0.982743095283	4.714276629070	-6.495673527667
H	2.463596881435	5.314657084786	-5.703874572505
O	-3.384340791088	3.074461763591	3.394625438227
C	-4.259581715152	2.453731718765	4.324129568250
H	-5.306301576545	2.515026383776	3.994035819447
H	-4.002379576301	1.395585457223	4.475975805839
H	-4.153208756317	2.984744405055	5.270543492969

Pin_TS1-F3500

($E_F = -929.91038704$ a.u.; $G_F = -929.52340277$ a.u.)

0 1

C	-1.788859080878	1.972638183711	-0.150762451333
C	-1.660790665608	3.442146390478	0.415498481783
C	-2.116036173898	3.886724214271	1.807071338883
C	-1.740216687769	2.004217386963	2.797999062802
C	-0.614079574645	1.310063022351	2.042247919281
C	-0.431298749235	1.697616873777	0.573998446770
H	-2.030874220241	4.173476305205	-0.307150647331
H	-2.723672194965	1.742594768603	2.437588535967
H	0.317876972344	1.485286389648	2.589189887948
H	-0.812445655623	0.230194645411	2.118724736981
H	0.258405515502	1.007052276719	0.079107328401
C	-0.121573861017	3.212086485932	0.473938979168
H	0.401674435784	3.496648727451	-0.437559669751
H	0.378862751714	3.664683596080	1.329470213705
C	-1.587301808355	2.051508482565	-1.680095400838

H	-0.779674213617	2.721044511659	-1.977700645178
H	-1.360490727558	1.058410526137	-2.079427090256
H	-2.504278263603	2.405496137245	-2.162075102884
C	-3.011303108796	1.068423628143	0.058285068590
H	-2.928255391965	0.186198970588	-0.583825332337
H	-3.149479596736	0.703089414855	1.072258666323
H	-3.924208941232	1.596327188165	-0.235161840341
C	-3.601686907254	4.017266525494	2.055221493318
H	-4.018599544901	4.806625277509	1.418657059786
H	-4.141277122119	3.095301857663	1.833271917866
H	-3.782681487653	4.292314965046	3.095859043352
O	-1.514844229182	5.228772982216	2.047595216971
O	-1.662007607723	1.548857363911	4.177542261967
C	-1.543935005429	6.193693468261	0.901252633374
H	-2.519562131739	6.143771006741	0.411151310236
H	-0.780478544586	5.903875436983	0.176534299871
C	-1.292791701093	7.729989577250	1.207799431444
H	-2.062697162314	8.111370799613	1.889410560982
H	-0.310223769016	7.866391957877	1.675312035913
C	-2.436302974544	0.315504355370	4.493023149441
H	-2.761117523822	-0.160344823930	3.563266556773
H	-3.325035695109	0.615190655005	5.054349578262
C	-1.677324462959	-0.792909810028	5.349853722219
H	-0.802569499518	-1.146258241916	4.789019449063
H	-1.329411690361	-0.346007795895	6.289352329643
O	-1.353097171614	8.419861380288	-0.080861806175

C	-1.159918707693	9.892328203934	-0.238773267200
H	-1.925563201049	10.449301327529	0.311182218888
H	-0.163066712944	10.195218499505	0.097960954863
H	-1.265068996302	10.060375272762	-1.308412325130
O	-2.598826141292	-1.893418217217	5.612608578324
C	-2.209820469309	-3.098635871209	6.406091982666
H	-1.387205207395	-3.635816474060	5.922652724167
H	-1.926177127539	-2.819845015802	7.426213937770
H	-3.108027658329	-3.712191235904	6.417066809191

Pin_Int1-F3500

($E_F = -930.25646431$ a.u.; $G_F = -929.87912396$ a.u.)

0 1

C	-2.024755013146	2.759570810052	0.914339921068
C	-1.260729971035	4.185709415807	1.080739477610
C	-1.886810529935	5.554774898302	0.747655872699
C	-1.430237641554	-0.343572432145	3.222833641250
C	-1.764629872728	1.170196417570	3.274876290929
C	-1.205449209407	2.194271070369	2.165811159454
H	-0.334577200975	4.112719730983	0.502915455403
H	-1.497610327026	-0.885295519626	2.280045558150
H	-2.857365834079	1.291890977267	3.330913237032
H	-1.393250313797	1.535482379415	4.240112481869
H	-0.261177725695	1.790016086381	1.786929187461
C	-0.970242166395	3.697796424506	2.564064304122
H	0.003408653309	3.956201090845	2.987570781591

H	-1.746022631258	4.043232310482	3.252662161840
C	-1.765853609270	2.062569123736	-0.416078501049
H	-0.693832742845	1.983592611626	-0.617870443930
H	-2.186327800979	1.050736465780	-0.416115997095
H	-2.224692704500	2.619521157629	-1.239948745266
C	-3.526321354713	2.850502242816	1.180696453883
H	-3.980076243200	1.855650737549	1.135546411055
H	-3.755493126420	3.268683871585	2.163233432841
H	-4.007820833343	3.479765837241	0.426862093859
C	-2.873346078650	6.185395620519	1.680056188343
H	-3.686639690732	6.699207865847	1.157061150484
H	-3.327908416282	5.429756077123	2.318458580905
H	-2.399218618770	6.927921423106	2.342411267870
O	-1.204770346591	6.432852383226	-0.151631195350
O	-1.683794078146	-1.120026440338	4.372878476056
C	-1.842248553379	7.718161359380	-0.533390927082
H	-2.045438549000	8.306085126818	0.364158250557
H	-2.793404532121	7.503249279157	-1.029041661686
C	-0.986229006007	8.640435491882	-1.500851591162
H	-0.018993474474	8.858287665448	-1.030843363460
H	-0.803363377726	8.114658380675	-2.446027086224
C	-1.478781788554	-2.584677612848	4.297565091689
H	-0.441623820209	-2.779205146361	4.010689382331
H	-2.138364763159	-2.992788027803	3.525125983176
C	-1.773121430202	-3.348153645915	5.659474082858
H	-1.112855949827	-2.949693344682	6.440009369615

H	-2.812630130400	-3.159873618564	5.956418007732
O	-1.737129297114	9.870099240912	-1.731432418794
C	-1.233480873016	10.974070430650	-2.603107007083
H	-0.295191082338	11.382541430312	-2.213749554116
H	-1.092101201303	10.626624954307	-3.631748750526
H	-2.019111681990	11.725294643971	-2.562162297110
O	-1.542818812124	-4.774173032030	5.468726717425
C	-1.728708145342	-5.767227810667	6.570289445192
H	-1.049925518870	-5.557541065658	7.403370855463
H	-2.765206821113	-5.769413218352	6.923091006359
H	-1.482466222590	-6.722688180086	6.112376534068

Pin-F3500

($E_F = -929.91631340$ a.u.; $G_F = -929.52715028$ a.u.)

0 1

C	-1.755403063013	1.831923798647	-0.152824005252
C	-1.793449873457	3.325614213053	0.389680747893
C	-2.135265050144	3.653325345819	1.877666079295
C	-1.711439996733	2.199472714086	2.622848391838
C	-0.453534126966	1.548705895811	2.027132771990
C	-0.337722716649	1.776092049336	0.509647413332
H	-2.343467384141	4.003310176347	-0.264126970712
H	-2.565547341760	1.670878884356	2.219289981350
H	0.436188220505	1.930575212388	2.536659320446
H	-0.513170047057	0.478494551436	2.255564119519
H	0.414906340611	1.125081665700	0.055492217922

C	-0.233594480143	3.300381992114	0.286742981488
H	0.142534935614	3.582796302804	-0.694222841506
H	0.298563502095	3.865413270452	1.050040977158
C	-1.674390876833	1.896731674422	-1.693111742808
H	-1.027944691869	2.688560053016	-2.070705962238
H	-1.304580414630	0.945781046427	-2.088607964407
H	-2.673839727286	2.064035652516	-2.107332678267
C	-2.816352157673	0.756978680800	0.163124065542
H	-2.844204683915	0.015321606222	-0.639539209532
H	-2.632581990029	0.201894057715	1.082014674179
H	-3.816204158316	1.197574078537	0.224174115018
C	-3.618454941216	3.861569150675	2.171481870864
H	-4.007681952337	4.730227150245	1.638016499500
H	-4.213348459368	2.994374990175	1.874251807653
H	-3.753749778138	4.023736157486	3.242792104914
O	-1.473814614108	5.002079494530	2.151586220832
O	-1.759948349222	1.875511685958	4.057602425385
C	-1.631630545683	6.018973225642	1.073969406607
H	-2.678200232846	6.067522911573	0.761927496798
H	-1.037637142731	5.724220433745	0.207181541779
C	-1.196585284753	7.516091801866	1.373844215361
H	-1.812162759233	7.943029621661	2.174759041081
H	-0.144986456184	7.547426508200	1.684138828592
C	-2.485399818675	0.634371405029	4.421569161306
H	-2.959993945122	0.210896503607	3.531267434713
H	-3.276825536298	0.932985292949	5.112954893287

C	-1.683107559889	-0.547625198821	5.135822909463
H	-0.920639870095	-0.945966006157	4.453851430086
H	-1.179254954826	-0.154010956882	6.027280737636
O	-1.389014745854	8.253956260259	0.124294886268
C	-1.089619487134	9.707899155630	-0.031912413622
H	-1.707751559037	10.310692099833	0.641598431345
H	-0.029509255162	9.912186384368	0.151213389091
H	-1.341871210164	9.921185426321	-1.068453505507
O	-2.637905272001	-1.590291793567	5.500375548563
C	-2.241075706724	-2.840630091119	6.215539729017
H	-1.531772891182	-3.423964498186	5.619152884977
H	-1.806204932072	-2.610170552038	7.193634148466
H	-3.173957371798	-3.387214452182	6.335389510170

Pin_TS1-F3000

($E_F = -929.74250747$ a.u.; $G_F = -929.35546060$ a.u.)

0 1

C	-1.780589962779	1.993924435061	-0.162134778523
C	-1.605184197573	3.458423937546	0.394899654051
C	-2.122710380079	3.940356106535	1.743280996882
C	-1.753000134428	1.932410670540	2.846380130726
C	-0.673494617922	1.221685894463	2.046369398920
C	-0.457530969530	1.655413736058	0.597991369481
H	-1.895204939111	4.195640212195	-0.359322823414
H	-2.764911733632	1.733381640848	2.523809763024
H	0.266250251418	1.325193066690	2.598629495276

H	-0.924936513604	0.148774849487	2.078635659185
H	0.217472545954	0.954680284237	0.096832354608
C	-0.084024412345	3.159026080089	0.533032663742
H	0.499417022061	3.428233822232	-0.346607845640
H	0.388418598268	3.581181056153	1.419746746899
C	-1.526568648976	2.044430088160	-1.684285279133
H	-0.659571749867	2.648483674168	-1.955355117368
H	-1.361422132087	1.034124930811	-2.070660810742
H	-2.396638607312	2.463688954989	-2.199682421202
C	-3.047051092822	1.152054027427	0.024894191167
H	-2.944141956361	0.210045374749	-0.523112551321
H	-3.280921088702	0.893753727642	1.053703755755
H	-3.912481877293	1.676734891919	-0.392074803058
C	-3.612325574411	4.028293409719	1.961182699513
H	-4.039428639805	4.787934747819	1.292467724473
H	-4.122084316141	3.086952519582	1.756379198751
H	-3.822319693361	4.331878970036	2.988330884655
O	-1.552521661156	5.265471861948	2.004148981811
O	-1.623536135044	1.508713963098	4.209718894482
C	-1.523778460846	6.216505328923	0.859467254355
H	-2.458582749056	6.138893539995	0.297892970885
H	-0.700233700695	5.949545226159	0.193315397927
C	-1.348682329468	7.743741811991	1.195493920912
H	-2.175168303503	8.092406327843	1.827400123580
H	-0.404482433572	7.913499612513	1.727714043314
C	-2.448720526275	0.357507797892	4.635446211696

H	-2.999471029207	-0.039009989912	3.777430089416
H	-3.170687571226	0.720680513932	5.370999198053
C	-1.650807631631	-0.838518566479	5.295223999535
H	-0.951821715446	-1.261395528091	4.561467352397
H	-1.070329856637	-0.458537327406	6.145647662723
O	-1.350703014216	8.429572189467	-0.087997007996
C	-1.204339887142	9.895732948721	-0.200439195276
H	-2.024317771925	10.414779537000	0.308395762055
H	-0.244965555845	10.229612992448	0.210361713767
H	-1.242433690338	10.094844487946	-1.269670409337
O	-2.607609237442	-1.839459970878	5.729281396648
C	-2.168142865756	-3.078489424872	6.407190879665
H	-1.513675632348	-3.671317065317	5.758264979348
H	-1.649850208796	-2.850724177744	7.345366343294
H	-3.087490905200	-3.624245645353	6.610371524224

Pin-F3000

($E_F = -929.75639076$ a.u.; $G_F = -929.36554571$ a.u.)

0 1

C	-1.736922912855	1.787207352425	-0.158617569132
C	-1.802775098964	3.288611689327	0.361098079066
C	-2.149263340135	3.611182569245	1.851129810905
C	-1.706382106964	2.209224171799	2.603478735772
C	-0.430577288225	1.570225567244	2.028472073431
C	-0.318866938610	1.768639163582	0.505771509583
H	-2.366624922724	3.950144026014	-0.297950702797

H	-2.541937132722	1.630892357420	2.227200890849
H	0.448977031441	1.986182149018	2.528812115148
H	-0.464572198194	0.504939321677	2.280999211193
H	0.445766402368	1.123141542157	0.064034734192
C	-0.242692214080	3.290235311249	0.255248307352
H	0.125605663560	3.561956070942	-0.731649383725
H	0.282689438181	3.876144691102	1.007349421752
C	-1.656715353972	1.826580847319	-1.699702831322
H	-1.027156576679	2.625134298703	-2.091262260642
H	-1.266901101541	0.876875311501	-2.078730929277
H	-2.659374813412	1.965494163670	-2.116635205016
C	-2.776518017581	0.696703622677	0.175387976840
H	-2.780882999530	-0.063963855883	-0.609846361407
H	-2.589021409444	0.167692907940	1.109001810053
H	-3.786229971795	1.116499313968	0.217514182501
C	-3.639055218977	3.803169949997	2.132713929112
H	-4.033649365675	4.672570502465	1.604874114392
H	-4.221251677176	2.932726652949	1.820329859227
H	-3.784949624005	3.952591785116	3.204591513079
O	-1.493631553802	4.938590140219	2.154319975210
O	-1.748604842887	1.981481775663	4.042575247161
C	-1.659640459954	5.965146314339	1.104706990570
H	-2.709883282153	6.031627986641	0.807461781057
H	-1.082346195510	5.686288122298	0.220999220708
C	-1.205627912780	7.435555839521	1.438078791468
H	-1.804242281926	7.852768832825	2.257407388767

H	-0.148854697951	7.450083660681	1.733511980938
C	-2.493363627065	0.802639067949	4.505603569860
H	-3.189604746743	0.474510874830	3.726324983062
H	-3.083660347522	1.143134597304	5.358877596145
C	-1.689405202532	-0.472864894679	5.000362626581
H	-1.143177399677	-0.929228976801	4.163915810197
H	-0.961289054599	-0.168109643684	5.763137386721
O	-1.410196100641	8.191593032851	0.210195257324
C	-1.090033548141	9.629138080151	0.102307029730
H	-1.687257766613	10.221639211603	0.804571669914
H	-0.024153270994	9.811552295942	0.280046219410
H	-1.347984052576	9.892865720961	-0.921600286281
O	-2.652518557017	-1.411012692598	5.548996641353
C	-2.231039459310	-2.705400545237	6.125926954294
H	-1.734560018145	-3.329163258879	5.374001338472
H	-1.562399023927	-2.556070654569	6.981100053531
H	-3.155611459375	-3.177796402641	6.452055464496

Pin_Int1-F3000

($E_F = -930.03841463$ a.u.; $G_F = -929.65981688$ a.u.)

0 1

C	-2.009451465239	2.752724406610	0.926491946305
C	-1.263511801911	4.182119311808	1.094015421074
C	-1.907093503713	5.532207207769	0.765207645891
C	-1.448561669085	-0.306287354864	3.194842097569
C	-1.743182752444	1.201798467141	3.286618507021

C	-1.188735877500	2.206599986082	2.179948880026
H	-0.337249737272	4.123312454286	0.514658298988
H	-1.570957683381	-0.835470329111	2.250392196087
H	-2.829989412289	1.353929995226	3.379818145923
H	-1.330617455984	1.540879302902	4.245049148815
H	-0.241033477041	1.804229071971	1.807127128710
C	-0.965628699816	3.708035241960	2.575024494549
H	0.006753099432	3.976485142680	2.995110399677
H	-1.742945882205	4.048441107997	3.264498894573
C	-1.736266993890	2.054734579808	-0.400812374844
H	-0.662401446161	1.986573276162	-0.596779840993
H	-2.145917624877	1.038480896261	-0.400658749463
H	-2.196570423902	2.604579468419	-1.228644253113
C	-3.513417366009	2.825072195680	1.185369073714
H	-3.953104237768	1.823662646649	1.145689801026
H	-3.753122411338	3.247283482988	2.163582634553
H	-4.000068629960	3.442329799100	0.424961237686
C	-2.897971737381	6.157223048362	1.697175675010
H	-3.712850241649	6.668342211506	1.174318722858
H	-3.350016347903	5.398290294405	2.333243004003
H	-2.427623954010	6.900232116665	2.361828254235
O	-1.220341691388	6.405499789200	-0.123062857912
O	-1.671459815167	-1.078994382556	4.344982181320
C	-1.864911467348	7.671490530110	-0.513399886536
H	-2.086405803328	8.265456364807	0.376322943827
H	-2.807835345248	7.448383611028	-1.022201072884

C	-0.998873073668	8.579226334924	-1.464479797311
H	-0.038475550040	8.802514735048	-0.981923641934
H	-0.799624890541	8.051774636400	-2.405990363289
C	-1.504314469236	-2.536149725209	4.243553165256
H	-0.486102738636	-2.755715894568	3.909034670605
H	-2.207466927030	-2.925698213392	3.499779775939
C	-1.756122741797	-3.283084829232	5.607938638185
H	-1.050648198015	-2.906076694485	6.359781494822
H	-2.775701289774	-3.068227989583	5.953883925240
O	-1.752590076886	9.796478882330	-1.704005963947
C	-1.224340746783	10.875298687201	-2.565859615323
H	-0.288908746016	11.279196172516	-2.162763827603
H	-1.062033775404	10.518515208441	-3.589081282181
H	-1.997433624561	11.641078175502	-2.555305563301
O	-1.572970824026	-4.705257689636	5.396846187957
C	-1.736788681304	-5.666792139456	6.508896089419
H	-1.016361281317	-5.467687635173	7.310082108432
H	-2.755528305713	-5.633297478090	6.910987273600
H	-1.541962662518	-6.640542546366	6.063877800067

Pin_TS1-F2500

($E_F = -929.57531037$ a.u.; $G_F = -929.18840772$ a.u.)

0 1

C	-1.760991427530	1.988152154243	-0.171371315278
C	-1.581781605626	3.457462480313	0.369367136940
C	-2.138636934646	3.959979834325	1.689802077818

C	-1.745925099792	1.883213255044	2.869399530913
C	-0.677921320757	1.182333953194	2.049191542916
C	-0.452566975153	1.640703282245	0.609987923324
H	-1.835866262150	4.186852179140	-0.406657023447
H	-2.768909408235	1.703362689709	2.567663986538
H	0.263560268800	1.267680680062	2.601827543170
H	-0.935002456218	0.109577304002	2.059171890848
H	0.225685570379	0.943566319879	0.108050553466
C	-0.068657072432	3.142718169992	0.554920806274
H	0.544134806711	3.404482777043	-0.307227607971
H	0.379526121332	3.562656752039	1.455141384592
C	-1.482086237244	2.015089946144	-1.689279351714
H	-0.599183866602	2.600406375701	-1.951051871576
H	-1.328340269459	0.997523064046	-2.061213454987
H	-2.335249584891	2.444238386866	-2.224460261037
C	-3.036462784522	1.161018517523	0.012451563191
H	-2.927057174286	0.201082925768	-0.502422846566
H	-3.293171677706	0.938323396435	1.044121351182
H	-3.889423655084	1.676705903575	-0.439826201689
C	-3.629339874741	4.014178216250	1.895146952397
H	-4.070469810547	4.753952655341	1.211330150568
H	-4.115910611280	3.058810393713	1.702176036993
H	-3.854773230242	4.330152443403	2.915414797932
O	-1.588523907372	5.272702142998	1.969715356595
O	-1.582883712107	1.509823560224	4.225417836412
C	-1.526278692298	6.215830627678	0.833982170500

H	-2.437505905146	6.131408432521	0.235016725815
H	-0.674149776505	5.963769278705	0.197758270895
C	-1.386722344284	7.728078365825	1.198801228204
H	-2.240744332890	8.056795153457	1.805108832855
H	-0.465037073675	7.905927831908	1.767564801879
C	-2.442276834274	0.449130028866	4.763995860468
H	-3.194379297559	0.163746794085	4.021915948856
H	-2.955852160936	0.856779788895	5.637629573201
C	-1.671813643392	-0.842775254036	5.219392398079
H	-1.193941393023	-1.316327597057	4.350709105452
H	-0.885787819074	-0.559183316681	5.931767951879
O	-1.353669479450	8.421581567975	-0.072252375089
C	-1.230909193584	9.878899666211	-0.134211868170
H	-2.077779745542	10.370681801520	0.359110368819
H	-0.294504924704	10.218951283970	0.323875054784
H	-1.231328815861	10.119373686501	-1.196015475985
O	-2.624517653907	-1.738403670378	5.831262954655
C	-2.172271113411	-3.019862132660	6.380614030296
H	-1.734059787822	-3.652902986813	5.599744758507
H	-1.439700856732	-2.869629539923	7.182558532496
H	-3.067878657728	-3.492108016808	6.780705007987

Pin_Int1-F2500

($E_F = -929.82282428$ a.u.; $G_F = -929.44321691$ a.u.)

0 1

C	-2.390584824247	2.918391305804	1.166995473015
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C	-1.357035090368	4.139023425239	0.939184210768
C	-1.747454947108	5.607866643490	1.019279280021
C	-1.562167476308	-0.408828711813	2.767457882638
C	-1.335120996717	1.081229386329	3.022376842484
C	-1.200879390332	2.074257209742	1.800550748574
H	-0.896826613597	3.985838537626	-0.041552649700
H	-2.313327133853	-0.743039661802	2.052398165237
H	-2.114444407150	1.462113616899	3.701598857228
H	-0.401962725513	1.161565188486	3.594343177801
H	-0.697559099404	1.541771624648	0.986603506684
C	-0.464838262152	3.434420340867	2.034438171919
H	0.616890978378	3.453325474954	1.881299443667
H	-0.677361656133	3.825454815280	3.033197719528
C	-2.993874331176	2.358592085460	-0.116302698406
H	-3.570219746426	1.448848781488	0.085477477194
H	-3.666654216934	3.089257823644	-0.577828630811
H	-2.214782304521	2.111259202369	-0.843047061319
C	-3.495418680884	3.241375750071	2.171667534745
H	-4.109098062545	2.354492717833	2.357687767451
H	-3.104822025642	3.574896682576	3.135321586698
H	-4.144044943928	4.030741447350	1.781534117895
C	-1.948543425488	6.286104749841	2.338866401921
H	-2.765002133288	7.015153953446	2.324683766691
H	-2.185148716065	5.553672046639	3.108501436255
H	-1.044041566147	6.823285392386	2.668365969746
O	-1.410124469865	6.428456497795	-0.083567861316

O	-1.329616226072	-1.271854341221	3.840645134008
C	-1.849546391389	7.823867186691	-0.073568461644
H	-1.454792565458	8.337466992853	0.806562322922
H	-2.943018479989	7.857692915907	-0.029261687543
C	-1.382201301394	8.636692998070	-1.323723684897
H	-0.287438565285	8.596391390577	-1.401010269450
H	-1.809559358375	8.204443008704	-2.238016428332
C	-1.635033396314	-2.687664811674	3.651740806886
H	-1.053826371545	-3.073654793685	2.808536303400
H	-2.700049540471	-2.801733618174	3.421258423144
C	-1.303871629615	-3.537387517515	4.922069728788
H	-0.236049124505	-3.436384847337	5.158098750807
H	-1.881480745478	-3.156943034024	5.775344573212
O	-1.837831143835	9.994211660841	-1.132041485459
C	-1.555272809081	11.016484188941	-2.142246769888
H	-0.475669487002	11.155305172456	-2.274721274191
H	-2.011065504465	10.758786284661	-3.105638465044
H	-2.001043504057	11.931172317795	-1.755174521103
O	-1.642257514509	-4.911398402265	4.642566398608
C	-1.422692406544	-5.934343993577	5.668936246068
H	-0.362117450114	-6.002835279350	5.938574377567
H	-2.015539359630	-5.726767403641	6.567667442083
H	-1.750776204673	-6.868565592197	5.216566954971

Pin-F2500

($E_F = -929.59973253$ a.u.; $G_F = -929.20834560$ a.u.)

0 1

C	-1.713355699509	1.742462388975	-0.166603075874
C	-1.810963627847	3.250585768532	0.328473390846
C	-2.167471224828	3.568137253622	1.817602530384
C	-1.702421943532	2.215088665099	2.585549547633
C	-0.407461445224	1.594062097028	2.030077251589
C	-0.297337985335	1.764143651710	0.502879218681
H	-2.387948312587	3.894182285261	-0.337555044144
H	-2.518704375402	1.587182020249	2.244958658115
H	0.458230465413	2.047870997431	2.521445920846
H	-0.410101771626	0.534709425224	2.306576391918
H	0.481308094896	1.126101141431	0.075073075458
C	-0.251165009125	3.282150121084	0.223868758337
H	0.111818530753	3.542532166158	-0.768006907874
H	0.263600797903	3.890813144788	0.965054475573
C	-1.629171317339	1.754940672335	-1.707843517204
H	-1.015637368116	2.559314608127	-2.112625800514
H	-1.218294557014	0.806856677639	-2.068321809898
H	-2.633324711765	1.864789297899	-2.129851128747
C	-2.731073644759	0.636674742704	0.184707261854
H	-2.716699557933	-0.138220690722	-0.586398111905
H	-2.535248567313	0.129072151956	1.128545029923
H	-3.749657342605	1.035237739074	0.216269585774
C	-3.664423281412	3.738292204053	2.083188611245
H	-4.066853572405	4.605410201214	1.557844508074
H	-4.228963692966	2.861782774576	1.756055748634

H	-3.824196429119	3.876300290230	3.154661074487
O	-1.521731015182	4.876947271390	2.150373065324
O	-1.730505774600	2.087496846229	4.026712354551
C	-1.698910854732	5.915981332369	1.131571507774
H	-2.754808213752	6.007738483923	0.860893027399
H	-1.149072127804	5.651413395938	0.225724250185
C	-1.210561512868	7.354582313550	1.498104206282
H	-1.779655535316	7.761010811581	2.344023307831
H	-0.146169843315	7.341807060369	1.766927964215
C	-2.484747389759	0.966882911706	4.574003900319
H	-3.328272202119	0.727123602406	3.916418438377
H	-2.891414536754	1.327715952584	5.520616613094
C	-1.724710120350	-0.375452855829	4.896587863425
H	-1.376922226516	-0.856510097080	3.971865701724
H	-0.848656671345	-0.156643350636	5.521721183941
O	-1.432752474150	8.138659698858	0.299342902482
C	-1.076669277427	9.556282897133	0.243338419529
H	-1.637704390566	10.138023056538	0.984585880737
H	-0.001713704693	9.703536437938	0.403041216728
H	-1.348005462195	9.878534904285	-0.760639010375
O	-2.656773225167	-1.234046841186	5.590778498047
C	-2.239282421949	-2.563386134467	6.042790086039
H	-1.939511875255	-3.193935682572	5.197051412343
H	-1.411531656989	-2.496281195640	6.758798844649
H	-3.115518399558	-2.988987740812	6.528919378599

Pin_TS1-F2000

($E_F = -929.40981328$ a.u.; $G_F = -929.02270349$ a.u.)

0 1

C	-1.750396410461	1.970868170324	-0.189423670530
C	-1.573588127293	3.446250526174	0.334222170765
C	-2.159457601259	3.960684745862	1.634115047511
C	-1.734155938913	1.846733857914	2.875839137771
C	-0.676312330064	1.150968830188	2.040716079537
C	-0.449947906399	1.624937797919	0.606253107189
H	-1.804983306033	4.167421444419	-0.457734933057
H	-2.765861306299	1.671678256239	2.598300746368
H	0.268186493433	1.227167866685	2.589551184267
H	-0.934483694224	0.078129153844	2.035912832764
H	0.232794328574	0.932280052690	0.104133569223
C	-0.065512460826	3.127313693993	0.553549637788
H	0.566162991046	3.384000115076	-0.296699076837
H	0.364024868841	3.550411316454	1.461343136114
C	-1.456886721810	1.975197361261	-1.704277219257
H	-0.564766256924	2.548244372231	-1.962824532894
H	-1.309573975133	0.951586402320	-2.062156265061
H	-2.299629971868	2.406858858197	-2.253759696903
C	-3.028229926059	1.149950341664	-0.000740206903
H	-2.908858096771	0.172700298371	-0.479780823640
H	-3.301681912416	0.964250907374	1.033894358317
H	-3.873827763575	1.648457491248	-0.484935457534
C	-3.650228633275	3.990259450279	1.832882587461

H	-4.102022088191	4.721897680117	1.146054888670
H	-4.121009732865	3.027270582194	1.640719730269
H	-3.884956655454	4.305482317873	2.851492434389
O	-1.619727592077	5.258563683276	1.938933077899
O	-1.536770408107	1.536407785648	4.230324358661
C	-1.529744986399	6.201467426417	0.818654382830
H	-2.422797738925	6.121491544977	0.191537401854
H	-0.658140671507	5.962958186535	0.202940577817
C	-1.411990206374	7.694967522124	1.221049901589
H	-2.285362995251	8.004982536863	1.810211865183
H	-0.508230187446	7.867732229481	1.820210901531
C	-2.408167665989	0.551388691278	4.858629053561
H	-3.282319239063	0.361160516791	4.227621990218
H	-2.749640613607	0.978335464927	5.803896393971
C	-1.698048004491	-0.804004217819	5.169152437022
H	-1.397979540262	-1.294493042648	4.232258771357
H	-0.791585218841	-0.606953262898	5.757556142436
O	-1.348989143196	8.408306926554	-0.030429280060
C	-1.245439049418	9.856006355024	-0.030493307882
H	-2.112887967546	10.318956538441	0.456584857145
H	-0.328838706742	10.191548575522	0.470673822450
H	-1.216266006065	10.147407659917	-1.079495884230
O	-2.621063239047	-1.625486395446	5.902553077227
C	-2.177499434422	-2.935965673368	6.349397136525
H	-1.908925587325	-3.576310363610	5.499812908655
H	-1.317949070717	-2.854599116209	7.026374509004

H	-3.023772286151	-3.368359909706	6.881218483629
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Pin_Int1-F2000

($E_F = -929.60961342$ a.u.; $G_F = -929.22906870$ a.u.)

0 1

C	-2.367085839042	2.906132668206	1.175997683440
C	-1.352143475307	4.135808735261	0.953241117040
C	-1.763020784343	5.589279659332	1.048558676628
C	-1.577900342604	-0.363259395143	2.755648150953
C	-1.288166454587	1.104080980979	3.020859393266
C	-1.164891800459	2.082600516378	1.802742715706
H	-0.895622136568	3.998749208808	-0.031563866714
H	-2.372227241452	-0.664332754856	2.073181121706
H	-2.027732647498	1.509382044373	3.730253413179
H	-0.332102813199	1.144184522038	3.558546798747
H	-0.659400202940	1.551294302988	0.989231505342
C	-0.442139229888	3.445209226253	2.036431182442
H	0.637663657060	3.477511221504	1.872858396090
H	-0.650196380037	3.830506609964	3.038391684045
C	-2.963769144753	2.342112270653	-0.108803748610
H	-3.529016522610	1.424860374904	0.090206077874
H	-3.645537918436	3.065700627712	-0.568318832681
H	-2.181808517054	2.106305495188	-0.836321594934
C	-3.476260548844	3.208401670007	2.182571778670
H	-4.072919752018	2.310104614307	2.369258404581
H	-3.090708982111	3.548885473895	3.145718379670

H	-4.139793524545	3.985947990278	1.793853977235
C	-1.961705689279	6.262254574809	2.371380458090
H	-2.779101955768	6.990105800264	2.362147999642
H	-2.195334077633	5.526453788450	3.138625294915
H	-1.056638942726	6.799052771770	2.700282488838
O	-1.423833637598	6.404917294900	-0.048890880645
O	-1.324324570139	-1.235549380229	3.808093195035
C	-1.877234059352	7.786029012090	-0.042204527775
H	-1.493213626150	8.310570413891	0.836695089210
H	-2.971670899224	7.812091731310	-0.006009951879
C	-1.403199077434	8.577124436169	-1.290553988966
H	-0.307366379683	8.538350991521	-1.359382674781
H	-1.821892172628	8.135122864555	-2.204706863896
C	-1.677531729154	-2.630960131634	3.617203888710
H	-1.146020732527	-3.027902939128	2.746294148118
H	-2.754937702901	-2.716433349612	3.435171615673
C	-1.309278780757	-3.479711546606	4.864527595674
H	-0.229108633460	-3.405598528992	5.051231340681
H	-1.836293352247	-3.085888792057	5.744626487874
O	-1.863104457125	9.928240806102	-1.112157863958
C	-1.559743246274	10.914683693684	-2.134284750568
H	-0.476791949189	11.042133213459	-2.256239511140
H	-2.001683221928	10.637653556588	-3.099564280547
H	-2.000990446060	11.846529721370	-1.783575453331
O	-1.694309373364	-4.837289124736	4.598390246724
C	-1.441832081831	-5.837854778184	5.622178062437

H	-0.369910859283	-5.921265488065	5.840712614791
H	-1.982462592577	-5.604746399164	6.548019177170
H	-1.806562278156	-6.778127487359	5.211405977803

Pin-F2000

($E_F = -929.44642381$ a.u.; $G_F = -929.05440689$ a.u.)

0 1

C	-1.695780545593	1.703410210708	-0.187094134289
C	-1.824805938286	3.214608306429	0.288982775359
C	-2.190436146717	3.520848250184	1.777398128610
C	-1.699677364916	2.213323616367	2.561081178684
C	-0.389249094086	1.612335826260	2.017016735377
C	-0.282207518685	1.762384106943	0.486538440541
H	-2.415676918844	3.842006378557	-0.380922159023
H	-2.498058289862	1.539932551154	2.264901701558
H	0.463031491140	2.099311944316	2.499829978795
H	-0.361291808453	0.558352203723	2.311148684543
H	0.509953238867	1.134502273673	0.068721367794
C	-0.266272449972	3.277377973065	0.185172093862
H	0.091679569599	3.529658618839	-0.810566381632
H	0.236745836426	3.906662109054	0.916999464614
C	-1.607274353062	1.694767119731	-1.728095484005
H	-1.009470384191	2.505589601620	-2.143351035949
H	-1.176040797919	0.750123005676	-2.073572507905
H	-2.612324019450	1.777554018551	-2.154159636937
C	-2.693131780203	0.583870333631	0.176960676940

H	-2.651913549425	-0.207523170732	-0.576275367102
H	-2.498858842174	0.102104961476	1.134225400410
H	-3.720337529682	0.960644362974	0.186985066100
C	-3.693689177005	3.664219761190	2.029426135043
H	-4.108849006845	4.525004617647	1.503841335156
H	-4.237087073339	2.778303968800	1.692503876481
H	-3.865144766126	3.793721831129	3.100143887974
O	-1.555472978406	4.811379547876	2.143344402419
O	-1.706121365338	2.186097376553	4.000233322687
C	-1.756642168541	5.871753857607	1.167251868182
H	-2.822359092681	6.007216382267	0.959222301304
H	-1.267993334187	5.619855121510	0.223178717553
C	-1.196283130395	7.265387507871	1.558053655331
H	-1.700294132803	7.661517315437	2.449413092711
H	-0.119374392140	7.203798461400	1.765161685590
C	-2.462664002764	1.119465041934	4.621001188830
H	-3.390487955706	0.940563901557	4.064379572781
H	-2.733091611328	1.494874214796	5.609525558855
C	-1.752329929714	-0.258092495519	4.837047276804
H	-1.537871935104	-0.743263069193	3.874126995009
H	-0.799819769074	-0.101283189606	5.361862371460
O	-1.455772469757	8.092897253029	0.404555809659
C	-1.035128900881	9.480914834561	0.398667311525
H	-1.523109408050	10.051492873248	1.198988782113
H	0.053456951982	9.569882115393	0.505499900045
H	-1.340528031370	9.875542204261	-0.569521176612

O	-2.648316670729	-1.068587042960	5.617349551584
C	-2.241192816623	-2.415581006358	5.978460032077
H	-2.073486656525	-3.033747311481	5.087354744381
H	-1.328638756191	-2.405764298049	6.587538041536
H	-3.065267342804	-2.827024121447	6.559577394180

Pin_TS1-F1500

($E_F = -929.24611715$ a.u.; $G_F = -928.85894930$ a.u.)

0 1

C	-1.742957882035	1.947630127753	-0.207689270893
C	-1.571469364046	3.432142017352	0.291367211361
C	-2.189055441895	3.964044743809	1.564920130495
C	-1.711889308955	1.803757112317	2.885638270433
C	-0.667181336285	1.116971686686	2.030599686552
C	-0.447500003129	1.609547427575	0.600349259538
H	-1.779229925279	4.140447628785	-0.520195949430
H	-2.753275693736	1.635772156654	2.637839014254
H	0.282746172505	1.186394483771	2.570939399091
H	-0.922125094883	0.043175774797	2.009832848482
H	0.241300805206	0.924677580512	0.095765368700
C	-0.068512738239	3.113690896421	0.547611021821
H	0.582355324107	3.366119343140	-0.289699282585
H	0.339111297424	3.543257862911	1.462462432424
C	-1.439041833406	1.923587036399	-1.719661607640
H	-0.540697430263	2.486861750948	-1.979280104469
H	-1.295186704177	0.893242972148	-2.059349307414

H	-2.274325412759	2.351811291887	-2.283067925369
C	-3.020125634012	1.130076710505	-0.006183065050
H	-2.891449261412	0.136815835798	-0.448673486305
H	-3.303223637118	0.981292035008	1.031844364644
H	-3.862296126853	1.607654363271	-0.516702942944
C	-3.678195837050	3.965925901243	1.762609264786
H	-4.145597432062	4.684684455101	1.071247213529
H	-4.131009639916	2.993312177293	1.578202648947
H	-3.918947602819	4.284724025454	2.778923857725
O	-1.659051964449	5.246114796178	1.895017563241
O	-1.472106579383	1.564017557107	4.236768376350
C	-1.534937997432	6.190464343908	0.791923865454
H	-2.407536475000	6.119441532059	0.134859450466
H	-0.643300049954	5.963315485046	0.200065309288
C	-1.436609617204	7.662245522241	1.239030597296
H	-2.330652494753	7.952124379806	1.807891390051
H	-0.554506342637	7.820673672108	1.874187004462
C	-2.347477463818	0.656656802541	4.950385596758
H	-3.311511166295	0.570642833415	4.437989302088
H	-2.516947574112	1.087311148232	5.939025433270
C	-1.728757797629	-0.754514003186	5.131123962649
H	-1.602971364915	-1.240478095578	4.152433857353
H	-0.735841957659	-0.653443232380	5.591141669165
O	-1.335283719787	8.406390915846	0.015439400708
C	-1.254757631271	9.842525829576	0.091620227793
H	-2.146537972956	10.269902431318	0.568748026999

H	-0.363770529076	10.166415644742	0.645413328949
H	-1.189863015089	10.195186205786	-0.937224775229
O	-2.609223631572	-1.512133736436	5.966247728327
C	-2.192958962484	-2.849412369275	6.314872813773
H	-2.084143861175	-3.479661113690	5.422468544368
H	-1.242719950750	-2.840272262277	6.864527354335
H	-2.978089832703	-3.254620131650	6.952217265592

Pin-F1500

($E_F = -929.30036002$ a.u.; $G_F = -928.90823334$ a.u.)

0 1

C	-1.524270734859	1.993233611409	-0.288044493284
C	-1.708717441858	3.413086623107	0.385948880723
C	-2.241224937794	3.454489295872	1.845407386923
C	-1.754698451811	2.116153666859	2.561024385581
C	-0.423582404557	1.559687087235	2.009900363697
C	-0.188777838160	1.936803732734	0.534503199235
H	-2.233410988221	4.158835106644	-0.218634938367
H	-2.534490172819	1.416322155481	2.270475035114
H	0.398060518217	1.950116658188	2.617327771118
H	-0.430560050074	0.472681188549	2.143930263903
H	0.644221197992	1.374242939131	0.103298042335
C	-0.154234036143	3.482636822927	0.464911470209
H	0.308555282140	3.875113258693	-0.438372081250
H	0.256118639617	4.000503941104	1.329400522162
C	-1.257992659907	2.181121596449	-1.796312783346

H	-0.589765573411	3.010910077517	-2.025281892800
H	-0.816185928303	1.272375089812	-2.216740150051
H	-2.201597573811	2.365231763201	-2.319780669774
C	-2.558992102013	0.862764952009	-0.190261658675
H	-2.254942061987	0.034902162096	-0.838250160305
H	-2.693684775031	0.445308217882	0.804384262496
H	-3.535379392610	1.208104114473	-0.544572384572
C	-3.772228461309	3.476820093724	1.925175935228
H	-4.201211001565	4.348105577708	1.429658476069
H	-4.191807552541	2.592779399114	1.441151129923
H	-4.081065569474	3.484880431319	2.973224158299
O	-1.687510018418	4.637867845373	2.485781064788
O	-1.747260653287	2.125664358309	3.994618450034
C	-2.088220601645	5.944683515441	2.022707611001
H	-2.190197655101	6.556433688763	2.922103407955
H	-3.064470401387	5.923673344777	1.534551491974
C	-1.122200139502	6.702986456086	1.069111764130
H	-0.129876443896	6.803216018371	1.530484122364
H	-1.004998913271	6.172605403218	0.115290339719
C	-2.530511714303	1.117750149283	4.656212663797
H	-3.453981765296	0.917808917455	4.099046964010
H	-2.810017684394	1.542906119115	5.622336102113
C	-1.820760939323	-0.235554408163	4.932854282925
H	-1.576612177871	-0.747875678791	3.990267562457
H	-0.882346547132	-0.053432794484	5.475286584967
O	-1.724532854532	7.988705262673	0.860220824960

C	-1.047856267117	8.914462353917	-0.011923162148
H	-0.049283249802	9.167221627586	0.368300122372
H	-0.950226273938	8.509894370797	-1.028242003785
H	-1.663928412339	9.812828009773	-0.037150629400
O	-2.728035601082	-1.020849022716	5.715152597079
C	-2.281437242787	-2.319422182235	6.154089910294
H	-2.056528194441	-2.975179552149	5.302486432112
H	-1.389800542903	-2.241637483091	6.789886378360
H	-3.102836986603	-2.743288042772	6.730837085751

Pin_Int1-F1500

($E_F = -929.39872210$ a.u.; $G_F = -929.01764381$ a.u.)

0 1

C	-2.335266995172	2.891635889888	1.188484430558
C	-1.344710580325	4.134314175799	0.969841924818
C	-1.781752818462	5.570873903057	1.081263570381
C	-1.591318981222	-0.312379827002	2.746154498394
C	-1.225620248694	1.127205588082	3.019387355916
C	-1.116231552109	2.093416035256	1.805385926631
H	-0.893718900336	4.015750719574	-0.019818452357
H	-2.433665256729	-0.570246148703	2.104795581116
H	-1.915802923539	1.559313942126	3.762410288160
H	-0.246249557901	1.118579708218	3.515151212377
H	-0.608392139936	1.565290872631	0.991187752710
C	-0.411543685730	3.461200697932	2.038393955502
H	0.665335295650	3.511678102471	1.861412862778

H	-0.613964147140	3.839398586160	3.044241869261
C	-2.925511116320	2.322722262979	-0.097421260744
H	-3.476910819978	1.396464777007	0.098461253835
H	-3.618738620576	3.037705987856	-0.553298472151
H	-2.141241735365	2.101318873998	-0.826990198731
C	-3.447600922242	3.167197083472	2.199522738808
H	-4.022262832832	2.254916787535	2.387519914586
H	-3.066784298779	3.515747394450	3.161541285757
H	-4.130342728518	3.929618919934	1.814211236682
C	-1.979367254723	6.237787560855	2.407384378312
H	-2.799523931110	6.962372318911	2.403069223286
H	-2.207978081256	5.497972670974	3.172223961917
H	-1.075019794776	6.776543802186	2.735390201032
O	-1.443644258706	6.383335680569	-0.010795339799
O	-1.317171165474	-1.199898878478	3.772327703677
C	-1.913987880032	7.749736738781	-0.009114704486
H	-1.541583629240	8.287030902118	0.867547509184
H	-3.009272188655	7.765542032627	0.018868967663
C	-1.433408052389	8.516422106132	-1.258089791027
H	-0.336494505228	8.479848316955	-1.316782808162
H	-1.841694412615	8.059646774675	-2.170164907956
C	-1.732740727302	-2.570064815904	3.583386900369
H	-1.267413891502	-2.978219504105	2.680005253830
H	-2.821638515935	-2.616521484669	3.464437760930
C	-1.319351430684	-3.424809758071	4.799764959844
H	-0.227701889180	-3.386618214973	4.921482299258

H	-1.778338021482	-3.015321369250	5.710769523221
O	-1.898428444522	9.862116909210	-1.101279724036
C	-1.569484567394	10.807652720574	-2.138660085586
H	-0.482880347704	10.922666461516	-2.245401655012
H	-1.993738890670	10.505746771505	-3.105155371070
H	-2.006541534419	11.757057457416	-1.831339195947
O	-1.763834639732	-4.761925950670	4.555696771670
C	-1.470553686869	-5.743448449932	5.571886502205
H	-0.388549330545	-5.849674328257	5.723836602197
H	-1.942331176371	-5.481686366948	6.527979397901
H	-1.880964765278	-6.685391061247	5.209998548626

Pin_TS1-F1000

($E_F = -929.08430440$ a.u.; $G_F = -928.69748796$ a.u.)

0 1

C	-1.735529465071	1.918607208484	-0.233489086273
C	-1.578466726654	3.415253738792	0.234447735020
C	-2.237533232030	3.968025154513	1.472097558833
C	-1.665481971409	1.741588783994	2.895370099848
C	-0.640803617851	1.073986491173	2.007451429196
C	-0.440504579077	1.598171785557	0.583923758902
H	-1.759860720039	4.104944885719	-0.601200823907
H	-2.718073946028	1.584934901556	2.687397143125
H	0.318886830762	1.135271967034	2.531374992014
H	-0.888852168412	-0.001159777540	1.961886823461
H	0.259019089131	0.930944671671	0.070426292506

C	-0.080478467472	3.107392893863	0.535294350133
H	0.591809902276	3.362968038908	-0.284463028112
H	0.296450947434	3.544692295787	1.459624054485
C	-1.425381604694	1.862299860584	-1.742469456089
H	-0.524798706309	2.420599274965	-2.006633631597
H	-1.279403030131	0.825300079363	-2.060518620038
H	-2.257050019930	2.279748551057	-2.319185810056
C	-3.005693303465	1.097470132557	-0.010072895044
H	-2.862641379769	0.088197692117	-0.410058377455
H	-3.292964452820	0.990136513663	1.031991095126
H	-3.849510212778	1.544289478623	-0.545106540350
C	-3.723040509786	3.931590456644	1.673216935205
H	-4.215395097804	4.626819134391	0.973532887280
H	-4.149863192120	2.944446575434	1.507298306255
H	-3.969064745420	4.260534792677	2.685312328151
O	-1.721296653480	5.234047490120	1.831909662965
O	-1.367026752580	1.581629204103	4.237269091855
C	-1.551207686069	6.183184610685	0.750839642708
H	-2.399696097034	6.130113312580	0.060543020285
H	-0.638687821980	5.963612128123	0.187635195950
C	-1.466921096542	7.627446645305	1.255006223082
H	-2.382198692807	7.896087487648	1.800883963555
H	-0.610882811239	7.755950055734	1.932034645956
C	-2.244452632984	0.770375702173	5.042669984152
H	-3.268757504722	0.802805680320	4.655551016031
H	-2.238286896607	1.196704678252	6.047087876019

C	-1.756902258130	-0.690088937472	5.117456168119
H	-1.796791308736	-1.153031818567	4.119828037229
H	-0.710241879314	-0.699950129590	5.453614701147
O	-1.316559764182	8.418239144385	0.073542407472
C	-1.255771632672	9.836917955117	0.248394245542
H	-2.173351964761	10.225313029722	0.711242044172
H	-0.396231244458	10.130815783152	0.866245732817
H	-1.145755267852	10.266174731536	-0.747399699697
O	-2.598148964909	-1.384066992748	6.034068140975
C	-2.238844797914	-2.748017156962	6.292254261700
H	-2.280179011459	-3.353955384765	5.376952756528
H	-1.230267035710	-2.821128968581	6.720834817214
H	-2.964653537579	-3.129722278890	7.009910887821

Pin_Int1-F1000

($E_F = -929.19018418$ a.u.; $G_F = -928.80869475$ a.u.)

0 1

C	-2.289602026866	2.876583714511	1.211289482776
C	-1.331235319348	4.137157514295	0.995739486787
C	-1.801900043663	5.554294847553	1.123708105356
C	-1.591520958183	-0.253053840713	2.738149907241
C	-1.141746917301	1.151973940506	3.021850034278
C	-1.048376612102	2.110356707112	1.814483558691
H	-0.887670720840	4.039606634153	0.000587759743
H	-2.476911494129	-0.456630642385	2.136519081124
H	-1.776822438619	1.607938859374	3.799360331056

H	-0.142594700856	1.087895836163	3.471990949002
H	-0.537203171459	1.589315646425	0.997781042691
C	-0.368946392610	3.486893573692	2.047181341572
H	0.703576117230	3.562267146644	1.854179421452
H	-0.565389939383	3.856293840976	3.057487745741
C	-2.873569267534	2.300201224869	-0.074416769062
H	-3.403093406183	1.360833775458	0.119191667623
H	-3.584973636678	3.001524704368	-0.523498274315
H	-2.088211108744	2.099827729649	-0.808889720498
C	-3.403130467720	3.118847250071	2.229973130509
H	-3.951130123765	2.190642938995	2.419468458956
H	-3.026407198566	3.475788508963	3.190408668966
H	-4.108982507068	3.863030801797	1.850786939957
C	-1.999489348619	6.215310170844	2.452715366774
H	-2.824289688667	6.934438662519	2.452797929664
H	-2.220794805277	5.471483084362	3.215800077719
H	-1.097187790152	6.758789308483	2.778897248329
O	-1.469796534716	6.364707645354	0.036077415831
O	-1.309531157143	-1.163243485676	3.733847652746
C	-1.960564660068	7.715580390833	0.029509878654
H	-1.599204306680	8.269328413436	0.901060405822
H	-3.056479393522	7.718385676188	0.051123522315
C	-1.475359524167	8.451129490418	-1.225269378854
H	-0.377439514026	8.417453774477	-1.273089482166
H	-1.872118287873	7.970756302728	-2.130720233566
C	-1.796014479659	-2.502213380340	3.544037808128

H	-1.400536174780	-2.917380345677	2.610738799274
H	-2.891241983717	-2.501623652990	3.487774156816
C	-1.345333283566	-3.371823503561	4.724515645657
H	-0.247356369899	-3.374536281455	4.781208949385
H	-1.732617754766	-2.949615917002	5.663048502716
O	-1.946066670213	9.792433636797	-1.103972011201
C	-1.585834641932	10.686390753139	-2.163118297043
H	-0.495473494967	10.788276311084	-2.248990927878
H	-1.987262158709	10.348882769027	-3.128279970668
H	-2.019228750538	11.654206187795	-1.911946632848
O	-1.852252025717	-4.684523468210	4.503345590744
C	-1.520806673717	-5.652123309842	5.507591793332
H	-0.433854508769	-5.785194022788	5.592442494412
H	-1.920742079936	-5.364044366910	6.489198184761
H	-1.975656002542	-6.591605794330	5.194705615556

Pin-F1000

($E_F = -929.15396719$ a.u.; $G_F = -928.76146386$ a.u.)

0 1

C	-1.498087097637	1.981447376163	-0.313784991221
C	-1.702164062315	3.395772230347	0.362283003919
C	-2.262540745458	3.406025408121	1.809703658353
C	-1.751742145570	2.098568062577	2.547143319263
C	-0.419878031400	1.540901930664	1.993059425535
C	-0.173062137564	1.931388809515	0.524734710377
H	-2.224454637318	4.141627867785	-0.244265194756

H	-2.525370453716	1.367208110657	2.319910171117
H	0.397742387573	1.926669445408	2.608567240274
H	-0.426233079683	0.452902013166	2.117307810736
H	0.669646641064	1.379470812532	0.098724289747
C	-0.150807714623	3.478295602108	0.467438242879
H	0.323078104226	3.882185282523	-0.425138447648
H	0.241237430078	3.992275085594	1.343010856181
C	-1.211659352060	2.168084010405	-1.817713921647
H	-0.524086460829	2.985337770267	-2.034809500328
H	-0.781502510139	1.252499084296	-2.235480495662
H	-2.144603476127	2.371938604435	-2.352774940037
C	-2.526039585370	0.846568155391	-0.222054909321
H	-2.171046872057	-0.012511840628	-0.800063717956
H	-2.725747319338	0.487412057666	0.784105557532
H	-3.479238560247	1.159805260366	-0.659640599679
C	-3.795521281383	3.394090588153	1.852315857224
H	-4.230139178973	4.258139258893	1.348503372069
H	-4.184143959918	2.503085454369	1.355928928780
H	-4.130654571824	3.393618732360	2.892273287162
O	-1.749574183001	4.575248912816	2.495327942032
O	-1.699843300113	2.206394956186	3.971231059670
C	-2.153468646012	5.878598571654	2.050805581082
H	-2.299024990017	6.474578517135	2.955241968523
H	-3.108107830227	5.857786280396	1.520710682239
C	-1.148949945994	6.639913347667	1.157466781081
H	-0.177640632405	6.729219026730	1.664407882389

H	-0.989720718720	6.120677602453	0.203656733132
C	-2.493590443208	1.273498664680	4.708955475098
H	-3.479433927872	1.142432252569	4.244951770690
H	-2.645347037210	1.719830062420	5.693678044023
C	-1.851642640826	-0.115414037270	4.908424374984
H	-1.716740416169	-0.623904625015	3.941471514594
H	-0.861110901937	0.000873878492	5.371364275559
O	-1.733306653743	7.925664499040	0.936742999309
C	-1.003379207159	8.816577684387	0.087315012329
H	-0.011570438430	9.045369160108	0.500763603124
H	-0.877416773850	8.398299338287	-0.920990489431
H	-1.587088239549	9.734964024300	0.025061813228
O	-2.732315072460	-0.857883640950	5.749805446992
C	-2.298902648925	-2.173926156002	6.112204746230
H	-2.174339002911	-2.814221461200	5.228083254858
H	-1.350127215977	-2.145675944547	6.665003591199
H	-3.076176510464	-2.591645093746	6.751861642760

Pin_TS1-F500

($E_F = -928.92458323$ a.u.; $G_F = -928.53922463$ a.u.)

0 1

C	-1.730214795313	1.888279548111	-0.275237432370
C	-1.616133043485	3.403291690159	0.149861745674
C	-2.343409103103	3.980517481200	1.328505662201
C	-1.533592654005	1.632202706573	2.904671392095
C	-0.554942158525	1.017842828051	1.940379776930

C	-0.418274864673	1.613930023310	0.534953931234
H	-1.767568377084	4.060747194828	-0.719709751605
H	-2.601733547411	1.513615050069	2.759026261412
H	0.428494214437	1.065084814959	2.420247399154
H	-0.788518356167	-0.057789472973	1.843970593587
H	0.302960040673	0.997719658782	-0.011377546451
C	-0.120646916334	3.137232222304	0.509264583272
H	0.575100406326	3.425375483619	-0.280351363965
H	0.201631482557	3.579203536946	1.452025946954
C	-1.432336088264	1.796149503272	-1.783508677200
H	-0.543656437652	2.366237523172	-2.064972879140
H	-1.266609968169	0.754387331646	-2.075549047195
H	-2.275224996090	2.182722382620	-2.365491886396
C	-2.970603765770	1.039239567377	-0.002125877770
H	-2.793740353223	0.014866018912	-0.346562107599
H	-3.245604297353	0.982248688943	1.047560448122
H	-3.832806468620	1.426238610140	-0.554074202619
C	-3.819874252081	3.870129424388	1.541534957590
H	-4.362475952410	4.507081463105	0.821890718131
H	-4.191736794035	2.854719029663	1.423083287045
H	-4.075392868641	4.226513114793	2.542383231578
O	-1.862704242785	5.233753715787	1.728139655992
O	-1.137665840150	1.533977268939	4.219102345018
C	-1.586665565814	6.187083973471	0.684128371920
H	-2.379649752585	6.170936328344	-0.071592406010
H	-0.636179758420	5.961895356509	0.189134993698

C	-1.521110005021	7.592811171648	1.267771011472
H	-2.474766683887	7.843125218824	1.754241742157
H	-0.723920110014	7.661623932819	2.021768645283
C	-2.026328920556	0.880834404396	5.135887919536
H	-3.072746158556	1.085394401846	4.883177500830
H	-1.820009983130	1.290778660985	6.125481621615
C	-1.765692776189	-0.628705665071	5.142228010715
H	-1.983969377715	-1.050234940834	4.148511922430
H	-0.701534474621	-0.805457786955	5.356342002731
O	-1.263444608095	8.452461225456	0.163123286925
C	-1.228179511695	9.840096138153	0.474096671042
H	-2.187402799261	10.185933820676	0.884442169525
H	-0.433392872092	10.072460208986	1.196770950273
H	-1.027559426062	10.368221070575	-0.458327123737
O	-2.592693540759	-1.213874117274	6.135654830385
C	-2.380217738537	-2.611411417757	6.319700437347
H	-2.593740581710	-3.175268873671	5.400874369392
H	-1.347388914430	-2.822051168657	6.629994423776
H	-3.063464136685	-2.935656798194	7.104769829230

Pin_Int1-F500

($E_F = -928.98417295$ a.u.; $G_F = -928.60279607$ a.u.)

0 1

C	-2.207957428035	2.865167530733	1.256344960958
C	-1.292139895840	4.149692515934	1.045694825849
C	-1.807806891123	5.542621936042	1.190636939874

C	-1.561461484517	-0.179038957872	2.732086247170
C	-1.013318460218	1.178890342883	3.034216824273
C	-0.938208510949	2.139029990986	1.840015745874
H	-0.857187751710	4.077260899206	0.044744993163
H	-2.482431714003	-0.309603217012	2.164723273410
H	-1.584337257924	1.652686861886	3.850166433800
H	0.001118655404	1.047039556844	3.432210198850
H	-0.421495770631	1.633284398821	1.017218313043
C	-0.295095722147	3.528612269583	2.077275109861
H	0.771062493679	3.638890601077	1.867454793936
H	-0.487354263665	3.884527526855	3.093176689051
C	-2.786214638577	2.282550350153	-0.029287387192
H	-3.289261026565	1.328024814102	0.159908228407
H	-3.519253175483	2.968302968352	-0.467559789333
H	-2.001339279185	2.108801016402	-0.771038865386
C	-3.319415235016	3.064758626156	2.287200735968
H	-3.833556939750	2.117847725436	2.478663020952
H	-2.945904017058	3.431286720741	3.245217960074
H	-4.053903771370	3.785782493359	1.917873879588
C	-2.000924664756	6.201865475736	2.520770265341
H	-2.835470703755	6.909526095380	2.527256164967
H	-2.204395369782	5.455815741480	3.286807490588
H	-1.102675233799	6.758277408249	2.836601176710
O	-1.500106463219	6.348870707796	0.100523438227
O	-1.295599770894	-1.123453239007	3.691501930495
C	-2.022845896028	7.679839111946	0.078296977989

H	-1.667043853404	8.262013257674	0.934053595236
H	-3.118772927582	7.660706012402	0.106125711369
C	-1.550100136497	8.369397281401	-1.197103537260
H	-0.451658748503	8.341291142232	-1.244604454583
H	-1.942207884517	7.848872711008	-2.082623641510
C	-1.867842415088	-2.419382289279	3.489197588014
H	-1.538161788972	-2.835500526137	2.530833389812
H	-2.962978603369	-2.356737405853	3.483665638067
C	-1.407363520029	-3.319676519417	4.631254164109
H	-0.309023434678	-3.375604756512	4.635069376195
H	-1.727101398079	-2.890067705520	5.592004812676
O	-2.028517028614	9.705879077042	-1.130706786456
C	-1.647313701857	10.528083923604	-2.228561226359
H	-0.554523381244	10.616954223292	-2.304283027129
H	-2.034772237797	10.136441289166	-3.179469532382
H	-2.074499653830	11.514673819817	-2.048317483706
O	-1.986111320182	-4.598623918316	4.422691152809
C	-1.634008705164	-5.565069945868	5.408708858974
H	-0.548987527688	-5.737239491110	5.433144227202
H	-1.963986335720	-5.256077156622	6.410343052914
H	-2.137393350538	-6.492848639864	5.136724882270

Pin-F500

($E_F = -929.01075085$ a.u.; $G_F = -928.61714900$ a.u.)

0 1

C	-1.472453332155	1.964037340577	-0.345173516328
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C	-1.704681726894	3.372815110432	0.331512897747
C	-2.295632854975	3.353295662890	1.764009558986
C	-1.750427538018	2.080757893113	2.526802986767
C	-0.417751615417	1.522646604812	1.968662918367
C	-0.158208014304	1.928546252062	0.508577053548
H	-2.225155510819	4.115905853262	-0.280070848139
H	-2.514992930332	1.321887172013	2.362405460067
H	0.396405067156	1.900845844171	2.593102700365
H	-0.425640299408	0.433424633324	2.081073997987
H	0.697533223669	1.391925978529	0.089046130310
C	-0.157335950931	3.475736453057	0.465009423441
H	0.325973885011	3.894729318994	-0.415713070833
H	0.212770701176	3.986284776086	1.352468770630
C	-1.171351103701	2.152148922070	-1.844909876814
H	-0.478881558762	2.968240923381	-2.051736207537
H	-0.738699886479	1.236560305868	-2.260194728565
H	-2.097872967244	2.359869949215	-2.389573740298
C	-2.483413874521	0.815483536191	-0.253697790838
H	-2.091826741805	-0.056165563146	-0.787815047617
H	-2.713480078545	0.489889681619	0.757617339775
H	-3.425360237574	1.095505627427	-0.735781941472
C	-3.828731495438	3.294096575597	1.769976366864
H	-4.274946977882	4.146574834900	1.256058791690
H	-4.181964272827	2.392710979031	1.266804371239
H	-4.188211241373	3.285953593642	2.801654293729
O	-1.840331003427	4.520211559887	2.482819193089

O	-1.654023287057	2.280198209087	3.935665925040
C	-2.254210897647	5.810815889803	2.031906007404
H	-2.515939097863	6.387705876646	2.923212654847
H	-3.144102375665	5.769690641010	1.399470307181
C	-1.174353917158	6.590235886297	1.269762191142
H	-0.262645140861	6.671705637535	1.879094850551
H	-0.911710838855	6.086315812238	0.330542421900
C	-2.458901059024	1.427294168182	4.742477990480
H	-3.477341276680	1.341368650206	4.342149703064
H	-2.524335838321	1.904906502839	5.721943170164
C	-1.872192768385	0.021060376199	4.919553797947
H	-1.795697223742	-0.491087567487	3.947564838633
H	-0.858815401259	0.095815612533	5.340705815025
O	-1.733337679376	7.873556766737	1.007880166648
C	-0.903867157536	8.738936110135	0.241724547606
H	0.046713779018	8.945217296444	0.753535116882
H	-0.683313412509	8.314317381090	-0.748090000723
H	-1.450469834424	9.673817715844	0.114961363646
O	-2.742576248586	-0.686594941937	5.791721546066
C	-2.324404495568	-2.012511034960	6.098598897938
H	-2.260392856194	-2.634497388479	5.194479169996
H	-1.346312465588	-2.020114360982	6.599580211528
H	-3.072916631207	-2.434468634175	6.769609220591

Pin_TS1-F200

($E_F = -928.83008680$ a.u.; $G_F = -928.44725113$ a.u.)

0 1

C	-1.727006764590	1.836510251124	-0.323768191807
C	-1.695877003783	3.378267505959	0.024133233290
C	-2.544202522865	3.974493572929	1.102235138193
C	-1.243349158009	1.512489699261	2.898660577490
C	-0.359166658743	0.978869951249	1.815511260741
C	-0.368447013450	1.669142684856	0.444938521307
H	-1.817543247417	3.978964737890	-0.892898753221
H	-2.324709692162	1.501880796165	2.831336157432
H	0.665783618198	1.022830763319	2.200805875511
H	-0.571176468075	-0.095202164655	1.663439219572
H	0.379933696350	1.155170342093	-0.166460755496
C	-0.207603469637	3.211962059023	0.463338125431
H	0.509221246993	3.584287380034	-0.270801915906
H	0.015820633838	3.647748777277	1.437272807094
C	-1.488604125388	1.667294708544	-1.832690268082
H	-0.634140602217	2.257665005025	-2.175397773197
H	-1.288878585355	0.618222383931	-2.073772635449
H	-2.367484853872	1.987709292313	-2.401578794820
C	-2.896787124001	0.941916026175	0.078974932019
H	-2.630958603579	-0.105647134034	-0.097615494977
H	-3.175007215711	1.037472196110	1.126149235791
H	-3.782497956140	1.160764016915	-0.525282549424
C	-4.033754491261	3.865942259385	1.162328161608
H	-4.501400805303	4.555329963033	0.437620706760
H	-4.396820693244	2.864541608616	0.940711027417

H	-4.389212707026	4.160151566814	2.153807074154
O	-2.088654743194	5.188736669090	1.608702769277
O	-0.729022617276	1.374149841523	4.163179522022
C	-1.692748907651	6.181084811109	0.647877966445
H	-2.427645219002	6.248403168238	-0.162518846906
H	-0.718107664168	5.940938432285	0.210020716824
C	-1.613706871202	7.524130494056	1.352287908004
H	-2.593658002195	7.777934375133	1.782003543861
H	-0.884026304215	7.478774807255	2.173957742831
C	-1.628687932266	0.947033362652	5.189297625118
H	-2.622877588977	1.386953949112	5.052079692625
H	-1.220037042136	1.299063055096	6.137261050041
C	-1.714566863730	-0.576915239812	5.195037766975
H	-2.117863863478	-0.930042832359	4.232898254083
H	-0.702036512862	-0.991927246769	5.307503896758
O	-1.223287257918	8.468912197780	0.367839105525
C	-1.157480775631	9.802459662088	0.846483633350
H	-2.134165544742	10.147614603365	1.214912884990
H	-0.422193262060	9.905299395026	1.657293443765
H	-0.851819342756	10.429412196203	0.008297028033
O	-2.549687960096	-0.965733058498	6.270130932407
C	-2.632465251891	-2.374463216645	6.434312079993
H	-3.050800993280	-2.860241708336	5.541369443169
H	-1.646291916270	-2.812908500924	6.642114849809
H	-3.291634689727	-2.560935913051	7.282484413793

Pin-F200

($E_F = -928.92669706$ a.u.; $G_F = -928.53345353$ a.u.)

0 1

C	-1.675512517115	1.544645402611	-0.498636647667
C	-1.788226582595	3.047816829452	-0.028927453079
C	-2.250000080362	3.269562666438	1.433969889931
C	-1.707853850751	2.096119314045	2.327494905998
C	-0.451372337686	1.388270179828	1.759883549810
C	-0.294716288315	1.563981604160	0.241470051896
H	-2.329741183649	3.712196629117	-0.707002598146
H	-2.519032943640	1.368410241204	2.347936401292
H	0.425545998516	1.806356955282	2.261461431786
H	-0.496769453607	0.328134121829	2.029276461834
H	0.498340517248	0.924911879034	-0.157208178541
C	-0.231313934679	3.086090218593	-0.037580648836
H	0.189352375994	3.342727465483	-1.007770407419
H	0.237873807653	3.698921831446	0.731158784407
C	-1.500099424102	1.493104487959	-2.029000312205
H	-0.793789738644	2.229593411976	-2.412185376568
H	-1.145739137010	0.503399974105	-2.333727506937
H	-2.460932588626	1.669984280934	-2.522662908505
C	-2.724215595882	0.480830118301	-0.154089218061
H	-2.417796177139	-0.481590721668	-0.576296843934
H	-2.884532832397	0.323879194171	0.909480430744
H	-3.689717015903	0.738539661739	-0.600733598280
C	-3.775878263680	3.339288438561	1.562572444668

H	-4.184674307728	4.176804343551	0.994124116282
H	-4.242403662460	2.426660531642	1.186569031481
H	-4.047556368604	3.469383201318	2.612718143357
O	-1.678669074884	4.490782709500	1.952319173190
O	-1.478304763594	2.513281854705	3.671983244010
C	-1.830943067680	5.653761694394	1.150674245558
H	-2.877769890723	5.836369118434	0.881726410557
H	-1.254183609336	5.585582533206	0.220688294767
C	-1.315930169834	6.846310789185	1.940346858332
H	-1.905646865482	6.979764644951	2.858724675738
H	-0.268821092620	6.677737130617	2.231492956392
C	-2.218219920995	1.811212120263	4.661156600458
H	-3.283361813448	1.752740968276	4.400265426817
H	-2.129916314638	2.392073383094	5.581196038621
C	-1.688374897040	0.397662505458	4.907167815705
H	-1.746866508515	-0.199924107159	3.984525385776
H	-0.631149977478	0.445135380051	5.208034025628
O	-1.436180436384	7.971501441383	1.082137773907
C	-0.964696645460	9.181337359761	1.650155464030
H	-1.523532654898	9.446943367753	2.559098628400
H	0.103455223775	9.119741333428	1.903655233164
H	-1.107993512600	9.964047997145	0.904401529688
O	-2.487675934075	-0.184129946349	5.923374579644
C	-2.130303596277	-1.524230468328	6.225769477189
H	-2.239833827332	-2.178046619694	5.348540369917
H	-1.094182446452	-1.593973873607	6.586139879606

H	-2.803987470786	-1.867673592548	7.011391795500
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Pin_Int1-F200

($E_F = -928.86202465$ a.u.; $G_F = -928.48106209$ a.u.)

0 1

C	-2.095585786346	2.881130513083	1.322360611852
C	-1.199686530751	4.177133359919	1.125436426942
C	-1.743821793127	5.554082107162	1.279170743716
C	-1.498655515408	-0.121668395684	2.733492035935
C	-0.889523392417	1.197385192893	3.070065889826
C	-0.813615653749	2.172499658560	1.895219369839
H	-0.763746774942	4.120942084893	0.123840688782
H	-2.423219700018	-0.193745401378	2.162095734049
H	-1.428683565929	1.670317052566	3.908106049172
H	0.126385503806	1.016997209624	3.444309125416
H	-0.290152815179	1.683699753284	1.066448404538
C	-0.192091322478	3.567101121446	2.149668524334
H	0.871573524191	3.697997879240	1.939522743315
H	-0.389173873307	3.908439938051	3.169541479532
C	-2.670936320572	2.305381208553	0.032461624179
H	-3.169255115567	1.346663283499	0.212141781204
H	-3.407657031225	2.991278665964	-0.399457306648
H	-1.885295935219	2.142725723032	-0.711019751482
C	-3.205912031412	3.061359241500	2.358551742543
H	-3.707066570043	2.107818885659	2.550577943819
H	-2.833665030446	3.432393865701	3.315431494359

H	-3.951159997244	3.773319479677	1.993235149563
C	-1.912564548006	6.227914409787	2.604438397588
H	-2.759355416396	6.920747992151	2.623095170720
H	-2.082336589769	5.488790398018	3.385696572180
H	-1.016534622359	6.804987615525	2.888344328993
O	-1.491771905132	6.344031198366	0.168101511458
O	-1.278932234651	-1.098731151074	3.666498136988
C	-2.059284464200	7.651791884946	0.124242640750
H	-1.687095277967	8.278496237597	0.941168542224
H	-3.152214359302	7.600958396253	0.197328368469
C	-1.652788294214	8.283561913803	-1.197584581624
H	-0.556237961319	8.274993646396	-1.284322980812
H	-2.063267791726	7.705255345297	-2.038077536739
C	-1.918052248635	-2.353243115096	3.429013548292
H	-1.610909356093	-2.761821438977	2.459835806766
H	-3.008643283655	-2.234247890416	3.427691648092
C	-1.499609978926	-3.294219629876	4.547617580370
H	-0.405129778163	-3.403554420192	4.546029036817
H	-1.794365856325	-2.868416137029	5.518214227040
O	-2.156794742194	9.608583695766	-1.189721066713
C	-1.819013362627	10.352487892793	-2.350137151737
H	-0.729865322111	10.448476383852	-2.464146661251
H	-2.226437886628	9.888955157994	-3.259814413924
H	-2.253428697490	11.345526616322	-2.232051153881
O	-2.139744619720	-4.536348915491	4.316648214105
C	-1.819904837963	-5.522494908749	5.287163097244

H	-0.742533786931	-5.739804401631	5.300241662202
H	-2.126503460358	-5.209679359834	6.295323235957
H	-2.362582703106	-6.428016940166	5.014914542560

Cam_TS3C-F4000

($E_F = -930.58403049$ a.u.; $G_F = -930.20874739$ a.u.)

0 1

C	-0.780299288590	1.707264054645	-3.865086228052
C	-0.474488327989	2.504210952205	-4.933192192959
C	-3.531912062041	1.447094577525	1.698003143281
C	-3.161972080592	1.452537418061	-0.353389911819
C	-1.859655719231	1.418655871246	-1.254969222920
C	-1.934587618843	2.006061196585	-2.793282729619
H	-0.941999048134	3.478027127505	-5.064104632208
H	-2.588223387964	1.251714803515	2.195669059154
H	-4.005463194793	0.911254094018	-0.772090976759
H	-1.044249555665	1.938773447763	-0.746075641249
H	-1.547532636970	0.374386455891	-1.342274681784
H	-2.100567840998	3.085656265800	-2.734756553028
H	-2.849302243468	1.579112139470	-3.221814307350
C	-3.580695506261	2.517412124700	0.650131086038
C	-4.972574474586	3.105462713048	0.409696685066
H	-4.954857086084	3.740450387969	-0.479967013526
H	-5.712996919933	2.317189440545	0.260785962530
H	-5.292681852907	3.706973339628	1.265895460134
C	-2.548836182460	3.622913027167	0.884040852988

H	-2.441469182390	4.228790791251	-0.022259851116
H	-2.861794928665	4.273007645513	1.705649049140
H	-1.565137538530	3.214387731420	1.128838214717
O	0.447183497489	2.166323357077	-5.970884321209
O	-4.686368452322	1.094229829803	2.431089785749
C	-0.126188846027	0.353545253461	-3.739160496345
H	0.447112982859	0.276669140205	-2.808847265388
H	-0.880509703108	-0.442057303249	-3.710101510478
H	0.547846844999	0.158729541323	-4.573381703302
C	0.630679004832	3.076821091275	-7.132243145150
H	0.977768467227	4.049250595993	-6.770701666190
H	-0.331454224727	3.210283458708	-7.635242974359
C	1.686692797138	2.544344433695	-8.215869358329
H	2.655667854623	2.408262817113	-7.720528553719
H	1.345246297984	1.569645788230	-8.584823972434
C	-4.592009016514	0.506887081217	3.801286709048
H	-3.755165008977	0.975831787135	4.325656693464
H	-4.400141810032	-0.564521476386	3.707967279454
C	-5.918326135967	0.710603046072	4.683479214311
H	-6.107518224105	1.786539856403	4.780595124890
H	-6.762456085146	0.256001076082	4.151178385582
O	1.803507635486	3.500140886436	-9.320553625826
C	2.716093482493	3.295840297626	-10.509407013969
H	3.760729115721	3.237785397261	-10.189587867353
H	2.436785182522	2.393112732722	-11.060764276305
H	2.549036750605	4.182921103652	-11.115582968277

O	-5.748802500925	0.095955249076	6.001380795183
C	-6.818455422499	0.107419315598	7.072551244124
H	-7.061286920641	1.133341938756	7.364279263652
H	-7.716397090628	-0.412859756325	6.726798250682
H	-6.357762160638	-0.428501542426	7.898728897124

Cam_Int2C-F4000

($E_F = -930.59651628$ a.u.; $G_F = -930.21925561$ a.u.)

0 1

C	-0.901297224606	1.654193239991	-3.737783921864
C	-0.518585867341	2.482752710383	-4.755774143868
C	-3.337557601637	1.345045188299	1.385386086038
C	-3.255995441123	1.480383584733	-0.209644677537
C	-1.974665827639	1.311825821475	-1.153684821973
C	-1.994788702044	2.014371157687	-2.622267660030
H	-0.869417851788	3.511463236740	-4.808795312953
H	-2.378890814028	1.197639719561	1.882032968066
H	-4.161046447121	1.116559586962	-0.691554034725
H	-1.087569876529	1.661833258054	-0.619787104880
H	-1.835513093074	0.237567538947	-1.302379081461
H	-2.015819833458	3.099076777486	-2.482219798810
H	-2.962170849388	1.747283201671	-3.065670494896
C	-3.527892463888	2.677265893822	0.698290584610
C	-4.936001782427	3.245691948480	0.670474751986
H	-5.071127177887	3.895394409183	-0.199797680524
H	-5.681271728758	2.449827060284	0.631704225536

H	-5.128977734765	3.840222538643	1.569649210277
C	-2.445146159757	3.727172951886	0.876832070969
H	-2.433628340900	4.418480266907	0.027454190370
H	-2.626004008712	4.310995915082	1.784779560784
H	-1.450302192989	3.284195166742	0.958255027556
O	0.342307561133	2.113993689564	-5.832544474851
O	-4.424193400880	0.688466659180	2.110923237177
C	-0.412329468499	0.227215240613	-3.717652317962
H	0.156769356707	0.016747776145	-2.805526307080
H	-1.255720770390	-0.473829523935	-3.731034690665
H	0.225474765825	0.013897913715	-4.575444883776
C	0.611883948697	3.074669696580	-6.936078796987
H	1.066901823520	3.977402342918	-6.518144599272
H	-0.335556463446	3.344323391931	-7.411413537624
C	1.591087704117	2.503992909765	-8.071153855591
H	2.546087013727	2.234245073221	-7.604290077380
H	1.142444102681	1.596801247119	-8.493621565895
C	-4.566664588012	1.055521512215	3.547167945302
H	-4.810953497835	2.119703681319	3.620925642465
H	-3.610553524722	0.884373266161	4.053721795926
C	-5.693355453310	0.232454624912	4.338708011339
H	-6.660349960729	0.401805995380	3.849401232091
H	-5.455127176413	-0.836232902043	4.274815382720
O	1.795194744396	3.511208132654	-9.115494929509
C	2.667534843130	3.289837103420	-10.331408342681
H	3.704001426290	3.103840170967	-10.034895312866

H	2.289020653987	2.457893744384	-10.932571063685
H	2.586689551934	4.226290636403	-10.877924766621
O	-5.746923477496	0.663743339149	5.740113909178
C	-6.704608910936	0.086331738783	6.757110347081
H	-7.741861958442	0.264890392594	6.458011756866
H	-6.528000987894	-0.985105317694	6.891237598091
H	-6.469710759196	0.630517277496	7.668768453220

Cam_Int3C-F4000

($E_F = -930.62424940$ a.u.; $G_F = -930.25416985$ a.u.)

0 1

C	-0.618246038777	2.055842513113	-4.068919877770
C	-0.634976082287	2.239025735250	-5.423734102346
C	-4.354572060289	0.902489133168	1.648325257745
C	-3.108803500773	1.408984957196	-0.701056115291
C	-1.980939964297	2.027489569883	-1.613504239222
C	-1.882876093216	1.626685715716	-3.183494734123
H	-1.565763198751	2.207147521792	-5.986458597181
H	-4.251699016765	-0.177983318993	1.549344996525
H	-3.886376498111	0.827128862436	-1.190673845644
H	-2.049004246907	3.123249759184	-1.554887098209
H	-1.015491652098	1.785049715535	-1.153777738256
H	-2.796425105672	1.963863063443	-3.681909990830
H	-1.905069100703	0.530450580699	-3.214984730237
C	-3.394706137381	1.840915419730	0.804526600985
C	-4.044536883646	3.248744848824	0.769675281830

H	-3.376472424658	3.973089154499	0.296744508438
H	-4.983084527640	3.225551056688	0.210747718021
H	-4.261149578947	3.587986927917	1.785814386564
C	-2.050689231513	1.928870858766	1.572116286814
H	-1.375131079202	2.651246364457	1.104359825973
H	-2.230728732258	2.244628528132	2.602330451194
H	-1.551401176797	0.956542100843	1.591157900649
O	0.517315604343	2.472341653249	-6.232274777580
O	-4.762353730522	1.342713415877	2.932473159075
C	0.698605328045	2.082895695104	-3.333020870230
H	0.710518161767	2.870714424627	-2.571823072302
H	0.871629579108	1.135228609852	-2.808655621839
H	1.530962627698	2.255095622054	-4.015327470962
C	0.385269472768	2.575456182475	-7.710636684153
H	-0.284776169100	3.406139827520	-7.950464052449
H	-0.050389440644	1.648239406353	-8.093771550730
C	1.775342596416	2.822180954530	-8.472211418042
H	2.219039736302	3.751500039561	-8.095026034830
H	2.453218517824	1.992929499197	-8.236426193675
C	-5.540846619144	0.423570464630	3.814218996078
H	-4.931517834664	-0.463452891017	4.009836196425
H	-6.444998710679	0.120680557233	3.280429974739
C	-5.976876485454	1.055048235413	5.222224085881
H	-5.074321062566	1.362797794294	5.764060671808
H	-6.588553201097	1.945103148867	5.031669055893
O	1.551596409121	2.908568531910	-9.917632054512

C	2.658813152003	3.136361828335	-10.922850562336
H	3.152594405802	4.095918805247	-10.743409492546
H	3.387575831151	2.321250565709	-10.886757457274
H	2.139285609300	3.144711381131	-11.877949767931
O	-6.731618776583	0.068564503471	5.999243240627
C	-7.297102356350	0.341512837442	7.375809711962
H	-6.495994702993	0.573488933891	8.083697055599
H	-8.022263197932	1.159798483512	7.340530123041
H	-7.785305275572	-0.593032618904	7.641112301050

Cam_TS3C-F3000

($E_F = -930.12314988$ a.u.; $G_F = -929.74694894$ a.u.)

0 1

C	-0.814268652954	1.673428512697	-3.844660348746
C	-0.485458316296	2.501772038767	-4.869984404646
C	-3.510716689548	1.492369385319	1.714903434792
C	-3.121865268048	1.461769030954	-0.419195587348
C	-1.829392539787	1.437075079592	-1.282456282824
C	-1.954424704112	1.974037922157	-2.803304797962
H	-0.931844765763	3.489342687425	-4.968883572569
H	-2.563988346816	1.263485751659	2.191781219418
H	-3.940913488406	0.856069032038	-0.796002114043
H	-1.031460969570	2.000784149499	-0.791698998728
H	-1.478106518408	0.402342190278	-1.343176622680
H	-2.153128407176	3.049780765075	-2.773934870483
H	-2.862429040308	1.507824152304	-3.207451497088

C	-3.552146223458	2.498164353811	0.603739551780
C	-4.950713644494	3.071057972450	0.348473850388
H	-4.931857938847	3.695720102569	-0.548209483922
H	-5.681340919335	2.273343644057	0.201220289268
H	-5.283686729117	3.678102848716	1.195784841031
C	-2.538640198850	3.627432424946	0.820022014428
H	-2.432361324525	4.213278329033	-0.099558490908
H	-2.870265730446	4.290907658540	1.623190721734
H	-1.551144036358	3.240622454335	1.084176251727
O	0.440770787153	2.181122309604	-5.886074493595
O	-4.658161767264	1.169308955228	2.431240392274
C	-0.194405745121	0.300487176283	-3.761841317059
H	0.411312699605	0.191947835813	-2.855505208346
H	-0.970070410166	-0.473328372285	-3.716659371227
H	0.443760849977	0.100778159065	-4.622552100926
C	0.561928359727	3.076193835880	-7.040925350571
H	0.846047532893	4.077737589835	-6.700834556059
H	-0.401647423896	3.142692899289	-7.556425557614
C	1.643192047861	2.575912281514	-8.072639041708
H	2.615299180405	2.507429444677	-7.567045218344
H	1.365728862385	1.572995674357	-8.422576129324
C	-4.561510881282	0.498960630376	3.738278321739
H	-3.682414073948	0.873776455417	4.270725798979
H	-4.448482008449	-0.576904878033	3.580410932212
C	-5.838136271003	0.758088475733	4.628185736119
H	-5.950154020777	1.839757067387	4.779235462096

H	-6.725200772204	0.391252545747	4.095689552169
O	1.702799186177	3.509171302103	-9.179780375150
C	2.632217702742	3.287735805940	-10.308928170511
H	3.673119394418	3.283655005363	-9.966530947588
H	2.408681031906	2.346414890745	-10.823402555259
H	2.461585206813	4.129226864097	-10.977573198246
O	-5.676724204541	0.074126613007	5.893871985323
C	-6.730123190518	0.143718820344	6.931574207063
H	-6.893324518737	1.177292281418	7.256181121716
H	-7.670509360492	-0.282396254789	6.565131124287
H	-6.345212106414	-0.451983298313	7.756750350230

Cam_Int2C-F3000

($E_F = -930.14871828$ a.u.; $G_F = -929.76876579$ a.u.)

0 1

C	-0.967892225288	1.613766092632	-3.685694868208
C	-0.543193996566	2.468417913676	-4.652427038987
C	-3.283335708620	1.382428251346	1.327676706489
C	-3.238955294754	1.492618926581	-0.232343926748
C	-1.975135221325	1.303191842128	-1.148852099498
C	-2.033511882575	1.989701808189	-2.591034568891
H	-0.846272948698	3.513645525547	-4.659695009334
H	-2.318772286998	1.249222808178	1.818718539269
H	-4.145953902021	1.113151786477	-0.698709944384
H	-1.082869190933	1.658259853524	-0.625976441886
H	-1.837099589246	0.226764965306	-1.286468734286

H	-2.053771096702	3.076058192622	-2.460021261764
H	-3.009639634321	1.718737570171	-3.015770933252
C	-3.503352039428	2.714940814246	0.644815561202
C	-4.916912643699	3.268363983143	0.633217613074
H	-5.076888290712	3.895643583273	-0.249396631555
H	-5.654738393564	2.464595084249	0.627108225549
H	-5.098946305281	3.883420448040	1.520840883020
C	-2.426725784713	3.775622609556	0.786811262422
H	-2.435844992072	4.455345515269	-0.071969362419
H	-2.596358995485	4.371714481907	1.689101527205
H	-1.426445199808	3.343479705155	0.857713851040
O	0.306447634591	2.104784620408	-5.718057697220
O	-4.349067298142	0.712114798735	2.034590750379
C	-0.549920353662	0.164947267324	-3.726602186886
H	0.035595846544	-0.105048228882	-2.840938962253
H	-1.427600520532	-0.492578264754	-3.736522792384
H	0.051712498374	-0.049500108018	-4.609649047519
C	0.552029369609	3.074886565136	-6.790258773111
H	0.996794407749	3.982422609898	-6.368671546710
H	-0.396239450457	3.340082204256	-7.268673269766
C	1.524072734023	2.510615967709	-7.895034381039
H	2.481752525204	2.246116471203	-7.428034092366
H	1.086726247094	1.599435804647	-8.323637384533
C	-4.496398108762	1.107675262769	3.440073275635
H	-4.762123329026	2.168707446662	3.497306175610
H	-3.541897608250	0.966041506707	3.961050847546

C	-5.596420195291	0.277498166929	4.204408155468
H	-6.566028154513	0.420697135895	3.709408755062
H	-5.339766403205	-0.788855030298	4.155339846277
O	1.710386151671	3.521788564551	-8.916028317089
C	2.577591023841	3.266470076104	-10.086917550506
H	3.610453830267	3.073290103915	-9.776370133179
H	2.204298952877	2.421132363944	-10.675691109935
H	2.528033525888	4.181811845832	-10.673325068300
O	-5.652482879358	0.730473629707	5.581698453724
C	-6.601060541258	0.128189228973	6.542192053374
H	-7.637491814680	0.277079199181	6.218617031001
H	-6.405267105841	-0.942368679729	6.670824545299
H	-6.422368429348	0.655617915348	7.477252745791

Cam_Int3C-F3000

($E_F = -930.14753855$ a.u.; $G_F = -929.77416771$ a.u.)

0 1

C	-0.632428836752	1.988473111901	-3.988118336734
C	-0.674116278576	2.268409771911	-5.316767205477
C	-4.286109613886	0.933332358049	1.574251751075
C	-3.078737319320	1.438755556525	-0.707176172011
C	-1.954673009071	2.035592311604	-1.592284266474
C	-1.894594493249	1.613456181003	-3.128959392323
H	-1.618650530757	2.350681780389	-5.851053127153
H	-4.137359163875	-0.142587509946	1.482078534161
H	-3.845226408714	0.840002158840	-1.193647747228

H	-1.998811799125	3.133878993987	-1.540526591837
H	-0.991594055206	1.777673504269	-1.133852912624
H	-2.797273173130	1.978445116416	-3.628718423347
H	-1.958538146741	0.517183961528	-3.147395816677
C	-3.372700202619	1.898604430034	0.758658991457
C	-4.079807837570	3.280325008471	0.694330102261
H	-3.439658820396	4.019748329603	0.206456133185
H	-5.015378793225	3.207293169223	0.134731873213
H	-4.311245451140	3.632267400849	1.702698829857
C	-2.039595496330	2.059562328220	1.537108635900
H	-1.394088787837	2.806765704421	1.066431816597
H	-2.244990812603	2.379659983159	2.560946680044
H	-1.496043893398	1.111707200001	1.573643052890
O	0.466127617765	2.477111083051	-6.120083550961
O	-4.713219236214	1.369489439793	2.836982645750
C	0.699006585017	1.853658129473	-3.291428458145
H	0.824177803201	2.621251037127	-2.519731731019
H	0.776887377326	0.883042028864	-2.787052797239
H	1.525567381827	1.944077494507	-3.995946350394
C	0.299850311860	2.581066401356	-7.573722659087
H	-0.375656831876	3.410763826741	-7.806948326038
H	-0.137809180823	1.654799024271	-7.959491644231
C	1.668571808651	2.829631718571	-8.314570808959
H	2.114763074088	3.759823653212	-7.939236139450
H	2.353462223556	2.002615981011	-8.086099278414
C	-5.451604481068	0.428854202894	3.692007920814

H	-4.815588592221	-0.437622954977	3.900483354165
H	-6.343043945836	0.088010601509	3.157674569655
C	-5.899380694134	1.065342062992	5.062123170916
H	-5.010950428288	1.411132146280	5.606655559227
H	-6.540572173800	1.933619375553	4.861891319658
O	1.421730464598	2.914840966191	-9.739838097607
C	2.532875777105	3.141284151896	-10.689692955655
H	3.029239421795	4.098158716255	-10.493216455343
H	3.265123907000	2.327724581163	-10.639242451324
H	2.060354974646	3.159187906313	-11.669796873793
O	-6.613653196509	0.062629765077	5.826333433012
C	-7.164753293926	0.375389767466	7.163154222399
H	-6.368150499194	0.657089478247	7.860709461344
H	-7.906318021349	1.179812009412	7.104188654916
H	-7.639184959311	-0.547790619042	7.489898307759

Cam_TS3C-F2500

($E_F = -929.89597364$ a.u.; $G_F = -929.51844085$ a.u.)

0 1

C	-0.836415979691	1.652952864922	-3.841103235643
C	-0.490983010774	2.500675793071	-4.839150334392
C	-3.496843513428	1.514846261472	1.723304716048
C	-3.108751865785	1.470143250554	-0.451194008554
C	-1.821767538641	1.442438079669	-1.300170985299
C	-1.971312205387	1.953533801704	-2.813836299276
H	-0.926696151904	3.494782172232	-4.919814115134

H	-2.550424636197	1.259093441781	2.186853603261
H	-3.917894013388	0.836779468486	-0.803373318477
H	-1.029340358879	2.024285797619	-0.821655769209
H	-1.456873545594	0.411144598445	-1.347261016128
H	-2.185675151627	3.026689683310	-2.798520754459
H	-2.875259209025	1.468132589601	-3.205505325192
C	-3.533011653926	2.492409184585	0.586043247721
C	-4.932818091219	3.066161360603	0.330920121466
H	-4.914088267580	3.688231235522	-0.567475051043
H	-5.663823482208	2.268376192897	0.185843156323
H	-5.264792828259	3.675480717712	1.176965256166
C	-2.521159067204	3.626860980666	0.791848978808
H	-2.415647567554	4.205130886721	-0.132619239438
H	-2.854974866036	4.296285933947	1.589032213061
H	-1.533086533141	3.244641293147	1.060561918027
O	0.446351357324	2.195064037706	-5.839194269550
O	-4.643481135702	1.206378203917	2.431932904883
C	-0.234591209808	0.271028231343	-3.781539918095
H	0.389240888556	0.146082174380	-2.889675313417
H	-1.020516975695	-0.491475141024	-3.725789502444
H	0.382841110157	0.069670114967	-4.656910801002
C	0.517038251837	3.065913961388	-7.005706665176
H	0.735516421562	4.092373568285	-6.690604910651
H	-0.443191545669	3.060529995656	-7.532314463797
C	1.632292008820	2.601241038149	-7.999014791397
H	2.601288234626	2.605606500750	-7.481991364690

H	1.421103272077	1.573334634995	-8.323194578552
C	-4.545746051716	0.501275226028	3.709903785118
H	-3.653750748475	0.839919905273	4.245770390141
H	-4.460178300841	-0.573110648944	3.524343063982
C	-5.803068848290	0.775561871988	4.601465542703
H	-5.887650245539	1.856797468045	4.775323823306
H	-6.703754783009	0.442494290830	4.068625541258
O	1.644163292730	3.503431288124	-9.124167447902
C	2.598679526577	3.285044218341	-10.214607428677
H	3.632341818274	3.346307883114	-9.853891207524
H	2.436070549756	2.312249376712	-10.693712235106
H	2.407299342840	4.085322996940	-10.927394318148
O	-5.646121285105	0.063655918126	5.844231815255
C	-6.693714782517	0.159285501808	6.866301102569
H	-6.824418633949	1.194817340269	7.201803882951
H	-7.648328969304	-0.227114125912	6.490462825263
H	-6.343861387453	-0.456880817893	7.692607275361

Cam_Int2C-F2500

($E_F = -929.92889740$ a.u.; $G_F = -929.54776088$ a.u.)

0 1

C	-1.006541453771	1.591217899080	-3.669356580345
C	-0.549381202252	2.461752333089	-4.600508843097
C	-3.254127721576	1.400759924559	1.304408005827
C	-3.229830317557	1.495046720480	-0.241871258962
C	-1.975807650322	1.296492639418	-1.149751116296

C	-2.056326582904	1.975052603984	-2.581006192266
H	-0.819979841674	3.515688575696	-4.576749455059
H	-2.285824383767	1.276855310165	1.791239049996
H	-4.138115687312	1.104432323982	-0.696450453746
H	-1.080102102381	1.655823921072	-0.635372040264
H	-1.837474584107	0.219167910749	-1.281805050600
H	-2.075040232880	3.062099875037	-2.454375599139
H	-3.037606097028	1.702276141032	-2.993976861287
C	-3.491387742942	2.730074570101	0.618699558571
C	-4.908126011191	3.274710566835	0.615848223521
H	-5.082519824028	3.887441983505	-0.274301071848
H	-5.641113824383	2.466574827813	0.629987338373
H	-5.084013961929	3.902603501591	1.495701526052
C	-2.419247538678	3.797626573626	0.738456235174
H	-2.442054388167	4.470374335712	-0.125570852956
H	-2.581795609002	4.400602864076	1.637540210037
H	-1.415600919796	3.372243373168	0.801626650375
O	0.300501401240	2.104081039174	-5.658155337864
O	-4.308340929377	0.724173522386	2.005898672227
C	-0.636547674779	0.131270268535	-3.751189408108
H	-0.037345021939	-0.177120093708	-2.887435723630
H	-1.535311027047	-0.497004064673	-3.751977881225
H	-0.064097296300	-0.082581517623	-4.653578742195
C	0.519103735909	3.073489512719	-6.724790307945
H	0.938798139761	3.995763568299	-6.308101234737
H	-0.432980486140	3.312335128236	-7.210310202553

C	1.504250291932	2.520900022310	-7.806673974750
H	2.465459790601	2.281917309559	-7.332114242984
H	1.091730790016	1.595690784754	-8.231029009185
C	-4.457670566307	1.134161245989	3.397380455886
H	-4.733654419722	2.193388285887	3.445730295493
H	-3.503998178203	1.006641400855	3.924465431021
C	-5.545867361997	0.300115933142	4.149676363430
H	-6.515784417357	0.430265429169	3.650641486469
H	-5.279467746149	-0.764644838695	4.108058634631
O	1.668801744546	3.526612681695	-8.826978762775
C	2.544310040655	3.257794158825	-9.971323113181
H	3.576838001681	3.082491500610	-9.646701940848
H	2.190166762265	2.393606998270	-10.545793492737
H	2.496535990250	4.155368036746	-10.585445018655
O	-5.606399341726	0.762701159465	5.516195288309
C	-6.551971864776	0.145461881698	6.449016145539
H	-7.586745369936	0.279114697385	6.111227917853
H	-6.344782517842	-0.924172924539	6.573876736184
H	-6.402160065139	0.663788296025	7.394658452986

Cam_Int3C-F2500

($E_F = -929.91339329$ a.u.; $G_F = -929.53890838$ a.u.)

0 1

C	-0.638186448349	1.958151637530	-3.952836621089
C	-0.692794577695	2.268973178110	-5.269791633207
C	-4.262975114653	0.952643429340	1.536383715256

C	-3.068118996402	1.457446963969	-0.711632394814
C	-1.945754032821	2.042641030699	-1.586457861262
C	-1.893662740396	1.592993352237	-3.103115250039
H	-1.641768011486	2.376581043825	-5.791673219732
H	-4.108764363448	-0.121993651053	1.437350296700
H	-3.839525835965	0.865499249700	-1.198638159914
H	-1.989192036185	3.142225376932	-1.552596295963
H	-0.983612798225	1.791718370676	-1.121816342424
H	-2.796782234226	1.949104817242	-3.608865356440
H	-1.957176685026	0.496052310503	-3.102410790607
C	-3.357567083967	1.924134384950	0.740493994594
C	-4.070660690640	3.303691146361	0.674810263900
H	-3.433011516248	4.044631896142	0.186011603870
H	-5.005855005807	3.226238109051	0.115168555079
H	-4.303268352700	3.655943067484	1.682739652752
C	-2.027219810010	2.092059103519	1.523425544902
H	-1.385830592295	2.845795649252	1.057754365778
H	-2.238455516258	2.406819599818	2.547630187080
H	-1.477018325418	1.147952807204	1.558184075624
O	0.438974924054	2.484113936068	-6.070467208456
O	-4.690470545901	1.381381777332	2.793930834351
C	0.697113794585	1.787843256023	-3.271860823045
H	0.853225134129	2.552250210194	-2.502639570056
H	0.754169766329	0.815754272052	-2.767754721261
H	1.517123619020	1.856130324654	-3.986414551888
C	0.257231758246	2.569785181718	-7.514506368484

H	-0.434711074192	3.384721518566	-7.753918459151
H	-0.164514970591	1.632279144258	-7.891874490325
C	1.613877351649	2.835553475136	-8.246234320075
H	2.044395766903	3.776725129603	-7.878666067859
H	2.314975602491	2.023158815287	-8.012265441700
C	-5.423189074594	0.433632330474	3.629486467762
H	-4.787526804107	-0.434617183240	3.834014723260
H	-6.314612712912	0.094615110367	3.093139243995
C	-5.863708716183	1.067182931192	4.989692412385
H	-4.975100842045	1.411710603356	5.535712351330
H	-6.504993216131	1.936940083663	4.793632516407
O	1.359798553566	2.903784140968	-9.664079735408
C	2.474111628491	3.139374549720	-10.586576066882
H	2.955130371494	4.104386374490	-10.387551176220
H	3.219850304121	2.338440802084	-10.518552398950
H	2.027534624351	3.146113688868	-11.579346218835
O	-6.573517538176	0.062820140936	5.742700708563
C	-7.110173398047	0.394472408808	7.065792330318
H	-6.308919053494	0.680994084378	7.757227395156
H	-7.845558180822	1.205230248668	7.002324554902
H	-7.592691480575	-0.516574711412	7.415318201569

Cam_TS3C-F2000

($E_F = -929.67067114$ a.u.; $G_F = -929.29277164$ a.u.)

0 1

C	-0.857220537238	1.630387411891	-3.845199597933
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C	-0.505104978314	2.494868439768	-4.820754087758
C	-3.483990178247	1.536275042617	1.739678846627
C	-3.099641293437	1.483095656789	-0.489266734982
C	-1.818393592587	1.451542900321	-1.325999453441
C	-1.995179584351	1.922315835437	-2.837116616547
H	-0.945910864898	3.487524622680	-4.892233939819
H	-2.540887770922	1.231556305323	2.179597947521
H	-3.896244045955	0.817635615883	-0.810130011000
H	-1.034494815751	2.059565591821	-0.866404641278
H	-1.434557835034	0.425622889715	-1.351094577131
H	-2.239230314326	2.989286706313	-2.844186425502
H	-2.886870056186	1.403211862637	-3.214391565442
C	-3.510636874747	2.482591394987	0.573689201592
C	-4.910107545518	3.064363466248	0.323376315234
H	-4.890244396369	3.688509606143	-0.573409948664
H	-5.644856587338	2.270169262883	0.177353423461
H	-5.237384773959	3.672687422834	1.171899860264
C	-2.496074773024	3.618472498056	0.771216240855
H	-2.390473388639	4.191949803034	-0.156269424258
H	-2.828963788302	4.292199472169	1.564967886193
H	-1.508451573071	3.236559693782	1.042185779488
O	0.447901537081	2.209379723711	-5.801942047741
O	-4.631670482846	1.246763143309	2.440837085720
C	-0.250710252792	0.250523936582	-3.794423230846
H	0.380850308087	0.124311629192	-2.908188692652
H	-1.034051369338	-0.514238081313	-3.735180774575

H	0.361264710777	0.054495931316	-4.674811477528
C	0.478203742615	3.061555598540	-6.974271061884
H	0.647510641773	4.103161361396	-6.677551953291
H	-0.477553490100	3.003236666379	-7.506459374784
C	1.615051569317	2.625166757957	-7.938401094943
H	2.578867945144	2.680569805826	-7.413813270370
H	1.452002327214	1.582718706013	-8.244842891474
C	-4.534653680793	0.509420541266	3.690953457341
H	-3.634226493244	0.817459723317	4.231702147674
H	-4.469889250089	-0.561958831726	3.479043600481
C	-5.777196972375	0.792078543745	4.581229810330
H	-5.840715238574	1.871583710209	4.776203798904
H	-6.687236921121	0.487301968675	4.046458606932
O	1.594605324250	3.504174646638	-9.073603384796
C	2.568554402955	3.284378189337	-10.129957974941
H	3.593901875415	3.388099666120	-9.753457675480
H	2.448078928681	2.291677847964	-10.581463208953
H	2.372561423070	4.052822671826	-10.876301677354
O	-5.625725522340	0.055247963352	5.802752504499
C	-6.669693228538	0.174936926349	6.808608588394
H	-6.772297135711	1.211680350818	7.152335043268
H	-7.634743700464	-0.175944411658	6.422668015634
H	-6.353859795236	-0.457115584452	7.637125150258

Cam_Int2C-F2000

($E_F = -929.71157193$ a.u.; $G_F = -929.32946528$ a.u.)

0 1

C	-1.048243960458	1.568395123853	-3.657715087462
C	-0.562170835793	2.453465510148	-4.553885092623
C	-3.225635625150	1.419829184709	1.282420616340
C	-3.223818458628	1.500118499128	-0.251472021116
C	-1.982239392932	1.288820198966	-1.155180321175
C	-2.087702574287	1.955922620661	-2.577915156239
H	-0.809798075388	3.512210277652	-4.503899401623
H	-2.253219363776	1.300096145592	1.762680212451
H	-4.136035715093	1.102538102885	-0.691907858076
H	-1.081253878560	1.653147780249	-0.653436179815
H	-1.844982377309	0.210195113598	-1.279427345093
H	-2.111074880859	3.043737994581	-2.457853741814
H	-3.071839829609	1.674765463241	-2.979467814442
C	-3.475448337185	2.747151836779	0.595109856695
C	-4.892658263432	3.289825329021	0.604656853209
H	-5.080097754826	3.890463555201	-0.291138111696
H	-5.624347640608	2.481057514648	0.638685678085
H	-5.058015240430	3.929492301868	1.478058592946
C	-2.402910919176	3.816302127621	0.691910382402
H	-2.437292728397	4.482528306578	-0.176789263098
H	-2.554577938189	4.426395399969	1.588147575828
H	-1.397949485538	3.392850776640	0.745928455973
O	0.294876507653	2.104501912413	-5.599520148923
O	-4.270443411750	0.740944586960	1.980235898498
C	-0.712137704333	0.102811073359	-3.773000070506

H	-0.105546047732	-0.235860854172	-2.925894553084
H	-1.624761899601	-0.504944915277	-3.770723866950
H	-0.158563796914	-0.105343957559	-4.688417288751
C	0.483971356137	3.071624806433	-6.663152131276
H	0.875199915968	4.009686788623	-6.252762488311
H	-0.471909691113	3.279916641465	-7.155975762278
C	1.484673940090	2.532410547706	-7.721549996325
H	2.448527815890	2.321939634821	-7.237941847250
H	1.099763514328	1.592396698846	-8.140371959250
C	-4.417193963748	1.161762099362	3.359982326988
H	-4.695355279259	2.220970906721	3.403129829940
H	-3.464804922779	1.039059001282	3.891393441658
C	-5.499950310138	0.328739024104	4.098461889477
H	-6.469023188772	0.455212063989	3.595890523335
H	-5.231522014120	-0.736051598183	4.059496255528
O	1.627424537769	3.530757827312	-8.743465667627
C	2.514050214082	3.248652206344	-9.860403533230
H	3.545404905698	3.093370211913	-9.519914618853
H	2.180846340056	2.365105736644	-10.419046037338
H	2.468148985091	4.127137104762	-10.502317340222
O	-5.562406812161	0.794626242599	5.457006380473
C	-6.509632585266	0.163778464101	6.359759322854
H	-7.541253374106	0.291717930345	6.008118170141
H	-6.298173769067	-0.906853460391	6.474699955328
H	-6.384592425096	0.666508432681	7.317781766557

Cam_Int3C-F2000

($E_F = -929.68183678$ a.u.; $G_F = -929.30625486$ a.u.)

0 1

C	-0.641949090196	1.919467173335	-3.920325194778
C	-0.709753329713	2.276725463268	-5.220549799828
C	-4.236869581042	0.974782490192	1.502371953041
C	-3.055211845608	1.477751270285	-0.714496383378
C	-1.932034744182	2.046875680766	-1.580188320218
C	-1.892053400502	1.570512499889	-3.077880875977
H	-1.663008562351	2.423447562818	-5.725024338139
H	-4.071773031906	-0.097956395234	1.399430434158
H	-3.829963764228	0.889734414686	-1.200892747818
H	-1.969475510161	3.147557965911	-1.563911612303
H	-0.971445282508	1.797952386282	-1.110745454323
H	-2.794115410521	1.923838814396	-3.587750422077
H	-1.961574843596	0.473691451206	-3.058873944049
C	-3.342750292410	1.954547573303	0.723281904226
C	-4.067362427650	3.328515568328	0.651593197977
H	-3.435180989010	4.071788695226	0.159222978828
H	-5.001807910799	3.240935744846	0.092196463399
H	-4.302598361635	3.683629690915	1.657876109130
C	-2.016283801581	2.136761935776	1.510371377949
H	-1.381404816353	2.897174001433	1.046765626781
H	-2.234614926280	2.449513517138	2.533622228409
H	-1.456352091679	1.198456852340	1.547369197921
O	0.413263024320	2.500929094734	-6.018961535350

O	-4.668237872215	1.396950874031	2.753610966037
C	0.696031662562	1.694341734623	-3.261453539579
H	0.896495217952	2.450453175201	-2.494257965509
H	0.721269266921	0.719867191996	-2.759696594715
H	1.506214628804	1.731601280430	-3.989478033694
C	0.217253994706	2.557653611331	-7.454607887518
H	-0.499953090095	3.347804197691	-7.704822920914
H	-0.177037087226	1.602468440029	-7.818013463375
C	1.559660173488	2.852333818363	-8.178250472599
H	1.962327542227	3.810891991645	-7.822973036944
H	2.285457842481	2.064687081154	-7.933225551550
C	-5.390019219079	0.439315255990	3.572473473019
H	-4.748449762554	-0.425208318575	3.776477879086
H	-6.278126108542	0.094263898631	3.033755811531
C	-5.829822549152	1.071627520882	4.921012942812
H	-4.943936999080	1.423504251352	5.467660232095
H	-6.477248582616	1.937339500135	4.724863380030
O	1.301468078136	2.892823897379	-9.589983246230
C	2.418416182588	3.145968890755	-10.485235659242
H	2.871809363730	4.125445486031	-10.288201678108
H	3.185816522006	2.367258390816	-10.393230174249
H	1.999790466680	3.131291241190	-11.490440251914
O	-6.528949377217	0.063952363457	5.667458512372
C	-7.055046101340	0.416794935435	6.975933425644
H	-6.251432517338	0.717004001635	7.659883913637
H	-7.789985102197	1.228106390739	6.903152276792

H	-7.538822152187	-0.483655178261	7.351399742608
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Cam_TS3C-F1000

($E_F = -929.22296996$ a.u.; $G_F = -928.84506730$ a.u.)

0 1

C	-0.826513967476	1.607914831308	-3.924447132299
C	-0.623396867060	2.441231006145	-4.957149127608
C	-3.630313450028	1.263766176572	1.668527435184
C	-3.104720509710	1.627797023258	-0.694115398947
C	-1.823276321061	1.676903801060	-1.489137727042
C	-2.058777290647	1.730812197636	-3.033394927852
H	-1.294826661560	3.272527727042	-5.165421372722
H	-2.801410282559	0.625566026612	1.963145212860
H	-3.892243072676	0.979878742837	-1.071880219439
H	-1.207906085415	2.530962138684	-1.192435694666
H	-1.214815593993	0.784577490041	-1.271753652484
H	-2.607232377234	2.647325960131	-3.272731344069
H	-2.729754186882	0.896855076082	-3.284659090503
C	-3.432142014689	2.333473835944	0.618954878504
C	-4.740292413757	3.138846892795	0.427116488639
H	-4.590910990724	3.906450212593	-0.335523082043
H	-5.556152696845	2.486146913736	0.107896258798
H	-5.040597610644	3.619562294789	1.360829741065
C	-2.311718243861	3.298833341396	1.067132516903
H	-2.142342691957	4.078092941682	0.316413486139
H	-2.593887086836	3.782345964068	2.005604191352

H	-1.368538230154	2.769485917513	1.226253681992
O	0.452878122603	2.329748234493	-5.819463561534
O	-4.639690067243	1.430954121455	2.587279566198
C	0.096826921660	0.444927189259	-3.668013735741
H	0.693235848609	0.599301749227	-2.761961369283
H	-0.476626343433	-0.476831509353	-3.516437965061
H	0.784936255208	0.296252881768	-4.500279156915
C	0.291816683539	2.935411948525	-7.112508500425
H	0.082839415528	4.007315045744	-7.009648242399
H	-0.540930278724	2.470471881747	-7.652327727993
C	1.583813366391	2.747706533384	-7.917405026944
H	2.424327289885	3.208636400865	-7.379009929603
H	1.797427299083	1.674784023093	-8.026460208826
C	-4.739770341068	0.462761898425	3.644255637791
H	-3.770823195414	0.348102681015	4.144051557573
H	-5.039496106436	-0.509135985878	3.237583660105
C	-5.780382109157	0.948943051976	4.661581259051
H	-5.481422060524	1.935012596942	5.045609079150
H	-6.756893530575	1.058733530929	4.168542900364
O	1.384952147494	3.363365700802	-9.186732156871
C	2.487444517390	3.273015361351	-10.098033475828
H	3.383744644797	3.761796658701	-9.692803425854
H	2.728898230079	2.227436888382	-10.332434069325
H	2.178854812632	3.784670765876	-11.009318000866
O	-5.838134979394	-0.014422303714	5.708619938976
C	-6.756792942671	0.281875246147	6.768720905637

H	-6.497791755159	1.223542347433	7.271293686445
H	-7.788309363934	0.349464050417	6.397686608609
H	-6.682952200742	-0.539316899465	7.481143127249

Cam_Int2C-F1000

($E_F = -929.28407320$ a.u.; $G_F = -928.90116516$ a.u.)

0 1

C	-1.186860304741	1.513413832766	-3.675448563883
C	-0.600298790794	2.426247589478	-4.465440880128
C	-3.158197869160	1.463429566231	1.232801854569
C	-3.226229002703	1.527683773154	-0.277739043084
C	-2.035502273317	1.257392566594	-1.201402096476
C	-2.196384185727	1.913764490807	-2.602812459409
H	-0.771542190103	3.493869922837	-4.337499706905
H	-2.174200642635	1.315098573656	1.681397545830
H	-4.167139820499	1.149546380243	-0.672290095220
H	-1.103469977891	1.602099904015	-0.744142093851
H	-1.935495197704	0.173256845761	-1.317455409830
H	-2.210987699236	3.002255337861	-2.486345149241
H	-3.192837747791	1.633472518166	-2.974831076428
C	-3.400253089125	2.798504997341	0.553605128012
C	-4.797505349928	3.386162438088	0.617547238285
H	-5.007484663293	3.975835751753	-0.280658750990
H	-5.551883832239	2.601976977557	0.699359564219
H	-4.903392850361	4.047379782594	1.484129725880
C	-2.290594871968	3.832342959250	0.590492369256

H	-2.341083661593	4.491328635632	-0.282945672816
H	-2.383237381518	4.456182154506	1.485395216430
H	-1.298120806082	3.377628381513	0.606175959465
O	0.279355779203	2.093117094505	-5.480435424089
O	-4.196087415984	0.809002384551	1.936098814202
C	-0.960318135339	0.038845133170	-3.889861414100
H	-0.360260613248	-0.396081294960	-3.082964508201
H	-1.914592529689	-0.500395633942	-3.900640596221
H	-0.441725464971	-0.147744662472	-4.830239271694
C	0.421076723333	3.056369486843	-6.537014071877
H	0.759475429215	4.019276016161	-6.134802037833
H	-0.537255195024	3.211085004775	-7.045704796738
C	1.452649269203	2.540076308198	-7.547843873797
H	2.415932407265	2.379744186620	-7.042666509147
H	1.117922899182	1.575338871579	-7.955283440585
C	-4.305898886411	1.238622776581	3.301174179440
H	-4.544010479351	2.307786399449	3.350497706712
H	-3.356933298104	1.077720116398	3.829972272503
C	-5.408288242501	0.439742723552	4.007163573929
H	-6.370749439718	0.605973260796	3.501763288225
H	-5.177872059028	-0.634012945747	3.953248835527
O	1.566379568505	3.520044997808	-8.575617602770
C	2.478864672918	3.203068194422	-9.634508170026
H	3.503001124356	3.078935445887	-9.257522318700
H	2.180360348433	2.285547319148	-10.159373131665
H	2.449966647944	4.041630099009	-10.329790562497

O	-5.456074126142	0.888227843626	5.360088813726
C	-6.430596194116	0.248447156971	6.192279563203
H	-7.449558867509	0.409981431767	5.814764400740
H	-6.247995412797	-0.832288801027	6.266414905552
H	-6.337818301593	0.697734713306	7.180829393765

Cam_Int3C-F1000

($E_F = -929.22614616$ a.u.; $G_F = -928.84969605$ a.u.)

0 1

C	-0.620991525431	1.836621172204	-3.855236626108
C	-0.732554136045	2.270059033254	-5.120686752707
C	-4.174312502848	1.026057297983	1.434407368253
C	-3.012642908026	1.521230680587	-0.720680923525
C	-1.889720255202	2.056860707517	-1.574464896150
C	-1.845761030112	1.481099941085	-3.017320950173
H	-1.700709278763	2.440455526781	-5.588550651894
H	-3.990234489577	-0.042570390455	1.319880940713
H	-3.795925527836	0.942608000695	-1.204718585052
H	-1.942651490055	3.156638439978	-1.632747209120
H	-0.931886568849	1.851963173780	-1.078698520263
H	-2.759948669845	1.770979739080	-3.545793779552
H	-1.876009623860	0.385650452114	-2.927486838799
C	-3.299846033667	2.022738030546	0.688734619305
C	-4.046963705952	3.384521169951	0.601022789170
H	-3.424130477141	4.131836390901	0.102754288178
H	-4.977852189372	3.276209563698	0.039336949898

H	-4.290849003690	3.746346599742	1.602848765884
C	-1.983817943279	2.233497288544	1.486584925229
H	-1.361048517723	3.006605168856	1.027732937076
H	-2.218358251920	2.542975111913	2.507111378983
H	-1.404891775433	1.307045167115	1.530308401824
O	0.361338968536	2.556953107839	-5.917443586139
O	-4.612336015249	1.431073685504	2.675484448828
C	0.730636788080	1.580799173332	-3.238723108247
H	0.971690816052	2.329272518991	-2.475682251349
H	0.749492163364	0.603913524280	-2.742025786460
H	1.518586033573	1.606595389743	-3.991451652022
C	0.138799937545	2.533198271428	-7.336638282908
H	-0.645814612596	3.248041553439	-7.613503439957
H	-0.173664578457	1.533481952259	-7.659183612848
C	1.442600503408	2.911382952234	-8.050623231366
H	1.763114754600	3.911980293619	-7.726727954052
H	2.232248605457	2.196741995022	-7.777612888720
C	-5.317272939120	0.452597675639	3.458125053516
H	-4.668354255770	-0.409211174947	3.653719687705
H	-6.201920509207	0.105391774056	2.913958818188
C	-5.748295628521	1.079323070026	4.789919477386
H	-4.862919769837	1.435963497485	5.335847936582
H	-6.400376479820	1.943402812748	4.597924492538
O	1.184386831883	2.880954862263	-9.451251686708
C	2.302320314260	3.191076949782	-10.292906734144
H	2.676830436794	4.206248366995	-10.104235133837

H	3.124006263629	2.476978704480	-10.146891535072
H	1.944813493290	3.124036355070	-11.320105455901
O	-6.434135690722	0.070255077987	5.525225538823
C	-6.930071610426	0.468089864621	6.809841145683
H	-6.114481813782	0.784689057252	7.473882181677
H	-7.655544254584	1.288092589744	6.722764022042
H	-7.422889078885	-0.405540378520	7.235570039407

cisCydiol_TS1-F4000

($E_F = -774.03158332$ a.u.; $G_F = -773.73146081$ a.u.)

0 1

C	-4.490401945921	-1.746770169603	-2.885138039478
C	-3.209892617966	-0.919130794918	-1.231525430977
C	-4.115581589692	-1.196906658452	-0.048374299388
C	-4.385742188383	-2.699649759710	0.144710971906
C	-5.059210744743	-3.392472265499	-1.047008720001
C	-4.328109888785	-3.170822186615	-2.379785929979
H	-3.882198828487	-1.479210156934	-3.749854828900
H	-2.511811783173	-1.724996770397	-1.459230341166
H	-3.631037374016	-0.805615691475	0.855961653802
H	-5.052840610953	-0.642853904500	-0.159771657723
H	-5.002814004139	-2.838881638038	1.038767729222
H	-3.428110701237	-3.195149989546	0.350276850148
H	-5.127899989004	-4.465932831152	-0.842962065922
H	-6.082652324777	-3.023563089232	-1.159213777946
H	-4.747629709753	-3.846748065106	-3.137528478538

H	-3.271229485512	-3.440431155530	-2.293820606122
O	-5.905917928476	-1.519083633062	-3.146311077971
O	-2.442029723375	0.302040031809	-1.040265536155
C	-6.462716026173	-2.051493710798	-4.439094756978
H	-5.842668229500	-2.881141764056	-4.786785367616
H	-6.408773174382	-1.245917128679	-5.175438242396
C	-7.981090176116	-2.574123725721	-4.395064362546
H	-8.046223747105	-3.412366464176	-3.690443191623
H	-8.623988116449	-1.763390022046	-4.032185966628
C	-1.133600134113	0.104600808222	-0.325158625421
H	-0.425857447717	-0.348312257304	-1.025862080597
H	-1.289958531524	-0.587652868023	0.507197569959
C	-0.454757119453	1.422139135364	0.286787935793
H	-0.253921970186	2.132390235745	-0.523948993101
H	-1.157697299900	1.884961373515	0.989760811644
O	-8.395696836520	-2.998890374482	-5.736745152150
C	-9.769559114695	-3.541490859221	-6.062948588060
H	-9.963354251723	-4.463411343255	-5.506677214227
H	-10.541290843591	-2.797245127379	-5.845436164707
H	-9.718388219650	-3.740723697152	-7.130579388633
O	0.791090508570	1.055294533413	0.969736796180
C	1.695501901589	2.048520946697	1.665405544477
H	2.074786144669	2.789613602387	0.955687551489
H	1.167676932796	2.543534099022	2.485864002844
H	2.505845246810	1.431906086695	2.046568739175

cisCydiol-F4000

($E_F = -774.04373482$ a.u.; $G_F = -773.73988006$ a.u.)

0 1

C	-4.182446739614	-1.695069230042	-2.691073956405
C	-3.400981053448	-1.123781998859	-1.349107637029
C	-4.368942663389	-1.261237061921	-0.174064122450
C	-4.637509341307	-2.757808663633	0.083752568451
C	-5.096432138456	-3.510171642433	-1.177088331655
C	-4.224216451589	-3.216391470763	-2.412241504981
H	-3.584628034908	-1.453779571559	-3.575416491264
H	-2.636644305832	-1.901761853944	-1.256591505749
H	-3.938936887156	-0.801877141602	0.719484321092
H	-5.295959696782	-0.729843241741	-0.406460425582
H	-5.383433304223	-2.875907937826	0.875755648431
H	-3.710237859037	-3.210620783654	0.457297920508
H	-5.106919067104	-4.587268263446	-0.983328761075
H	-6.122327581817	-3.216517324211	-1.411796756082
H	-4.640246604925	-3.729947143099	-3.283313620693
H	-3.211758174490	-3.610635055593	-2.279582638106
O	-5.599343478699	-1.308631534565	-2.953307474847
O	-2.602832860927	0.140425174741	-1.279079243607
C	-6.225549693284	-1.769279926204	-4.226008128740
H	-5.527539546162	-2.400985679566	-4.781197559166
H	-6.409762418235	-0.870185871240	-4.818602963592
C	-7.630800214006	-2.554550924983	-4.139635491896
H	-7.478069901383	-3.519446530353	-3.639899366033

H	-8.326916919753	-1.957800128006	-3.537774457262
C	-1.418316990010	0.003516488466	-0.380266223360
H	-0.708045915657	-0.688157090205	-0.847272262126
H	-1.736691132376	-0.431268401060	0.572696594402
C	-0.610993510510	1.339039610977	-0.016784750113
H	-0.232607775836	1.796689128181	-0.938543133604
H	-1.292224347681	2.047130042831	0.470098653117
O	-8.164467344523	-2.760349840631	-5.491141935267
C	-9.480268755919	-3.444378672255	-5.786363231804
H	-9.467300147381	-4.479080620770	-5.430838940806
H	-10.311524598021	-2.897407098069	-5.331563030675
H	-9.547607947175	-3.412264970486	-6.871113561703
O	0.500840294233	0.995440243667	0.879687798236
C	1.485745163744	2.000786282641	1.431166830208
H	2.036857665876	2.488203026136	0.621356014736
H	0.974182527301	2.748051025827	2.045131565536
H	2.153738604732	1.396301382353	2.040019616867

cisCydiol_Int1-F4000

($E_F = -774.43982816$ a.u.; $G_F = -774.14960896$ a.u.)

0 1

C	-6.805104652048	-2.262905237891	-3.786537041002
C	-1.392835819100	-0.377795358526	0.079202271071
C	-2.677584757406	-0.145246763812	-0.786041657611
C	-3.483819203117	-1.438864299196	-1.338455078980
C	-4.782861737045	-1.200441315834	-2.273288033965

C	-5.575435799929	-2.494361964844	-2.844407369968
H	-6.773240586789	-1.438869779659	-4.498530685356
H	-0.735055472417	-1.209479695351	-0.171026677881
H	-3.370205097391	0.471152174144	-0.201836242959
H	-2.404523253399	0.467469065170	-1.659605558302
H	-3.791661571476	-2.034325962211	-0.473245661504
H	-2.775626320617	-2.056616922839	-1.901287084899
H	-5.498876667885	-0.591588907365	-1.712426274784
H	-4.470627243432	-0.596061421167	-3.131870412773
H	-5.911717930947	-3.097747537914	-1.993634595758
H	-4.840713594812	-3.119667173881	-3.375654663561
O	-7.604044053867	-3.360153284069	-4.192829957173
O	-0.743358640320	0.720876651783	0.694296304234
C	-8.695023786857	-3.122666194556	-5.185653861681
H	-8.246204263994	-2.729145517979	-6.102518423253
H	-9.374468030302	-2.371160877976	-4.775567743401
C	-9.556467449183	-4.419327847786	-5.569081431798
H	-8.883011014664	-5.180484428625	-5.981284644735
H	-10.015281134664	-4.818446438363	-4.656519663561
C	0.546238326824	0.481574591106	1.409833452393
H	1.267892025182	0.078708417295	0.693013447894
H	0.372195928389	-0.263146251629	2.190610010156
C	1.193486777161	1.779836690798	2.092476489390
H	1.370448784053	2.534637376879	1.316734883550
H	0.479643691210	2.187798930400	2.818134846261
O	-10.586355767778	-4.059544690840	-6.547720856217

C	-11.580324400818	-5.046205878567	-7.119700557403
H	-11.064991212332	-5.840842087390	-7.667184384992
H	-12.202060903244	-5.472308655738	-6.326862700738
H	-12.180507012634	-4.441435675648	-7.795083920188
O	2.450167466950	1.418333902570	2.754178058708
C	3.317087107292	2.405985611860	3.503634140433
H	3.670044260261	3.196221145777	2.834491182511
H	2.770446688927	2.837930457508	4.347032213968
H	4.148898273643	1.800293755404	3.854908597303

cisCydiol_TS1-F3500

($E_F = -773.86050841$ a.u.; $G_F = -773.56061157$ a.u.)

0 1

C	-4.534959298223	-1.781021047460	-2.912525466766
C	-3.174723179298	-0.904115445503	-1.193874457684
C	-4.087037907872	-1.194472864351	-0.021545837301
C	-4.374428354499	-2.695265130388	0.158290253772
C	-5.080236518823	-3.374382545619	-1.022190169091
C	-4.359498479094	-3.183082776012	-2.365103828961
H	-3.911230884546	-1.513034532923	-3.765650848678
H	-2.492441263031	-1.711959799755	-1.458927639007
H	-3.597238317370	-0.819647012123	0.888433519883
H	-5.018015415941	-0.627502358016	-0.121463153150
H	-4.976776520873	-2.832787710624	1.062762069020
H	-3.420731189697	-3.206323005573	0.343288047606
H	-5.174468576868	-4.444207528179	-0.808825232004

H	-6.095772889731	-2.980789678557	-1.124333481175
H	-4.778455832042	-3.884827552594	-3.101462041342
H	-3.299692481596	-3.440685723497	-2.278224871661
O	-5.933228742010	-1.552913895629	-3.175491804056
O	-2.424286636175	0.306753376407	-0.998997001980
C	-6.470362315581	-2.066438478275	-4.471419393502
H	-5.855915533150	-2.902271385882	-4.815644231240
H	-6.402560129669	-1.260659410045	-5.207154955082
C	-7.979272844508	-2.569253622136	-4.424953469682
H	-8.056594727349	-3.401102030195	-3.713135401874
H	-8.619963602557	-1.751188532484	-4.073028371155
C	-1.097070308519	0.109677118272	-0.342995108713
H	-0.396957688376	-0.285176029569	-1.085661145081
H	-1.205046434295	-0.626999060463	0.458693676205
C	-0.459821865361	1.412923293141	0.305055832044
H	-0.303091641564	2.168748736929	-0.474383032646
H	-1.159037969880	1.818775392313	1.046802010097
O	-8.377511306332	-2.997789322276	-5.760929473255
C	-9.742997640709	-3.525895028950	-6.061883215253
H	-9.944516573344	-4.436656801544	-5.488411067935
H	-10.508634867684	-2.772656541663	-5.849257586557
H	-9.714673881579	-3.747077586642	-7.126542986177
O	0.805788066914	1.049788735132	0.932791847707
C	1.665640349165	2.044599424867	1.643684942724
H	1.995282848558	2.834389745773	0.960894443074
H	1.133671659171	2.482952869645	2.494312014308

H	2.517116951580	1.462196495248	1.988573886254
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cisCydiol-F3500

($E_F = -773.88178717$ a.u.; $G_F = -773.57666459$ a.u.)

0 1

C	-4.162029960583	-1.718384822953	-2.672450283504
C	-3.406191258280	-1.162064758653	-1.342032110271
C	-4.382585008016	-1.282390719317	-0.171040736939
C	-4.677224223467	-2.773766696979	0.086222165440
C	-5.140458830125	-3.516409626907	-1.178684178091
C	-4.248713516843	-3.240189353691	-2.403768770703
H	-3.546165375787	-1.492287250288	-3.549383384539
H	-2.642323775129	-1.939104897258	-1.227517047873
H	-3.949382562236	-0.828701258367	0.723873612832
H	-5.298768676572	-0.735790663613	-0.410249761114
H	-5.430087248461	-2.879548140626	0.873321110268
H	-3.760281765110	-3.242838746831	0.465260614442
H	-5.176816532345	-4.593096390337	-0.985932748162
H	-6.157673289325	-3.200145046009	-1.421887507736
H	-4.668352457654	-3.737542180300	-3.282613532486
H	-3.248084450682	-3.660748018650	-2.261766798648
O	-5.550248301204	-1.279598478742	-2.937482757967
O	-2.624346475125	0.100076944631	-1.299592666320
C	-6.177130615612	-1.713958876474	-4.204869183574
H	-5.469634010911	-2.301799151570	-4.796254280307
H	-6.403273584840	-0.802754408729	-4.763936835239

C	-7.542159645111	-2.539254536717	-4.111435383605
H	-7.352521748059	-3.519435568094	-3.654790836648
H	-8.243375624497	-1.989189272229	-3.471053305534
C	-1.446419098163	-0.022842279753	-0.409494287362
H	-0.730900549673	-0.715609328992	-0.868240055700
H	-1.756252316926	-0.448083889442	0.551125095845
C	-0.660340079890	1.314392499595	-0.071892386060
H	-0.283543821794	1.765731992009	-0.998071564938
H	-1.343231311730	2.025930759391	0.408843811456
O	-8.089235831754	-2.701455015450	-5.454180920982
C	-9.377131525278	-3.410435594337	-5.720281800654
H	-9.321495616104	-4.455995748752	-5.399508857964
H	-10.210329167125	-2.908953602088	-5.216987500641
H	-9.496489218500	-3.351712786639	-6.799935718642
O	0.444399661252	0.975907274023	0.821796159791
C	1.403179378069	1.993941682604	1.346010243305
H	1.946525994733	2.477976769506	0.527751211877
H	0.883980498258	2.747708554172	1.947109192069
H	2.087591521253	1.420423902828	1.967342900837

cisCydiol_Int1-F3500

($E_F = -774.21441073$ a.u.; $G_F = -773.92265363$ a.u.)

0 1

C	-6.773931766614	-2.248672740813	-3.757986447562
C	-1.428002584659	-0.403200154277	0.053550541480
C	-2.706153498299	-0.160486270930	-0.794541969371

C	-3.489003056044	-1.449450421185	-1.346441432215
C	-4.780859276285	-1.202693263771	-2.262510245266
C	-5.550051933124	-2.491612456699	-2.833387966022
H	-6.750306877241	-1.415032548514	-4.459281650004
H	-0.767222935248	-1.228706353211	-0.209593665008
H	-3.400437020269	0.444213566938	-0.199444549686
H	-2.442632347084	0.465222292803	-1.662616857472
H	-3.787264159969	-2.057676531400	-0.486313428237
H	-2.778348680330	-2.055522778652	-1.919584225887
H	-5.499412524882	-0.605505379400	-1.691739306248
H	-4.477834140409	-0.585629485220	-3.115881886434
H	-5.878367581024	-3.107700198305	-1.988126107354
H	-4.812541954242	-3.106033075017	-3.374708209088
O	-7.558719979124	-3.344171442166	-4.169966174470
O	-0.788964948980	0.690349792425	0.671142633756
C	-8.647570297585	-3.094267039395	-5.144065732257
H	-8.211081746484	-2.681137316592	-6.058957065646
H	-9.333542183296	-2.356119472022	-4.719442713598
C	-9.483461455797	-4.388182522404	-5.531828035920
H	-8.805011865620	-5.137161306343	-5.959474312523
H	-9.933369475237	-4.807442699518	-4.623172321131
C	0.492342309326	0.442995199814	1.373963034821
H	1.215759460281	0.046598006060	0.654423352091
H	0.324970101067	-0.307466923765	2.151424573391
C	1.122030803620	1.733739149561	2.052731047633
H	1.294340802511	2.495232039872	1.281643189352

H	0.409056173549	2.136061725466	2.783269612692
O	-10.514069756646	-4.018415756831	-6.493248663302
C	-11.478951037820	-5.013604839956	-7.052589312968
H	-10.953415192019	-5.797454327430	-7.607715642978
H	-12.084382624541	-5.459825227919	-6.256943560162
H	-12.105550185238	-4.429740448973	-7.723155525565
O	2.373583059262	1.366877738790	2.702485752521
C	3.211135679996	2.360213659406	3.441477714486
H	3.550716238209	3.158315275022	2.773269873919
H	2.657611913243	2.787238882560	4.284062433391
H	4.058620693617	1.780185023064	3.800017654830

cisCydiol_TS1-F3000

($E_F = -773.69059800$ a.u.; $G_F = -773.39025005$ a.u.)

0 1

C	-4.543337403197	-1.808373181465	-2.920160407861
C	-3.160995696064	-0.910555091997	-1.168037696438
C	-4.090701648274	-1.199133093394	-0.010448961850
C	-4.386247552206	-2.698319028827	0.167820031327
C	-5.097935891617	-3.375528613163	-1.010324388199
C	-4.374410568259	-3.201843920422	-2.354332773170
H	-3.905499679761	-1.540216964043	-3.762794772312
H	-2.484752165736	-1.721671736792	-1.438794598043
H	-3.610784642309	-0.825129376470	0.905681669029
H	-5.018677831911	-0.628869264453	-0.121492286684
H	-4.988979673214	-2.832039762137	1.072631365894

H	-3.435730891112	-3.215294782050	0.352894670004
H	-5.204466297333	-4.442862717512	-0.790162963323
H	-6.109265892275	-2.971593715346	-1.115290826643
H	-4.795116376875	-3.911570757706	-3.083011293551
H	-3.315354527621	-3.460992326014	-2.262570886459
O	-5.926820863331	-1.562463100110	-3.182917677775
O	-2.423656581982	0.296096873686	-0.979557588480
C	-6.452114736534	-2.046680105086	-4.482353842661
H	-5.833399599628	-2.871549486489	-4.846124996471
H	-6.393735638088	-1.226867494599	-5.203920091298
C	-7.944448890449	-2.556470991176	-4.426876706168
H	-8.011171461967	-3.400260577606	-3.727308698146
H	-8.590979058136	-1.749994146916	-4.057607577183
C	-1.090424907016	0.100743406126	-0.361235805317
H	-0.396920924962	-0.268795854005	-1.123544406475
H	-1.169677518908	-0.652356148193	0.428973924178
C	-0.477640743042	1.396855594829	0.292702916728
H	-0.343576102895	2.170652877812	-0.474000351215
H	-1.172701463539	1.778523128727	1.051773522124
O	-8.338992122029	-2.963404744262	-5.762294664291
C	-9.692972727794	-3.493700191574	-6.032851249949
H	-9.876793503325	-4.411972913861	-5.463782983989
H	-10.461750912105	-2.750572871231	-5.793289681424
H	-9.698561769076	-3.707212853379	-7.099914438231
O	0.794594334468	1.037171488730	0.890748742112
C	1.618988660857	2.038467728099	1.601831730738

H	1.917293402340	2.851327523529	0.930307960339
H	1.081729891284	2.449552179084	2.463880162675
H	2.496238030862	1.487527760470	1.935323190149

cisCydiol-F3000

($E_F = -773.72245034$ a.u.; $G_F = -773.41619818$ a.u.)

0 1

C	-4.143746032874	-1.743949062318	-2.652919729028
C	-3.407992646647	-1.203366370557	-1.331019323918
C	-4.389826902299	-1.310196296199	-0.162517429267
C	-4.712185631066	-2.796183675822	0.089960527778
C	-5.185691843868	-3.523327270757	-1.179910299400
C	-4.276490499865	-3.264494403014	-2.395612472490
H	-3.509923369236	-1.533484451387	-3.521803626713
H	-2.643566411672	-1.978701313248	-1.200363436656
H	-3.950964578425	-0.865725298789	0.734321990048
H	-5.294831219128	-0.746631949058	-0.404261620413
H	-5.469028785754	-2.890628043299	0.874622340961
H	-3.805506885186	-3.284638058289	0.469306210447
H	-5.251270939926	-4.599387214712	-0.991574413344
H	-6.193065618521	-3.180117034327	-1.427818156919
H	-4.699176683211	-3.745063373812	-3.282377357640
H	-3.288519309807	-3.711557062273	-2.245416043971
O	-5.501269506796	-1.250278316817	-2.920584741799
O	-2.643863842899	0.058159881706	-1.313601506113
C	-6.129084069962	-1.656841897367	-4.184157530316

H	-5.416212666067	-2.206645338608	-4.805915212263
H	-6.387936447206	-0.735199534601	-4.711313461228
C	-7.460418386066	-2.511981678213	-4.087730882956
H	-7.243200274636	-3.502970484354	-3.667346719892
H	-8.164017270525	-2.000409494309	-3.417737202447
C	-1.468483908879	-0.050115472667	-0.435980682199
H	-0.746568128181	-0.738918879655	-0.891968433392
H	-1.765392406765	-0.470636478383	0.531285054446
C	-0.707574595200	1.291607820020	-0.121001773226
H	-0.338161079748	1.741469822215	-1.051456875847
H	-1.394310614574	2.001071217686	0.358443022624
O	-8.018257319477	-2.638177031644	-5.421512667328
C	-9.280568663764	-3.370020043363	-5.660175020511
H	-9.187831939183	-4.421765278172	-5.366456516294
H	-10.112365237610	-2.907400849071	-5.117120169573
H	-9.446472153712	-3.294798472347	-6.733090887489
O	0.395921416563	0.961849814269	0.765401796374
C	1.325576633058	1.996781587930	1.263894378262
H	1.855447529325	2.482735603495	0.436870799233
H	0.795442678868	2.751217360580	1.856076868039
H	2.030265722761	1.455870634446	1.892535010711

cisCydiol_Int1-F3000

($E_F = -773.99178424$ a.u.; $G_F = -773.69875552$ a.u.)

0 1

C	-6.745089983075	-2.223100626335	-3.733233529164
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C	-1.455505142809	-0.419947305047	0.027125778714
C	-2.731162441043	-0.166697935626	-0.799665166904
C	-3.488946872727	-1.450693606550	-1.358790388209
C	-4.778379633834	-1.195176689086	-2.251978438254
C	-5.522344208404	-2.478586334789	-2.830694696888
H	-6.734447297277	-1.375605340894	-4.418277355853
H	-0.789407410167	-1.234576259905	-0.256327201667
H	-3.427528415085	0.419490243696	-0.188105852887
H	-2.481428407831	0.478225610345	-1.658394442464
H	-3.773114173120	-2.078098288793	-0.507328433281
H	-2.775346536321	-2.038227772317	-1.948017249880
H	-5.500041885106	-0.616764741412	-1.665439763469
H	-4.489187352834	-0.558797471445	-3.096362770593
H	-5.837955939213	-3.114143342700	-1.994652298177
H	-4.781533671265	-3.075057022323	-3.388453809276
O	-7.513229406655	-3.316968693065	-4.156483451699
O	-0.828882894252	0.666852665399	0.653092412083
C	-8.604831281202	-3.052983838063	-5.107505555999
H	-8.184905806011	-2.612430956099	-6.017969951188
H	-9.298556616936	-2.334541426764	-4.661047838849
C	-9.411952985252	-4.345524763500	-5.506995743920
H	-8.726507773078	-5.075536316001	-5.957090406866
H	-9.847458084279	-4.792672089235	-4.603998177091
C	0.447793879861	0.411929701937	1.339240454527
H	1.172189999161	0.029057097985	0.612604410608
H	0.291090731077	-0.349385004853	2.108977858986

C	1.057939617014	1.694227609986	2.021214087364
H	1.220743722406	2.467092952484	1.258653899590
H	0.345696493241	2.083599635195	2.760224476430
O	-10.449121998718	-3.965646717756	-6.445681728611
C	-11.382459153188	-4.971486738435	-6.998107359389
H	-10.843626397764	-5.737783993868	-7.566473604227
H	-11.966976365715	-5.444843028989	-6.201370135427
H	-12.038009720478	-4.407486801192	-7.658638516532
O	2.308031053393	1.324489262117	2.655012164421
C	3.114963519512	2.323818370142	3.388671888150
H	3.436167065757	3.134077784784	2.724678240369
H	2.553942226013	2.738528044186	4.233514821339
H	3.979793908993	1.770462024390	3.749267325990

cisCydiol_TS1-F2500

($E_F = -773.52204696$ a.u.; $G_F = -773.22266781$ a.u.)

0 1

C	-4.548166773530	-1.844892916212	-2.924201546941
C	-3.147142865307	-0.918593950022	-1.127866874161
C	-4.107700471174	-1.196003773656	0.005454755827
C	-4.417689104170	-2.691847228258	0.186856563469
C	-5.129792109813	-3.371486375113	-0.989757970905
C	-4.394717887500	-3.226469554777	-2.331081135809
H	-3.891202192081	-1.583949427573	-3.754362642840
H	-2.478377255899	-1.736505070207	-1.395663749492
H	-3.646064896339	-0.819240725003	0.930218439047

H	-5.029778495763	-0.620900370955	-0.129546872783
H	-5.027434410655	-2.814778283162	1.088528984322
H	-3.473564687484	-3.217017476393	0.381563736959
H	-5.254003199073	-4.434277629391	-0.756915564163
H	-6.134541562725	-2.954287451656	-1.106693051591
H	-4.814874294988	-3.947894893067	-3.049645384386
H	-3.337786319115	-3.489769402115	-2.226000487177
O	-5.915392443967	-1.575650949631	-3.195087015080
O	-2.423591418357	0.282770387427	-0.944476713529
C	-6.426356336534	-2.035983984657	-4.497538477299
H	-5.807187489750	-2.856179098566	-4.872028891069
H	-6.368462271783	-1.207366316657	-5.209669854710
C	-7.906907894374	-2.542835188380	-4.436551424827
H	-7.971098240699	-3.392781741083	-3.743463885476
H	-8.554785047988	-1.740982826114	-4.058191738657
C	-1.059700068279	0.102232654424	-0.419954814760
H	-0.389599667537	-0.167581598821	-1.242812352630
H	-1.057592937769	-0.713083484854	0.310324869159
C	-0.496546529220	1.372154735356	0.299346238796
H	-0.440932240297	2.209833665134	-0.408317800665
H	-1.174767560633	1.654781462452	1.115512042566
O	-8.297379752260	-2.935854380004	-5.769771467621
C	-9.643030436877	-3.463953284812	-6.010015245798
H	-9.815190450090	-4.383810005109	-5.438412767403
H	-10.410533018162	-2.724709432269	-5.751666819581
H	-9.680046658259	-3.678543182612	-7.076645448458

O	0.813021957609	1.037657849722	0.807450867630
C	1.584047224290	2.034242975936	1.555797182776
H	1.796456795664	2.915578546159	0.939100526443
H	1.054245109852	2.343501025762	2.464643591167
H	2.514413958279	1.535099449580	1.821109471344

cisCydiol_Int1-F2500

($E_F = -773.77171783$ a.u.; $G_F = -773.47774159$ a.u.)

0 1

C	-6.723192484512	-2.205985467453	-3.701961026591
C	-1.476065193777	-0.443872221369	-0.000461452633
C	-2.755801321676	-0.181364921054	-0.797526821528
C	-3.484489046019	-1.459887895450	-1.373282670980
C	-4.779172592943	-1.196711112265	-2.234519134275
C	-5.493320045438	-2.473702662078	-2.831547089566
H	-6.736086476023	-1.337837958862	-4.360818112314
H	-0.801064715695	-1.239579215734	-0.315357606267
H	-3.454309635271	0.375449845875	-0.161000543341
H	-2.528261367709	0.491735986403	-1.641263733658
H	-3.745489911711	-2.115931066905	-0.535784931173
H	-2.767904228374	-2.017702744600	-1.987771677266
H	-5.504262674395	-0.649071596811	-1.622747967491
H	-4.513164527440	-0.530862383462	-3.064046033346
H	-5.786260069561	-3.139404635083	-2.010514972328
H	-4.748959353922	-3.039952849971	-3.416352278902
O	-7.469288307909	-3.298922107911	-4.144557746729

O	-0.865378123271	0.634048905583	0.641509554810
C	-8.573138492454	-3.020054394408	-5.061981883950
H	-8.180130033550	-2.537832851874	-5.963857996258
H	-9.276974085020	-2.334194594870	-4.580495105247
C	-9.343243409155	-4.313428648999	-5.484537865473
H	-8.647490459869	-5.011227047486	-5.969720566893
H	-9.753005808161	-4.802567755717	-4.590737927873
C	0.412730153518	0.374323699096	1.302476153835
H	1.136423411866	0.017051628568	0.561543590740
H	0.275515291842	-0.405682774571	2.057654661166
C	0.998523718268	1.646647310336	1.997053398254
H	1.141941951756	2.438294034931	1.249316547055
H	0.287782282455	2.010668730245	2.750978637537
O	-10.397787866928	-3.924589960933	-6.388966665291
C	-11.293430372708	-4.944447166139	-6.941776045097
H	-10.737402192403	-5.679623459393	-7.535583433292
H	-11.845435571620	-5.459313438793	-6.146545722815
H	-11.986467702757	-4.400277784791	-7.580996548468
O	2.253637198174	1.279459196425	2.606239389058
C	3.026309018816	2.285330291097	3.340483907883
H	3.319091448825	3.114880152907	2.685979536678
H	2.458301451111	2.675598457000	4.193252319052
H	3.913033533029	1.762385043137	3.694452665622

cisCydiol-F2500

($E_F = -773.56559010$ a.u.; $G_F = -773.25835727$ a.u.)

0 1

C	-4.124342984837	-1.779613032290	-2.631786966715
C	-3.405859366492	-1.249637272818	-1.318114215513
C	-4.392993138929	-1.336358926291	-0.151886147093
C	-4.748850935961	-2.814151097106	0.100551208970
C	-5.236119875497	-3.527240193048	-1.171768218033
C	-4.308293589484	-3.295152918200	-2.378272092415
H	-3.471003138863	-1.592069805203	-3.492234040368
H	-2.641934781856	-2.023508112461	-1.169722813608
H	-3.946897896065	-0.899994785979	0.745461400875
H	-5.284380119460	-0.753370046134	-0.397550666136
H	-5.509217212065	-2.891448248606	0.883626956391
H	-3.854744306492	-3.324515466820	0.480983510260
H	-5.336498468111	-4.600759442106	-0.984419596189
H	-6.230877305779	-3.152880908173	-1.425810161918
H	-4.732866805938	-3.762851762600	-3.270904633515
H	-3.335163309205	-3.770053427074	-2.216170934849
O	-5.447106543501	-1.226987724073	-2.906990435828
O	-2.657898152141	0.010772192357	-1.330121682081
C	-6.074258614509	-1.608364438578	-4.167601317397
H	-5.361248839402	-2.136454130180	-4.808685674960
H	-6.348658452201	-0.678832113613	-4.672832857528
C	-7.385016050827	-2.473844442763	-4.067947156805
H	-7.157080694402	-3.470961359551	-3.667792777215
H	-8.088205215895	-1.981812823724	-3.382204312885
C	-1.483352196193	-0.079466145748	-0.465824608106

H	-0.755134642430	-0.764910761978	-0.918027455544
H	-1.766072785793	-0.492002551799	0.509559799433
C	-0.748484686451	1.269211136697	-0.178973728089
H	-0.389474832327	1.714280130693	-1.116296682923
H	-1.439835111544	1.976748969570	0.297650144427
O	-7.947096810012	-2.578220358300	-5.394217777081
C	-9.189633481710	-3.325318753945	-5.604028878693
H	-9.071718787679	-4.378209365389	-5.320709662933
H	-10.017154362017	-2.885208669483	-5.034844756434
H	-9.393123857709	-3.250054389390	-6.670873591281
O	0.356968943654	0.955107932826	0.699668102233
C	1.255717351307	2.011547867212	1.167993507052
H	1.768593151164	2.497634998646	0.329402092110
H	0.712697550869	2.766105358865	1.749680407682
H	1.982164359402	1.507584963527	1.803277759616

cisCydiol_TS1-F2000

($E_F = -773.35580468$ a.u.; $G_F = -773.05503275$ a.u.)

0 1

C	-4.506901489860	-1.924630542046	-2.895120576850
C	-3.152921121109	-0.875538046528	-1.022617688717
C	-4.250498893635	-1.058971726139	-0.001447664808
C	-4.570538412255	-2.540028819300	0.269137059474
C	-5.202291310764	-3.313731619709	-0.896238214249
C	-4.396461530015	-3.261962015476	-2.203319054346
H	-3.811607613717	-1.725670853299	-3.711778160149

H	-2.480398941125	-1.718103970988	-1.179190741278
H	-3.911828383766	-0.594080939902	0.935556212452
H	-5.154153061358	-0.520197295280	-0.303962218998
H	-5.244063206950	-2.595155072141	1.131278308539
H	-3.643928671965	-3.044062668091	0.573385655074
H	-5.332999541513	-4.357444294839	-0.590876683304
H	-6.201601549622	-2.917840079631	-1.100698552592
H	-4.780213809515	-4.037808027982	-2.886480820145
H	-3.346590278532	-3.515652268170	-2.023818175072
O	-5.851837021887	-1.632770636770	-3.226446983702
O	-2.469408875342	0.322170828358	-0.857012526317
C	-6.322086238804	-2.151831247117	-4.509912648054
H	-5.754730904371	-3.046023941607	-4.785684804390
H	-6.165878464326	-1.393774259522	-5.284630110891
C	-7.828710944880	-2.534497841587	-4.473710723424
H	-7.988602398546	-3.311688445267	-3.713278886211
H	-8.428820824008	-1.656633376487	-4.197699591990
C	-1.015324887192	0.343562682596	-0.794985660675
H	-0.631974247026	0.822635628030	-1.699403043625
H	-0.624254969041	-0.677095432739	-0.744745720764
C	-0.519318995605	1.144053007754	0.446711200372
H	-0.956055493236	2.151744853184	0.421687744635
H	-0.864186002641	0.645021896405	1.363335154241
O	-8.187573229434	-3.013879943056	-5.780873088237
C	-9.551225934887	-3.462673905928	-6.004774913054
H	-9.803843898967	-4.309046618946	-5.353518908923

H	-10.270481257369	-2.651161664398	-5.836917066031
H	-9.590891134568	-3.777528590096	-7.046615700160
O	0.914119436702	1.201705399258	0.401654089452
C	1.605360243989	1.916588131100	1.463124716491
H	1.310953017746	2.973122973777	1.486656359237
H	1.405898903973	1.463479536629	2.442217009496
H	2.666119992693	1.836021956778	1.230582689232

cisCydiol_Int1-F2000

($E_F = -773.55403352$ a.u.; $G_F = -773.25932649$ a.u.)

0 1

C	-6.699822476624	-2.206478962166	-3.655507660401
C	-1.480651336883	-0.446185176514	-0.042081910966
C	-2.777059298741	-0.186405668042	-0.792976220591
C	-3.463977141782	-1.462346618598	-1.395328703200
C	-4.777374955812	-1.203172450135	-2.207924122529
C	-5.448917264341	-2.475821112672	-2.834138588539
H	-6.756901080344	-1.311981940235	-4.275838959597
H	-0.787952958596	-1.205051864781	-0.406040826257
H	-3.478088233566	0.320752493362	-0.118509310914
H	-2.591448709090	0.527414660197	-1.613721055390
H	-3.681989532774	-2.160084525068	-0.579246174677
H	-2.743886180520	-1.969987495841	-2.048435557871
H	-5.506480758020	-0.707490051049	-1.557480366125
H	-4.554565961706	-0.494339789310	-3.014568677409
H	-5.698976720731	-3.185738443225	-2.036033576982

H	-4.700075491814	-2.990385717947	-3.460289551181
O	-7.412051671063	-3.303260886189	-4.123871563197
O	-0.896774017830	0.622972485600	0.625360139076
C	-8.541589299105	-3.018861647990	-4.993463549804
H	-8.192735679801	-2.481010300854	-5.882432431919
H	-9.258945482668	-2.383746810509	-4.463906134157
C	-9.259250436828	-4.318856169447	-5.446863700278
H	-8.548241866715	-4.966211559802	-5.978592786713
H	-9.625783698564	-4.863477020876	-4.565956548537
C	0.394699210899	0.373160817994	1.243923904320
H	1.114553389887	0.065749766807	0.476743539958
H	0.299129949176	-0.437304526011	1.973543904350
C	0.941102643493	1.635828911272	1.963449683092
H	1.041451261579	2.457582709197	1.240965333687
H	0.234054312143	1.949851097853	2.743484593613
O	-10.345563154763	-3.933157513637	-6.303764048613
C	-11.190843652696	-4.976193701182	-6.860705108733
H	-10.612021713856	-5.663376967984	-7.490402364079
H	-11.692247868057	-5.546798440130	-6.069056424699
H	-11.933590384374	-4.460510170136	-7.467523694868
O	2.214491924646	1.289566778599	2.530580341190
C	2.940761334575	2.306835995206	3.272386109750
H	3.180678944590	3.167921805635	2.636178438027
H	2.367768667017	2.649186926400	4.143114635024
H	3.861043003846	1.828414842772	3.604151620957

cisCydiol-F2000

($E_F = -773.41005530$ a.u.; $G_F = -773.10308315$ a.u.)

0 1

C	-4.101596777786	-1.868173657086	-2.536361393004
C	-3.408498811996	-1.212369792564	-1.282630122680
C	-4.395597412708	-1.172427047012	-0.115354863020
C	-4.814641601234	-2.605139952842	0.263699364595
C	-5.334978315623	-3.401030735443	-0.943769346250
C	-4.372265118395	-3.336880125669	-2.141517269561
H	-3.409841532774	-1.805845326570	-3.385832272660
H	-2.621771272698	-1.937510880949	-1.035159850274
H	-3.920567331881	-0.675351154041	0.734766130337
H	-5.264354951160	-0.576355610150	-0.407893698384
H	-5.574844067999	-2.578966160441	1.050276213818
H	-3.944225576912	-3.122881959062	0.687314622659
H	-5.507263369497	-4.443939914495	-0.660604719289
H	-6.299539541931	-2.989018268489	-1.252392757984
H	-4.795864824080	-3.871022303793	-2.996800258734
H	-3.427419562082	-3.837306034413	-1.902295400204
O	-5.366050721080	-1.261246803926	-2.910749146463
O	-2.750624645321	0.061608277071	-1.463460814753
C	-5.935369162120	-1.683520471926	-4.175050525160
H	-5.229280391552	-2.310094944172	-4.730083321271
H	-6.112247189620	-0.780724177319	-4.766198577689
C	-7.295820639303	-2.443931431068	-4.076952270164
H	-7.161394053611	-3.409078265441	-3.568883133546

H	-8.004886419802	-1.844559086384	-3.489086101577
C	-1.339913058777	0.143559918997	-1.155305024321
H	-0.852642301048	0.629534715907	-2.005050389557
H	-0.909399380962	-0.859240054553	-1.053325106258
C	-0.964092990746	0.966364390244	0.117686797417
H	-1.414540317021	1.966268620023	0.052780087732
H	-1.351320245797	0.473677478567	1.021340423501
O	-7.775599691112	-2.639529399028	-5.418364886267
C	-9.049642882245	-3.310050544422	-5.611847031138
H	-9.027081111200	-4.331962269944	-5.212417829808
H	-9.867894698042	-2.755037658596	-5.135947177413
H	-9.206386017262	-3.341569281599	-6.689140636512
O	0.471844804395	1.046893255482	0.155076624925
C	1.106808288149	1.803681851351	1.219601142494
H	0.799691959947	2.856879846736	1.197219304539
H	0.872343535358	1.380864572040	2.204775535274
H	2.177801663653	1.730510819669	1.035559278975

cisCydiol_TS1-F1500

($E_F = -773.19013179$ a.u.; $G_F = -772.88971768$ a.u.)

0 1

C	-4.519338548648	-1.981400361471	-2.901823882657
C	-3.135618839713	-0.869200307078	-0.962347366876
C	-4.261493755221	-1.054565205850	0.023053877491
C	-4.583889701749	-2.534531868715	0.296154803624
C	-5.218471979272	-3.314233548109	-0.863911890564

C	-4.408289963850	-3.293432334080	-2.169895796935
H	-3.805946404399	-1.780037884995	-3.701654603373
H	-2.457404550772	-1.707225519358	-1.117936422257
H	-3.955224982282	-0.580471634379	0.967199513805
H	-5.159478116617	-0.523027286179	-0.309323923961
H	-5.259260905964	-2.584819796917	1.157126698364
H	-3.659498363023	-3.040004954026	0.604808669710
H	-5.362919453912	-4.351978111384	-0.544534322043
H	-6.212815298547	-2.910166220403	-1.077204132390
H	-4.787208036870	-4.091061683132	-2.831689707505
H	-3.357581661404	-3.535734391426	-1.979703949336
O	-5.849274462375	-1.679291289079	-3.239280788264
O	-2.482312429276	0.337833681443	-0.808753601049
C	-6.299457518367	-2.161092274056	-4.535375058397
H	-5.736072328068	-3.053853997718	-4.824783749742
H	-6.132380928089	-1.387925146226	-5.293165108039
C	-7.799250874525	-2.529355616230	-4.501386352530
H	-7.963994624083	-3.315567903688	-3.750865380548
H	-8.393770266146	-1.651494896760	-4.212062328097
C	-1.036487308254	0.395952495485	-0.829902768412
H	-0.718465506535	0.951342627013	-1.715866809856
H	-0.613081277272	-0.612084421920	-0.876290383044
C	-0.514947486818	1.118338787694	0.436358192928
H	-0.988406012358	2.107629441298	0.506488479322
H	-0.798090183773	0.541935751216	1.329080323810
O	-8.157858913128	-2.986166366482	-5.809994282423

C	-9.517479914787	-3.426939705318	-6.003150641864
H	-9.757784936517	-4.278333881842	-5.352811228063
H	-10.232367665900	-2.616563101570	-5.809431138050
H	-9.591133701595	-3.734278795180	-7.045725084677
O	0.905712684816	1.233437087998	0.329305657678
C	1.586764774182	1.899663265507	1.414204272785
H	1.241365774613	2.935806148120	1.524700325838
H	1.438367617790	1.369195790510	2.363900555374
H	2.645094105967	1.894326178123	1.156056601957

cisCydiol -F1500

($E_F = -773.25901380$ a.u.; $G_F = -772.95127131$ a.u.)

0 1

C	-4.078138461281	-1.909730225937	-2.497032700029
C	-3.402806568274	-1.222037834777	-1.268493788916
C	-4.382861186977	-1.166077271421	-0.096077971466
C	-4.808893851418	-2.589157023736	0.307147278592
C	-5.348755295133	-3.392167560314	-0.886502603579
C	-4.381989837785	-3.364199737109	-2.081335288090
H	-3.373685608900	-1.879326670259	-3.338445298042
H	-2.586040295747	-1.906643238078	-1.000225390200
H	-3.903656383629	-0.655213277488	0.743637662214
H	-5.249828879771	-0.571313128099	-0.396328309178
H	-5.560402521483	-2.545259424578	1.101209507001
H	-3.939502784249	-3.111187185927	0.727823476446
H	-5.543649524897	-4.426788655888	-0.588224356700

H	-6.304199763809	-2.963391859361	-1.201572204474
H	-4.808560504320	-3.904586459918	-2.931280343490
H	-3.446474306469	-3.875676779550	-1.827600354030
O	-5.309255179208	-1.264585416520	-2.889456492016
O	-2.819178096661	0.067223169139	-1.522366202970
C	-5.859921691254	-1.665527246567	-4.159602160803
H	-5.158674961781	-2.304143453742	-4.707733377939
H	-6.014414088329	-0.758923378446	-4.751695630346
C	-7.223231892613	-2.399076958641	-4.063586125552
H	-7.109220356327	-3.359736467286	-3.541536456139
H	-7.930008059587	-1.782488217671	-3.490240377389
C	-1.409859018812	0.219771397731	-1.287431031172
H	-1.031922964526	0.879674559400	-2.072147646278
H	-0.891686068872	-0.742121738571	-1.383297346933
C	-1.023942542926	0.856135586989	0.074757057465
H	-1.560494538118	1.807503075541	0.197168564102
H	-1.307644970831	0.194355823748	0.906893099769
O	-7.687331753985	-2.602327212684	-5.403071940240
C	-8.962462404280	-3.254508924401	-5.569445079995
H	-8.952492679974	-4.267476182798	-5.145637041268
H	-9.770403631877	-2.678821809787	-5.099032503337
H	-9.135863004033	-3.312462723373	-6.643473207256
O	0.393625188305	1.060606066405	0.047036633233
C	0.998085440632	1.710265518095	1.183068871005
H	0.590446410026	2.719021424238	1.330159148854
H	0.851619495780	1.128556410842	2.102815396819

H	2.062951730384	1.777590249072	0.962631685870
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cisCydiol_Int1-F1500

($E_F = -773.33859758$ a.u.; $G_F = -773.04324928$ a.u.)

0 1

C	-6.676931495362	-2.189578772132	-3.635682444540
C	-1.505012705171	-0.465156166782	-0.057023603559
C	-2.796966405525	-0.196340213877	-0.794159187343
C	-3.467028817132	-1.467541662933	-1.399666182595
C	-4.775592744233	-1.201502022774	-2.198351524474
C	-5.429848746547	-2.468934612901	-2.828552593438
H	-6.738244111306	-1.289885317513	-4.248245770789
H	-0.808409488768	-1.213476045599	-0.435427343959
H	-3.497910909164	0.299318751673	-0.110865794093
H	-2.618392380989	0.527654339988	-1.607996449176
H	-3.677784207202	-2.174944601573	-0.589797941659
H	-2.745962191950	-1.964008955593	-2.060581441507
H	-5.506062491070	-0.717513455053	-1.540394425529
H	-4.559788111317	-0.482623090237	-2.998260819894
H	-5.674105947981	-3.189008529096	-2.037577710652
H	-4.679970744452	-2.972465315476	-3.462990869277
O	-7.378903146061	-3.283769838803	-4.107964861676
O	-0.932513142405	0.597974121012	0.617515246106
C	-8.507437610203	-2.992537580683	-4.963497385431
H	-8.168869459719	-2.441171638456	-5.848601261627
H	-9.229384389651	-2.370656476360	-4.423908421698

C	-9.200546648535	-4.293241831934	-5.418989326741
H	-8.482280609193	-4.927070995564	-5.958004923772
H	-9.556437350171	-4.850652841481	-4.541247895745
C	0.354791025502	0.344795655514	1.225044370716
H	1.076364144367	0.048931977332	0.454438885652
H	0.267508077647	-0.472156852332	1.948927900860
C	0.878962821191	1.604526755696	1.944780567571
H	0.967415569962	2.432172405968	1.226884332235
H	0.169390410904	1.906086683418	2.727968597323
O	-10.289639942651	-3.913935699539	-6.265411193210
C	-11.099531893246	-4.976380423630	-6.810058293933
H	-10.503540123850	-5.651096985164	-7.438353317943
H	-11.580744106593	-5.559894773716	-6.014400569367
H	-11.862884316545	-4.492920600722	-7.418504776357
O	2.152162559342	1.268912646625	2.503972848134
C	2.839565132714	2.301934221337	3.239940713339
H	3.056335166287	3.169452996809	2.603050884648
H	2.253080347640	2.632164015082	4.107176826802
H	3.774472158601	1.858858971355	3.580957310499

cisCydiol_TS1-F1000

($E_F = -773.02540082$ a.u.; $G_F = -772.72663295$ a.u.)

0 1

C	-4.604682296866	-2.146301779771	-2.874882282955
C	-3.106866196382	-0.870542341796	-0.925399877726
C	-4.284889281573	-0.960975685837	0.006368374955

C	-4.643305459813	-2.407941413919	0.390517152867
C	-5.306619129454	-3.260124324036	-0.700731622574
C	-4.513882904747	-3.374369219171	-2.013404992752
H	-3.910948079446	-2.037796457154	-3.707217343647
H	-2.441386853655	-1.729582184189	-1.001981351750
H	-4.027011242473	-0.406839474979	0.921540444235
H	-5.159478890848	-0.455433502687	-0.419440133564
H	-5.317309499150	-2.376065735168	1.253468984369
H	-3.731831562163	-2.912787563721	0.736395831993
H	-5.472159240541	-4.264811134190	-0.296817476318
H	-6.294607300788	-2.851987084235	-0.934647184686
H	-4.913945019360	-4.228196873921	-2.587947495732
H	-3.463547500002	-3.608538295375	-1.811655146310
O	-5.911723375832	-1.779079411068	-3.153276500076
O	-2.451261056314	0.340200603176	-0.856322884119
C	-6.400742169440	-1.841029373352	-4.509456417642
H	-5.639079376561	-2.253493437069	-5.178057301240
H	-6.650506026477	-0.830373720443	-4.844544388012
C	-7.663964103341	-2.718584210498	-4.561351195518
H	-7.410853233713	-3.747011479791	-4.263898651711
H	-8.401894452690	-2.330969951480	-3.844329465917
C	-1.014180639379	0.380464439263	-0.908859520162
H	-0.709354709038	0.958423110671	-1.785107951423
H	-0.599043162702	-0.628667267847	-0.993792154645
C	-0.475270331758	1.060190216594	0.362403849116
H	-0.946833970589	2.047418222615	0.469704941053

H	-0.744875949419	0.458901166750	1.243424395838
O	-8.173219448493	-2.681246272173	-5.891619478926
C	-9.374979913558	-3.431193196227	-6.112148940869
H	-9.224760952142	-4.499499253306	-5.904859418690
H	-10.198324326370	-3.061049995246	-5.486269215088
H	-9.634095892223	-3.301092154035	-7.162653144229
O	0.938467624048	1.177020006719	0.235242811873
C	1.603013357595	1.820183884669	1.331140624243
H	1.244973268744	2.849514017178	1.467240818842
H	1.457017988716	1.266840752577	2.268676162517
H	2.664209365466	1.837049123297	1.084114416117

cisCydiol_Int1-F1000

($E_F = -773.12533226$ a.u.; $G_F = -772.83038674$ a.u.)

0 1

C	-6.690001494503	-2.139372314423	-3.583142881179
C	-1.529247101019	-0.515551110631	-0.050648290387
C	-2.851356262149	-0.240689858064	-0.711178624529
C	-3.421506949061	-1.455121180615	-1.487863128135
C	-4.797726784271	-1.199795656235	-2.145953742065
C	-5.367872939391	-2.414223360255	-2.922646958852
H	-6.877116171519	-1.173362008947	-4.052646889727
H	-1.342176909640	-1.481542438735	0.418911097824
H	-3.591612115343	0.077820919916	0.043405567969
H	-2.738170351612	0.614206814589	-1.389760674167
H	-3.508445656766	-2.306945945216	-0.802065124345

H	-2.701219883192	-1.753746561221	-2.257994556156
H	-5.518014842280	-0.901178337228	-1.375819876527
H	-4.710791387511	-0.347965727696	-2.831745861833
H	-5.481029692388	-3.269133726418	-2.244076460828
H	-4.627628063948	-2.732709558447	-3.677252412418
O	-7.324703155782	-3.218807703639	-4.157077615545
O	-0.894519159187	0.563892238378	0.523242745234
C	-8.534929099380	-2.920750780266	-4.875633394982
H	-8.322704703349	-2.221943411643	-5.693730525507
H	-9.263945453093	-2.455432434503	-4.203554738655
C	-9.127294229997	-4.210480444323	-5.456093583487
H	-8.397102499501	-4.686836329236	-6.126057636852
H	-9.353701798555	-4.915120965201	-4.643178262832
C	0.315656060123	0.265824094086	1.241879747700
H	1.044671318758	-0.199609513405	0.569878279317
H	0.103348236828	-0.432889095892	2.060036581595
C	0.908081045336	1.555570998552	1.822241497588
H	1.134589450977	2.260112445097	1.009265635684
H	0.177882208381	2.032050152704	2.492113420421
O	-10.309033569080	-3.840700545493	-6.161543964547
C	-11.026523580569	-4.915289739133	-6.781234258900
H	-10.409668976940	-5.429923525949	-7.530289142313
H	-11.369385171337	-5.648981943498	-6.039249996803
H	-11.890692644100	-4.468132476237	-7.271804595988
O	2.089751361445	1.185775005041	2.527801865700
C	2.807290798313	2.260378923433	3.147410467154

H	3.150264416287	2.993956187134	2.405356569986
H	2.190427685329	2.775157377889	3.896366487644
H	3.671391740810	1.813203567539	3.638091792760

cisCydiol-F1000

($E_F = -773.11081334$ a.u.; $G_F = -772.80261922$ a.u.)

0 1

C	-4.068581944945	-1.950633682302	-2.449442568005
C	-3.405571992016	-1.224655038251	-1.251500385880
C	-4.385980390910	-1.119412044214	-0.082827108431
C	-4.843332686085	-2.519557966583	0.361492518968
C	-5.408325154752	-3.337476223018	-0.809863587463
C	-4.432610191456	-3.377731504054	-1.996121902517
H	-3.347629420619	-1.975698523899	-3.277427966711
H	-2.573729527837	-1.877272380009	-0.950078303798
H	-3.901229860628	-0.590289846524	0.742337038185
H	-5.239905558523	-0.518110687466	-0.406166920474
H	-5.589733331845	-2.435126783627	1.157050401844
H	-3.985926072281	-3.053260044336	0.792235879895
H	-5.642319371134	-4.355214425461	-0.483149090398
H	-6.345997709941	-2.883227812248	-1.143054755157
H	-4.867908330277	-3.927696114862	-2.835577403633
H	-3.517160494646	-3.912216821187	-1.716537422430
O	-5.252271582328	-1.255027786743	-2.876859619503
O	-2.869494863146	0.060689345584	-1.590053868366
C	-5.779951341140	-1.638646025473	-4.153558801682

H	-5.095317886110	-2.313789349360	-4.679020251189
H	-5.883768424729	-0.733620157349	-4.759511818215
C	-7.163770375916	-2.310522708099	-4.060407934507
H	-7.095663334135	-3.260111033804	-3.510224089210
H	-7.854906485394	-1.652118148737	-3.514480767439
C	-1.464454851770	0.246408531366	-1.407311086656
H	-1.153155022854	0.995099649570	-2.139212142750
H	-0.912100312054	-0.677785390661	-1.620222219750
C	-1.060843987639	0.758497898406	-0.009153861865
H	-1.619962233487	1.677819590009	0.216886056350
H	-1.304803193679	0.013678454348	0.764006652550
O	-7.611775508313	-2.530637682751	-5.396801759005
C	-8.902043205692	-3.137279001329	-5.532632287204
H	-8.928185141319	-4.133957572757	-5.071001542783
H	-9.687013248213	-2.516861120232	-5.079116118366
H	-9.090460497667	-3.231202807459	-6.601970205220
O	0.343849069558	1.004451198002	-0.051844247407
C	0.922993679872	1.571938260085	1.128465744304
H	0.478795571825	2.548771639994	1.363229183276
H	0.799427003142	0.909478423860	1.996225376700
H	1.985598245767	1.699676901652	0.922495795006

cisCydiol_TS1-F500

($E_F = -772.86221468$ a.u.; $G_F = -772.56392193$ a.u.)

0 1

C	-4.655333936871	-2.476305287491	-2.792760622036
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C	-3.065377774146	-0.764379937799	-0.863556997650
C	-4.251316325987	-0.854602427347	0.048006183070
C	-4.523696051303	-2.279627366113	0.560661673901
C	-5.179976155258	-3.259895735790	-0.422308044488
C	-4.414147560776	-3.510755520336	-1.736753919120
H	-3.968572735954	-2.384218976067	-3.631510315645
H	-2.316476954023	-1.555065463578	-0.847840981737
H	-4.059187037354	-0.199807626462	0.913326765187
H	-5.147855505005	-0.450526567886	-0.438213595134
H	-5.172273228212	-2.206064207466	1.440257998030
H	-3.579016741711	-2.709588406408	0.918855548674
H	-5.305957111513	-4.216762343068	0.095918384053
H	-6.186839939156	-2.911759958589	-0.672211408780
H	-4.732552459116	-4.489903826791	-2.135178743750
H	-3.339604356799	-3.589742976202	-1.546589332714
O	-5.991255510402	-2.350866473892	-3.099289801586
O	-2.568572785513	0.505935405551	-1.027362099782
C	-6.386938512398	-2.053316936540	-4.441575505074
H	-5.639127555871	-2.412977091404	-5.156334087873
H	-6.507786218535	-0.973157988385	-4.573061529446
C	-7.713637477799	-2.773164351826	-4.682387029750
H	-7.566705624402	-3.852126606638	-4.526812403881
H	-8.457212989377	-2.426529900506	-3.949858055214
C	-1.148726409683	0.663722528352	-1.123429429271
H	-0.961258836601	1.496001104165	-1.803911575001
H	-0.679236329873	-0.235268157694	-1.536989048292

C	-0.555597508871	0.987604498547	0.250659010517
H	-1.063243092681	1.872786189291	0.660628638697
H	-0.730459371869	0.147908081926	0.941117490449
O	-8.137001573671	-2.501800866623	-6.008795599258
C	-9.346521089955	-3.163447307446	-6.370861959088
H	-9.239772702015	-4.255409773972	-6.310503383779
H	-10.181379604071	-2.855448920053	-5.726352202308
H	-9.566890968308	-2.881703398569	-7.400485701465
O	0.832615043830	1.226694015570	0.077193888099
C	1.507113757933	1.641289912436	1.262241074241
H	1.091653687279	2.580899317062	1.651949417179
H	1.445839652779	0.876380524288	2.048896213447
H	2.552533950528	1.795625574584	0.994788358319

cisCydiol_Int1-F500

($E_F = -772.90446825$ a.u.; $G_F = -772.61078810$ a.u.)

0 1

C	-6.424661637136	-1.609892373652	-3.845554576189
C	-1.774973998571	-0.828912286505	0.058288504987
C	-3.014100612530	-0.646130392613	-0.761193643627
C	-3.775927668334	-1.975940645163	-0.939805824414
C	-5.147229673396	-1.877480740946	-1.637564329738
C	-5.091698168838	-1.712296375402	-3.176537524864
H	-6.702353658921	-0.745660505057	-4.443985456529
H	-1.736824745124	-1.605526655975	0.822604035357
H	-3.681714654807	0.086849736677	-0.275932385031

H	-2.754222414552	-0.210076603234	-1.734247196670
H	-3.934015284902	-2.407526036370	0.055469264732
H	-3.139780790090	-2.686989871543	-1.480380916116
H	-5.718754868674	-2.785704843387	-1.420597601149
H	-5.718388974768	-1.045549992981	-1.209703058759
H	-4.535670100149	-2.564479310847	-3.595245605873
H	-4.520241755499	-0.811543793782	-3.424155643438
O	-7.061672208531	-2.785705299167	-4.154690043803
O	-1.035333441079	0.297548120490	0.315705338498
C	-8.330314030262	-2.629988804355	-4.801394776660
H	-8.237053998414	-1.950398049756	-5.657413717995
H	-9.059708262279	-2.206014892497	-4.102608424267
C	-8.816834301246	-3.987246208331	-5.296834767910
H	-8.079234301114	-4.416286225833	-5.990676941379
H	-8.932025837466	-4.680923025760	-4.451384783580
C	0.088320375820	0.095319600220	1.181361094343
H	0.810400048548	-0.580869276274	0.710710868712
H	-0.239231668369	-0.352992733478	2.127449526142
C	0.750658022355	1.438525065331	1.466412783558
H	1.096735977517	1.894837931595	0.527665053381
H	0.023724157214	2.122201693230	1.928797685680
O	-10.059107880597	-3.753927273453	-5.945014001638
C	-10.662667569079	-4.915436476574	-6.505658814304
H	-10.021049505370	-5.371949682506	-7.272121836665
H	-10.880328044419	-5.668043810852	-5.735134269766
H	-11.597206456533	-4.595041191148	-6.966234095221

O	1.837478909092	1.173672058710	2.341674689147
C	2.579638782714	2.325857709701	2.728482173083
H	3.027456069794	2.826813316604	1.858941394234
H	1.949549224921	3.048813959836	3.265090094432
H	3.373871242516	1.982533816607	3.391414851132

cisCydiol -F500

($E_F = -772.96547629$ a.u.; $G_F = -772.65718030$ a.u.)

0 1

C	-4.056825416068	-2.009990667709	-2.408535952978
C	-3.423684556316	-1.234241196727	-1.238142149830
C	-4.406299556026	-1.112546287575	-0.073223515273
C	-4.855309000180	-2.503521646733	0.404633240377
C	-5.423475838371	-3.345341870178	-0.747813871136
C	-4.441114540698	-3.420130632543	-1.926196169281
H	-3.321099151671	-2.065483457507	-3.222342926178
H	-2.561419141564	-1.832496296635	-0.910426386465
H	-3.929757411711	-0.556636048679	0.739083567597
H	-5.264249538467	-0.527663660660	-0.415314472482
H	-5.598069086743	-2.403595901788	1.201758031541
H	-3.994917169599	-3.026772319683	0.842394944212
H	-5.666627006042	-4.353213917157	-0.398144982417
H	-6.356420097318	-2.891730258193	-1.095669872365
H	-4.872815381633	-3.986030960216	-2.757040692200
H	-3.531392820888	-3.953872723769	-1.626000124699
O	-5.212609024017	-1.298133996840	-2.866158860427

O	-2.967039390369	0.057213965855	-1.650159397743
C	-5.707701247343	-1.671662348267	-4.151244932834
H	-5.030163452326	-2.371024096478	-4.654217811675
H	-5.774638934780	-0.770481245405	-4.768666281826
C	-7.100038648150	-2.303307900640	-4.060142250511
H	-7.059517465030	-3.240858652961	-3.486379688240
H	-7.780461841258	-1.616760705898	-3.535199458857
C	-1.568773831031	0.294351472762	-1.538235079054
H	-1.334037853042	1.106654477516	-2.229326726423
H	-0.986758970350	-0.584791268977	-1.845477332028
C	-1.138004451168	0.716323658089	-0.128174301469
H	-1.711751383331	1.603728749586	0.176810633447
H	-1.346818917264	-0.085728718243	0.597166428964
O	-7.539327037584	-2.543098345488	-5.390439819891
C	-8.836566395686	-3.121330713241	-5.488011106852
H	-8.879442490517	-4.101327216350	-4.991883979691
H	-9.602244987714	-2.469782629914	-5.044000518222
H	-9.048669046531	-3.249356861715	-6.549724993783
O	0.254126705070	0.996330634342	-0.184198576188
C	0.811216395228	1.484077804848	1.031706398724
H	0.338656432422	2.426828817869	1.340975820108
H	0.703663853536	0.753963488402	1.846408085078
H	1.871453242439	1.659263721929	0.847697477407

transCydiol_TS1-F4000

($E_F = -774.04729761$ a.u.; $G_F = -773.74861605$ a.u.)

0 1

C	-1.077780016770	-0.419261289721	0.533447646962
C	1.077780664887	-0.418966126486	-0.533652019327
C	0.837625414371	0.846488367137	-1.307942131504
C	0.653279052284	2.077890630278	-0.400617568766
C	-0.653329638670	2.077672786541	0.401712296026
C	-0.837655776999	0.845796156714	1.308396391102
H	-0.980964485150	-1.357024795578	1.079046895692
H	1.691381593251	1.026349903003	-1.980738151637
H	-0.050327731656	0.703772750631	-1.933377496912
H	0.688602907958	2.980339205791	-1.019172154266
H	1.506593385127	2.129361493071	0.283896554822
H	-0.688666165608	2.979798687967	1.020736684193
H	-1.506645674241	2.129487011112	-0.282773834817
H	-1.691420358736	1.025290082198	1.981279868856
H	0.050295864222	0.702778484142	1.933764721247
O	-2.310806138189	-0.356836924887	-0.224855925789
C	-3.577924720516	-0.796015163722	0.454008470081
H	-3.587212656287	-0.398051285795	1.472066391571
H	-3.581044380284	-1.888659136366	0.503867745446
C	-4.932880972903	-0.321922003668	-0.262263461598
H	-4.937558283517	0.773841365108	-0.309077708119
H	-4.947515707650	-0.714001878068	-1.286320910399
O	-6.093378738494	-0.808781503954	0.491138667860
C	-7.527283782451	-0.537264227424	0.092930673938
H	-7.732481591118	0.537397367428	0.095307145431

H	-7.742642379251	-0.963002162861	-0.891624410169
H	-8.105909731234	-1.040441759289	0.863790202534
H	0.980979600654	-1.356447938909	-1.079737586874
O	2.310808893089	-0.356912869530	0.224678391006
C	3.577933861416	-0.795718659762	-0.454414218985
H	3.581076428251	-1.888337637544	-0.504831696659
H	3.587210550054	-0.397234063072	-1.472269309855
C	4.932882373778	-0.321963819069	0.262097180418
H	4.937544802010	0.773777163362	0.309459566539
H	4.947520599522	-0.714556026157	1.285959511791
O	6.093388052045	-0.808431548982	-0.491546689016
C	7.527288456017	-0.537080746517	-0.093208122366
H	7.732467211775	0.537587012153	-0.095067166528
H	7.742655354059	-0.963289574001	0.891143023737
H	8.105922864936	-1.039877325296	-0.864311465609

transCydiol_Int1-F4000

($E_F = -774.43983505$ a.u.; $G_F = -774.14950871$ a.u.)

0 1

C	-3.449044744805	-0.040988046767	-0.228165692665
C	3.449038494052	-0.041035306978	0.228158061716
C	2.068289552605	0.003589198553	-0.510013227148
C	0.713790541848	0.015727943974	0.380859811137
C	-0.713797231072	0.015835977021	-0.380848775106
C	-2.068296224814	0.003418060863	0.510020605816
H	-3.537558766304	-0.628496141594	-1.141400094600

H	2.062602969468	0.885276627464	-1.160849149244
H	2.006121615459	-0.862164198237	-1.188008037819
H	0.751572569566	0.893742389598	1.033248749246
H	0.741319211687	-0.858974077882	1.039698758069
H	-0.751586796784	0.894046096498	-1.032974333000
H	-0.741318340534	-0.858668600438	-1.039950390923
H	-2.062614194100	0.884908021662	1.161125185826
H	-2.006124037382	-0.862541659618	1.187752322944
O	-4.652064136624	0.083347210912	0.509773941997
C	-5.952494416584	-0.079997695216	-0.207632589608
H	-5.978752351051	-1.080654491845	-0.649122591927
H	-5.996478297693	0.660295377888	-1.010461137567
C	-7.257688039791	0.095760394796	0.706672173781
H	-7.222410747965	-0.642700927713	1.516763118636
H	-7.243578632433	1.098826534628	1.149675183601
O	-8.462291149483	-0.090594830311	-0.107003025332
C	-9.868478517585	0.014477625719	0.441042743778
H	-10.039634333383	-0.740412276334	1.214100415472
H	-10.054066882419	1.016039051462	0.839987951367
H	-10.495534596712	-0.175447431943	-0.426641119360
H	3.537559054509	-0.628836429430	1.141202076369
O	4.652056443030	0.083548344070	-0.509741371926
C	5.952488513978	-0.080014620666	0.207613029719
H	5.996467169148	0.660024822034	1.010677979597
H	5.978754086990	-1.080813181487	0.648785522167
C	7.257680190116	0.096044073578	-0.706637898007

H	7.222408554993	-0.642162953517	-1.516965311249
H	7.243562248505	1.099253082214	-1.149324840415
O	8.462284043556	-0.090559046162	0.106981469439
C	9.868469448295	0.014695805462	-0.441033492859
H	10.039633237861	-0.739959605455	-1.214325627576
H	10.054048433162	1.016385647549	-0.839674665876
H	10.495528245316	-0.175489178343	0.426596289664

transCydiol-F4000

($E_F = -774.07765103$ a.u.; $G_F = -773.77362826$ a.u.)

0 1

C	-0.634834263967	-0.467697573224	0.501663849848
C	0.634827262609	-0.467446162216	-0.501881275744
C	0.535895202028	0.782977851188	-1.376094051780
C	0.561378927066	2.061078981085	-0.524225367298
C	-0.561386403732	2.060821750306	0.525263501282
C	-0.535913825740	0.782295051409	1.376495790208
H	-0.594062814367	-1.376707141919	1.110932880166
H	1.333815172905	0.795029558643	-2.123192675655
H	-0.411535285846	0.717493926609	-1.920583697339
H	0.473520573493	2.939509519961	-1.170858387531
H	1.529884401656	2.130026460340	-0.017659410199
H	-0.473520374458	2.938928121540	1.172335670119
H	-1.529891645249	2.130032228912	0.018732210615
H	-1.333843201337	0.793976272038	2.123590269157
H	0.411509545958	0.716542233168	1.920965264569

O	-1.926131161286	-0.492560782362	-0.268987956833
C	-3.188571164267	-0.546316937529	0.507394780188
H	-3.256155152526	0.324727418268	1.165082461135
H	-3.187873895747	-1.447115591306	1.131439497485
C	-4.530200467535	-0.556496241253	-0.372543055163
H	-4.529616050409	0.329193608825	-1.019846845302
H	-4.536329474165	-1.450634873758	-1.007449361415
O	-5.702541777911	-0.545874941773	0.510304324180
C	-7.130100953677	-0.552067903923	0.013481939217
H	-7.335107191978	0.338933461362	-0.587582393934
H	-7.334417427369	-1.456527174818	-0.567347110624
H	-7.719162679135	-0.542030125123	0.927371023457
H	0.594060432739	-1.376154947858	-1.111599094734
O	1.926127491081	-0.492684563739	0.268754053289
C	3.188567697930	-0.545955052519	-0.507663104168
H	3.187872810205	-1.446367139663	-1.132271746131
H	3.256149938819	0.325502525641	-1.164809339117
C	4.530197240815	-0.556675768478	0.372271220941
H	4.529584836733	0.328588863046	1.020164377714
H	4.536355593549	-1.451238284592	1.006587923129
O	5.702537497731	-0.545433716112	-0.510573687792
C	7.130097767086	-0.551947422677	-0.013755357873
H	7.335099075323	0.338651446537	0.587899022811
H	7.334422109693	-1.456787363336	0.566469839980
H	7.719157241582	-0.541298016867	-0.927632782815

transCydiol_TS1-F3500

($E_F = -773.87511743$ a.u.; $G_F = -773.57557655$ a.u.)

0 1

C	-1.095487674984	-0.410227789141	0.542758208182
C	1.095483540487	-0.409950380200	-0.542939656127
C	0.836729952668	0.854587267681	-1.311721768150
C	0.652330505686	2.084417886318	-0.402239698655
C	-0.652377877023	2.084216325098	0.403263889119
C	-0.836762840293	0.853944282899	1.312151528508
H	-0.989565317319	-1.351400873645	1.080920500030
H	1.684404785503	1.041576640716	-1.991084563728
H	-0.054413140759	0.706682399939	-1.931086492016
H	0.685544025439	2.987655033167	-1.019849428550
H	1.507250677209	2.136492691456	0.280272825874
H	-0.685601300155	2.987154048429	1.021310875835
H	-1.507299181974	2.136611339004	-0.279222687181
H	-1.684450615341	1.040588441896	1.991593559307
H	0.054376329053	0.705762013497	1.931454998431
O	-2.316569151257	-0.342443475331	-0.211724426551
C	-3.564172258071	-0.815686419515	0.453007007811
H	-3.576818142809	-0.455062957093	1.485439550348
H	-3.562625894863	-1.910007203361	0.464951852850
C	-4.902587103691	-0.320900773140	-0.247331171543
H	-4.910026646404	0.776392351552	-0.258538639104
H	-4.918032674602	-0.677917557595	-1.284776405764
O	-6.049804959724	-0.835391730488	0.491103458785

C	-7.458593154199	-0.540766743724	0.087914025343
H	-7.656681468075	0.535681642850	0.119120552586
H	-7.667879951802	-0.930999886408	-0.913475135580
H	-8.062196189925	-1.058637698303	0.829984248611
H	0.989572015236	-1.350865487613	-1.081556275132
O	2.316568600373	-0.342518973819	0.211573149255
C	3.564184436905	-0.815343895578	-0.453427710389
H	3.562651351264	-1.909652555010	-0.466036567290
H	3.576836490299	-0.454095880484	-1.485636218566
C	4.902588158475	-0.320969048724	0.247215590891
H	4.910007335675	0.776311257880	0.259103695352
H	4.918041464611	-0.678627244468	1.284433398211
O	6.049815116297	-0.834977566876	-0.491534431279
C	7.458598460682	-0.540576083767	-0.088168897229
H	7.656663861519	0.535890480962	-0.118692729216
H	7.667898274397	-0.931437559636	0.912963869674
H	8.062209161477	-1.057956319442	-0.830567882891

transCydiol-F3500

($E_F = -773.91489982$ a.u.; $G_F = -773.60973186$ a.u.)

0 1

C	-0.622932455391	-0.460856238233	0.504847033538
C	0.622932294621	-0.460589081572	-0.505064540796
C	0.522736374987	0.790857477859	-1.380191904503
C	0.556931800086	2.068917118287	-0.528918092680
C	-0.556973589683	2.068642289105	0.529984880862

C	-0.522764114817	0.790149236108	1.380608457676
H	-0.574230881305	-1.368570554192	1.116669104241
H	1.316315386476	0.799999235171	-2.131839519240
H	-0.427356006952	0.727753095403	-1.919723328752
H	0.464522409481	2.947626694398	-1.174543459519
H	1.529628904470	2.137448805285	-0.030210819001
H	-0.464572013375	2.947023269660	1.176058447488
H	-1.529671995330	2.137420824991	0.031313424969
H	-1.316347691904	0.798895647071	2.132255959352
H	0.427325840168	0.726787972099	1.920114214088
O	-1.902432336917	-0.490683531862	-0.261819753903
C	-3.150033224504	-0.553609578506	0.516187613615
H	-3.223624563290	0.312976428960	1.179830255478
H	-3.147171875314	-1.457830340115	1.136370778877
C	-4.472083297308	-0.562729405879	-0.366383866273
H	-4.472703177687	0.325600512417	-1.011078859748
H	-4.477366519311	-1.454166404478	-1.006085761603
O	-5.633434490041	-0.557166330340	0.516837789943
C	-7.034711502157	-0.560999356107	-0.000084565810
H	-7.231692859166	0.331811988776	-0.602806916865
H	-7.231190398789	-1.461637553640	-0.591171458102
H	-7.650356003151	-0.555395870382	0.896754321909
H	0.574247613600	-1.367995472546	-1.117344326051
O	1.902435504466	-0.490773408827	0.261581828469
C	3.150034050281	-0.553307053914	-0.516460007540
H	3.147195254466	-1.457242758900	-1.137055624090

H	3.223598537138	0.313582937382	-1.179705787688
C	4.472087754252	-0.562794312516	0.366100401933
H	4.472689192733	0.325243135908	1.011194531490
H	4.477393330316	-1.454517543516	1.005399167095
O	5.633436484947	-0.556806579177	-0.517120089802
C	7.034714604156	-0.560841718388	-0.000203516050
H	7.231683177737	0.331710871183	0.602903666675
H	7.231208745023	-1.461731203535	0.590492644671
H	7.650357208128	-0.554840990644	-0.897040221278

transCydiol_Int1-F3500

($E_F = -774.21441621$ a.u.; $G_F = -773.92260216$ a.u.)

0 1

C	-3.402313054657	-0.039586339567	-0.229816028925
C	3.402306614679	-0.038646224538	0.229907021885
C	2.038852882836	0.004601652809	-0.512403161952
C	0.704786056708	0.018823195506	0.381376206761
C	-0.704816716199	0.016915039768	-0.381458448296
C	-2.038875439348	0.006336298677	0.512365224422
H	-3.488664667636	-0.628569962867	-1.142536167353
H	2.033831604946	0.885410636527	-1.165080153237
H	1.975833025626	-0.862328106678	-1.189869660689
H	0.743359491506	0.898316715396	1.032324452983
H	0.732995081921	-0.854390530345	1.042836938722
H	-0.743616584083	0.893462363260	-1.036359632524
H	-0.732791078865	-0.859275722023	-1.038981262005

H	-2.033732208503	0.889712811958	1.161583354305
H	-1.975988267770	-0.857916073427	1.193253067079
O	-4.596492440123	0.083854006906	0.508042643347
C	-5.881382434288	-0.076490729791	-0.213308753710
H	-5.909870453911	-1.075096718041	-0.660712953420
H	-5.927413996039	0.666940201857	-1.013819132807
C	-7.167763899537	0.095102846522	0.702669969708
H	-7.132960049222	-0.646813071353	1.510429989877
H	-7.154790171113	1.096260315894	1.151443807667
O	-8.360812067213	-0.088158320593	-0.113603561994
C	-9.740214997644	0.018175609974	0.452358871198
H	-9.903516407577	-0.737748650304	1.227371626724
H	-9.918288620225	1.018153406426	0.861023801387
H	-10.392514298190	-0.164839841243	-0.398642304193
H	3.488935055767	-0.625427217246	1.143984898829
O	4.596452394006	0.083726712344	-0.508173124789
C	5.881356485919	-0.077338939978	0.212994636401
H	5.926907968608	0.664496470076	1.015017659980
H	5.910319373072	-1.076837645374	0.658357729088
C	7.167751848347	0.096679355230	-0.702521704463
H	7.132239215636	-0.642175898151	-1.513077619652
H	7.155528285708	1.099544350212	-1.147527711793
O	8.360755328943	-0.090561717958	0.112913493604
C	9.740192335542	0.018249481473	-0.452505069333
H	9.903257038361	-0.733686402950	-1.231466093301
H	9.918583423139	1.020310208507	-0.855940632354

H	10.392431262385	-0.169418046080	0.397546173599
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transCydiol_TS1-F3000

($E_F = -773.70440642$ a.u.; $G_F = -773.40471209$ a.u.)

0 1

C	-1.115341441689	-0.398868283979	0.554228863411
C	1.115119085878	-0.399348741753	-0.553891596470
C	0.834645578319	0.863219198683	-1.316946861685
C	0.650963390331	2.092013606221	-0.405800430425
C	-0.650738642395	2.092329137227	0.404693731893
C	-0.834577529991	0.864074217962	1.316541468841
H	-1.000828422202	-1.343759133747	1.084045082607
H	1.674304743878	1.057748084251	-2.004937994753
H	-0.060943714064	0.708698261298	-1.927954543190
H	0.680958998273	2.995614380824	-1.023146879189
H	1.508448829752	2.145434098823	0.273415245916
H	-0.680614722059	2.996279899784	1.021531958472
H	-1.508223769699	2.145484807287	-0.274543161874
H	-1.674222794125	1.059077069436	2.004417790131
H	0.061023945529	0.709748613659	1.927579098092
O	-2.326049023742	-0.323464258664	-0.195183901998
C	-3.553745807389	-0.840953801878	0.448355481355
H	-3.568722097778	-0.532190578291	1.497870515192
H	-3.545880348596	-1.934970618235	0.406980235250
C	-4.878119099388	-0.317724042248	-0.228027841610
H	-4.889928033937	0.779308346989	-0.185961326474

H	-4.892439558622	-0.622545046408	-1.282566206193
O	-6.013489129099	-0.872298997188	0.483840082600
C	-7.398958342295	-0.545538640874	0.081912102975
H	-7.589354555428	0.530380187792	0.165488371439
H	-7.600205294257	-0.877846419780	-0.942699801659
H	-8.026802186955	-1.092259397500	0.782713824819
H	1.000466280425	-1.344498264322	-1.083238065362
O	2.325835999108	-0.323958592711	0.195648599467
C	3.553770090621	-0.839447937006	-0.449063548293
H	3.545761813036	-1.933585510887	-0.411285345443
H	3.569207269370	-0.527289921123	-1.497552343314
C	4.877994657765	-0.318565115990	0.229365735712
H	4.889440940916	0.778614620877	0.191786435576
H	4.892563419545	-0.627694193230	1.282624575177
O	6.013457600701	-0.869819731244	-0.484931100998
C	7.398889086837	-0.544917125204	-0.081393001425
H	7.588999049335	0.531490938593	-0.158992886471
H	7.600356771735	-0.882875272239	0.941315838134
H	8.026785962337	-1.087545845243	-0.785312200179

transCydiol-F3000

($E_F = -773.75424071$ a.u.; $G_F = -773.44825176$ a.u.)

0 1

C	-0.611658230625	-0.452691868837	0.508447085158
C	0.611663185663	-0.452587615726	-0.508542939921
C	0.510166686261	0.799766937194	-1.384416049173

C	0.552625182304	2.077789223533	-0.533776941873
C	-0.552928705068	2.077691526720	0.533826534785
C	-0.510316371299	0.799625039568	1.384391923283
H	-0.554697430254	-1.359086820244	1.122576102457
H	1.299665282687	0.806189473693	-2.140302441594
H	-0.442453389326	0.738966743381	-1.919263113545
H	0.456077866735	2.956746383299	-1.178466511172
H	1.529207334092	2.145746484538	-0.042483171273
H	-0.456487836634	2.956623003689	1.178567035729
H	-1.529519038277	2.145559080294	0.042536630748
H	-1.299817384402	0.805907902857	2.140277001599
H	0.442309916210	0.738910263353	1.919237725708
O	-1.880981082126	-0.487634575378	-0.253798316592
C	-3.114429570039	-0.564405283205	0.526201646992
H	-3.193990792671	0.294211186926	1.200067959835
H	-3.108437230427	-1.475360163130	1.137433980761
C	-4.418348280477	-0.568458263937	-0.359679136564
H	-4.420020194935	0.326142928712	-0.996549405824
H	-4.421159165675	-1.453544295490	-1.009026080022
O	-5.571107784943	-0.573839093962	0.522080648065
C	-6.947217640481	-0.571966393377	-0.017417702661
H	-7.134430083065	0.326553350934	-0.616268036976
H	-7.133927281301	-1.465124389084	-0.624334125134
H	-7.589505513563	-0.576154609137	0.861098313201
H	0.554813605187	-1.358954618828	-1.122723376569
O	1.880991169195	-0.487415959482	0.253699015986

C	3.114448520603	-0.563994544852	-0.526305696593
H	3.108573561165	-1.474924569435	-1.137575355377
H	3.193898091304	0.294659572687	-1.200136596900
C	4.418368289397	-0.567917293571	0.359573457980
H	4.419934888438	0.326666659356	0.996468897907
H	4.421283545515	-1.453021424673	1.008895980768
O	5.571128120090	-0.573138198510	-0.522188149428
C	6.947237894249	-0.571094891903	0.017311141637
H	7.134338230732	0.327451568756	0.616165085417
H	7.134059198507	-1.464234400081	0.624228969065
H	7.589526057207	-0.575202085372	-0.861209562211

transCydiol_Int1-F3000

($E_F = -773.99178846$ a.u.; $G_F = -773.69873877$ a.u.)

0 1

C	-3.359982414398	-0.037455694266	-0.231825436934
C	3.359943672957	-0.037666892589	0.231808304141
C	2.012472293199	0.008129223578	-0.514705531059
C	0.696741541776	0.019935587914	0.382042533386
C	-0.696783286979	0.020361717373	-0.381987111045
C	-2.012512829509	0.007442473428	0.514745188635
H	-3.444383991990	-0.626625578774	-1.144740674140
H	2.008306846723	0.891509589018	-1.164438572708
H	1.948779491657	-0.856528722776	-1.195895277062
H	0.736280673832	0.897476587933	1.036060457032
H	0.725430263294	-0.855397343471	1.041251625668

H	-0.736354806175	0.898675209915	-1.034964437658
H	-0.725439551416	-0.854190179217	-1.042232274651
H	-2.008356424747	0.890030915489	1.165552868995
H	-1.948810404295	-0.858041026837	1.194882103572
O	-4.545882361975	0.084519738699	0.506070230779
C	-5.816602722650	-0.074681736637	-0.219006404591
H	-5.847211979613	-1.072737290469	-0.668766984851
H	-5.864005027372	0.669486937026	-1.019384400617
C	-7.085550213384	0.096200931801	0.698718488356
H	-7.049910254362	-0.645524878152	1.507348336767
H	-7.073587264027	1.097500700573	1.148481707893
O	-8.269077072481	-0.088150884392	-0.117659983009
C	-9.623060084710	0.022252185430	0.467654943956
H	-9.776303296465	-0.730322698990	1.249156160937
H	-9.792753655851	1.023154778928	0.879876973155
H	-10.300112478625	-0.159375557288	-0.364688441528
H	3.444379859464	-0.628064832716	1.143921593411
O	4.545837405914	0.085367202258	-0.505918609356
C	5.816563635147	-0.074885308036	0.218912369116
H	5.863967369799	0.668090493680	1.020387354214
H	5.847183584237	-1.073599479148	0.667187083274
C	7.085504833888	0.097364343618	-0.698554665901
H	7.049944071864	-0.643255503951	-1.508192734192
H	7.073453621945	1.099271305104	-1.146946087870
O	8.269039189368	-0.087991609744	0.117590071402
C	9.623016682900	0.023116173120	-0.467625130721

H	9.776245614859	-0.728531460524	-1.250021356073
H	9.792716673379	1.024506091446	-0.878666194847
H	10.300072332771	-0.159508276239	0.364478473062

transCydiol_TS1-F2500

($E_F = -773.53498853$ a.u.; $G_F = -773.23556733$ a.u.)

0 1

C	-1.136945867788	-0.381663244128	0.568590128734
C	1.137270649903	-0.380484319664	-0.569415402395
C	0.825555568899	0.878700737524	-1.324452570903
C	0.646316894574	2.106349665280	-0.410620593384
C	-0.646855571282	2.105562872845	0.413665046566
C	-0.825809724331	0.876478259202	1.325612024601
H	-1.016654050461	-1.332451170642	1.086095625469
H	1.650653288298	1.083050404801	-2.027861246837
H	-0.078991366268	0.714476671699	-1.919244189679
H	0.667381728633	3.010217381238	-1.028079701027
H	1.510878115492	2.162872368844	0.259293896664
H	-0.668155852311	3.008490449120	1.032491659194
H	-1.511415467830	2.162870904058	-0.256184451764
H	-1.651067615730	1.079512326010	2.029216967861
H	0.078680249185	0.711682053595	1.920334740379
O	-2.339645784902	-0.289511920292	-0.171736553635
C	-3.544026327836	-0.882525648732	0.424942621707
H	-3.559955538728	-0.674281158484	1.499206139764
H	-3.525905659673	-1.968002257678	0.280775569319

C	-4.857884400865	-0.306732212670	-0.200272460243
H	-4.876658069680	0.781735859876	-0.054583793380
H	-4.869413944218	-0.508978560328	-1.279701976916
O	-5.981919082300	-0.932856763014	0.453191528733
C	-7.345462444629	-0.555070377383	0.071265204765
H	-7.527578069817	0.510148141691	0.257117220409
H	-7.537461915142	-0.779495317786	-0.984704551024
H	-7.996711795485	-1.157580847168	0.702043611246
H	1.017215490209	-1.330540053275	-1.088291743454
O	2.339969382705	-0.288865685469	0.170813656609
C	3.544096481429	-0.883335612013	-0.424898342569
H	3.525972068157	-1.968478253767	-0.278226301813
H	3.559717355924	-0.677520112876	-1.499638970227
C	4.858099025936	-0.306130649132	0.198757489168
H	4.877034893613	0.781963847683	0.050211982909
H	4.869580350998	-0.505542319218	1.278731259410
O	5.982037958326	-0.934151309745	-0.453045864886
C	7.345623266603	-0.555322052657	-0.072269494664
H	7.527836476119	0.509320420603	-0.261411457748
H	7.537595308624	-0.776511741459	0.984407451162
H	7.996812995610	-1.159850776522	-0.701198158055

transCydiol_Int1-F2500

($E_F = -773.77172343$ a.u.; $G_F = -773.47767887$ a.u.)

0 1

C	-3.320975435747	-0.036326544645	-0.235941406384
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C	3.321021612347	-0.035665878794	0.235914688335
C	1.988853571711	0.009467783086	-0.515934066728
C	0.689273912602	0.022815978411	0.382959681875
C	-0.689228765989	0.022055168756	-0.383119029795
C	-1.988802733990	0.010293640423	0.515809357468
H	-3.402859801811	-0.629092196624	-1.146902489067
H	1.986067948441	0.892603778896	-1.166439341341
H	1.925036369055	-0.855985630225	-1.196868072796
H	0.729337229777	0.901390339883	1.035967125821
H	0.718084998192	-0.851712954410	1.043714006590
H	-0.729352614600	0.899411947574	-1.037763331499
H	-0.717982523226	-0.853707310550	-1.042245136039
H	-1.986069821617	0.894646715654	1.164668650633
H	-1.924924630969	-0.853885639088	1.198361862593
O	-4.499458385776	0.086510006087	0.501045238408
C	-5.756894318363	-0.072860261285	-0.227970944305
H	-5.788973175622	-1.070943176678	-0.678671246122
H	-5.805470289426	0.671233701151	-1.028888752846
C	-7.009428265343	0.098218542142	0.691951417570
H	-6.972379967390	-0.642966523631	1.501666905772
H	-6.997474692908	1.099861256599	1.142085657160
O	-8.185407312112	-0.087019270977	-0.122916476136
C	-9.514593943727	0.027971716425	0.483653604315
H	-9.656422735044	-0.721556242059	1.271279326506
H	-9.674313327167	1.029802773254	0.899610724996
H	-10.216295718211	-0.151652996784	-0.328980739255

H	3.402936158349	-0.626785881249	1.147955665659
O	4.499505088759	0.085916630006	-0.501298175866
C	5.756944676917	-0.071985795562	0.228055155566
H	5.805475958892	0.673660823227	1.027565928061
H	5.789074649364	-1.069224222110	0.680679473003
C	7.009475809516	0.097416407341	-0.692190175708
H	6.972661743741	-0.645506956279	-1.500294287848
H	6.997279396051	1.098065171789	-1.144476196208
O	8.185463243380	-0.085736312623	0.123103920430
C	9.514646518204	0.027948904874	-0.483691778959
H	9.656649319551	-0.723592134023	-1.269353553634
H	9.674176630640	1.028717091597	-0.902254596286
H	10.216361494294	-0.149412250869	0.329436978103

transCydiol-F2500

($E_F = -773.59551785$ a.u.; $G_F = -773.28888056$ a.u.)

0 1

C	-0.601210865125	-0.442966507251	0.511783892209
C	0.601218713162	-0.442613561645	-0.512083130339
C	0.499585264191	0.811320839657	-1.387568857028
C	0.549464058347	2.088569018542	-0.536464661322
C	-0.549195302355	2.088204183262	0.538181316563
C	-0.499484001349	0.810267239691	1.388265102369
H	-0.536094784293	-1.348481100857	1.127341708106
H	1.286053712663	0.815591458344	-2.146580623636
H	-0.454872325671	0.753536913799	-1.919066540887

H	0.449995351555	2.968323849948	-1.179629010912
H	1.529225014185	2.155099488485	-0.051215450112
H	-0.449618937638	2.967428438881	1.182054372153
H	-1.528946863418	2.155247202462	0.052984453907
H	-1.285991974558	0.814018324286	2.147239266574
H	0.454939712902	0.751966920306	1.919766692705
O	-1.861234445666	-0.482408644690	-0.246430271163
C	-3.081369373151	-0.580673751893	0.534743272999
H	-3.167412763317	0.263790282803	1.226022690278
H	-3.071480341220	-1.503646570752	1.128543269500
C	-4.367578177879	-0.572535980035	-0.355881625414
H	-4.369859701926	0.334149168760	-0.976265187659
H	-4.365517692214	-1.444921942925	-1.022963884402
O	-5.514732463008	-0.598248536509	0.521278250083
C	-6.865505443552	-0.584546418498	-0.044388172358
H	-7.040775926016	0.325969420042	-0.630016841326
H	-7.039860549827	-1.463578607749	-0.676477187724
H	-7.535615363671	-0.607236042207	0.813338392776
H	0.536022662409	-1.347630937617	-1.128363940746
O	1.861240213136	-0.482792476701	0.246099699879
C	3.081392591934	-0.580010150090	-0.535173146719
H	3.071433280344	-1.502074895303	-1.130367261546
H	3.167542816340	0.265486438557	-1.225164744294
C	4.367579702417	-0.573338019824	0.355487011043
H	4.369886692009	0.332356689123	0.977298421822
H	4.365474270197	-1.446770931048	1.021181548111

O	5.514746640904	-0.597708000936	-0.521688463070
C	6.865514823611	-0.585009023856	0.044006541785
H	7.040845412139	0.324545304970	0.631091138789
H	7.039802570006	-1.465058709894	0.674679664317
H	7.535630284215	-0.606369727989	-0.813741651550

transCydiol_TS1-F2000

($E_F = -773.36681842$ a.u.; $G_F = -773.06897582$ a.u.)

0 1

C	-1.158026905571	-0.338990330580	0.595828857541
C	1.157480586037	-0.339806686702	-0.595141184066
C	0.784657977424	0.904560458293	-1.346828872101
C	0.629150730290	2.140576851360	-0.439468463995
C	-0.628382390030	2.141080870491	0.438605388890
C	-0.784388261655	0.905637571809	1.346676453582
H	-1.050532942742	-1.298429381278	1.098430223729
H	1.569695639063	1.117239780221	-2.092708444396
H	-0.145268715280	0.716524592391	-1.892986449012
H	0.616136654350	3.037559820423	-1.067375975165
H	1.520475650210	2.213911459167	0.192408324459
H	-0.614966056616	3.038386962504	1.066041822973
H	-1.519693432341	2.214489146846	-0.193281899206
H	-1.569180499184	1.119133902870	2.092568095324
H	0.145556986685	0.717395977276	1.892720460697
O	-2.358846352879	-0.192766090280	-0.116100655287
C	-3.515309026162	-0.990529611229	0.268440719796

H	-3.508010633998	-1.162279607870	1.349254430837
H	-3.483979741509	-1.959876111979	-0.240041947880
C	-4.834152387160	-0.256708518894	-0.108061674190
H	-4.865624592603	0.711505168482	0.410581204491
H	-4.849404387717	-0.065113212016	-1.189910984346
O	-5.939593566956	-1.085662177005	0.283172430365
C	-7.285568275704	-0.587001681893	0.052520356263
H	-7.463111957495	0.346001223076	0.601975639538
H	-7.469338782672	-0.417689942252	-1.015856421886
H	-7.954930345966	-1.362823097005	0.421248984462
H	1.049638830376	-1.299470210010	-1.097268760573
O	2.358297986070	-0.193985933426	0.117108596286
C	3.515271362303	-0.989635520239	-0.270429166338
H	3.483969528758	-1.961331922310	0.233590851606
H	3.508573284548	-1.156483732228	-1.352025901445
C	4.833793197130	-0.257256122839	0.109896258174
H	4.865157782238	0.713418013364	-0.404147753215
H	4.848813283534	-0.070800981957	1.192654182480
O	5.939490740174	-1.084120684946	-0.285087805066
C	7.285335507978	-0.586278007911	-0.051972371374
H	7.462709664967	0.349406267027	-0.596928901245
H	7.469024922089	-0.422061539591	1.017224894196
H	7.954887939985	-1.360176961213	-0.424398544849

transCydiol_Int1-F2000

($E_F = -773.55404079$ a.u.; $G_F = -773.25921514$ a.u.)

0 1

C	-3.283966762826	-0.037167279191	-0.254026689266
C	3.283876373699	-0.036465141385	0.254059138727
C	1.969245071889	0.009030246159	-0.508646951815
C	0.680657384001	0.022718836157	0.386950981119
C	-0.680752857134	0.021969426803	-0.387020858107
C	-1.969339969386	0.009761411842	0.508598910275
H	-3.359795805513	-0.632681654243	-1.163867118860
H	1.970691035911	0.892834973214	-1.158586832243
H	1.908326777399	-0.856346917782	-1.190593625433
H	0.718495555272	0.901417565622	1.040259191015
H	0.706693165631	-0.851993728254	1.047982354426
H	-0.718668862635	0.899498468338	-1.041894109700
H	-0.706710802118	-0.853922139289	-1.046491746683
H	-1.970853389735	0.894703514265	1.156985330995
H	-1.908357378896	-0.854412493910	1.192061115797
O	-4.458377156931	0.085952540497	0.477539292327
C	-5.700816110978	-0.072205291793	-0.260269085229
H	-5.732548678446	-1.069451409631	-0.713842868584
H	-5.747642110309	0.673596062821	-1.060194856758
C	-6.940512390931	0.097327540213	0.658950042590
H	-6.903903719910	-0.645258084960	1.467995324831
H	-6.928840701625	1.098218751770	1.111785415895
O	-8.108393749902	-0.086180597146	-0.156832343268
C	-9.414777386822	0.031901240213	0.469275434290
H	-9.546392300631	-0.717616216023	1.259630274713

H	-9.564130988220	1.033186974990	0.892134744574
H	-10.138806826795	-0.142222196169	-0.325259545807
H	3.359747302077	-0.630337921117	1.164966488340
O	4.458276908173	0.085453864276	-0.477723246344
C	5.700727177968	-0.071559594052	0.260324505363
H	5.747459178772	0.675342320610	1.059244978763
H	5.732569592485	-1.068193063403	0.715260261192
C	6.940417939010	0.096846411038	-0.659114693087
H	6.903706397479	-0.646617986010	-1.467350485212
H	6.928848174403	1.097250683099	-1.113039446460
O	8.108297280516	-0.085894266365	0.156836743217
C	9.414684284619	0.031727341372	-0.469343563460
H	9.546298993650	-0.718358746731	-1.259183009961
H	9.564039618022	1.032733148577	-0.892905691275
H	10.138710975103	-0.141843903655	0.325333457551

transCydiol-F2000

($E_F = -773.43861637$ a.u.; $G_F = -773.13140121$ a.u.)

0 1

C	-0.594070663638	-0.433405745238	0.512021758435
C	0.593907273887	-0.432977262635	-0.512665675407
C	0.497385839400	0.822451050224	-1.388173334338
C	0.549417456107	2.098954116440	-0.536361970799
C	-0.549054206933	2.098505598252	0.538413360189
C	-0.497326644655	0.821077587203	1.388859690054
H	-0.523669110337	-1.337871072811	1.129361643024

H	1.285596532430	0.824588199006	-2.145381605753
H	-0.455666091513	0.767715985760	-1.922206275941
H	0.451109634209	2.979457959795	-1.178687157615
H	1.529313629993	2.163949730405	-0.051069467665
H	-0.450539067349	2.978294030058	1.181686716887
H	-1.528934990548	2.164259498200	0.053191670271
H	-1.285572951762	0.822572781971	2.146032899228
H	0.455687374559	0.765580347090	1.922880559938
O	-1.841681817909	-0.478075953860	-0.248691697259
C	-3.053045368423	-0.602171110346	0.526750859271
H	-3.150943491704	0.226064007623	1.236324556625
H	-3.040181973975	-1.538151201064	1.100596248483
C	-4.316987491267	-0.582063343178	-0.376478785607
H	-4.316874782490	0.337531402509	-0.978317096367
H	-4.303511603646	-1.440027169491	-1.062538778133
O	-5.465858851886	-0.631365222771	0.486684798369
C	-6.787472800171	-0.604497785662	-0.115176347953
H	-6.946552981370	0.319193666489	-0.685906403160
H	-6.942849230473	-1.467314934638	-0.775135937927
H	-7.490778005468	-0.647553417448	0.715236050418
H	0.523333547079	-1.336774912066	-1.130963347804
O	1.841514506917	-0.478691503691	0.247993417856
C	3.052865128253	-0.601977370976	-0.527602810380
H	3.039840225390	-1.537197552956	-1.102699284081
H	3.150921848596	0.227191151505	-1.236077350963
C	4.316802899921	-0.583295557988	0.375670920103

H	4.316846386955	0.335503033063	0.978742174135
H	4.303175224000	-1.442180939486	1.060589965514
O	5.465670135828	-0.631641255919	-0.487562184448
C	6.787287254518	-0.605807981723	0.114342606581
H	6.946524480266	0.317097986359	0.686320278751
H	6.942515359877	-1.469547728892	0.773147993248
H	7.490586404633	-0.647866561424	-0.716135226273

transCydioI_TS1-F1500

($E_F = -773.19996489$ a.u.; $G_F = -772.90053071$ a.u.)

0 1

C	-1.187230746526	-0.301787771311	0.629582798264
C	1.187476745125	-0.300844499310	-0.630006716527
C	0.753822931265	0.932226803675	-1.365846146807
C	0.614036913948	2.170438341678	-0.458176084327
C	-0.614570157465	2.169812935521	0.460316905034
C	-0.754015267576	0.930652943324	1.366734471040
H	-1.085112898399	-1.269184942678	1.116949774886
H	1.499187387688	1.160339431774	-2.147469266312
H	-0.194886560797	0.722312473454	-1.869477192139
H	0.573390331820	3.064192192203	-1.089721031798
H	1.524506070721	2.256057454829	0.143886152610
H	-0.574181894082	3.062953558246	1.092745023912
H	-1.525060791933	2.255765410478	-0.141666606534
H	-1.499507771036	1.157742017085	2.148538446442
H	0.194720772664	0.720534472057	1.870234656034

O	-2.387910123830	-0.115005543669	-0.053283226386
C	-3.494103223018	-1.020592293575	0.163087902430
H	-3.467083392518	-1.416285311574	1.183410716376
H	-3.438428693194	-1.858723454615	-0.539610168016
C	-4.822213334455	-0.257063331946	-0.046398367487
H	-4.871010441004	0.578165983795	0.666548948843
H	-4.845416347189	0.162062528929	-1.062312120670
O	-5.903573509699	-1.169810288378	0.157319084844
C	-7.236814022499	-0.631136797370	0.032620281906
H	-7.415998969100	0.164013514268	0.768084168684
H	-7.413832235528	-0.232995129260	-0.975035889092
H	-7.917763314755	-1.460408331974	0.220537641971
H	1.085559101902	-1.267774139798	-1.118337273373
O	2.388209559325	-0.114365791719	0.052787763786
C	3.494129367908	-1.020395897151	-0.163143745195
H	3.438407602979	-1.857999817330	0.540261641885
H	3.466800541987	-1.416895433102	-1.183204881070
C	4.822446120513	-0.256916750468	0.045501942716
H	4.871301167968	0.577773033829	-0.668154180653
H	4.845881046929	0.163038166877	1.061124150144
O	5.903597232745	-1.170059793983	-0.157651038025
C	7.236956587542	-0.631540665827	-0.033446360080
H	7.416271416885	0.162990565089	-0.769574499823
H	7.414096443009	-0.232618210155	0.973898559210
H	7.917725351648	-1.461117631953	-0.220730236642

transCydiol_Int1-F1500

($E_F = -773.33860086$ a.u.; $G_F = -773.04326734$ a.u.)

0 1

C	-3.249203307697	-0.035947384164	-0.273075004132
C	3.249230059333	-0.036201478756	0.273048949356
C	1.951527187957	0.009960990822	-0.500668674381
C	0.672476106039	0.023136537016	0.391222290133
C	-0.672450200278	0.023514428171	-0.391184579170
C	-1.951501601509	0.009458338601	0.500691253243
H	-3.319405387384	-0.633004813002	-1.182486780259
H	1.957344250556	0.894945459124	-1.149243085589
H	1.894005103961	-0.854872433614	-1.184152134645
H	0.707882049116	0.901238315395	1.045748452287
H	0.695289134892	-0.852549335946	1.051425865697
H	-0.707861253513	0.902255480185	-1.044850930222
H	-0.695257403836	-0.851524582191	-1.052244108597
H	-1.957320017183	0.893807726422	1.150132520611
H	-1.893979362614	-0.856043907358	1.183328178981
O	-4.419646740908	0.086968350590	0.453596669841
C	-5.648623773871	-0.067928468945	-0.292081082918
H	-5.680722572010	-1.063299685766	-0.750615883304
H	-5.694302278457	0.681598190144	-1.089028919371
C	-6.874301041433	0.098441590174	0.629701546502
H	-6.835650257679	-0.647159145995	1.436410143180
H	-6.861036366601	1.097620138467	1.087192628341
O	-8.037676765277	-0.081262183732	-0.183119900573

C	-9.319532067000	0.039067874054	0.467785514470
H	-9.437608145334	-0.711905482101	1.259799081461
H	-9.456117140406	1.039129849692	0.899433434614
H	-10.068037475983	-0.128094595466	-0.305795305272
H	3.319447480295	-0.634193739765	1.181840301979
O	4.419670842782	0.087490931411	-0.453493305294
C	5.648650590989	-0.068195785961	0.292012188846
H	5.694297926570	0.680438534313	1.089799015961
H	5.680783756633	-1.064078447681	0.749430062170
C	6.874324948954	0.099249384182	-0.629580949046
H	6.835653851068	-0.645392415302	-1.437178239770
H	6.861077367603	1.098974953699	-1.085884128784
O	8.037701425756	-0.081438974057	0.183024575850
C	9.319557783224	0.039693773958	-0.467728889046
H	9.437655694577	-0.710337532699	-1.260632718326
H	9.456122379524	1.040271504402	-0.898189744456
H	10.068063180426	-0.128367136397	0.305660251408

transCydiol-F1500

($E_F = -773.28345786$ a.u.; $G_F = -772.97618395$ a.u.)

0 1

C	-0.585472310667	-0.403415571743	0.514719341111
C	0.585517118508	-0.403046336067	-0.515026716943
C	0.492341041089	0.853791625931	-1.390144188310
C	0.548195890100	2.129526665929	-0.537660951452
C	-0.548002794705	2.129152319348	0.539299867792

C	-0.492262630181	0.852751415324	1.390797198617
H	-0.507073100222	-1.306646474379	1.133593352819
H	1.281228528960	0.853764792697	-2.146703192712
H	-0.460218506882	0.802303823123	-1.925197574962
H	0.449911559724	3.010780183113	-1.178971962187
H	1.529166006481	2.192744033445	-0.054251390548
H	-0.449646443528	3.009897158742	1.181298446480
H	-1.528966399313	2.192831364622	0.055938278978
H	-1.281190845518	0.852190607831	2.147314301521
H	0.460265249087	0.800800305732	1.925861340744
O	-1.824091340412	-0.453930695502	-0.243928189387
C	-3.023361502042	-0.617586393410	0.528670426707
H	-3.132446717903	0.183958383889	1.267146500120
H	-3.001891280129	-1.573412663718	1.069322904848
C	-4.268510243320	-0.576859836527	-0.382857506586
H	-4.270922260885	0.363806086834	-0.951941231746
H	-4.240630207847	-1.409211925319	-1.099982439164
O	-5.418494577512	-0.666814590214	0.465444173410
C	-6.711439509933	-0.618024578234	-0.170566946452
H	-6.856662905632	0.327617850291	-0.709400892556
H	-6.844927214220	-1.452474860547	-0.871592762958
H	-7.446044445706	-0.696011552874	0.630144633761
H	0.507082883958	-1.305799996583	-1.134592924535
O	1.824135963991	-0.454198014744	0.243579487565
C	3.023423817296	-0.616978311372	-0.529176504715
H	3.001937580542	-1.572156911838	-1.070973403018

H	3.132558123549	0.185446094244	-1.266690252667
C	4.268553238696	-0.577377295667	0.382426467688
H	4.270960066873	0.362593558634	0.952662888235
H	4.240660006030	-1.410609503827	1.098532458160
O	5.418548463622	-0.666295404285	-0.465974596553
C	6.711487627374	-0.618302210638	0.170110050919
H	6.856696807956	0.326654794170	0.710154564915
H	6.844981840698	-1.453648050537	0.870071978394
H	7.446099074589	-0.695256083418	-0.630696834988

transCydiol_TS1-F1000

($E_F = -773.03413633$ a.u.; $G_F = -772.73421152$ a.u.)

0 1

C	-1.224887960702	-0.239490620722	0.688485645207
C	1.224824816360	-0.239240355534	-0.688594943299
C	0.713658181664	0.979998750778	-1.394014070776
C	0.596144258729	2.218472937954	-0.482409136308
C	-0.596085804974	2.218281616298	0.483355795747
C	-0.713639334047	0.979414413140	1.394423867449
H	-1.120389735906	-1.215035793889	1.158326966448
H	1.404113259236	1.228289581380	-2.219165320416
H	-0.256455729942	0.744519223957	-1.841678673423
H	0.524489397035	3.110072226160	-1.114448676973
H	1.528350877757	2.314671293080	0.083335164966
H	-0.524399296289	3.109603972809	1.115782236495
H	-1.528289467875	2.314759266657	-0.082345181087

H	-1.404058951830	1.227380349784	2.219701537229
H	0.256476048495	0.743688480401	1.841953920753
O	-2.439138683422	-0.011144140085	0.062369582654
C	-3.473163701816	-1.007145104290	0.101966130594
H	-3.427246830359	-1.572536280947	1.038870619385
H	-3.363733926774	-1.705317265880	-0.734930702192
C	-4.825374162516	-0.282579058642	0.008634832350
H	-4.915231574188	0.414947797416	0.853895425564
H	-4.860369893449	0.305920532554	-0.919595919471
O	-5.862524496665	-1.257524612976	0.036569805823
C	-7.195069710026	-0.729122158036	-0.004475188957
H	-7.394740239580	-0.080343777689	0.859063321752
H	-7.371004314391	-0.157500920751	-0.925740163831
H	-7.869533896758	-1.584562636686	0.023346435754
H	1.120292082622	-1.214571251389	-1.158872063153
O	2.439053612408	-0.011255253618	-0.062290429832
C	3.473170522306	-1.007131826313	-0.102779452519
H	3.363625967635	-1.706256628349	0.733307883863
H	3.427489709393	-1.571470558469	-1.040328594709
C	4.825315194940	-0.282582897439	-0.008405137586
H	4.915157920076	0.416065138610	-0.852740250136
H	4.860234496654	0.304689877737	0.920603452850
O	5.862532340841	-1.257421778627	-0.037591523747
C	7.195042687290	-0.728993986866	0.004225630509
H	7.394667702627	-0.078930736547	-0.858356023786
H	7.370944993117	-0.158720162683	0.926330176257

H	7.869562642276	-1.584347652342	-0.024860979394
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transCydiol-F1000

($E_F = -773.13000645$ a.u.; $G_F = -772.82354313$ a.u.)

0 1

C	-0.575578918196	-0.354471325432	0.519514763885
C	0.575492283218	-0.355111937782	-0.519538907168
C	0.484530810201	0.902652659901	-1.394437545416
C	0.546205236904	2.177984832554	-0.541965366594
C	-0.546050046563	2.178720405981	0.538799128548
C	-0.484802697228	0.904407189753	1.392847176988
H	-0.486124133329	-1.255711945210	1.140342844705
H	1.273134731487	0.899605469773	-2.151410755419
H	-0.468444626089	0.854748512192	-1.929047491221
H	0.447385268501	3.059722020560	-1.182539049338
H	1.529039116218	2.239056943038	-0.062045664976
H	-0.447101981532	3.061205356990	1.178323142759
H	-1.528831116506	2.239383638726	0.058736763019
H	-1.273842276997	0.902400504339	2.149385070239
H	0.467899180139	0.857124846778	1.928003864004
O	-1.808636555730	-0.412575452988	-0.232216907123
C	-2.991396878639	-0.629329832215	0.539808493630
H	-3.112165094602	0.136695353410	1.313810150085
H	-2.953361242442	-1.608296745234	1.037076640468
C	-4.221349012791	-0.565886677033	-0.375515830788
H	-4.234806396030	0.401129069589	-0.899138461780

H	-4.172825553425	-1.361523682871	-1.132702133684
O	-5.371323253110	-0.715331257395	0.454729093771
C	-6.636041630629	-0.639353978475	-0.212980193872
H	-6.773501930427	0.334538240371	-0.702450181157
H	-6.741480233876	-1.431983614663	-0.966280776677
H	-7.399886923773	-0.767985115509	0.553606951721
H	0.486074277616	-1.257095682263	-1.139312855227
O	1.808468352455	-0.412555972473	0.232391946079
C	2.991875732106	-0.624807944475	-0.539861206538
H	2.954017436679	-1.600525148558	-1.043440170515
H	3.113594521560	0.146126561727	-1.308781006224
C	4.221114519255	-0.567505913662	0.376780473323
H	4.233711546610	0.395634151978	0.907476717859
H	4.172577855304	-1.368695172366	1.128050355515
O	5.371658387816	-0.710255794260	-0.453870907179
C	6.635983034740	-0.638780462721	0.215054438227
H	6.772806135367	0.331490943450	0.711838023182
H	6.741336279463	-1.436958477789	0.962488712693
H	7.400283296922	-0.761412640054	-0.552066897436

transCydiol_Int1-F1000

($E_F = -773.12530289$ a.u.; $G_F = -772.82975480$ a.u.)

0 1

C	-3.216668720311	-0.032287577510	-0.293851254117
C	3.216652327989	-0.032474033784	0.293794308456
C	1.935358240213	0.012057588811	-0.491225762102

C	0.664253691436	0.026020038672	0.396000290365
C	-0.664270593027	0.026271913515	-0.396016965018
C	-1.935375671145	0.011742241977	0.491199144193
H	-3.282412432624	-0.633487830635	-1.200991312030
H	1.945599858789	0.896928506402	-1.140090071810
H	1.882149626648	-0.853648959852	-1.174420450166
H	0.696544868706	0.904614410493	1.050247056721
H	0.683266173489	-0.849581905759	1.056709279581
H	-0.696562425654	0.905283638094	-1.049702913726
H	-0.683281961893	-0.848908173758	-1.057284701508
H	-1.945617353791	0.896198731827	1.140628609767
H	-1.882168324186	-0.854400655132	1.173840966519
O	-4.382766704414	0.093733317634	0.428480747263
C	-5.600686228426	-0.057627933106	-0.322224146781
H	-5.635009808294	-1.051482298954	-0.784645155286
H	-5.646604507944	0.695182083756	-1.116452149513
C	-6.809200691765	0.107390846897	0.607011803206
H	-6.764888155531	-0.640676305390	1.411640882485
H	-6.790550608242	1.105077426910	1.068418858602
O	-7.973626104463	-0.067605709439	-0.195685762239
C	-9.226685364071	0.055795587691	0.488483688236
H	-9.325982729771	-0.696778080045	1.282363010742
H	-9.346159509574	1.054612991788	0.929459153822
H	-10.003983659974	-0.103689509123	-0.258363051082
H	3.282401103914	-0.634265001218	1.200541896360
O	4.382748757810	0.094024700795	-0.428456876289

C	5.600670103909	-0.057841720118	0.322142710252
H	5.646584926261	0.694424938601	1.116885731328
H	5.635000247468	-1.052012157604	0.783883041886
C	6.809182051912	0.107819103378	-0.606982566431
H	6.764864912230	-0.639690415121	-1.412129869383
H	6.790533053522	1.105825465568	-1.067697933114
O	7.973609084592	-0.067736129589	0.195590570566
C	9.226667720675	0.056137420564	-0.488494330857
H	9.325963676486	-0.695886312452	-1.282892879115
H	9.346142358613	1.055257868847	-0.928778903275
H	10.003966636180	-0.103864012649	0.258240053430

transCydiol_TS1-F500

($E_F = -772.86913597$ a.u.; $G_F = -772.56951581$ a.u.)

0 1

C	-1.282826120240	-0.140829940714	0.803463745623
C	1.282711486661	-0.141049317520	-0.804189585072
C	0.646215711156	1.053936609828	-1.440176317375
C	0.569229308114	2.287798140058	-0.515349234445
C	-0.568773498281	2.287832488930	0.514636954270
C	-0.645863807639	1.053924646860	1.439415118190
H	-1.139030767909	-1.133663504201	1.224652336955
H	1.235019975258	1.335509367136	-2.330915764439
H	-0.352600271905	0.776789029112	-1.788985315800
H	0.459115816132	3.181593934229	-1.138841038575
H	1.530590676355	2.388483325101	-0.001755854288

H	-0.458563035961	3.181599160985	1.138153516816
H	-1.530129799699	2.388632904834	0.001055933610
H	-1.234383958922	1.335578355913	2.330311270855
H	0.352965248123	0.776491194399	1.787950879949
O	-2.546034057380	0.131126216385	0.328654058274
C	-3.470390741110	-0.943087702194	0.152567744686
H	-3.423650083803	-1.636513055417	1.000407110255
H	-3.248855864493	-1.497970098508	-0.766008411035
C	-4.861771415690	-0.317464258644	0.078137340367
H	-5.042157491125	0.258857869114	0.997407320818
H	-4.906023804086	0.381078358175	-0.770356551429
O	-5.813131052592	-1.359465209157	-0.066652892362
C	-7.163038200208	-0.902416285688	-0.096231466872
H	-7.430127751569	-0.380685830033	0.833290686429
H	-7.339480988482	-0.224886672806	-0.943208152114
H	-7.794418977785	-1.784149667601	-0.206066944125
H	1.139010987830	-1.133738528948	-1.225737460547
O	2.545635807081	0.130553172103	-0.328405586143
C	3.470392283230	-0.943663054077	-0.154363721988
H	3.247897530432	-1.501601048372	0.762119975463
H	3.425261358569	-1.634400688871	-1.004469125606
C	4.861323645564	-0.317527294488	-0.076143146588
H	5.042039930899	0.262747370721	-0.992832657257
H	4.904566786289	0.377447552318	0.775306052609
O	5.813170719119	-1.359581898880	0.064933639491
C	7.162799990287	-0.901932241247	0.097435315454

H	7.430155894953	-0.375823191818	-0.829512353768
H	7.338347403946	-0.228189684688	0.947592225544
H	7.794610128831	-1.783790522396	0.203636354231

transCydiol-F500

($E_F = -772.97829547$ a.u.; $G_F = -772.67101977$ a.u.)

0 1

C	-0.560029307848	-0.276561122377	0.530125409116
C	0.560046861278	-0.276354445372	-0.530844607048
C	0.463316790279	0.984329424875	-1.401404361727
C	0.539286539604	2.257422575408	-0.547036968262
C	-0.539431905777	2.257223038756	0.547099783968
C	-0.463414561935	0.983865479608	1.401071855316
H	-0.451483940840	-1.175846975581	1.151402704473
H	1.243807596834	0.979280465356	-2.166869972272
H	-0.495590100819	0.941445629236	-1.925764976465
H	0.434678259069	3.141034023494	-1.184086341025
H	1.528154306544	2.315086048193	-0.079052098333
H	-0.434868914857	3.140638432578	1.184428593688
H	-1.528300337976	2.314986269366	0.079129994288
H	-1.243946691446	0.978531246786	2.166494446300
H	0.495468650902	0.940884439581	1.925467718794
O	-1.795203530192	-0.346441688543	-0.201965342202
C	-2.957628299163	-0.582187458081	0.583431487302
H	-3.102821000113	0.199061952684	1.338436844270
H	-2.887081912153	-1.547260168555	1.104491873829

C	-4.171511798074	-0.579696584823	-0.341139287984
H	-4.207738882896	0.373268642717	-0.889491687214
H	-4.088838548886	-1.391311375006	-1.078585409153
O	-5.322105766554	-0.743375978458	0.476435913112
C	-6.556239860698	-0.706957989534	-0.232259172681
H	-6.697821860991	0.255136178449	-0.744507373190
H	-6.618128689110	-1.513287598049	-0.976580517956
H	-7.349035560145	-0.839690777637	0.504168278131
H	0.451578060567	-1.175457815623	-1.152400722211
O	1.795219485198	-0.346372670894	0.201234904725
C	2.957725872775	-0.581359866751	-0.584267525961
H	2.887299946658	-1.545992938325	-1.106162223879
H	3.102920047837	0.200550180087	-1.338590591346
C	4.171539091681	-0.579553907513	0.340398763126
H	4.207586981139	0.372910936171	0.889636476274
H	4.088934807739	-1.391864660785	1.077088634903
O	5.322212783558	-0.742307043425	-0.477251592941
C	6.556293052757	-0.706401497980	0.231562767926
H	6.697711587737	0.255222456830	0.744743221200
H	6.618239557453	-1.513436427338	0.975117732941
H	7.349157166160	-0.838322986609	-0.504938495331

transCydiol_Int1-F500

($E_F = -772.91409918$ a.u.; $G_F = -772.61871156$ a.u.)

0 1

C	-3.187070226421	-0.023382409052	-0.310600395099
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C	3.187030096003	-0.023022060881	0.310334872563
C	1.919727587032	0.016369170256	-0.483234050850
C	0.656580941732	0.030237182232	0.400372538476
C	-0.656626319038	0.030159119951	-0.400642082425
C	-1.919771059615	0.016166253210	0.482964852623
H	-3.253885029085	-0.631341935904	-1.213278860393
H	1.932214378938	0.900407954345	-1.133304600327
H	1.871516223759	-0.851050778333	-1.165022184827
H	0.685669373904	0.909340027490	1.054266565517
H	0.672482696766	-0.845330326783	1.061429431392
H	-0.685811116856	0.909248707759	-1.054548828749
H	-0.672432279479	-0.845419827812	-1.061685469600
H	-1.932355939103	0.900214739727	1.133018721488
H	-1.871462097767	-0.851234899188	1.164768371229
O	-4.345586789981	0.112083904729	0.411818780925
C	-5.558694480894	-0.032551507109	-0.335409325935
H	-5.601708574573	-1.024929723558	-0.800923669494
H	-5.608721250989	0.723699570241	-1.126472850513
C	-6.740640132661	0.134956035812	0.613248137247
H	-6.683055516451	-0.615477144214	1.415286076094
H	-6.707385339302	1.131044685763	1.078057847370
O	-7.917406314950	-0.031503213147	-0.163662042403
C	-9.130571655280	0.097582996857	0.571467995886
H	-9.201196142701	-0.657420183232	1.366841486306
H	-9.222676818084	1.094829518938	1.023735096806
H	-9.946488373628	-0.050907759187	-0.135913324661

H	3.253910399710	-0.630952949032	1.213029748288
O	4.345532936448	0.112552919791	-0.412086535602
C	5.558655446422	-0.031882596573	0.335157337193
H	5.608597272691	0.724446475953	1.126153793046
H	5.601779242337	-1.024215371430	0.800762412825
C	6.740583436068	0.135671673364	-0.613514741303
H	6.683094925317	-0.614851821766	-1.415473854784
H	6.707206455443	1.131707190946	-1.078427848019
O	7.917368090726	-0.030562058030	0.163414219260
C	9.130519062283	0.098599037224	-0.571726258907
H	9.201228636797	-0.656465727656	-1.367037593666
H	9.222511094489	1.095820601940	-1.024078549456
H	9.946453493230	-0.049740367332	0.135670770182

Cam_TS1

($E_F = -929.38447827$ a.u.; $G_F = -928.99726281$ a.u.)

0 1

C	-1.794727207069	0.967238200281	-2.633387759132
C	-1.080788462354	2.250912988802	-2.197308653341
C	-2.183494124714	1.987796456883	0.068788197438
C	-2.773446044563	0.723076325695	-0.493895567929
C	-1.708290885724	-0.396505348891	-0.571852752789
C	-1.069326593882	-0.239009089748	-1.970980336946
H	-0.103011678173	2.120026744387	-1.734723666457
H	-1.217169777992	1.916128835772	0.568293065239
H	-3.628273651486	0.443792027258	0.132683315282

H	-0.978116533836	-0.313113234041	0.236638063143
H	-2.183092866181	-1.373746845280	-0.464473758263
H	-1.223857422379	-1.135639002842	-2.575284768144
H	0.010529554498	-0.077570183209	-1.928366032951
C	-3.223801319584	0.912233599848	-1.974568489883
C	-4.058619364827	-0.294185042296	-2.445513541671
H	-4.388455091557	-0.161255034094	-3.478821744058
H	-3.521752387222	-1.242876743941	-2.388214604512
H	-4.956438139906	-0.382912900674	-1.826755809253
C	-4.053032451428	2.181316379782	-2.205612429279
H	-4.291177141161	2.291810956163	-3.267656070769
H	-4.996564649191	2.122192714247	-1.655001297883
H	-3.525407247379	3.075851991009	-1.877842447174
O	-1.085834221065	3.274746960113	-3.142711906162
O	-3.101174010055	2.765606826538	0.773779564608
C	-1.812512804186	0.842645205167	-4.163176113481
H	-0.792674829401	0.832748668317	-4.556703009178
H	-2.291241975274	-0.090474618091	-4.466814348307
H	-2.341473617655	1.675757472491	-4.625842243741
C	0.172941776064	3.663918935172	-3.766561834292
H	0.956971656393	2.946130541337	-3.508895727805
H	0.462054571084	4.647997620872	-3.387444767480
C	0.056995721059	3.740568634114	-5.315232819702
H	-0.212324779452	2.756083423079	-5.717196429821
H	-0.736760907397	4.449697941687	-5.587976451833
C	-2.998092439916	2.846066482094	2.222484183143

H	-3.016898395461	3.903931606331	2.493737042366
H	-2.050375942581	2.416088942384	2.560792442567
C	-4.174110216374	2.137570435885	2.954979631401
H	-5.125289849652	2.530347707436	2.569948252890
H	-4.144661381256	1.056498254310	2.756155488390
O	1.326746830216	4.167282769399	-5.829580125571
C	1.469439792210	4.261003775972	-7.268992453282
H	1.305158731940	3.287924120085	-7.749157485115
H	0.770172000594	4.993303234386	-7.691921851846
H	2.492861276952	4.588225993276	-7.446975348302
O	-4.036662189058	2.403207443844	4.358021175500
C	-5.055271409326	1.886946997202	5.250230484241
H	-6.043455040314	2.296618299272	5.005153881719
H	-5.100643816201	0.790990201253	5.212316604319
H	-4.765211758974	2.205945280937	6.250461180186

Cam_Int1

($E_F = -929.50587285$ a.u.; $G_F = -929.12223898$ a.u.)

0 1

C	-1.489993171916	1.814075943249	-2.520171888190
C	-0.986492587656	2.774155830448	-3.594152083015
C	-3.278531335944	2.013311060139	0.956500142539
C	-2.608635465422	1.488727527392	-0.294730673606
C	-1.090072890162	1.138510154316	-0.124838305250
C	-0.381237975648	1.464629746456	-1.467560676087
H	-0.581469161999	3.738876526311	-3.296341085046

H	-2.908918805992	2.924891025453	1.423260438444
H	-3.143965660555	0.573387406116	-0.564795824798
H	-0.659998107668	1.731866537117	0.686018526314
H	-0.975492209763	0.090517791127	0.160156253824
H	0.238136817883	0.639249097816	-1.826558592788
H	0.284193828020	2.321935195399	-1.341388855032
C	-2.627634084666	2.438773914438	-1.567263674592
C	-4.012029864771	2.463915865370	-2.221571545469
H	-3.987288803120	3.038969523040	-3.152254234782
H	-4.375049138436	1.459860930798	-2.450037716490
H	-4.736359814200	2.930742498795	-1.548017767107
C	-2.259730629924	3.880076174956	-1.160302323833
H	-2.259305143040	4.539179139743	-2.031027418623
H	-2.999168669451	4.273072556902	-0.459078573315
H	-1.278241252835	3.945477794307	-0.683705922860
O	-0.443417224677	2.264755460693	-4.765435559985
O	-3.856718678371	1.107930833068	1.835323728059
C	-1.967094772101	0.514657491959	-3.198674533090
H	-1.134931790950	0.055151032549	-3.734780289063
H	-2.336698703743	-0.206233041710	-2.466548183619
H	-2.758714410166	0.707152440364	-3.924742249844
C	0.110380873301	3.244858075751	-5.679784400077
H	0.916650804983	3.795739598903	-5.182014581972
H	-0.669803465954	3.957590347009	-5.966242977571
C	0.677650976811	2.578981441714	-6.957211866965
H	1.460871168691	1.858343184943	-6.683520609161

H	-0.122129224833	2.034611464973	-7.477987455718
C	-4.361506747147	1.678297711536	3.071032057915
H	-5.115219632144	2.438161399727	2.840050897665
H	-3.539877362000	2.160221893490	3.613155651044
C	-4.996356968884	0.605038172383	3.988255628097
H	-5.837856313468	0.123681549856	3.471218944540
H	-4.252521769482	-0.167956122159	4.226409253906
O	1.206898678888	3.628805275551	-7.778493399291
C	1.795819428531	3.264789119250	-9.051368608560
H	2.654567431629	2.594987621463	-8.916210500107
H	1.060777659353	2.780379461779	-9.706589489123
H	2.128357033542	4.198442985389	-9.502897637881
O	-5.437432659033	1.279954553712	5.174672817010
C	-6.085755507572	0.494021237864	6.204753510684
H	-7.002666037732	0.022736463280	5.828675429853
H	-5.415644031360	-0.282550817873	6.594919413428
H	-6.335120935013	1.194698593526	7.000390362122

Cam

($E_F = -929.41833017$ a.u.; $G_F = -929.02438381$ a.u.)

0 1

C	-1.837428138740	0.806105876940	-2.546438018874
C	-1.199680694235	2.024144040938	-1.784887677487
C	-1.919870042456	1.909581904095	-0.314064832057
C	-2.803125934358	0.652094247735	-0.504621180487
C	-1.872735431852	-0.579215164815	-0.527601212298

C	-1.199449471310	-0.466980687757	-1.925667184622
H	-0.145783553272	1.805540178044	-1.588620497520
H	-1.107927312897	1.700336353043	0.393188231839
H	-3.595744696261	0.598896987345	0.240682193108
H	-1.151039079103	-0.556246153667	0.292903877435
H	-2.439121502303	-1.506548565867	-0.426598474558
H	-1.412582482140	-1.340811065645	-2.545001806285
H	-0.111263822067	-0.380069800177	-1.867998753084
C	-3.291746156789	0.766889113258	-1.971622684473
C	-4.129438959817	-0.436211602700	-2.434808999663
H	-4.388152322491	-0.335780940750	-3.492713366623
H	-3.632510418719	-1.398329977616	-2.308345171121
H	-5.067665428475	-0.472055955606	-1.872550408786
C	-4.109590246311	2.036527016623	-2.263602032342
H	-4.357357529659	2.083662234666	-3.328346488770
H	-5.049634054175	2.009142290528	-1.704023565682
H	-3.592783327539	2.955616260639	-1.999207116757
O	-1.235884493577	3.246656307827	-2.544369747000
O	-2.667870713008	3.007148531290	0.218746894515
C	-1.712796372861	0.860318828983	-4.059069398271
H	-0.666021943100	0.880704813648	-4.375780376665
H	-2.173726758988	-0.024361849175	-4.506303566303
H	-2.206942359539	1.744238697394	-4.461418495017
C	-0.020526008223	3.534850962166	-3.288737038622
H	0.628094437854	2.654597613083	-3.315202626895
H	0.520485947562	4.334894734168	-2.772674468873

C	-0.247329484035	3.972104302660	-4.763641380179
H	-0.830667179813	3.214567448104	-5.298478913492
H	-0.800162670926	4.920679826154	-4.800458900446
C	-2.736071745357	3.087050014550	1.659772414255
H	-2.960370861110	4.133123455742	1.875111359910
H	-1.756408613049	2.853418343998	2.095308644787
C	-3.819032633211	2.236144517866	2.399188594732
H	-4.793635379914	2.381661538944	1.911861781199
H	-3.572325928559	1.166342511466	2.364581883967
O	1.055331428548	4.114349195396	-5.355549136754
C	1.128847709212	4.441359835641	-6.764448487213
H	0.643192129750	3.671471790820	-7.377915612097
H	0.664363177599	5.413316994494	-6.974473556960
H	2.190120413726	4.484828598543	-7.005897094044
O	-3.847962098266	2.691928126223	3.760249684932
C	-4.747179911794	2.025740271134	4.680190442536
H	-5.792308305904	2.129890336670	4.361887798477
H	-4.504394476158	0.959270004855	4.773156637268
H	-4.607886659608	2.517004728958	5.642297004159

Cam_TS2A

($E_F = -929.46746296$ a.u.; $G_F = -929.08756704$ a.u.)

0 1

C	-1.542532888962	1.706036456951	-2.548818528669
C	-1.065478804891	2.673140466090	-3.616134697419
C	-3.367237047958	1.766108991271	0.874847875268

C	-2.951808263213	1.380058384908	-0.381019886402
C	-0.786876324185	0.580174808576	-0.387911320984
C	-0.320912517029	1.267983859747	-1.621603109649
H	-0.703259766317	3.657029310235	-3.327773078401
H	-3.160905563749	2.750009373391	1.283686786698
H	-3.328488858875	0.410730487671	-0.693083424306
H	-0.461717126900	0.938943555992	0.580055335426
H	-1.033061590854	-0.474495191508	-0.430606022667
H	0.323462826388	0.630789720703	-2.239406683117
H	0.261095077426	2.157942029786	-1.372057038877
C	-2.624142931140	2.359130900185	-1.544407607858
C	-3.941986961806	2.648060035543	-2.298883644560
H	-3.748667107196	3.251371684929	-3.190796822499
H	-4.441456387860	1.728655140447	-2.609823471653
H	-4.631805182672	3.192819029475	-1.649365287965
C	-2.099109765746	3.694430042932	-0.979420352318
H	-1.898112952802	4.409107627547	-1.778572233676
H	-2.849233653393	4.155577311149	-0.333133894809
H	-1.187931562402	3.563012245428	-0.392666924861
O	-0.471131600382	2.168013569523	-4.763656835089
O	-3.988981518116	0.895367962263	1.757897797022
C	-2.095234641995	0.441347751631	-3.237267179854
H	-1.314705579580	-0.011491520582	-3.850731982028
H	-2.425437466503	-0.301574203476	-2.509955858870
H	-2.931951820229	0.676650300437	-3.896477497340
C	0.081775190953	3.154793563379	-5.672424318764

H	0.870701700370	3.719744098159	-5.163087777213
H	-0.705510716152	3.853548747705	-5.973200703071
C	0.678507895417	2.496366354664	-6.940106233547
H	1.472133414112	1.791857057656	-6.654795103952
H	-0.103987453192	1.935391764025	-7.469440728761
C	-4.356841906296	1.448244428733	3.047464593922
H	-4.993366009011	2.328692880476	2.905874651376
H	-3.456228930767	1.754840652500	3.590891936810
C	-5.128199764138	0.414480111389	3.903661193571
H	-6.038218354039	0.101991192178	3.373089174312
H	-4.502716169612	-0.474483825126	4.064259713149
O	1.197191264212	3.554890709952	-7.756931584179
C	1.808829444675	3.200598660294	-9.021905058695
H	2.679378350241	2.548818090930	-8.874951475975
H	1.091762031059	2.700034557778	-9.684828291762
H	2.127581017864	4.140070756100	-9.471290964948
O	-5.448655618809	1.052115385465	5.147475092412
C	-6.187333218872	0.287306600537	6.132028303426
H	-7.167872391230	-0.018046465216	5.745272928562
H	-5.629484255546	-0.604650222395	6.444263264127
H	-6.321480487624	0.951414940093	6.984767109779

Cam_Int2A

($E_F = -929.47416039$ a.u.; $G_F = -929.09666943$ a.u.)

0 1

C	-1.540922724569	1.707325288460	-2.528371734381
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C	-1.240163685554	2.631282762833	-3.683258172547
C	-3.435234000012	1.740204429020	0.880007653299
C	-3.103821859669	1.413863925077	-0.383602421989
C	-0.185818617134	0.548362199173	-0.612520491624
C	-0.108263768979	1.393066210607	-1.809499403257
H	-1.150049860144	3.703012589986	-3.522901985130
H	-3.209655492819	2.714402437233	1.305223820459
H	-3.396107803664	0.424180718446	-0.719836331058
H	-0.239781157755	0.983792668547	0.376415628757
H	-0.400251113319	-0.510668151300	-0.692598665870
H	0.479768354524	0.922130607253	-2.604389492864
H	0.358270183961	2.353706268316	-1.584211482842
C	-2.569381919327	2.383606493154	-1.472838698213
C	-3.826187472997	2.867117977889	-2.247938009364
H	-3.560452778064	3.569650347581	-3.041436440483
H	-4.362629468028	2.032944087425	-2.704301058477
H	-4.513535097208	3.361879321213	-1.557457400912
C	-1.918415124498	3.614315341383	-0.808772953896
H	-1.498999115598	4.297148476914	-1.549193053975
H	-2.661033354027	4.182235716042	-0.243188000495
H	-1.122038851124	3.327589778299	-0.120140053636
O	-0.471825670681	2.148577496755	-4.729733643129
O	-4.091795348631	0.883061826422	1.753862700297
C	-2.073755771196	0.370987694218	-3.080664293805
H	-1.398524822210	-0.001824450605	-3.852686836430
H	-2.142318852806	-0.385308926602	-2.297779784556

H	-3.059164184620	0.489994384041	-3.534609337998
C	-0.076050784342	3.125238193039	-5.729133326453
H	0.545450194953	3.895772911485	-5.259679637941
H	-0.969640287496	3.603437811562	-6.142389360339
C	0.720921680415	2.473382760656	-6.885071720390
H	1.626052971780	1.992484125816	-6.488974037205
H	0.106337065961	1.702024002440	-7.369272377814
C	-4.424105468650	1.428591805410	3.056152573735
H	-5.018027207007	2.341782467730	2.938591213226
H	-3.507426356989	1.678224700302	3.601902472532
C	-5.242097177287	0.415662826394	3.893881772741
H	-6.166592306353	0.157670287692	3.359104694767
H	-4.659266584244	-0.505031402147	4.034508880240
O	1.053511245352	3.521837660228	-7.804929118156
C	1.800987827592	3.170667525580	-8.995895515602
H	2.778969807749	2.743331140322	-8.740891421327
H	1.246603347561	2.456615643435	-9.617886127585
H	1.940542015554	4.101356614857	-9.543991734527
O	-5.530280581977	1.041578254495	5.151462562767
C	-6.301034565410	0.290818345563	6.122136779163
H	-7.295521432387	0.039164941070	5.732383581224
H	-5.784125904234	-0.632274561216	6.413528120027
H	-6.402387070036	0.942051030899	6.989196464145

Cam_TS2B

($E_F = -929.47716708$ a.u.; $G_F = -929.09753813$ a.u.)

0 1

C	-1.512338165489	1.742751721394	-2.646248500021
C	-1.035707579880	2.731340920070	-3.712324316139
C	-2.855146469685	1.399218296266	1.228714600916
C	-2.507972295819	1.010874612664	-0.070745699391
C	-1.013522959026	0.741849111831	-0.345887151828
C	-0.413840534055	1.464715804821	-1.578134916398
H	-0.756867079321	3.741367284530	-3.418712866656
H	-2.155827191922	1.955930453855	1.848884969521
H	-3.198604889276	0.293254942421	-0.507139573824
H	-0.426330345478	1.004847015690	0.538770980428
H	-0.895453305658	-0.340365829848	-0.465391887889
H	0.401304715426	0.881525687418	-2.017018224723
H	0.023220584021	2.416845216850	-1.265543468096
C	-2.694893218450	2.335438175611	-1.813579953775
C	-4.098981320185	2.121602468132	-2.319261175699
H	-4.271358860988	2.683724677999	-3.249039065287
H	-4.320490586592	1.072744208382	-2.525465417255
H	-4.824533819156	2.475769731711	-1.581357146798
C	-2.487419026140	3.715356420620	-1.233209339378
H	-2.643023950342	4.493687100537	-1.993953937134
H	-3.208696444728	3.894797118015	-0.430789469241
H	-1.489623125656	3.856583017554	-0.813447306340
O	-0.404930859559	2.252919819170	-4.851444167320
O	-4.063875359924	1.102462285977	1.838956814177
C	-1.893995868876	0.416125844506	-3.332759324673

H	-1.015637371369	-0.012346677361	-3.818362837004
H	-2.274978099937	-0.308787840238	-2.610974958202
H	-2.653842555492	0.567870589596	-4.101383567581
C	0.051890105942	3.252292832122	-5.797764762740
H	0.763942383206	3.925181505326	-5.306210072186
H	-0.801622502581	3.844211331191	-6.143896260288
C	0.743802499718	2.598171322457	-7.018906399514
H	1.599001491978	1.996553419860	-6.680591861617
H	0.036674573502	1.930619531795	-7.530453128316
C	-4.134657403223	1.398153512922	3.259334791414
H	-4.232354061094	2.479427478045	3.405145381386
H	-3.215416257267	1.063607514980	3.751433359284
C	-5.330363433426	0.687096049300	3.939191908237
H	-6.274150666605	1.018998949484	3.485018183811
H	-5.242675996269	-0.398526936202	3.794400087892
O	1.170005688718	3.658873398768	-7.884616559993
C	1.845508199333	3.299486949593	-9.115186080520
H	2.774153998199	2.750348966699	-8.914224970463
H	1.199905000325	2.691014637691	-9.761104815622
H	2.077727726022	4.240069602587	-9.612712126957
O	-5.278887189006	1.029276266919	5.331266537357
C	-6.285523653369	0.468243010276	6.209551178734
H	-7.293875976040	0.784641503739	5.914011796218
H	-6.240111235668	-0.628160619466	6.218361937945
H	-6.059293910115	0.851362380285	7.203629342246

Cam_Int2B

($E_F = -929.62117093$ a.u.; $G_F = -929.23874163$ a.u.)

0 1

C	-1.366770168210	1.803631106717	-2.768574035378
C	-0.731772430714	2.827660185201	-3.729551725411
C	-3.504279210521	0.919137650698	1.837307968843
C	-2.983580682877	1.758932469280	0.924743446124
C	-2.716390673423	1.408440100453	-0.546267904435
C	-1.491070760732	2.096768159418	-1.244393265007
H	-0.400429879703	3.771894494840	-3.294565298521
H	-3.686903370025	-0.128894081930	1.601061716443
H	-2.840026718662	2.796890730644	1.218620377532
H	-2.625138741391	0.322284073975	-0.647008720561
H	-3.606530357567	1.688309931679	-1.124693017300
H	-0.567794531821	1.764366029600	-0.755935476485
H	-1.553090634317	3.174013983078	-1.069702242369
C	-2.228592980900	2.585639166156	-3.776797003573
C	-2.806003241256	1.840054017818	-4.969201013144
H	-3.178199251464	2.550925437663	-5.713592848145
H	-2.067433239592	1.206997613964	-5.458779601086
H	-3.647776677512	1.211621423458	-4.661104546607
C	-3.143064890751	3.698389894662	-3.289006194191
H	-3.355141753129	4.392474995546	-4.108793105235
H	-4.099467068119	3.296580075594	-2.938288262832
H	-2.706965677455	4.277755834227	-2.474263713555
O	0.107472168759	2.390628662352	-4.795019930321

O	-3.868669051021	1.294441657553	3.121646978974
C	-1.086189516889	0.333306816697	-3.052743890929
H	-0.326130969509	-0.038664383145	-2.358821032873
H	-1.983975233281	-0.278287640997	-2.924474122378
H	-0.706793254397	0.179819183562	-4.061400954825
C	0.182129342851	3.320533877390	-5.899832498238
H	0.536584491011	4.297039198751	-5.545837680796
H	-0.809783821695	3.460407593014	-6.344326341451
C	1.155290487489	2.809775838815	-6.991255578981
H	2.152507278114	2.663687800121	-6.553214279830
H	0.805412027381	1.840251728140	-7.373224238837
C	-4.465850455413	0.270876551384	3.957883564010
H	-3.743438066963	-0.532114627320	4.140880093908
H	-5.342646412491	-0.156236803772	3.458931938724
C	-4.910846400061	0.863424357715	5.317607298736
H	-4.041172792257	1.289676150069	5.836424935149
H	-5.636293684087	1.670581587135	5.145696934041
O	1.191316032408	3.790222011309	-8.038312076816
C	2.047216220643	3.531009067062	-9.177535507349
H	3.098802707793	3.444769441272	-8.875123901417
H	1.747875716165	2.614118089807	-9.701470550443
H	1.927539278551	4.386097548000	-9.841627343251
O	-5.494547697333	-0.202131458795	6.078545033896
C	-5.997148409038	0.108464627753	7.401935740626
H	-5.196594980308	0.477272511023	8.055590708433
H	-6.799376971259	0.855918017261	7.357867113234

H	-6.390430053507	-0.826803988272	7.797849963312
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Cam_TS2C

($E_F = -929.47941076$ a.u.; $G_F = -929.10086023$ a.u.)

0 1

C	-1.153466665769	1.505628545480	-2.694403688311
C	-0.468363184895	2.368113610628	-3.570520900139
C	-3.385843187378	1.851432817989	0.969674200034
C	-2.789349439583	1.345047566278	-0.331144888923
C	-1.328123816456	0.774507945170	-0.200042424025
C	-0.420762257439	1.206091358938	-1.380667673303
H	0.210685583129	3.127788128355	-3.193208358995
H	-2.971114495988	2.740101599263	1.442803800790
H	-3.436003648169	0.524305248323	-0.658292186318
H	-0.876504300856	1.107200355241	0.738511671576
H	-1.384123235515	-0.315280608206	-0.138458231411
H	0.325374768705	0.421917065984	-1.563450540071
H	0.149052542661	2.095544604281	-1.096308543873
C	-2.778502084831	2.401779389697	-1.455638041575
C	-4.002468205371	2.470078340523	-2.327976874238
H	-3.811907907813	3.078709303369	-3.217803918984
H	-4.329660275030	1.479993296462	-2.654291552239
H	-4.843266094772	2.931117258694	-1.788057489381
C	-2.218330078235	3.755988289052	-1.092525469708
H	-1.956237064076	4.316748245067	-1.994589221112
H	-2.958922327997	4.350095985976	-0.539048049947

H	-1.325920330458	3.685816473624	-0.465661248466
O	-0.550443376326	2.285671115862	-4.952072648626
O	-3.984112467575	0.945710288690	1.834052706570
C	-1.861619087704	0.329124655110	-3.339670507792
H	-1.128334412503	-0.377882495958	-3.746722198216
H	-2.481304798484	-0.212550491045	-2.623386201740
H	-2.495794962841	0.653105865549	-4.166346356586
C	0.343923707641	3.150551318689	-5.698608562908
H	1.338986506333	3.135380039064	-5.241729733146
H	-0.033727984830	4.178354846381	-5.674559876985
C	0.480069708797	2.693594777036	-7.172100765209
H	0.851954268678	1.660063431919	-7.201724173785
H	-0.501540193355	2.719109425277	-7.665008914574
C	-4.473736359623	1.501568578124	3.082425689617
H	-5.220038984488	2.273941091834	2.869638131518
H	-3.643001961060	1.964426817388	3.627430426422
C	-5.113771246726	0.417563981570	3.983475118197
H	-5.963243011877	-0.045073245557	3.462326529345
H	-4.376054887664	-0.367397748864	4.200754497025
O	1.399715584360	3.592495474461	-7.806668301578
C	1.716831436209	3.367458815564	-9.202657944158
H	2.179458783710	2.383742476951	-9.352256878437
H	0.821322735486	3.443918602237	-9.832154454511
H	2.423757074379	4.149275624531	-9.476630809960
O	-5.540843037246	1.071544734341	5.186588761309
C	-6.189604511252	0.269239342218	6.203678987601

H	-7.113087080793	-0.185705904701	5.823517361981
H	-5.524025272893	-0.521562069689	6.572491025695
H	-6.427629988430	0.954566433618	7.016000396102

Cam_Int2C

($E_F = -929.62530924$ a.u.; $G_F = -929.24294992$ a.u.)

0 1

C	-1.068544298579	1.542510419622	-3.677677554099
C	-0.549825436730	2.432720615431	-4.547635345420
C	-3.201723202913	1.398049818637	1.256673778418
C	-3.213217932789	1.495262701441	-0.271250442618
C	-1.987141638811	1.257451200899	-1.182558773778
C	-2.090702527152	1.942333564752	-2.592351443141
H	-0.761436692236	3.497757116937	-4.471399613045
H	-2.229424462588	1.245455676085	1.727997300656
H	-4.139837393045	1.127216054466	-0.707226336157
H	-1.072085750804	1.592252711464	-0.685655740990
H	-1.880423558665	0.176746607107	-1.318991585038
H	-2.087969874400	3.028960636789	-2.459652907190
H	-3.084071891044	1.688301787232	-2.989615077690
C	-3.421812728013	2.741032885521	0.588972351562
C	-4.823161572419	3.322523939204	0.617926814790
H	-5.002914749598	3.936042800349	-0.270712481650
H	-5.576587355913	2.533986945624	0.652206960148
H	-4.962138064243	3.958834650900	1.498349125321
C	-2.319044731816	3.778734613218	0.686895534912

H	-2.342826353428	4.455430337103	-0.174044352661
H	-2.445432985130	4.382851742123	1.591084529477
H	-1.325741523983	3.327195773805	0.726855243928
O	0.300400892588	2.080891718889	-5.594395814725
O	-4.258797840282	0.737678765110	1.947869761655
C	-0.783510985332	0.069443744216	-3.827839267378
H	-0.181743489525	-0.308510301723	-2.994008129375
H	-1.716343078248	-0.506712530544	-3.830684920704
H	-0.244503026012	-0.136683587346	-4.752361350646
C	0.492449721081	3.053507026418	-6.648510664235
H	0.888566568202	3.987342316703	-6.232651808086
H	-0.462067982563	3.270066099429	-7.140679788424
C	1.488689530593	2.512533494405	-7.704195531963
H	2.450754415484	2.293467066334	-7.220468583292
H	1.098662579779	1.576728889479	-8.128096257849
C	-4.386629375321	1.145533586975	3.330107119964
H	-4.634567097468	2.211606143946	3.388653481066
H	-3.436583168117	0.988825839646	3.857070560627
C	-5.488328916540	0.333110099831	4.054736000064
H	-6.454729753307	0.493888158956	3.556479063142
H	-5.250058703223	-0.738258475606	3.999115794797
O	1.637661809656	3.514093841555	-8.718724666306
C	2.522456597434	3.221605699488	-9.828653205348
H	3.551154002824	3.054839999348	-9.484750936667
H	2.182317775556	2.340538678690	-10.387538721334
H	2.490615228605	4.098321655411	-10.474071594886

O	-5.533634351915	0.780412431847	5.417640869790
C	-6.496083360772	0.157017214325	6.302153530761
H	-7.523588155116	0.317269937599	5.950881763551
H	-6.312637472285	-0.921131037402	6.395450642874
H	-6.363646006873	0.634801527352	7.272039162774

Pin_TS1

($E_F = -929.50889790$ a.u.; $G_F = -929.12186947$ a.u.)

0 1

C	-1.744912223217	1.978153366229	-0.176808160212
C	-1.573600382156	3.451221781437	0.355772264342
C	-2.149297838989	3.958665934614	1.665021215870
C	-1.743683786001	1.871344435717	2.873585572108
C	-0.673427675007	1.174219309608	2.053972806490
C	-0.442257939713	1.636545362856	0.616818488664
H	-1.817599771673	4.175416465807	-0.428793292248
H	-2.768086471839	1.689341567508	2.576517495276
H	0.266313503263	1.259959871195	2.609519674335
H	-0.927712824461	0.100647581643	2.059074930529
H	0.242114861095	0.942200428150	0.119308558047
C	-0.062330448487	3.139726290119	0.561741008655
H	0.560886531180	3.399850982814	-0.293506021074
H	0.373348131746	3.563738510928	1.466164035319
C	-1.453144316960	1.994705332650	-1.692250469562
H	-0.567009464914	2.577271705102	-1.949527943254
H	-1.297327295679	0.974597785847	-2.056361994079

H	-2.300880012491	2.421652372716	-2.237719438144
C	-3.019696345930	1.149862572891	0.004055358496
H	-2.900783751718	0.182386230740	-0.494430788757
H	-3.287680310362	0.942782373897	1.036087521595
H	-3.868984247915	1.655446424752	-0.466172986081
C	-3.641235095038	3.998685672174	1.860444771338
H	-4.085510689400	4.732932908029	1.172242909590
H	-4.117596748731	3.038503752680	1.666688579565
H	-3.876370093796	4.314990614356	2.878506538662
O	-1.609088876104	5.267886175821	1.954813430541
O	-1.572790771340	1.525421076188	4.230503354811
C	-1.533755729853	6.208727620961	0.823632779586
H	-2.434393716420	6.121245873689	0.208973048507
H	-0.669696780097	5.964117035499	0.200320907285
C	-1.410555630358	7.714915765677	1.200562286015
H	-2.276898330151	8.034508958965	1.794492334452
H	-0.499809116748	7.895920796095	1.786075793524
C	-2.437395753416	0.493334868880	4.803763416026
H	-3.238144386191	0.240713271225	4.101695323084
H	-2.887947779663	0.911040900060	5.706682369696
C	-1.684697165562	-0.821507912072	5.205660067141
H	-1.271368959735	-1.304317307360	4.309222160658
H	-0.850901678396	-0.567399926125	5.873640335162
O	-1.361088435071	8.412916623142	-0.064518096351
C	-1.251415406661	9.866882264146	-0.105150913136
H	-2.111899192721	10.345187924358	0.378487220093

H	-0.327461044105	10.210629689873	0.375664554492
H	-1.233536283796	10.124691970995	-1.162919875649
O	-2.628177450360	-1.688527825858	5.864582690153
C	-2.175186438362	-2.979201794483	6.377373836456
H	-1.798842537469	-3.617576923881	5.568595563523
H	-1.391698332142	-2.851661237679	7.134346170374
H	-3.054093679855	-3.436266594050	6.829356703219

Pin

($E_F = -929.53801613$ a.u.; $G_F = -929.14579117$ a.u.)

0 1

C	-1.694003121042	1.722684443251	-0.171727178421
C	-1.809889577692	3.232872697403	0.312185369975
C	-2.177763545703	3.547914514666	1.798692659441
C	-1.702389240736	2.216506260636	2.577895436971
C	-0.397412832407	1.604861830311	2.034223281395
C	-0.282083843808	1.763867555814	0.505847738116
H	-2.390741773731	3.867438995040	-0.359369421684
H	-2.508745486189	1.567092765685	2.253000236844
H	0.459911212590	2.074859861354	2.524977965307
H	-0.386908165003	0.548162438174	2.320018220086
H	0.505367670012	1.130773529520	0.086935380138
C	-0.250139543130	3.280251406970	0.215103430854
H	0.114872268127	3.536476249913	-0.777090570931
H	0.255132668502	3.899645935228	0.953884510635
C	-1.601039156286	1.723900805175	-1.712521955989

H	-0.994019831017	2.531706233834	-2.120259660577
H	-1.177903643858	0.777527751668	-2.063207095848
H	-2.603904051165	1.819479313492	-2.141031591785
C	-2.702601396721	0.609601670445	0.182034249469
H	-2.670675489083	-0.174187410892	-0.579537423951
H	-2.511832177631	0.115624034519	1.133959011346
H	-3.725919745833	0.996762162180	0.197461808555
C	-3.679040949439	3.703044562687	2.051651677724
H	-4.085999245700	4.568430035439	1.527081408419
H	-4.231296151751	2.822358484216	1.715070424173
H	-3.849161337518	3.833581533833	3.122429131291
O	-1.542165003565	4.851990002767	2.145164520641
O	-1.727388225940	2.133237788890	4.019028175769
C	-1.724598124581	5.895767082718	1.138539308957
H	-2.782745855359	5.997229504176	0.879714001702
H	-1.186391059648	5.637135063850	0.223856714535
C	-1.221987763234	7.321325541692	1.517751212466
H	-1.778298931547	7.722542876474	2.374791394438
H	-0.154681300745	7.297246893848	1.774772577830
C	-2.481994694103	1.033830645773	4.596987497393
H	-3.364317193453	0.820226905170	3.982311312697
H	-2.829691260852	1.400993946969	5.564311125833
C	-1.741236144090	-0.324632626838	4.872003188869
H	-1.453974908883	-0.810076622129	3.928735357480
H	-0.828347031969	-0.131864988530	5.451752075513
O	-1.451583856623	8.117681782035	0.331700472039

C	-1.079654621712	9.526599941209	0.296543416969
H	-1.624638728022	10.103067370368	1.054148779545
H	-0.001143300021	9.658641958908	0.447452369404
H	-1.356559285907	9.872944685409	-0.698040849179
O	-2.657378277998	-1.160655311055	5.608053461021
C	-2.243198662177	-2.498158437238	6.021196166493
H	-2.004025043107	-3.125871826160	5.153922571369
H	-1.374370330403	-2.455907367143	6.689247756505
H	-3.097130569800	-2.914836266842	6.552952518044

Pin_Int1

($E_F = -929.73727343$ a.u.; $G_F = -929.35714613$ a.u.)

0 1

C	-1.984663482483	2.744046715898	0.949974076263
C	-1.267567394517	4.179854866297	1.114380564208
C	-1.939877925370	5.501949325454	0.789450580815
C	-1.474015481870	-0.251072803742	3.158634369963
C	-1.703375211196	1.248642634072	3.309734057217
C	-1.157510345507	2.229238180959	2.204872529516
H	-0.343020397622	4.142224764363	0.530571212793
H	-1.676879793229	-0.754814859885	2.213998869430
H	-2.776949742039	1.446507675430	3.459294920038
H	-1.229753210888	1.544395485319	4.254602475564
H	-0.205295429232	1.830663794631	1.838965186661
C	-0.953873415303	3.729090821793	2.592539892002
H	0.017238150166	4.014965672329	3.003753757197

H	-1.731876585049	4.062010813505	3.285032480766
C	-1.693232135564	2.043530167598	-0.372459248447
H	-0.617405053247	1.992713270590	-0.563006346476
H	-2.085367487387	1.020433377567	-0.369317626332
H	-2.158814478190	2.581083838048	-1.205413969795
C	-3.490985536659	2.786207106785	1.202629986102
H	-3.907883541821	1.774681061564	1.173871741684
H	-3.744089457256	3.214836785055	2.174521525826
H	-3.988432735357	3.383462294947	0.433324666595
C	-2.936963761296	6.118083437426	1.721135744620
H	-3.754545083616	6.624559722630	1.198397933555
H	-3.384532356263	5.354277264691	2.354295627930
H	-2.472227877120	6.862385197969	2.388490861564
O	-1.248536423367	6.370435561682	-0.084290333319
O	-1.655383531590	-1.025134386864	4.303783989062
C	-1.903912880024	7.609798052227	-0.488913568777
H	-2.150813890713	8.212565126378	0.388799136869
H	-2.834502561711	7.373333249442	-1.015572443637
C	-1.022299990681	8.496564522363	-1.418870359525
H	-0.072237576648	8.726521259165	-0.917791098758
H	-0.799972290203	7.963755182028	-2.352909920930
C	-1.541301895033	-2.471095386226	4.164724774359
H	-0.551886121164	-2.721642891660	3.769241616516
H	-2.298820936014	-2.830943540367	3.459426706783
C	-1.738866180796	-3.201096033276	5.528520675655
H	-0.979237583632	-2.852730079985	6.241383931215

H	-2.729135127624	-2.953877067620	5.934870942240
O	-1.775791421350	9.698880121147	-1.676597507741
C	-1.207066440405	10.741263303978	-2.525465905463
H	-0.276988432948	11.136972876775	-2.099622877519
H	-1.012934483133	10.367469520492	-3.538156402864
H	-1.959542764724	11.527403702776	-2.561111892450
O	-1.616370350798	-4.616581564931	5.295496290684
C	-1.752382043593	-5.536136750185	6.422171085771
H	-0.982782836447	-5.349823015442	7.181003982586
H	-2.744497404359	-5.455128270706	6.882645870178
H	-1.621577524161	-6.531534164267	6.000926212126

Pin_TS2A

($E_F = -929.70346814$ a.u.; $G_F = -929.32799679$ a.u.)

0 1

C	-1.848076562277	2.847725521239	0.764869255736
C	-1.197477255249	4.303286928535	1.038862886440
C	-1.905003900091	5.610889961714	0.726401547789
C	-2.096558757036	-0.417894531203	3.497252889638
C	-1.965768920043	0.997722173951	3.482708434389
C	-1.090346884865	2.333227555185	2.029108249852
H	-0.241139917191	4.324533428979	0.509429842572
H	-2.805476348208	-0.910837551721	2.836878735525
H	-2.913764462660	1.489344019268	3.288887025551
H	-1.413923866460	1.423646422962	4.316258483632
H	-0.157608911054	1.812822907587	1.818263613057

C	-0.942711393470	3.786826780663	2.519202431363
H	0.000112827605	4.076048930623	2.989258761321
H	-1.761341552393	4.077368490691	3.186728293308
C	-1.448126643500	2.215359589354	-0.563292963038
H	-0.361549281909	2.214270863418	-0.687104234365
H	-1.797467214309	1.178948165769	-0.622153885799
H	-1.884729253782	2.768998658043	-1.401557205782
C	-3.370692380038	2.836420298463	0.921532898487
H	-3.749152358802	1.813820539655	0.832158301611
H	-3.692940606899	3.223008823076	1.890777151026
H	-3.839065423894	3.447678985278	0.144709808695
C	-2.951122468777	6.171676100806	1.637949066872
H	-3.769050176879	6.661495897915	1.099905855631
H	-3.391253031136	5.378201589748	2.239690843130
H	-2.534120347880	6.916492386657	2.335672181629
O	-1.220034406337	6.515917775543	-0.113696589205
O	-1.398015337300	-1.273311015614	4.338558275286
C	-1.907521926835	7.735106539991	-0.526457212399
H	-2.195513141121	8.322965049779	0.349029436801
H	-2.816575971573	7.470987991007	-1.076967502720
C	-1.032576401987	8.654414261092	-1.430752495136
H	-0.104230788331	8.914524701786	-0.904381845718
H	-0.767976481505	8.131254282951	-2.359235736145
C	-1.870731597795	-2.657056518254	4.375241188690
H	-1.557810123588	-3.169033440669	3.459593021993
H	-2.964075432812	-2.664944131018	4.422849284281

C	-1.329913396769	-3.448976066524	5.604205025878
H	-0.232622488733	-3.482755306166	5.573823861716
H	-1.633605958264	-2.940220004029	6.529009928915
O	-1.818018362570	9.831770300989	-1.706887698232
C	-1.260335015254	10.893622148717	-2.538892419249
H	-0.355149478149	11.317898372126	-2.087673675197
H	-1.027218188889	10.528224079424	-3.546399704739
H	-2.036311473548	11.655417133650	-2.593866581898
O	-1.889504642367	-4.774310513237	5.534580423675
C	-1.562136422386	-5.746215179053	6.574775176597
H	-0.484411169091	-5.946738410120	6.605254018614
H	-1.896141761992	-5.399717826624	7.560208778543
H	-2.098480844983	-6.653338415363	6.301360668095

Pin_TS2B

($E_F = -929.70735797$ a.u.; $G_F = -929.33010741$ a.u.)

0 1

C	-1.584497735490	2.814512200501	1.098620055691
C	-1.348203397093	4.384852982751	1.132144359061
C	-2.004328008086	5.430755755597	0.463890811064
C	-1.425434438033	-0.135258933699	3.360102101717
C	-2.063999475720	1.245731723096	3.357032164559
C	-1.361973358098	2.476480021317	2.631234838907
H	-0.289599062883	4.600362642378	1.271750984315
H	-1.051328945182	-0.594640803946	2.446110655034
H	-2.159813499264	1.538661775910	4.409945914064

H	-3.101254285684	1.176103337280	2.994741646952
H	-0.283000272605	2.374188416948	2.789174711079
C	-1.798418731662	3.830196783803	3.166348378160
H	-1.198358224530	4.345505647261	3.909998870833
H	-2.868672610006	4.004776470688	3.243828967271
C	-0.531104671118	2.163034576547	0.189237657104
H	0.480543988852	2.445758132208	0.493151454053
H	-0.604924897667	1.071355184912	0.237288645569
H	-0.670547539259	2.469958788856	-0.851933179110
C	-2.972216109972	2.369097792332	0.627764744995
H	-3.174634583357	2.719386894795	-0.386964571844
H	-3.017810903610	1.276602875993	0.617285757994
H	-3.772495074501	2.721205498395	1.281998019656
C	-3.479484898901	5.503816803790	0.201031110551
H	-3.720114657259	5.629678494363	-0.859795357658
H	-3.986970370257	4.615639994696	0.558205327382
H	-3.911204689639	6.359908443796	0.733859525079
O	-1.289012265542	6.629312545365	0.225886745121
O	-1.898877504774	-1.018415595835	4.330220841065
C	-1.830682222395	7.595778343001	-0.725188153548
H	-2.828907153853	7.919454232242	-0.421650537072
H	-1.906422471210	7.131433863803	-1.713810908467
C	-0.961280826245	8.882163339519	-0.857162831791
H	-0.853543097915	9.358777856440	0.126407280134
H	0.039663392094	8.629268728556	-1.230804717333
C	-1.389437702874	-2.382707869454	4.319475202195

H	-0.301805417872	-2.366890489473	4.441643259580
H	-1.624689722303	-2.854100518256	3.358637303775
C	-2.015023868229	-3.236621452760	5.464876079521
H	-1.779451061509	-2.774090600332	6.432899242826
H	-3.107446965342	-3.254179083613	5.350527562136
O	-1.654695357236	9.747296715913	-1.779603764552
C	-1.088547469022	11.049328212392	-2.118762821469
H	-0.994242828410	11.685241982173	-1.230182095687
H	-0.106796099478	10.943768589947	-2.596103346391
H	-1.792299473894	11.496592791661	-2.818883422858
O	-1.467170549078	-4.565310307341	5.381890025016
C	-1.889846160947	-5.568368818334	6.355903483332
H	-1.630639439417	-5.263315496934	7.376921600586
H	-2.969488927710	-5.750985686678	6.293869408239
H	-1.346848221460	-6.474590284863	6.092763625634

Pin_Int2B

($E_F = -929.73653376$ a.u.; $G_F = -929.36088970$ a.u.)

0 1

C	-1.789187952283	2.958825577631	1.007588038429
C	-1.290380002937	4.440206765462	0.825170565293
C	-1.925287640995	5.609804298213	0.566660137716
C	-1.344704921343	-0.047731617923	3.742085579288
C	-1.896562354456	0.735786230506	2.560190549398
C	-1.414646419055	2.238907457864	2.432262007734
H	-0.212792753688	4.492303572489	0.677620968704

H	-0.308701130641	0.076904477882	4.054466231338
H	-2.990360533451	0.726643285311	2.638128599811
H	-1.663429123282	0.189594889637	1.635824365022
H	-0.312947955763	2.236016804123	2.450316280835
C	-1.915041650521	3.025740423627	3.589272988440
H	-1.611206164381	4.057948655645	3.716383532298
H	-2.665652228163	2.622794100778	4.257454605219
C	-1.030920617458	2.203169270546	-0.114263102605
H	0.050710240187	2.242991943276	0.044046343234
H	-1.328172376968	1.153358387136	-0.161828817302
H	-1.244888882362	2.655693539340	-1.086062397422
C	-3.296373876019	2.778480905090	0.756597894973
H	-3.609748610228	3.304813807805	-0.147270277224
H	-3.528023505575	1.720585360412	0.615977536406
H	-3.897040366237	3.133325088710	1.595847699641
C	-3.384842628830	5.911273952560	0.779100173266
H	-3.937713487484	6.010179071747	-0.160151071709
H	-3.863341500294	5.145738353783	1.378980091024
H	-3.477860917492	6.859046317270	1.317552077931
O	-1.158681091933	6.733127919885	0.158220065410
O	-1.894129500514	-1.309066371318	3.951611680152
C	-1.752455897653	7.681117367289	-0.780019835510
H	-2.718888736147	8.038514884369	-0.417473644495
H	-1.909237931572	7.187431493877	-1.745132875283
C	-0.863805179088	8.942543986392	-1.000755230152
H	-0.666333908583	9.422443760563	-0.032527826644

H	0.098007256006	8.657514975092	-1.447131769355
C	-1.300891522668	-2.147314114033	4.986346689662
H	-1.370790109175	-1.636863579414	5.951918153487
H	-0.242855254609	-2.315518391724	4.756998467319
C	-2.018700151579	-3.527835781424	5.090035612622
H	-3.079916362112	-3.369309484808	5.325134176640
H	-1.955492528418	-4.044976813593	4.122838922210
O	-1.598177590904	9.822969370569	-1.875094275181
C	-1.014426501632	11.102319025900	-2.266938210177
H	-0.831499985876	11.739668363607	-1.393271121036
H	-0.075498064701	10.959432638620	-2.815472911391
H	-1.752653724455	11.570266090070	-2.916209178932
O	-1.369616580792	-4.289272523923	6.124906187307
C	-1.858257948443	-5.631432282666	6.430932597984
H	-2.901602422472	-5.606127389308	6.767835357174
H	-1.773050685827	-6.292431404155	5.559923065232
H	-1.220006505961	-5.995734302650	7.234201549094

Pin_TS3B

($E_F = -929.72655743$ a.u.; $G_F = -929.35237684$ a.u.)

0 1

C	-1.776130576749	3.082665751544	0.872872328677
C	-1.274421515748	4.508718578089	0.653544836397
C	-1.905830168104	5.702095457462	0.464342561984
C	-1.355902898008	-0.145108415935	3.877727471815
C	-1.862631528353	0.680571540939	2.695544932544

C	-1.316749676794	2.144611544646	2.640804362943
H	-0.217633936680	4.546249030229	0.394780667708
H	-0.348883173543	0.007893604148	4.262053302175
H	-2.957875225290	0.715333934398	2.752247604780
H	-1.631260667096	0.148785821356	1.761881077288
H	-0.240126352411	2.182176133859	2.467070138960
C	-1.779212440881	2.981757579910	3.688771555639
H	-1.312305339938	3.940357528208	3.882457603674
H	-2.718730103770	2.773567142190	4.188694309413
C	-1.019073506458	2.195343916317	-0.118622760841
H	0.062301409261	2.253518643884	0.035379622497
H	-1.319525073749	1.149660622485	-0.035598560434
H	-1.221856037629	2.517938397428	-1.147683969723
C	-3.276399467765	2.854250188843	0.787707765579
H	-3.697777098151	3.326767451659	-0.107026419255
H	-3.493429364880	1.786019578091	0.727494952253
H	-3.801640892313	3.243148471044	1.661995949451
C	-3.330455601600	6.030658312606	0.811507816888
H	-3.940901773148	6.232604493361	-0.074063783443
H	-3.795196705706	5.229333474978	1.373646102562
H	-3.352940089474	6.929257224009	1.435812954294
O	-1.152673099362	6.790643169605	-0.031037188035
O	-1.872471099868	-1.429778155526	4.022075848489
C	-1.833452068662	7.845894292802	-0.777847958590
H	-2.608935355442	8.314480405607	-0.167391260577
H	-2.306388342722	7.417744211751	-1.667513256927

C	-0.865728670696	8.979875928170	-1.231886328469
H	-0.360257575525	9.404928738966	-0.354272023204
H	-0.101529279277	8.577224633358	-1.909632603184
C	-1.325152368927	-2.251259686491	5.095799319306
H	-1.470483689378	-1.740449367238	6.052703763566
H	-0.250197087617	-2.389903527877	4.935426096976
C	-2.006387422569	-3.652089146594	5.163949289414
H	-3.084316794308	-3.525766466990	5.333141620888
H	-1.868125233063	-4.173425478532	4.206914875373
O	-1.675062669950	9.971490252775	-1.894926056848
C	-1.045711860800	11.170378769744	-2.441397469545
H	-0.557780690649	11.756849812683	-1.653519107781
H	-0.310069963169	10.915801923023	-3.213892981370
H	-1.857396303841	11.747474332257	-2.881340476084
O	-1.397610526623	-4.385739247784	6.242953631599
C	-1.862124459512	-5.739623087495	6.533459429033
H	-2.923438792583	-5.743908755606	6.809926402746
H	-1.707062866467	-6.404796608755	5.675308264258
H	-1.260395982713	-6.077699641497	7.375481901285

Pin_TS2C

($E_F = -929.72195533$ a.u.; $G_F = -929.34517280$ a.u.)

0 1

C	-2.505246204207	2.705838272214	1.175186620126
C	-1.200009461543	4.282708807425	0.933124965452
C	-1.471400233660	5.675902481456	1.045715600589

C	-1.591289731692	-0.404011216189	2.784132505950
C	-1.325477340663	1.075552691884	3.033824570794
C	-1.244447988224	2.062498732412	1.801181679238
H	-0.837984033277	4.013029293017	-0.058472897860
H	-2.382387185887	-0.720729416482	2.105049540976
H	-2.068719320061	1.472891535480	3.744540307727
H	-0.365422139014	1.141077410651	3.561182913265
H	-0.696522057461	1.548185368791	1.003877635248
C	-0.553851728611	3.433105822746	2.061654331566
H	0.542307599413	3.421485471605	2.039219857860
H	-0.848145056265	3.808703478395	3.045731451576
C	-3.000017809377	2.160139484242	-0.136984949077
H	-3.522326051223	1.200423634363	0.005095987782
H	-3.707954672863	2.849079799908	-0.608860861258
H	-2.177618747429	1.983588721337	-0.835936868227
C	-3.597278534502	3.123147032825	2.125459241559
H	-4.209382376412	2.258618341030	2.423595193295
H	-3.207064613377	3.572057687853	3.041850227989
H	-4.264250812277	3.850049647264	1.652586508277
C	-1.831303715775	6.347578393184	2.335994570971
H	-2.801558573960	6.854864179428	2.281615996019
H	-1.893662970120	5.615362681794	3.138712297960
H	-1.092908678587	7.101872318206	2.636089766491
O	-1.428813042728	6.477150188988	-0.114809663987
O	-1.324190131094	-1.273139869188	3.841047205001
C	-1.836955580682	7.876335358856	-0.055281908415

H	-1.369419480595	8.377275161395	0.795141959642
H	-2.923338099789	7.939692318713	0.063510634259
C	-1.435164536451	8.676510238426	-1.331426336502
H	-0.348482351848	8.612774970193	-1.477594077935
H	-1.928185560070	8.252804867821	-2.216381158441
C	-1.665518698787	-2.678059553120	3.659394315865
H	-1.130437841088	-3.072847199625	2.789934836843
H	-2.741941663256	-2.771519587851	3.476767941502
C	-1.293399609216	-3.531315981853	4.910397099752
H	-0.214143159374	-3.450845349895	5.098307243445
H	-1.824395005512	-3.141464935429	5.789565639490
O	-1.849519644021	10.039850789878	-1.111856805930
C	-1.598381064626	11.045498787975	-2.140040965132
H	-0.524522703193	11.155244804609	-2.334197485644
H	-2.113193878877	10.794553192569	-3.075356745119
H	-1.997155077590	11.975474098726	-1.738006141840
O	-1.669914568715	-4.895324229989	4.644202706168
C	-1.419578006414	-5.912373489976	5.662225057166
H	-0.348609373078	-5.997030411223	5.883008631259
H	-1.965288256658	-5.690249817900	6.587337580813
H	-1.782866903373	-6.845502677555	5.234766140312

Pin_Int2C

($E_F = -929.75854409$ a.u.; $G_F = -929.38499278$ a.u.)

0 1

C	-2.945408966763	1.798368542371	1.207824609181
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C	-1.431199102167	4.555399235942	0.879593726052
C	-1.299985953680	5.899890373180	0.986673306168
C	-1.510952357712	-0.397334742350	2.829596189899
C	-1.310415023996	1.097005248979	3.034678379478
C	-1.553659720016	2.001388028638	1.746175339146
H	-1.642207051711	4.155620282493	-0.108134150517
H	-2.233690436456	-0.752421257327	2.096326192852
H	-1.990026091496	1.457046118177	3.824464400334
H	-0.297735882071	1.273972095014	3.419208287371
H	-0.837895309870	1.668975075731	0.986177938360
C	-1.251902567804	3.534034653014	2.039700895919
H	-0.222373031584	3.591720370573	2.414580869692
H	-1.890460367014	3.829093263930	2.880062856883
C	-3.145698449479	1.415302785841	-0.222812788769
H	-4.101970683191	0.902241617629	-0.374155535382
H	-3.158870987448	2.297900443153	-0.886236803351
H	-2.344542423559	0.763074366562	-0.584357721323
C	-4.109483459724	2.351453169833	1.967006750003
H	-5.035927506327	1.822027895273	1.723041852966
H	-3.962377182061	2.295991982176	3.050077191704
H	-4.277138811137	3.414843366589	1.726240576068
C	-0.989720402942	6.591597316966	2.286402255100
H	-1.761647064039	7.318780662299	2.554665779791
H	-0.913471851850	5.871766764028	3.098758162565
H	-0.038600081141	7.130653528330	2.226640045717
O	-1.381862872872	6.725572075005	-0.154853764641

O	-1.281412978238	-1.237731958653	3.915308722829
C	-1.575558158029	8.164115267373	-0.003642719447
H	-0.825726873928	8.587821641900	0.668196891396
H	-2.566764695432	8.362504304621	0.416827201341
C	-1.453341705803	8.928564019931	-1.356545818175
H	-0.472609964578	8.722908455719	-1.806227447566
H	-2.230934284504	8.591596897343	-2.054624390444
C	-1.533337594725	-2.659835371432	3.714026012394
H	-0.899141268792	-3.029079738768	2.901976859873
H	-2.581382712291	-2.806314403041	3.429783132920
C	-1.242849465261	-3.493712835527	4.998889705281
H	-0.191987409670	-3.362081802894	5.290308593919
H	-1.874808909874	-3.131492532168	5.821212062929
O	-1.601643130800	10.330437346242	-1.054656733648
C	-1.529523267626	11.312931632592	-2.132264804449
H	-0.553403778302	11.283799611196	-2.631434916346
H	-2.321685826915	11.149188292360	-2.872840163650
H	-1.668878411421	12.279791448985	-1.651374773642
O	-1.526116047716	-4.873767321110	4.700717632665
C	-1.329109824187	-5.880913609682	5.739886062307
H	-0.282229100035	-5.915719538925	6.064998056205
H	-1.972895641021	-5.687837074073	6.606599176746
H	-1.604135926783	-6.828800901403	5.280220396147

Pin_TS3CA

($E_F = -929.74236173$ a.u.; $G_F = -929.37056219$ a.u.)

0 1

C	-1.564257565763	1.566081493135	0.930735763853
C	-1.311616132819	5.101620811770	1.595332741718
C	-1.886924539890	5.903818994892	0.648733694532
C	-1.426339867241	-0.252730739472	3.515401782342
C	-1.886866013377	1.205070041532	3.451044189439
C	-1.272954035062	1.993899418029	2.254594923269
H	-0.323093582553	5.420203470782	1.920077767383
H	-0.417809893860	-0.509136800621	3.196007440265
H	-1.626506550164	1.723871860096	4.386854662497
H	-2.981733699076	1.228626231237	3.403077609595
H	-0.217415662393	2.210168882631	2.419418826237
C	-1.902451810638	3.959215408634	2.352739624764
H	-1.691228740828	4.049958412426	3.417305861506
H	-2.964047174971	3.794285276389	2.184909512970
C	-0.728166139772	2.093414126545	-0.196585719969
H	0.287852265665	2.336893882252	0.123881842983
H	-0.669583130884	1.377573831316	-1.023718505330
H	-1.164674601628	3.019620746208	-0.603222064944
C	-2.895243440646	0.989937430439	0.548878721416
H	-3.577644507955	1.781848248578	0.195646546070
H	-2.791956820061	0.282745431171	-0.280932897136
H	-3.388280026814	0.470373613279	1.371018911316
C	-3.230574663810	5.648288377612	0.031164158469
H	-3.140414381960	5.553715529790	-1.056430598939
H	-3.659701990886	4.722959083621	0.411191929996

H	-3.939826779661	6.457347789765	0.231374778958
O	-1.173310355345	7.015462105840	0.161386333282
O	-1.981077810469	-1.084715872797	4.484253706467
C	-1.896282582544	8.143592434495	-0.417550625750
H	-2.566453526227	8.576462413796	0.332091176009
H	-2.496328339495	7.819275993728	-1.271687117007
C	-0.934238956247	9.261457167361	-0.921659288179
H	-0.344846264250	9.655031511999	-0.082940279193
H	-0.241304818075	8.841808523923	-1.663404129042
C	-1.446881348899	-2.440780775476	4.559737504441
H	-0.375016707445	-2.395918605138	4.782760937969
H	-1.579180255406	-2.934976760370	3.592169916953
C	-2.149136282268	-3.294269459682	5.659119727975
H	-2.024701679838	-2.808941844614	6.636834323940
H	-3.224043019128	-3.358931811746	5.442190403889
O	-1.755697985291	10.291733101923	-1.505049983630
C	-1.124231839453	11.482695623199	-2.066602110324
H	-0.562473125939	12.032200444374	-1.301587634582
H	-0.453281963409	11.223230671282	-2.894453406836
H	-1.943615462260	12.097730029142	-2.435043525363
O	-1.541686595954	-4.600069356348	5.650743109282
C	-2.021633334965	-5.615732578915	6.584049559135
H	-1.883405504691	-5.295968227860	7.624096873151
H	-3.080384095507	-5.844350334571	6.411403699064
H	-1.416664965839	-6.499168456306	6.386467214593

Pin_TS3CC

($E_F = -929.75335703$ a.u.; $G_F = -929.37974463$ a.u.)

0 1

C	-2.827665553100	1.830202412640	0.934812610608
C	-1.410604074519	4.672638553213	0.817496926800
C	-1.300012779696	6.014884428997	0.963402802164
C	-1.925465576468	-0.241631434204	3.198284457393
C	-1.398130997691	1.140680185062	3.066386109999
C	-1.553535454300	2.112333821506	1.596383923825
H	-1.570880258066	4.290093480010	-0.186098982222
H	-2.995498486999	-0.392733278055	3.316646570427
H	-1.929337177671	1.795366699453	3.766989321621
H	-0.333310584410	1.160347952607	3.306934903003
H	-0.722624191082	1.745970233038	0.986875649246
C	-1.310051370277	3.620930415328	1.963569361288
H	-0.320076996000	3.687348950588	2.430305131818
H	-2.022262541018	3.887089816049	2.753384738887
C	-2.934359877690	0.512822237938	0.258802906104
H	-3.892479008018	0.363806104263	-0.244848681856
H	-2.126907752172	0.350374826856	-0.463438256375
H	-2.811363217615	-0.297808022954	1.016908987515
C	-4.074932179657	2.529962204378	1.384386624921
H	-4.925007509823	2.281103039854	0.744575401847
H	-4.352585672496	2.245419051063	2.414775572577
H	-3.960309385993	3.618065078610	1.383359432249
C	-1.070992347647	6.680317184619	2.293259859807

H	-1.871942952636	7.383571497463	2.539899169909
H	-1.019048314852	5.942053596801	3.091067111445
H	-0.130911253217	7.241607755020	2.294102508025
O	-1.326672475777	6.865440204923	-0.162823249509
O	-1.143135415395	-1.291415347625	3.676634783510
C	-1.575917384007	8.292975965320	0.005576450003
H	-0.884412388366	8.724778930725	0.732817120083
H	-2.597898217996	8.451174718512	0.365318239102
C	-1.392193761453	9.088950112257	-1.321992197119
H	-0.378951929291	8.921670453853	-1.711599324693
H	-2.112947676173	8.742564152835	-2.074350882793
C	-1.844009373778	-2.552773453583	3.893664607916
H	-2.114482126450	-2.985200310226	2.924676665416
H	-2.764865060307	-2.363628403817	4.456349075540
C	-0.994371750963	-3.588479626124	4.690694292781
H	-0.074589957048	-3.820849943354	4.137230391274
H	-0.712561209681	-3.160794611514	5.662512273369
O	-1.602834404322	10.479737472520	-1.005890376648
C	-1.493411369769	11.483493199634	-2.060462915831
H	-0.487112131063	11.493036389206	-2.496606542899
H	-2.231428768827	11.309352190615	-2.852862782737
H	-1.693281585167	12.436843528518	-1.573890530344
O	-1.805888646026	-4.766422410188	4.860457639239
C	-1.261353402433	-5.912642763049	5.583440845453
H	-0.369969244418	-6.310176420130	5.083236874822
H	-1.010296800394	-5.646558370450	6.617410340953

H	-2.052334442362	-6.660755938477	5.576870330515
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Cam_TS2C-F2500

($E_F = -929.76455870$ a.u.; $G_F = -929.38644387$ a.u.)

0 1

C	-1.200454790888	1.563772228832	-2.723142087807
C	-0.501223487509	2.418868652381	-3.624259329506
C	-3.380402624182	1.813339024476	1.015657687478
C	-2.789097329404	1.332150256233	-0.312673083978
C	-1.308390026635	0.799884198511	-0.222715746022
C	-0.435160520323	1.261139589533	-1.423044822863
H	0.166078653322	3.190749861955	-3.250175151630
H	-2.962569102792	2.696444972915	1.496050553471
H	-3.421460900201	0.498958514555	-0.635659594402
H	-0.842319939390	1.139856550683	0.706087099987
H	-1.333292152475	-0.291306435590	-0.166261644857
H	0.322539341143	0.493715393635	-1.628231344745
H	0.123181128127	2.158505751991	-1.140622402982
C	-2.803669822798	2.390656581691	-1.449815207930
C	-4.052481676170	2.440493144358	-2.289691998314
H	-3.904498733657	3.072391878719	-3.171032798696
H	-4.359056067224	1.447651815416	-2.627587172269
H	-4.890437592906	2.863927237100	-1.716065747704
C	-2.276725532517	3.757127482062	-1.077234536872
H	-2.052061313942	4.339709209462	-1.975320680528
H	-3.023096377556	4.317253968617	-0.497089941407

H	-1.369046153027	3.704512361616	-0.470909663117
O	-0.532679304879	2.296112120578	-5.012595377949
O	-3.999486761954	0.909558667442	1.880504951267
C	-1.883677075419	0.370751075651	-3.367642489846
H	-1.137334383394	-0.309572524239	-3.795697667572
H	-2.473842546566	-0.195174813475	-2.645089173191
H	-2.543297396889	0.682375466550	-4.179452790845
C	0.418769311016	3.115703116860	-5.764138059640
H	1.409431259217	3.029232387192	-5.306732575700
H	0.104944511969	4.163577303526	-5.720193819008
C	0.535285206983	2.688129250901	-7.263287260000
H	0.848040499153	1.636852134854	-7.318081169787
H	-0.443764030219	2.782162795478	-7.751594122980
C	-4.478576441196	1.456308622340	3.150882331999
H	-5.205304414693	2.248958018269	2.947628919367
H	-3.633736348631	1.891836149393	3.695550530928
C	-5.152563988671	0.381142377846	4.063427492201
H	-6.014808803541	-0.054999442295	3.541657277644
H	-4.435027463778	-0.423111183023	4.274497304149
O	1.508589784883	3.550470303558	-7.887998379945
C	1.833851585937	3.374862499174	-9.306390030953
H	2.249763904829	2.378343917029	-9.496252333647
H	0.950171966601	3.528499689195	-9.936905428038
H	2.581098121933	4.135857104384	-9.524205802186
O	-5.564227632217	1.037663359585	5.280780924506
C	-6.241409797212	0.270121007335	6.329499966912

H	-7.184396268926	-0.153177149182	5.963794775206
H	-5.600879304704	-0.536012277427	6.706432857678
H	-6.440938694855	0.986688384142	7.124318438689

Cam_TS2C-F2000

($E_F = -929.56042494$ a.u.; $G_F = -929.18201689$ a.u.)

0 1

C	-1.168254593137	1.524125234389	-2.703590619175
C	-0.479043359561	2.384464936507	-3.586506426078
C	-3.384752507891	1.839528398772	0.983227203631
C	-2.790172710765	1.340778729153	-0.325703717996
C	-1.322870136780	0.781613540842	-0.207623995408
C	-0.425951844075	1.223663765750	-1.393745333643
H	0.196165748792	3.147924971118	-3.209748936670
H	-2.969844365395	2.727128141906	1.458093964099
H	-3.432650911559	0.516274082731	-0.651459454140
H	-0.866782765799	1.115279348005	0.728411658864
H	-1.369458550045	-0.308767048116	-0.148890457214
H	0.324459395410	0.445235873583	-1.583544408401
H	0.139630289244	2.115846915014	-1.109449300435
C	-2.787665480034	2.398342032834	-1.453452300733
C	-4.019239646212	2.460886790671	-2.316059133406
H	-3.841710886985	3.077052661604	-3.203288379617
H	-4.339717015454	1.469835292619	-2.646120959430
H	-4.859648223004	2.910092623044	-1.765782470095
C	-2.237825623848	3.756478908154	-1.087534752592

H	-1.986752145027	4.323867629223	-1.988514082514
H	-2.980612645375	4.340385989884	-0.526296579999
H	-1.340918041271	3.691732902496	-0.466539514547
O	-0.545487055024	2.290114768147	-4.970297594631
O	-3.987729756454	0.933954833253	1.848098557171
C	-1.868640191857	0.342615659903	-3.348963540438
H	-1.131128288028	-0.356060196376	-3.762658281852
H	-2.479381983970	-0.206863404921	-2.630911409501
H	-2.510654341030	0.663123497906	-4.171064828028
C	0.370272691372	3.138032085351	-5.717085984224
H	1.364722593002	3.094781764220	-5.261005143794
H	0.017745876413	4.174326058073	-5.684652224939
C	0.496189482850	2.692395687667	-7.199072063348
H	0.845531903674	1.651599660522	-7.239231726754
H	-0.485367578375	2.744316883553	-7.689556864257
C	-4.475991170229	1.487735796434	3.101753490591
H	-5.218874329710	2.263589859085	2.890401216620
H	-3.642566291473	1.946032545511	3.646171225715
C	-5.122929631557	0.406069148455	4.007684794982
H	-5.974462051250	-0.052710347970	3.486841889644
H	-4.388746936669	-0.381826742068	4.225424232658
O	1.435456526732	3.577891136174	-7.829081431865
C	1.752483073626	3.368912272635	-9.232220280545
H	2.197441164736	2.379606132979	-9.396010564909
H	0.859885504883	3.472753803912	-9.861486054411
H	2.474187219458	4.142828809563	-9.488986767011

O	-5.548175721853	1.062390402625	5.212997054838
C	-6.203252140046	0.270513483465	6.240552107575
H	-7.130790210460	-0.179424395160	5.865156825893
H	-5.542573629374	-0.521753689858	6.614179298841
H	-6.433198236829	0.966243367520	7.046123736025

Cam_TS2C-F1500

($E_F = -929.35858975$ a.u.; $G_F = -928.97966773$ a.u.)

0 1

C	-1.129597695457	1.474598945564	-2.678865719503
C	-0.449854524859	2.339750956526	-3.545159823297
C	-3.388996029690	1.872025602378	0.947618737626
C	-2.787354594313	1.353883661535	-0.339987865089
C	-1.336371836230	0.765596142045	-0.185937847869
C	-0.412035878347	1.175579163563	-1.359305832750
H	0.235474353297	3.093367270072	-3.167427799824
H	-2.975987876545	2.763044087576	1.418017206678
H	-3.439977006223	0.539219624878	-0.670706024262
H	-0.891966581132	1.100687893352	0.755220929751
H	-1.407725686078	-0.322746746328	-0.115338622389
H	0.324269718848	0.379648911027	-1.530583251905
H	0.167720818511	2.059005192338	-1.076321460920
C	-2.760857274980	2.409191039563	-1.459616592623
C	-3.972101248319	2.488937183583	-2.347683308640
H	-3.759017612713	3.083900473213	-3.241821681656
H	-4.312633787720	1.501218028769	-2.667382823347

H	-4.811890624012	2.971459726946	-1.825062401718
C	-2.181951073235	3.755755190360	-1.100122375595
H	-1.902127384960	4.306122528676	-2.003379355635
H	-2.917463440691	4.366683214214	-0.558133472207
H	-1.296619655415	3.675167633263	-0.464512266177
O	-0.557278657939	2.276427334271	-4.922816507565
O	-3.979811114738	0.965845044907	1.811384608197
C	-1.851890167263	0.307091785268	-3.323608991882
H	-1.126756794416	-0.414050282944	-3.720411877761
H	-2.485902458364	-0.221112821843	-2.609847908938
H	-2.473544912548	0.637156767679	-4.157154023564
C	0.301670721346	3.168445864000	-5.669353185706
H	1.296276047527	3.198155131210	-5.211880759499
H	-0.116208246308	4.180901776473	-5.657579198432
C	0.454093415889	2.695417448604	-7.130129015131
H	0.865569101555	1.676422270881	-7.143941683279
H	-0.527395026788	2.674840397262	-7.624023684606
C	-4.475232563304	1.524608127125	3.050638206217
H	-5.230707454914	2.287140877562	2.833749527563
H	-3.651437706821	1.999805753941	3.596037656706
C	-5.099440711575	0.434943755697	3.945878353901
H	-5.941814798586	-0.039902145373	3.423671058117
H	-4.351691102383	-0.340322153244	4.164963378495
O	1.336873390090	3.618212026049	-7.774926063105
C	1.657686565881	3.366150401197	-9.158846047464
H	2.156908171314	2.396342199387	-9.282491811534

H	0.758559381395	3.389019883938	-9.788157396471
H	2.333878036087	4.164478280057	-9.462227075167
O	-5.535541647421	1.084405944118	5.144120928989
C	-6.169704048996	0.263478476910	6.146415435897
H	-7.082960557051	-0.206533064424	5.758763414192
H	-5.491084872746	-0.519105074134	6.510193087381
H	-6.425696594869	0.932600873126	6.967052900427

Cam_TS2C-F1000

($E_F = -929.15917502$ a.u.; $G_F = -928.78043433$ a.u.)

0 1

C	-1.078913330608	1.410306581288	-2.643527324487
C	-0.407067661965	2.276935456062	-3.496811129371
C	-3.398217375958	1.916656027043	0.904316031484
C	-2.773736414424	1.378087903463	-0.354144865773
C	-1.340663469635	0.768823907501	-0.144700833167
C	-0.386983590764	1.113218747171	-1.314306689272
H	0.292626807342	3.018189088980	-3.121689787375
H	-2.996792574722	2.815418396387	1.370386225203
H	-3.428900631091	0.569625703416	-0.695290352009
H	-0.910241201623	1.135868912507	0.791094504708
H	-1.436267263082	-0.313633255302	-0.028339777300
H	0.317773713010	0.284730960668	-1.461261211371
H	0.224952719914	1.978778457741	-1.044325305261
C	-2.714010326102	2.427073000014	-1.468280425519
C	-3.899722866170	2.529256968308	-2.386396947436

H	-3.640053938581	3.087434279718	-3.292258736035
H	-4.273257063588	1.547231379055	-2.685951056136
H	-4.731605389650	3.062458663238	-1.901540313405
C	-2.096362554855	3.756978827719	-1.116269516431
H	-1.786384820431	4.287847549591	-2.021556851507
H	-2.817961896729	4.399687094362	-0.592292721132
H	-1.222501133230	3.654779532651	-0.467909175646
O	-0.567104950025	2.250186044158	-4.865482963518
O	-3.977714231422	1.008888058391	1.765636113263
C	-1.831672900794	0.260542866506	-3.283350567684
H	-1.125041317670	-0.487061144346	-3.664248197582
H	-2.488320656365	-0.241132038557	-2.570996876560
H	-2.433729056794	0.601252754323	-4.126583369878
C	0.223028235322	3.191340643519	-5.612879807032
H	1.216220665040	3.294520478363	-5.162540506589
H	-0.262607892891	4.173402791769	-5.610580078947
C	0.393235897034	2.701521819713	-7.056657685894
H	0.868204095929	1.710044078725	-7.052501434391
H	-0.587967548151	2.607346689004	-7.543350142670
C	-4.494198528222	1.570150977222	2.986364851263
H	-5.272576788745	2.306091797375	2.757613634113
H	-3.690205142163	2.076552340375	3.533883882312
C	-5.081596886529	0.465287568782	3.872027662364
H	-5.902906550619	-0.040937600952	3.345050363083
H	-4.308254513453	-0.283152127806	4.097204886761
O	1.208949879267	3.661959648677	-7.722411591675

C	1.530285444386	3.368495093274	-9.087905498855
H	2.086241207062	2.425235285258	-9.174567261843
H	0.626233266860	3.306002786712	-9.708452308107
H	2.154209031718	4.188689157121	-9.442000414860
O	-5.545928432890	1.100575070327	5.060722212282
C	-6.144856219014	0.239964894484	6.037151758591
H	-7.031945442109	-0.267387105900	5.634542870984
H	-5.434185468448	-0.517782031188	6.393936218308
H	-6.441154459582	0.876607623896	6.870412184633

Cam_TS2C-F500

($E_F = -928.96260737$ a.u.; $G_F = -928.58457049$ a.u.)

0 1

C	-1.002447814216	1.297021532065	-2.578396914627
C	-0.316181016552	2.147155955474	-3.420712519519
C	-3.417803716973	1.990376059422	0.842595288356
C	-2.687882584095	1.443309257798	-0.344317646543
C	-1.252328214365	0.939157802940	-0.006629392480
C	-0.323635908910	0.957448909953	-1.252304266357
H	0.432852458563	2.841986279380	-3.052947916289
H	-3.101421130615	2.928432925151	1.296842697268
H	-3.273163438255	0.587187671000	-0.697416251511
H	-0.824938208012	1.580175448876	0.769796889456
H	-1.320233837495	-0.059497807683	0.430698608788
H	0.164248934620	-0.018299086708	-1.364188103357
H	0.484904383177	1.674310683594	-1.084267703705

C	-2.610213501146	2.457298222222	-1.477625129527
C	-3.784770369933	2.572222462391	-2.407038878914
H	-3.478864291931	3.022996864450	-3.357828729456
H	-4.237182900784	1.601008027529	-2.620217470454
H	-4.570954452752	3.214271892578	-1.982066739169
C	-1.924349053896	3.764872138175	-1.179902887695
H	-1.644452713699	4.271521891858	-2.108628489511
H	-2.588227447124	4.445386739920	-0.627253420157
H	-1.017349148558	3.635551968698	-0.583655529213
O	-0.567562824294	2.199461854968	-4.770197248509
O	-3.977222976420	1.070494845986	1.695940029304
C	-1.832629273565	0.200598681936	-3.216502656536
H	-1.174968101477	-0.587819896075	-3.602455845937
H	-2.512657259100	-0.263574644348	-2.500965821736
H	-2.417427956675	0.580486477796	-4.054631763915
C	0.177911035956	3.172891801248	-5.509042293310
H	1.193775711641	3.264098088538	-5.108953894999
H	-0.309545477082	4.152296858161	-5.444564685951
C	0.265603160452	2.725051761686	-6.964765052656
H	0.736926257226	1.732562582819	-7.011926998848
H	-0.741094889702	2.643709986597	-7.399759078603
C	-4.600928769006	1.622916340109	2.861185641007
H	-5.448986831170	2.253433987047	2.572128723066
H	-3.884493703184	2.239931930822	3.417213887049
C	-5.082013501468	0.484948452345	3.754472220124
H	-5.814553563734	-0.132903810685	3.215106501967

H	-4.232124157398	-0.157321866632	4.028120158933
O	1.043944638125	3.697985644950	-7.646072099249
C	1.290250786471	3.400218563579	-9.017165112749
H	1.841921288583	2.456583232890	-9.130250974316
H	0.354335596804	3.331528050832	-9.588929848900
H	1.892746835578	4.216897782949	-9.414906421195
O	-5.662283204967	1.087523046811	4.902213284261
C	-6.164014820755	0.164613407704	5.863828493100
H	-6.957553185429	-0.466575407852	5.440210352402
H	-5.367144865305	-0.485071893687	6.251893622364
H	-6.575465503359	0.754098901234	6.683223063061

Cam_Int1-F500

($E_F = -928.99139981$ a.u.; $G_F = -928.60773950$ a.u.)

0 1

C	-1.211703000816	1.509628830178	-2.381750771390
C	-0.373705956051	2.339872551016	-3.306323816400
C	-3.438304510306	1.966432514238	0.732470831695
C	-2.664411879787	1.361926124432	-0.392720605645
C	-1.255459644385	0.827836435778	0.027670492783
C	-0.324938896554	1.033373768066	-1.190008239192
H	0.249940922622	3.146720633523	-2.933287597051
H	-3.116302533636	2.902795548941	1.185874015711
H	-3.254597312408	0.510330751084	-0.746956567230
H	-0.887612579294	1.383028318277	0.894394601405
H	-1.323201463126	-0.218270283309	0.332084658508

H	0.222021929707	0.128167275725	-1.462942306759
H	0.427628451424	1.793404457344	-0.964342393880
C	-2.387466399329	2.290646646354	-1.621907937671
C	-3.634234232204	2.487190339124	-2.490312881234
H	-3.382115105505	3.030024021094	-3.406512208670
H	-4.090388596913	1.536542077346	-2.773256591496
H	-4.386810708176	3.064507030527	-1.945712978732
C	-1.897215755152	3.677994786676	-1.161263432479
H	-1.645143757658	4.300485537726	-2.022470463980
H	-2.682505625755	4.194935179341	-0.605201124666
H	-1.014457371235	3.620001250914	-0.519209369312
O	-0.637336568034	2.349679969731	-4.652680853653
O	-3.997323630095	1.061122814512	1.603609516829
C	-1.748346414549	0.283336222683	-3.149786287901
H	-0.909740970280	-0.298724243581	-3.539512987941
H	-2.337959674621	-0.368713399412	-2.502545522258
H	-2.364695986469	0.578861419854	-3.998639313354
C	0.308876780080	3.092712155932	-5.431902848978
H	1.328800834756	2.807382704431	-5.152558767516
H	0.186404338684	4.166895419107	-5.248759556606
C	0.098437237148	2.794246013144	-6.911851098718
H	0.213149947049	1.715527858747	-7.091796639782
H	-0.916110759698	3.085035434913	-7.220852962523
C	-4.580432149281	1.627495982560	2.782243613194
H	-5.412924959634	2.287017670646	2.512948407710
H	-3.833968583158	2.217357612309	3.328088871954

C	-5.082698545484	0.500203054131	3.677481634695
H	-5.844443531758	-0.089723291354	3.147386707939
H	-4.249546867242	-0.171337626098	3.931662336951
O	1.084371249126	3.541074688656	-7.610719377714
C	1.090632510159	3.343436556999	-9.020888916337
H	1.288871991375	2.293800605908	-9.278778431774
H	0.135387711254	3.642826606236	-9.474167467882
H	1.888323064510	3.967550708133	-9.423794240961
O	-5.622477848496	1.113324618205	4.839189405344
C	-6.137258076313	0.200207444618	5.803334685668
H	-6.958391199381	-0.401537593942	5.389575671796
H	-5.355418746807	-0.478029275798	6.172660978311
H	-6.514673800395	0.796742501719	6.633930013145

Cam_TS2C-F200

($E_F = -928.84708243$ a.u.; $G_F = -928.46838941$ a.u.)

0 1

C	-0.966477407026	1.027217474471	-2.566716782053
C	-0.191604879587	1.938512605714	-3.254274498338
C	-3.413614685966	2.030644851548	0.729960372262
C	-2.622317524616	1.383537561780	-0.358357099454
C	-1.140765437721	1.144948842798	0.000679953433
C	-0.426772250507	0.530927329036	-1.217068286038
H	0.563574613309	2.548287019522	-2.765406244795
H	-3.212564388233	3.055153801971	1.039073204703
H	-3.081028839783	0.401300992034	-0.533070944035

H	-0.678740137415	2.100317904389	0.269303930866
H	-1.058287238229	0.498778961524	0.879109246985
H	-0.550853102218	-0.556904616381	-1.191327607067
H	0.649396018805	0.713876287465	-1.146680365926
C	-2.688315449552	2.170689194607	-1.662266099723
C	-3.923279596152	1.993192874143	-2.505137818585
H	-3.746074057043	2.323242252878	-3.533956993806
H	-4.265790803088	0.956713318516	-2.532493008855
H	-4.752663876577	2.599132948934	-2.110429628096
C	-2.189476174403	3.594142081518	-1.639203978220
H	-2.017619705898	3.950903756286	-2.659128928335
H	-2.930158701515	4.264758306328	-1.179962241199
H	-1.252366471897	3.707570468195	-1.090898817437
O	-0.460321088646	2.249859994048	-4.563020106445
O	-3.878168620627	1.181339587375	1.699745159059
C	-1.748678647939	0.010724783776	-3.378262450692
H	-1.068172703415	-0.761537656657	-3.757541698993
H	-2.502423218902	-0.489760016941	-2.767827660450
H	-2.242749123016	0.468439339705	-4.234918759996
C	0.527212150329	3.052714378541	-5.210423906241
H	1.527256496186	2.632743272070	-5.053722645837
H	0.512759972141	4.075149113506	-4.813495220903
C	0.218833013886	3.064370019566	-6.698601268412
H	0.213690807391	2.032030512467	-7.077760609784
H	-0.777700749190	3.494987267078	-6.875896464048
C	-4.578803203476	1.798322240001	2.780588935280

H	-5.473401654802	2.312049050282	2.411194485401
H	-3.937510981518	2.533562116198	3.282277364448
C	-4.970419417644	0.706012777314	3.762577460122
H	-5.617898723583	-0.029244668702	3.262567357096
H	-4.068372795644	0.180646954475	4.109781924563
O	1.231137023887	3.835654116458	-7.321756726292
C	1.124038094734	3.874734453574	-8.736838515469
H	1.202596357730	2.869328918010	-9.174029142493
H	0.172860699490	4.322746676401	-9.057410255899
H	1.947423094612	4.488062862295	-9.103559200374
O	-5.643581781640	1.335745801774	4.838463065267
C	-6.069702889775	0.430560828720	5.845862697572
H	-6.775573546216	-0.312072920869	5.447847785989
H	-5.219097164357	-0.100710910921	6.295899193902
H	-6.569080830919	1.019557493977	6.615493511960

Pin_TS2C-F2500

($E_F = -929.80790720$ a.u.; $G_F = -929.43161500$ a.u.)

0 1

C	-2.514460679411	2.707020626613	1.172316625214
C	-1.211522247774	4.283743828126	0.924913359355
C	-1.476914274965	5.681894499854	1.033246624136
C	-1.584818779707	-0.419715475072	2.789695644539
C	-1.334068181126	1.067518800025	3.033589222722
C	-1.254465459719	2.060112022475	1.798845825137
H	-0.847779528545	4.010968132668	-0.065280336772

H	-2.366694077977	-0.745555016317	2.104333818357
H	-2.084927404901	1.458830043012	3.739392544586
H	-0.377690161313	1.144171368576	3.565962698843
H	-0.706624697672	1.546743754580	1.000965736536
C	-0.564646894804	3.434047977819	2.056769054232
H	0.531527269416	3.423406441648	2.035153871980
H	-0.860061524472	3.811368985064	3.039846668567
C	-3.011433842200	2.159624414436	-0.138471848232
H	-3.533184073308	1.200045698390	0.006207799480
H	-3.720243609390	2.847866710089	-0.609974292399
H	-2.190174151051	1.982262140176	-0.838531936746
C	-3.605658602120	3.124682156041	2.123615436184
H	-4.217751254183	2.260141586455	2.421615018841
H	-3.214518263952	3.572781086013	3.040006772494
H	-4.272599597821	3.852065860969	1.651522766362
C	-1.839407358601	6.354304474485	2.322476753851
H	-2.807412514056	6.865485756295	2.264191379676
H	-1.908193653913	5.621933230408	3.124589638786
H	-1.099465487151	7.105566558252	2.626262757701
O	-1.429004596935	6.487517643146	-0.127489410893
O	-1.320774372481	-1.286701919713	3.852560164432
C	-1.818352703079	7.895851493806	-0.063451035817
H	-1.332108701652	8.388250887574	0.781375464113
H	-2.901797651688	7.972103732161	0.071316344010
C	-1.427931552056	8.700586323010	-1.345509331828
H	-0.344232863910	8.628645490079	-1.507668664304

H	-1.937582096045	8.283257394007	-2.223831526314
C	-1.652649283483	-2.698043771631	3.674672066978
H	-1.108562428684	-3.091344577507	2.810345418412
H	-2.726951265892	-2.796980384869	3.483688146965
C	-1.286831901045	-3.553735256933	4.931383395314
H	-0.209692245406	-3.468242930310	5.127867768461
H	-1.827045743172	-3.166157817767	5.805681440376
O	-1.828122812791	10.069545529121	-1.117563679288
C	-1.590471451569	11.086881517257	-2.144621824865
H	-0.519914646969	11.193758284600	-2.356168658409
H	-2.123738144325	10.846122294020	-3.071912210629
H	-1.978863600597	12.012955517210	-1.724254319710
O	-1.654866087496	-4.922520791591	4.663705409514
C	-1.412291519728	-5.949658390719	5.680628241031
H	-0.343514928754	-6.034129147819	5.910427768290
H	-1.968004542241	-5.734303110632	6.601001325305
H	-1.770842483378	-6.878461338203	5.240378002282

Pin_TS2C-F2000

($E_F = -929.59372096$ a.u.; $G_F = -929.21660521$ a.u.)

0 1

C	-2.487768999994	2.704411055188	1.179449945683
C	-1.179805575058	4.282308517303	0.947344168552
C	-1.462166755658	5.667714072986	1.066151100227
C	-1.601413581577	-0.379641644880	2.776352033890
C	-1.310669703631	1.087792590962	3.035159360646

C	-1.226142164545	2.067002658539	1.805934726192
H	-0.819241756720	4.017768376419	-0.046046913120
H	-2.407493768406	-0.680814366081	2.107800029876
H	-2.041835722022	1.494861623857	3.753195460633
H	-0.345321737584	1.134881026403	3.554938048295
H	-0.676949823176	1.551644258502	1.010062147973
C	-0.535212676358	3.432952199692	2.071333980367
H	0.560930348309	3.420374007440	2.048553640071
H	-0.828858547853	3.805585311488	3.056728310209
C	-2.977424066772	2.161348220170	-0.135481914338
H	-3.500240332513	1.201138353115	0.001817429704
H	-3.683822254151	2.851117765193	-0.608572373647
H	-2.152415441580	1.986599019635	-0.831835613041
C	-3.582315674900	3.120439174833	2.127055690239
H	-4.194246179515	2.255544468990	2.424661156441
H	-3.194734202247	3.570721738005	3.043891977032
H	-4.249244531871	3.846274184081	1.652364215390
C	-1.820815470891	6.337814519840	2.357472349050
H	-2.796314358823	6.835476230715	2.308413810724
H	-1.870857743131	5.606241183107	3.161559759558
H	-1.087803947579	7.099655300458	2.651645994833
O	-1.429619227287	6.462048426756	-0.094503229769
O	-1.329733750713	-1.253316067606	3.823307861558
C	-1.864451488293	7.847657171164	-0.041438012455
H	-1.421251969494	8.361067909278	0.814679891074
H	-2.954041180266	7.892586833379	0.057750070243

C	-1.449953857274	8.639876673927	-1.310910495752
H	-0.359908548883	8.587324810771	-1.437124228767
H	-1.921571169054	8.206119708538	-2.202927156975
C	-1.688759247018	-2.647846788005	3.636477319215
H	-1.171080747184	-3.045158314366	2.757432673699
H	-2.768919240133	-2.730688792126	3.470176830889
C	-1.304492913217	-3.498956296059	4.877303515628
H	-0.221488570216	-3.428217407729	5.048215670652
H	-1.817401621987	-3.104698872070	5.765500897925
O	-1.882981411749	9.995467999484	-1.104594468108
C	-1.612913186308	10.982451472788	-2.135962841905
H	-0.535046584196	11.094143353220	-2.307727716890
H	-2.103607928060	10.716370776477	-3.080484847510
H	-2.023263613256	11.918995594501	-1.761158988256
O	-1.697321851575	-4.855149608110	4.615278149132
C	-1.433033058648	-5.857685021424	5.634093331567
H	-0.358306809926	-5.944731834022	5.836853525095
H	-1.959338621563	-5.624029243803	6.568009627107
H	-1.806665409542	-6.796330001542	5.227625998032

Pin_TS2C-F1800

($E_F = -929.50869156$ a.u.; $G_F = -929.13129005$ a.u.)

0 1

C	-2.474478444853	2.704634107058	1.183805532639
C	-1.164082462558	4.282392614656	0.957429986367
C	-1.453892019924	5.662624248848	1.080262559564

C	-1.609088869485	-0.362794331448	2.771483124056
C	-1.298845383225	1.095825916292	3.036297083563
C	-1.212134593890	2.070370619818	1.809463720353
H	-0.805275710495	4.021203902232	-0.037401198669
H	-2.426918387565	-0.651735696777	2.111835189507
H	-2.020216387592	1.510233229206	3.760210374735
H	-0.329442514302	1.128743890267	3.549636601952
H	-0.663069028650	1.554140424105	1.014002275207
C	-0.519932593790	3.432826885210	2.077833110712
H	0.576157263339	3.418987371667	2.053768423083
H	-0.812067279056	3.803562297794	3.064386903804
C	-2.962361736768	2.163793013674	-0.132531185054
H	-3.486290272437	1.203751417946	0.002019809233
H	-3.667532199235	2.854777526870	-0.605770164405
H	-2.136405624676	1.989496948056	-0.827889228637
C	-3.569524363177	3.120562553236	2.130677951563
H	-4.181646941184	2.255849012475	2.428504222442
H	-3.182514490351	3.571522278615	3.047425702581
H	-4.236368233138	3.846141264366	1.655390346827
C	-1.810921908303	6.332223648963	2.372109962270
H	-2.791034634760	6.821253024144	2.327977423530
H	-1.849588290634	5.601972617218	3.177975929373
H	-1.082600165817	7.101018775281	2.659860671885
O	-1.426413151254	6.452401251522	-0.080329118510
O	-1.333561211489	-1.240648998235	3.810636860056
C	-1.890649336249	7.825070764558	-0.036323057428

H	-1.478620586951	8.349681829095	0.828533740578
H	-2.983220837733	7.848200449655	0.036733480603
C	-1.458184779101	8.615792794945	-1.295912937112
H	-0.364472438941	8.579207418267	-1.394637383263
H	-1.900240722330	8.171565064415	-2.198055482684
C	-1.707782114086	-2.627456249526	3.621157065482
H	-1.205913871020	-3.026767979608	2.733727206198
H	-2.790971872134	-2.701017254195	3.469935368699
C	-1.312242913670	-3.478477534227	4.853392627878
H	-0.226128080696	-3.416583836913	5.008322396665
H	-1.808323792880	-3.080230925061	5.749540726031
O	-1.916337188779	9.962801144035	-1.105293633521
C	-1.624922580629	10.939480864634	-2.134384559292
H	-0.543207162964	11.060753952105	-2.274242519696
H	-2.082348888412	10.659392193991	-3.091782680983
H	-2.055296832765	11.876961356121	-1.784773324854
O	-1.719859015074	-4.828664986575	4.596242194819
C	-1.443471031625	-5.822171195845	5.614392919711
H	-0.365682511731	-5.913140453304	5.799891519299
H	-1.951697878631	-5.579494113012	6.556312413616
H	-1.827712602411	-6.763520787224	5.223972946089

Pin_Int1-F1800

($E_F = -929.52497837$ a.u.; $G_F = -929.14420874$ a.u.)

0 1

C	-2.355735893138	2.900521037204	1.180523743988
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C	-1.349781904952	4.134833396213	0.959189556018
C	-1.770268129663	5.581799180360	1.060867055919
C	-1.584058147254	-0.343643313423	2.751598755424
C	-1.265123154165	1.113265649952	3.020123474644
C	-1.147260572889	2.086474931712	1.803483883737
H	-0.895483425309	4.004792681616	-0.027567910341
H	-2.397506104077	-0.628594050518	2.084884452880
H	-1.985781829941	1.529293679707	3.742837789890
H	-0.299471968652	1.134747602583	3.541606917541
H	-0.641087070691	1.556069509940	0.989769385074
C	-0.430955244215	3.450773117127	2.036677091392
H	0.647779416783	3.489637202831	1.867832664296
H	-0.636620137618	3.833489471936	3.040133734550
C	-2.950168322201	2.334506702014	-0.104555027113
H	-3.510085519430	1.413804373333	0.093512177875
H	-3.636406832541	3.054756508542	-0.562677649265
H	-2.167407409512	2.104090391246	-0.832945792315
C	-3.466068246628	3.192962331497	2.188828692797
H	-4.054414302537	2.289348675712	2.376284035312
H	-3.082189326645	3.536719390999	3.151432434902
H	-4.136929406215	3.964771602092	1.801292341865
C	-1.967965148719	6.252506559782	2.385032686394
H	-2.786147365397	6.979413511706	2.377950641482
H	-2.199754236358	5.515225693450	3.151388259509
H	-1.062877618321	6.789684926751	2.713388343525
O	-1.431295065994	6.395884667846	-0.034525898123

O	-1.321825701367	-1.221220285522	3.794215741569
C	-1.890928228679	7.771235428846	-0.029505130610
H	-1.511128278360	8.300587572532	0.848527498066
H	-2.985707502481	7.793643043900	0.003725666349
C	-1.414540690882	8.552922269863	-1.277919144783
H	-0.318303430326	8.514801956920	-1.343260353684
H	-1.829649669730	8.105775499091	-2.191395687161
C	-1.698024956962	-2.607284910378	3.603618617506
H	-1.190776775833	-3.008793207948	2.720261933736
H	-2.780289170404	-2.678587894500	3.444927153269
C	-1.312614717798	-3.457359239296	4.839749282047
H	-0.227605496963	-3.396269943518	5.002537181476
H	-1.814834159929	-3.057497674462	5.731747640109
O	-1.876169086245	9.901813198419	-1.106838440980
C	-1.563538035954	10.872618406744	-2.134747935997
H	-0.479198015233	10.995118121907	-2.251679133779
H	-1.999335709966	10.586460711584	-3.100454979715
H	-2.002853418341	11.811471805482	-1.800223093677
O	-1.719628728093	-4.807422750242	4.581314355339
C	-1.451704279443	-5.799796909849	5.602873535631
H	-0.375430658328	-5.891184106185	5.796737783947
H	-1.966982520264	-5.555518618682	6.540529463826
H	-1.833556660827	-6.741402137505	5.210749445727

Pin_TS2C-F1500

($E_F = -929.38184067$ a.u.; $G_F = -929.00428929$ a.u.)

0 1

C	-2.448067151124	2.705245307807	1.190513000334
C	-1.135475021999	4.284085582855	0.975219619263
C	-1.439216654224	5.655937004009	1.103952938525
C	-1.620302798306	-0.335349677175	2.765035083713
C	-1.276840220327	1.108600512136	3.039598729631
C	-1.185014161621	2.076798084213	1.816722313552
H	-0.778272251612	4.028549468682	-0.021515873824
H	-2.456323647430	-0.602744096819	2.119197242064
H	-1.982132313015	1.535123586257	3.772546194318
H	-0.301640675191	1.117326720178	3.542933038009
H	-0.634615905338	1.559646065958	1.022698077013
C	-0.492166906009	3.434559955169	2.090701051233
H	0.603853240159	3.419716182956	2.065645754982
H	-0.783254089795	3.801958324926	3.078794434992
C	-2.930576517193	2.167476053809	-0.128800054581
H	-3.455039758814	1.206933967492	0.000515129091
H	-3.634057889793	2.859486865438	-0.603183519219
H	-2.101880120681	1.995131966783	-0.821409351877
C	-3.545675107436	3.119828966649	2.134690806829
H	-4.157429160457	2.254699999118	2.432179222553
H	-3.161288573611	3.572498907736	3.051712153512
H	-4.212594440100	3.844133398887	1.657441378212
C	-1.794488238710	6.324644780461	2.396445606638
H	-2.782845903773	6.797592136495	2.360593675973
H	-1.812874494105	5.597142729233	3.205462344198

H	-1.075430862161	7.106168529784	2.673106278841
O	-1.423371310113	6.438126099542	-0.057250318800
O	-1.341156820020	-1.221372432214	3.791370888776
C	-1.930474118496	7.790587431673	-0.026456299856
H	-1.560115475135	8.331702781261	0.847093486796
H	-3.025279613263	7.781286077052	0.014342815493
C	-1.478637631843	8.577769528567	-1.274486024853
H	-0.381629599437	8.562650806313	-1.339461294233
H	-1.882972359685	8.118386715202	-2.186974123550
C	-1.740702910643	-2.595595355889	3.597123410016
H	-1.263653065972	-2.997540966368	2.697053437962
H	-2.828031541685	-2.653190167235	3.468901142115
C	-1.329147217422	-3.448159676797	4.815623130973
H	-0.238915730491	-3.400077143185	4.946419051241
H	-1.799435305846	-3.044373711934	5.723429677509
O	-1.968883815497	9.912726481955	-1.107114603842
C	-1.649749362653	10.872355709404	-2.135151478218
H	-0.564533218932	11.004659894460	-2.235374052489
H	-2.064694399823	10.571924705956	-3.106087662234
H	-2.102923908025	11.812233988755	-1.821994618453
O	-1.759205006911	-4.789024382653	4.565890629986
C	-1.465266678469	-5.769473787927	5.582888075472
H	-0.383567226997	-5.866264610284	5.743393393637
H	-1.947050355815	-5.513521576307	6.535611270956
H	-1.864290378249	-6.714495403005	5.216236688465

Pin_TS2C-F1000

($E_F = -929.17232342$ a.u.; $G_F = -928.79435668$ a.u.)

0 1

C	-2.384966758814	2.710756456170	1.206768439054
C	-1.070473741196	4.293181005999	1.017083563282
C	-1.404744928197	5.649113097532	1.154699360476
C	-1.632795176917	-0.283334238355	2.755223833852
C	-1.228898208083	1.132099724696	3.051787072556
C	-1.122198814874	2.093113733672	1.837939878511
H	-0.713272599092	4.048241475805	0.017967350470
H	-2.494414599838	-0.507499176230	2.126796550178
H	-1.907705056610	1.578071268987	3.798440273392
H	-0.247349503823	1.094905078276	3.541334517842
H	-0.566022388417	1.576004740272	1.047816959480
C	-0.430381674873	3.443671560707	2.125564129362
H	0.665550107909	3.428306644462	2.101812922565
H	-0.723066601610	3.804098900774	3.115706391817
C	-2.853215968053	2.179078176453	-0.119655009121
H	-3.378237214186	1.217222922609	-0.002051225760
H	-3.552596940119	2.872829882908	-0.597789860941
H	-2.017334782413	2.011303896639	-0.804770524625
C	-3.490484432931	3.121585687729	2.142837534161
H	-4.102469060730	2.255366416157	2.436754939436
H	-3.113958165067	3.576523566302	3.062018905159
H	-4.155970689262	3.843994345876	1.660502713605
C	-1.761385306874	6.316386292694	2.446943862238

H	-2.767209210442	6.752147088229	2.425646328634
H	-1.737075408814	5.596876773843	3.262893968239
H	-1.066351202452	7.126558242469	2.701504578029
O	-1.418593688390	6.415441891841	-0.009743827008
O	-1.359568055199	-1.188351487781	3.758383820916
C	-1.995610927001	7.731486034593	-0.000392351007
H	-1.678828829441	8.302538467014	0.875421108310
H	-3.089818004660	7.667911985187	0.008216999751
C	-1.534898835915	8.504805545037	-1.242873120993
H	-0.436068062008	8.526188672260	-1.270839749272
H	-1.890491590169	8.012691094868	-2.159005656322
C	-1.805933636449	-2.538525393558	3.550405324385
H	-1.369169359550	-2.941665055015	2.630315616296
H	-2.898331526376	-2.564922365736	3.457211216823
C	-1.374257935425	-3.399628687671	4.744125763680
H	-0.279013845745	-3.376793868775	4.837367975290
H	-1.802354865481	-2.988511531843	5.669764586955
O	-2.074146335261	9.819490637979	-1.120616602054
C	-1.717425652238	10.743720435586	-2.155298600954
H	-0.630415541902	10.895114306041	-2.200189680068
H	-2.068610785884	10.401883479816	-3.138293392270
H	-2.202849754696	11.687542711952	-1.908098171654
O	-1.842586040135	-4.723465555706	4.504642762762
C	-1.521736921686	-5.685138226938	5.517921996433
H	-0.435336526533	-5.793152802990	5.638168845490
H	-1.960119475299	-5.408455931929	6.486316246360

H	-1.944142152856	-6.634295589533	5.189133333108
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Pin_TS2C-F500

($E_F = -928.96542963$ a.u.; $G_F = -928.58766836$ a.u.)

0 1

C	-2.263377927526	2.730823726989	1.241504231045
C	-0.949834193742	4.319187007439	1.095050674322
C	-1.330212860860	5.654465939461	1.236999428342
C	-1.625373510826	-0.210164506500	2.751072788006
C	-1.143846922687	1.164264402449	3.086281925732
C	-1.005802236443	2.125643029294	1.888643213572
H	-0.584958652598	4.086486920966	0.096124169816
H	-2.503733522044	-0.369845295944	2.126211480300
H	-1.794540457980	1.629939207346	3.846167247780
H	-0.162321330739	1.063781759813	3.566774344347
H	-0.434961549013	1.612254661238	1.106522923468
C	-0.320022704041	3.469762128663	2.200911604016
H	0.775888576227	3.455939630015	2.187891966486
H	-0.624199628423	3.820359451551	3.191048207461
C	-2.703990777092	2.208195808045	-0.097348096315
H	-3.231843088090	1.245624985180	0.000891920589
H	-3.393285733021	2.905645921577	-0.584958509068
H	-1.854256349640	2.045254134205	-0.766456634155
C	-3.385686519771	3.135770560886	2.159534417197
H	-3.999992286711	2.267955613630	2.443608475179
H	-3.025711665977	3.592760274801	3.084320969637

H	-4.045593892496	3.856297839329	1.666543150649
C	-1.695086457012	6.323895807084	2.524949282756
H	-2.724512150915	6.701542259324	2.521324802380
H	-1.608806648196	5.623484264689	3.353330996031
H	-1.041219052921	7.177170608171	2.745009455150
O	-1.386701403755	6.396718343182	0.065096876697
O	-1.389075012603	-1.147646678736	3.725319741871
C	-2.063413132763	7.656269696940	0.043350793505
H	-1.794980133653	8.277324761780	0.901723026145
H	-3.150338996211	7.511461769819	0.049060482336
C	-1.639497815669	8.400091035949	-1.219880270310
H	-0.542849055779	8.480494457623	-1.238571670103
H	-1.955022157038	7.849495867548	-2.117638630352
C	-1.895506636845	-2.463873694456	3.483199481695
H	-1.491095173179	-2.860785350965	2.545512263690
H	-2.989873106834	-2.444890381346	3.410357041309
C	-1.470016536238	-3.351585839366	4.648495560221
H	-0.372573958889	-3.363731459002	4.719128440770
H	-1.864511523874	-2.940129689615	5.589200090211
O	-2.248491615293	9.682399314377	-1.161109926098
C	-1.888725530502	10.556108945028	-2.226528839401
H	-0.806742032223	10.747989797533	-2.240698635340
H	-2.185914178339	10.146512179582	-3.201997854875
H	-2.416392392267	11.494973171838	-2.057965631475
O	-1.983103779478	-4.651589694254	4.401660310999
C	-1.653056592961	-5.607910648399	5.404983863190

H	-0.565453562257	-5.736052197819	5.495720053820
H	-2.056209445144	-5.317632599694	6.385225246380
H	-2.100511359755	-6.553994917882	5.100225647236

Pin_TS2C-F200

($E_F = -928.84310592$ a.u.; $G_F = -928.46576119$ a.u.)

0 1

C	-2.060686700554	2.782550415138	1.291627006781
C	-0.743694743665	4.369334704927	1.212950104245
C	-1.168399860636	5.686290157251	1.352517783030
C	-1.577834976727	-0.120863167916	2.760390102397
C	-1.019899615858	1.205623044810	3.148949779699
C	-0.824272155850	2.176857794784	1.974642263717
H	-0.354466739840	4.149188881876	0.220659939545
H	-2.454015349580	-0.203842793848	2.118018299971
H	-1.653814966567	1.687461127536	3.913149974392
H	-0.051578568430	1.035902559625	3.636377205735
H	-0.228657711534	1.667878633680	1.208315368777
C	-0.144465440431	3.512886392140	2.325667240529
H	0.951068655408	3.496179181534	2.341122868317
H	-0.475399606531	3.852933611279	3.310756217970
C	-2.453478806417	2.278159961919	-0.068490974310
H	-2.991538763843	1.318544532071	-0.003331214258
H	-3.118741959818	2.986696799966	-0.573437381518
H	-1.580106463007	2.116968241429	-0.706881327803
C	-3.212358995261	3.184506656234	2.173615100389

H	-3.838718544795	2.317572966729	2.432280342732
H	-2.881945091831	3.636446039905	3.111830377922
H	-3.852909650695	3.909962168610	1.662392995185
C	-1.558973440391	6.358516501760	2.630710973184
H	-2.614349558825	6.656601715291	2.642942458023
H	-1.399462061139	5.692279539339	3.476547978232
H	-0.967593252181	7.265900163951	2.805936184079
O	-1.238883615549	6.416120528931	0.177463672340
O	-1.414903439548	-1.099410794984	3.703711498298
C	-2.102483623551	7.548788143422	0.095562328646
H	-1.941049086940	8.246905362752	0.922036184662
H	-3.154428660176	7.238173687109	0.105123341287
C	-1.772156016005	8.266909831365	-1.203847119283
H	-0.696786960804	8.497553909535	-1.220279220685
H	-1.992712912065	7.621973216604	-2.066766004984
C	-1.995901414133	-2.369102431380	3.405799031553
H	-1.606892581935	-2.754971467442	2.456929271499
H	-3.086762966702	-2.283500101161	3.326890245812
C	-1.628023558082	-3.310885947808	4.541501741177
H	-0.533134282441	-3.383881774904	4.617283650629
H	-2.005381108304	-2.907461523213	5.492878708387
O	-2.550862986407	9.451044160795	-1.234109222364
C	-2.274013940390	10.280989480232	-2.351988957921
H	-1.225080373048	10.609803270533	-2.358632097680
H	-2.485186563450	9.765883885120	-3.299867350939
H	-2.920904355391	11.154917096751	-2.270735739125

O	-2.207245465560	-4.570674861538	4.252869450819
C	-1.920634657998	-5.557920147539	5.232602213506
H	-0.839697349651	-5.737590712150	5.318695478440
H	-2.307619612248	-5.269513466548	6.220181216981
H	-2.410296774716	-6.478172845126	4.913259908847

Camphanediol

(E = -542.51041820 a.u.; H = -542.22856734 a.u.)

0 1

C	-1.811229307931	0.798024401982	-2.550895596127
C	-1.160916037528	1.985245064328	-1.766751519597
C	-1.814684955324	1.879177066857	-0.343541445298
C	-2.738232988661	0.644397011137	-0.489010282065
C	-1.803629233544	-0.587397818986	-0.533811415981
C	-1.162198424749	-0.477505831177	-1.951346863648
H	-0.078644640844	1.815933068148	-1.687717684487
H	-1.035495827990	1.680216569619	0.404810567206
H	-3.506672591696	0.595164947786	0.287937423396
H	-1.058777728402	-0.559254775117	0.265644023331
H	-2.362213533142	-1.516663807335	-0.414063476936
H	-1.386420261759	-1.351638462470	-2.565966462683
H	-0.072655939322	-0.390158850914	-1.914631098173
C	-3.261485231704	0.738744342293	-1.952780319877
C	-4.071473644707	-0.494260880968	-2.394830152249
H	-4.332887715525	-0.413226201728	-3.453918161168
H	-3.558817476138	-1.445900878473	-2.256273495953

H	-5.009597038284	-0.540787958130	-1.833434843596
C	-4.136528387222	1.969545049548	-2.251281921326
H	-4.397649671982	1.987194236833	-3.314333826013
H	-5.072500725245	1.897476060282	-1.687245128722
H	-3.659693574121	2.910371085894	-2.000945427243
O	-1.390028860237	3.268020445841	-2.328445961177
O	-2.484121412418	3.085540782856	-0.008392003731
C	-1.677154823809	0.918745646858	-4.058347747953
H	-0.623088602362	0.941360033682	-4.358731308684
H	-2.141305881776	0.067615221490	-4.563496845229
H	-2.155955017960	1.829801650049	-4.424684726920
H	-0.844084926583	3.336537047495	-3.116440477605
H	-2.961791023743	2.922168355329	0.810239115266

Camphanediol_H2

(E = -543.72581137 a.u.; H = -543.42024775 a.u.)

0 1

C	-1.602140523483	1.804978803351	-2.553973309713
C	-1.061324174522	2.759936160430	-3.622540492102
C	-3.360807148495	2.019733443246	0.859625554148
C	-2.686731892766	1.509731809716	-0.403698154642
C	-1.204838419694	1.120279849212	-0.197874005686
C	-0.493369251137	1.401659190330	-1.544561383125
H	-0.620399262549	3.645135494670	-3.150297272091
H	-2.783738812881	2.848338412163	1.293355922799
H	-3.247273713440	0.612924499085	-0.686207464024

H	-0.765626667304	1.718753187147	0.606127507842
H	-1.117804966740	0.079253758917	0.114885187142
H	0.074602579871	0.546120410326	-1.911804764989
H	0.224792552694	2.219141146112	-1.435429703384
C	-2.698873322992	2.469956516033	-1.629807287472
C	-4.088922537949	2.549139389024	-2.279148882347
H	-4.056926495033	3.111639861559	-3.217227404184
H	-4.498254676542	1.560277787068	-2.492113331621
H	-4.793606649932	3.061705486502	-1.618050215208
C	-2.289966496357	3.898895414036	-1.206002774937
H	-2.287660188540	4.580582228750	-2.059736216451
H	-3.005388207578	4.303445057666	-0.485947835893
H	-1.300206061908	3.931652928431	-0.744624625470
O	-0.064297414818	2.068641046978	-4.381363022062
O	-3.421751737403	0.919805675128	1.772045028237
C	-2.135327727255	0.543273314578	-3.265840666074
H	-1.323135124780	0.076086209802	-3.822516239575
H	-2.528275361138	-0.189079766358	-2.557885914414
H	-2.926666862209	0.786022785631	-3.979541749103
H	0.298310553557	2.683092222970	-5.024767552230
H	-3.781950598720	1.239841378644	2.603692169378
H	-1.883372079859	3.093097228900	-4.274818033830
H	-4.370845742880	2.391354066624	0.631356289654

Pinanediol

(E = -542.48436261 a.u.; H = -542.20322834 a.u.)

0 1

C	-1.717126544362	1.750165685129	-0.240824960907
C	-1.772261221729	3.232563753912	0.292101799957
C	-2.192719950953	3.400172964070	1.773026133923
C	-1.621450012724	2.220500210401	2.629071125428
C	-0.429672440684	1.464512967149	1.972685620423
C	-0.314519435053	1.703573007768	0.459038637446
H	-2.314483483800	3.955612980994	-0.328624129299
H	-2.447768683999	1.509988297940	2.732157232666
H	0.489585285126	1.814502008878	2.452218852219
H	-0.523962594857	0.394693635336	2.191619202259
H	0.447688116550	1.061302611798	0.008254012373
C	-0.218999433844	3.235045092733	0.243631598289
H	0.184184863796	3.517578906692	-0.727347663355
H	0.276573563614	3.813814592189	1.021667678091
C	-1.587797195798	1.737512369845	-1.774935273968
H	-0.856017853992	2.450915927405	-2.154764933431
H	-1.290476498873	0.742395561442	-2.120766540183
H	-2.551583171416	1.975881844600	-2.236205768251
C	-2.782106821742	0.709964498557	0.118911338174
H	-2.495645144664	-0.264331742633	-0.290406445754
H	-2.936412527346	0.577610929062	1.186955387750
H	-3.746231704217	0.978417256235	-0.324646007493
C	-3.712409053701	3.484982292542	1.944324329787
H	-4.101012681794	4.363939664838	1.419648603772
H	-4.221492218041	2.605057305810	1.545260664503

H	-3.946114406735	3.586205345371	3.006137634181
O	-1.615381412638	4.611651509913	2.278393292790
O	-1.299631582479	2.711480431169	3.926325544264
H	-1.947078233416	5.329488523389	1.728722649133
H	-1.098688789056	1.946309218588	4.473707558563

Pinanediol_H2

(E = -543.70031681 a.u.; H = -543.39570535 a.u.)

0 1

C	-1.414831787491	2.664707691946	0.753568010114
C	-1.247760037126	4.155724638417	1.209460984917
C	-2.263239763269	5.244218025003	0.862841467939
C	-1.970712669770	0.895439008390	3.783775799213
C	-0.819742775157	0.957192698911	2.788739233898
C	-0.608506054159	2.282641980858	2.047697547786
H	-0.298739078193	4.514086745502	0.799534887305
H	-2.933068974751	1.078697929317	3.290784891415
H	0.086275737511	0.706544637724	3.350209219207
H	-0.954304126719	0.149246704502	2.060306795751
H	0.449953042492	2.333568527824	1.771472699956
C	-1.001250608698	3.658309809526	2.655518608855
H	-0.258788334723	4.186487159324	3.255875642223
H	-1.930401240872	3.599724994135	3.226521964189
C	-0.748716874339	2.299677258101	-0.571305776241
H	0.287838559973	2.646775741925	-0.600643871967
H	-0.746837383146	1.214832212293	-0.723187977598

H	-1.278709527992	2.751247809309	-1.416968833173
C	-2.859888598037	2.156798383408	0.754316459577
H	-2.880217306032	1.069801967111	0.632342680617
H	-3.389602262481	2.394257443714	1.676821817314
H	-3.423548546310	2.593519069691	-0.075708436907
C	-3.498085032482	5.329359445567	1.758970084897
H	-4.148620261583	6.144143624781	1.423633111893
H	-4.088113153763	4.412319333312	1.742045595980
H	-3.198358829059	5.539813002104	2.787886303550
O	-1.532896802892	6.481408545774	0.934892125859
O	-1.944976171196	-0.411475314086	4.362468945930
H	-2.142771461877	7.199095240307	0.737172627429
H	-2.650356745914	-0.464051888216	5.013327556263
H	-2.586781455512	5.073865465037	-0.176911874170
H	-1.834878544617	1.666714214315	4.555241887771

Transcyclohexanediol

(E = -386.44147288 a.u.; H = -386.25335164 a.u.)

0 1

C	-0.626160312053	-0.375628506316	0.400284171477
C	0.533750520978	-0.361173830914	-0.599175758244
C	0.550056469737	0.934091814955	-1.404845355268
C	0.602313379712	2.159676402893	-0.482096552969
C	-0.552221850567	2.145763828249	0.532417340763
C	-0.577106938235	0.833860151544	1.332593072886
H	1.399007577587	0.916039227259	-2.093369585101

H	-0.357076252617	0.959395697262	-2.019642522447
H	0.573322912836	3.077764573427	-1.075914340371
H	1.556882706858	2.168106633405	0.059177712066
H	-0.475102664785	2.998997321864	1.212619984830
H	-1.503341379389	2.255990792429	-0.002821273462
H	-1.429933163707	0.797042113094	2.015722771004
H	0.330656622035	0.765862571931	1.949173644359
H	1.471639773209	-0.429563097236	-0.015338252425
H	-1.559102790126	-0.368642151366	-0.172984422575
O	-0.650792328991	-1.624507821208	1.106546319490
H	0.097945812715	-1.630377313988	1.713914457314
O	0.436972085298	-1.458456007471	-1.494396483894
H	0.178536143969	-2.218015459748	-0.957522963077

cyclohexanediol_H2

(E = -387.63229706 a.u.; H = -387.42180155 a.u.)

0 1

C	-3.195897022324	0.059856101552	-0.327615320153
C	3.192931610325	0.085210983387	0.325917510951
C	1.901852407088	0.079566551695	-0.476281266392
C	0.649170564611	0.075906331900	0.403165408989
C	-0.652083059151	0.070081628294	-0.405156386284
C	-1.904692813844	0.066201612189	0.474405051836
H	-3.224561014476	-0.829436452737	-0.976037382092
H	1.900987528408	0.957468518858	-1.131598687501
H	1.907488935341	-0.799823510854	-1.129586018585

H	0.659250075334	0.954017946555	1.061331760500
H	0.665832278001	-0.800614786311	1.063319182214
H	-0.668841983903	0.946650293791	-1.065245783937
H	-0.662120120826	-0.807989582907	-1.063384232802
H	-1.910557315787	0.945681277123	1.127560653264
H	-1.903453550850	-0.811579743695	1.129859073820
O	-4.282959811130	0.056591220095	0.597017998760
H	3.228166025918	-0.801973729074	0.976966921754
O	4.280102181164	0.087457673037	-0.598504503449
H	5.100689562828	0.091417907974	-0.097908233722
H	3.222182734497	0.974639843661	0.974200421389
H	-5.103643161892	0.053413967684	0.096532174979
H	-3.231943807343	0.947113907260	-0.978470499290

Ciscyclohexanediol

(E = -386.44188437 a.u.; H = -386.25373293 a.u.)

0 1

C	-4.006268289005	-1.960699173913	-2.508526054866
C	-3.409125366444	-1.226355653119	-1.301093520013
C	-4.373578079878	-1.225893456089	-0.113815276501
C	-4.788089580873	-2.655980024466	0.264714790887
C	-5.397124810853	-3.385846379866	-0.940996716281
C	-4.433055820641	-3.379551003217	-2.135607135384
H	-3.241425952854	-1.992344600848	-3.297951332466
H	-2.473257630061	-1.731404864036	-1.017004583639
H	-3.907787199438	-0.718032946900	0.739533339040

H	-5.256714408955	-0.647669658297	-0.401463338622
H	-5.498344153592	-2.629858199462	1.096301601573
H	-3.908618762310	-3.208764791405	0.620498033488
H	-5.653839987556	-4.414962224460	-0.672352041030
H	-6.323942091779	-2.886032888734	-1.237219182640
H	-4.896748581032	-3.842081745205	-3.010862975031
H	-3.535846258262	-3.963284279596	-1.896431139217
O	-5.159649622051	-1.266766161627	-2.979709322846
O	-3.126576290475	0.102164746386	-1.764049739345
H	-4.906884191062	-0.336422692420	-3.026228365197
H	-2.944705748982	0.658736051225	-1.001010584843

Ciscyclopropanediol

(E = -268.40579358 a.u.; H = -268.30941431 a.u.)

0 1

C	-0.797567847682	0.005541794401	-1.575690773290
C	-1.727800764353	-0.017702624147	-0.378964340888
C	-0.266814821369	0.271118862389	-0.181155624521
H	-0.570041838328	-0.964909207631	-2.003319807376
H	-0.846700499505	0.829139514176	-2.278981809274
H	-2.441314051451	0.790926024893	-0.262390227531
H	0.053446174659	1.276306176408	0.082370930711
O	0.417957863784	-0.761345780853	0.490672487787
H	1.211165184600	-0.976906233050	-0.008956969358
O	-2.224581023948	-1.237748876050	0.082255837643
H	-1.482879767509	-1.682736749229	0.515185914681

Ciscyclopropanediol_H2

(E = -269.65003215 a.u.; H = -269.52893012 a.u.)

0 1

C	-1.938715601262	2.762233944632	-0.555124354086
H	-2.989987578768	2.752458369458	-0.227515329929
H	-1.463602954013	3.655346499075	-0.120147622961
C	-1.871700552571	2.829438339024	-2.072201124900
H	-0.823963256461	2.827748380724	-2.384793913982
H	-2.337238669351	1.933300342787	-2.491355209248
C	-2.559033618176	4.060097554974	-2.641045989858
H	-3.618714368687	4.068232324089	-2.341698322695
H	-2.092000161410	4.970563585528	-2.234191548833
O	-1.264345582739	1.573776008639	-0.147838105927
H	-1.300263296720	1.522006153125	0.811332004960
O	-2.428157951232	4.007658390228	-4.059925246177
H	-2.860245448644	4.782459167484	-4.429985783714

Ciscyclobutanediol

(E = -307.74426259 a.u.; H = -307.61763110 a.u.)

0 1

C	-2.058069361352	0.858672107785	-1.902161135908
C	-1.104433939681	1.099513758497	-0.705554261587
C	-2.271098479109	0.742162225450	0.253880397248
C	-3.242801166059	1.051026564363	-0.910747309908
H	-1.993433306644	-0.179032302124	-2.234614443673

H	-1.979737838045	1.528810128328	-2.759935270761
H	-0.827584908474	2.157550532908	-0.617813372072
H	-2.365309761024	1.334273289020	1.171293880249
H	-3.605777255424	2.081015886565	-0.886997366792
H	-4.084620412254	0.364932283229	-0.997280527959
O	0.027395325356	0.263023908085	-0.521640549262
H	0.469921387599	0.151033121667	-1.367783968316
O	-2.281334747400	-0.644135374456	0.542675027583
H	-1.356865756202	-0.926637645205	0.528416919887

Ciscyclobutanediol_H2

(E = -308.97928003 a.u.; H = -308.82821611 a.u.)

0 1

C	-2.503791518616	3.749218505141	-2.795948548576
H	-1.970418335433	2.864132368670	-2.439220996014
H	-1.956729415206	4.630528629311	-2.426853227202
C	-2.534928469025	3.758886722610	-4.323267676350
H	-3.102946871303	2.885104384470	-4.659942217463
H	-3.091515304502	4.644042760811	-4.660938967958
C	-1.138295899225	3.758144299742	-4.950916399470
H	-0.580078359973	2.870775119993	-4.633965148276
H	-0.571940134590	4.629267343147	-4.593567265828
C	-1.169333624839	3.783031985872	-6.478067892486
H	-1.712508677265	2.912166779063	-6.854467636238
H	-1.706473360709	4.678442518379	-6.827268980686
O	-3.803938604585	3.670826465959	-2.219581006330

H	-4.291770361511	4.456064204012	-2.486678915313
O	0.129938000160	3.703048702679	-7.056205237556
H	0.626489045617	4.476545120214	-6.771478869046

H₂

(E = -1.17957107 a.u.; H = -1.16619875 a.u.)

0 1

H	-0.300405579853	-0.001261525493	-1.302215418325
H	0.136204948853	0.448690953493	-0.901332330675

Azoalkane_TS-F4000

(E_F = -1375.67759959 a.u.; G_F = -1375.29557182 a.u.)

0 1

N	-0.569316893252	-1.175002294660	-0.150745983255
N	0.621696976501	-1.346630475615	-0.171075629653
C	-1.528868069266	-2.738504220303	0.009027867306
C	1.584179950658	0.222798609063	-0.323531475642
C	1.073680665708	0.812228309500	-1.623690524753
H	1.383911747231	0.207821591205	-2.479661594341
H	-0.017220005064	0.859983081585	-1.604083401730
H	1.449702316816	1.830616073914	-1.772542913032
C	1.174628765306	0.991583561517	0.917239240703
H	0.087316549703	1.086724968804	0.955576420934
H	1.516540874764	0.481964534638	1.821522846997
H	1.610783722812	1.995725400501	0.911427008789
C	-1.111825579478	-3.524279787289	-1.218719513874

H	-0.024169588510	-3.617735974776	-1.250098539834
H	-1.545809978636	-4.529175223028	-1.200783279783
H	-1.450030551221	-3.028332051926	-2.131920432123
C	-1.028585453073	-3.312532940831	1.320517245135
H	-1.412864000614	-4.325691120172	1.482459018776
H	0.062004262115	-3.367680522302	1.307553926253
H	-1.339352078725	-2.693316408793	2.165680045976
C	3.194610133017	0.017605406504	-0.352460854104
O	3.698726917312	-1.073033105666	-0.200993533629
N	3.992880540163	1.186829736859	-0.516385964732
H	3.504307000385	2.022354419261	-0.804984398982
C	-3.139754014614	-2.533142388221	0.027687924209
O	-3.643005823017	-1.442847304742	-0.128787100715
N	-3.938664160185	-3.701729477271	0.192410712211
H	-3.451010884745	-4.536696077365	0.484141067056
C	-5.443438455355	-3.705583397968	0.458582041338
H	-5.858683406729	-2.879418213240	-0.116266223261
H	-5.616238087686	-3.493697851981	1.517346742660
C	-6.214070350122	-5.056889713181	0.098543059130
H	-6.187198972103	-5.233946930797	-0.976755175783
H	-5.744712564689	-5.905345394704	0.599796989751
C	5.496940005213	1.191591339115	-0.786350331298
H	5.667047409449	0.984609114035	-1.846507107203
H	5.913343465057	0.362615427683	-0.216434153291
C	6.268904162031	2.540977694952	-0.421950574420
H	5.798753306508	3.391854022755	-0.918296591196

H	6.244503860559	2.713154908242	0.654191666374
O	7.721491516567	2.529474594179	-0.847529509446
O	-7.667554691473	-5.043986981268	0.520878966724
C	8.489827918081	3.683455744698	-0.626267483843
O	8.018603398939	4.672864818296	-0.124884010244
C	-8.435200263685	-6.198966962730	0.302313271769
O	-7.962733809033	-7.190050886476	-0.194535992793
C	9.972326134390	3.583700918519	-1.073198108361
H	10.220049838575	2.618164687226	-1.504514959582
C	10.959072370774	4.531248627215	-0.988149088637
H	10.773513699132	5.513229859179	-0.566973120855
H	11.953889365708	4.301877814506	-1.348494910992
C	-9.918554126137	-6.097991619355	0.746067383265
H	-10.167278283616	-5.131063351481	1.173644463203
C	-10.904930954425	-7.046046754291	0.662413453172
H	-10.718384401864	-8.029391756755	0.244901058230
H	-11.900460510732	-6.815686904697	1.020137426260

Azoalkane_R-F4000

($E_F = -1375.68034482$ a.u.; $G_F = -1375.29772992$ a.u.)

0 1

N	-0.589544527686	-1.210631270542	-0.160292266090
N	0.643857501830	-1.305196978822	-0.160313076641
C	-1.367445048348	-2.624616720985	0.014368117659
C	1.421757730566	0.108787615861	-0.334984208843
C	0.959019019996	0.702408652451	-1.666889140155

H	1.256567083677	0.061985324225	-2.500972480631
H	-0.128625099008	0.791743670316	-1.665679038233
H	1.384889339998	1.695610388247	-1.829341073555
C	1.029017456047	0.973518714972	0.863927762154
H	-0.055542538373	1.094902853741	0.887315525767
H	1.349836126727	0.505169217505	1.797697079180
H	1.491940134358	1.960928817157	0.802875865687
C	-0.974722827907	-3.489324173654	-1.184567205824
H	0.109836270252	-3.610714515941	-1.207969146280
H	-1.437650541519	-4.476732859545	-1.123531953565
H	-1.295548790467	-3.020952425157	-2.118322923266
C	-0.904689647995	-3.218266973833	1.346254272113
H	-1.330554500223	-4.211474338690	1.508687258889
H	0.182954812271	-3.307597988058	1.345030017139
H	-1.202230863287	-2.577864098835	2.180355811758
C	3.052446225558	-0.071572000740	-0.357586949966
O	3.564975860641	-1.162039125041	-0.238677250353
N	3.843699007636	1.103680808620	-0.496397965308
H	3.352053629751	1.946424457920	-0.756749139738
C	-2.998132976549	-2.444253497591	0.036997759172
O	-3.510660563852	-1.353781735704	-0.081873115512
N	-3.789386935995	-3.619507567204	0.175787739522
H	-3.297739258199	-4.462259005593	0.436107200139
C	-5.289199167228	-3.631203620320	0.465884604283
H	-5.712892354427	-2.787313750967	-0.075999705049
H	-5.444658871071	-3.452078855808	1.533406311875

C	-6.068099273282	-4.969566994522	0.077243349123
H	-6.059663719605	-5.113525374228	-1.003283200555
H	-5.592430645172	-5.833950300058	0.544155942904
C	5.343516923249	1.115371411848	-0.786467645004
H	5.498997509097	0.936204757990	-1.853979789905
H	5.767203974340	0.271504389657	-0.244541752396
C	6.122403582413	2.453753800776	-0.397864251054
H	5.646742168659	3.318116509794	-0.864823597613
H	6.113943446430	2.597756840739	0.682656785378
O	7.568632990404	2.451107518913	-0.844801088637
O	-7.514318700206	-4.966934880551	0.524212560792
C	8.343055119307	3.596831324836	-0.603189159470
O	7.881981743236	4.572911619306	-0.067411713379
C	-8.288750847742	-6.112644565358	0.282568690248
O	-7.827693877228	-7.088702619702	-0.253262182208
C	9.818381080381	3.506483376288	-1.075224605022
H	10.057088558408	2.552846134952	-1.537030297055
C	10.808715207140	4.449200973168	-0.978900378520
H	10.632106877017	5.419438178239	-0.527722712035
H	11.797331809806	4.227827913706	-1.360667298661
C	-9.764064857213	-6.022312780875	0.754643165523
H	-10.002757136615	-5.068696680633	1.216499061585
C	-10.754405242596	-6.965021721118	0.658299107224
H	-10.577812331283	-7.935237888422	0.207071157020
H	-11.743011374468	-6.743662996072	1.040100970496

Azoalkane_TS-F3000

($E_F = -1375.11163455$ a.u.; $G_F = -1374.73213159$ a.u.)

0 1

N	-0.554223645580	-1.157934536671	-0.147728715419
N	0.608933770382	-1.354669281489	-0.169262556449
C	-1.591380094333	-2.823305784286	0.001457639655
C	1.644735623891	0.307936553772	-0.320205233570
C	1.106192978496	0.873519416746	-1.612115920300
H	1.435066738034	0.286233735744	-2.472892633126
H	0.013888012807	0.881178809891	-1.586760081438
H	1.436271538147	1.909459280031	-1.762191858066
C	1.211133026668	1.030471352597	0.932333583766
H	0.121360444926	1.098397073627	0.969982459807
H	1.565630883789	0.512155082328	1.826701394992
H	1.619670174746	2.047973425889	0.949730402260
C	-1.158835970378	-3.541362108905	-1.253900941062
H	-0.069072310837	-3.608775898664	-1.293010571587
H	-1.567036992011	-4.558974767685	-1.274317804443
H	-1.514541251459	-3.020166984961	-2.146120870094
C	-1.050264617957	-3.391769384291	1.290833997884
H	-1.377836590161	-4.428968888063	1.437991534661
H	0.042050447287	-3.397102401654	1.264137969293
H	-1.379304516925	-2.808001809795	2.153928269085
C	3.209645269990	0.062781900234	-0.337249431722
O	3.702030637149	-1.026151361228	-0.126746130162
N	4.004670482155	1.206776353705	-0.554181595541

H	3.527108140048	2.034141461925	-0.881316168166
C	-3.156209259342	-2.578725298053	0.020657131437
O	-3.649215602603	-1.489982478332	-0.189567924291
N	-3.950727382027	-3.722980929858	0.238258369378
H	-3.472699799110	-4.550214642941	0.565095600053
C	-5.437930798136	-3.698062634979	0.468527287321
H	-5.837990315077	-2.884953714039	-0.135695154933
H	-5.643195439954	-3.462870601895	1.517526536402
C	-6.165214361934	-5.045752783292	0.115979750389
H	-6.110348806712	-5.245466993391	-0.955166461607
H	-5.701704528709	-5.883009248565	0.643054918565
C	5.491997626890	1.181458692001	-0.783651762058
H	5.697782906990	0.945305061494	-1.832323542933
H	5.891697312551	0.368883736428	-0.178485484819
C	6.219140450556	2.529434303288	-0.431933997602
H	5.755809541519	3.366239556024	-0.959867659766
H	6.163850798092	2.730029010667	0.639015699415
O	7.655480761043	2.488290874908	-0.824271194964
O	-7.601424566514	-5.004873700418	0.508897981235
C	8.408776842331	3.639436949466	-0.633963374198
O	7.932708173026	4.651709901230	-0.181663739624
C	-8.354791111260	-6.155898943864	0.318172570404
O	-7.878895229572	-7.167944992221	-0.134876702088
C	9.873711305494	3.496203973212	-1.048118360621
H	10.128053294504	2.514121615668	-1.434542346235
C	10.835958264149	4.453510553099	-0.972769796007

H	10.617185236388	5.444881399960	-0.591129695801
H	11.846324967977	4.236948508570	-1.296101911626
C	-9.819596165154	-6.012860504324	0.732902506233
H	-10.073793490525	-5.030977725677	1.119981766044
C	-10.781893544261	-6.970100464929	0.657313311499
H	-10.563265560599	-7.961275204823	0.275028205131
H	-11.792152783471	-6.753685341134	0.981108100251

Azoalkane_R-F3000

($E_F = -1375.12543091$ a.u.; $G_F = -1374.73928078$ a.u.)

0 1

N	-0.590782698700	-1.220866710282	-0.153712760579
N	0.644687902172	-1.294904955601	-0.163250955590
C	-1.312631924069	-2.605555861366	0.013013713236
C	1.366537492652	0.089784101631	-0.329982109024
C	0.897631507368	0.698197550679	-1.658083522794
H	1.198927437939	0.069962862373	-2.499982643528
H	-0.190596022814	0.776050119577	-1.651820182349
H	1.311509914481	1.697772019258	-1.809610536500
C	0.978663592037	0.959879138244	0.872379085392
H	-0.105811059133	1.079273674367	0.897964402123
H	1.302432821876	0.491375707510	1.805006428156
H	1.441587692150	1.946486357742	0.807788466164
C	-0.924767562573	-3.475639716748	-1.189358628741
H	0.159706589328	-3.595037135989	-1.214951609433
H	-1.387693934549	-4.462246225632	-1.124775359731

H	-1.248540894479	-3.007126099846	-2.121979183567
C	-0.843717255262	-3.213982986010	1.341105526925
H	-1.257594188416	-4.213559194473	1.492624194829
H	0.244510262660	-3.291834772747	1.334834649773
H	-1.145008230538	-2.585757628979	2.183013080230
C	2.965469734311	-0.107796653696	-0.348101958356
O	3.477318814167	-1.196969935609	-0.197058614462
N	3.743855654840	1.052453942131	-0.515927896316
H	3.258321850383	1.890165625472	-0.800633634953
C	-2.911563778771	-2.407973671716	0.031147146309
O	-3.423412776148	-1.318797915636	-0.119877656772
N	-3.689949953429	-3.568225531184	0.198963414831
H	-3.204415031354	-4.405941601847	0.483654101493
C	-5.171504429008	-3.557050231542	0.460938339967
H	-5.587194269629	-2.725656256121	-0.106549936845
H	-5.355571335477	-3.357747029044	1.521340478415
C	-5.904188098786	-4.893279194646	0.079058114604
H	-5.870220367287	-5.058586594198	-0.998795831992
H	-5.431042730080	-5.746994430320	0.570007803388
C	5.225412396992	1.041276880410	-0.777889760025
H	5.409489039263	0.841955430289	-1.838286841834
H	5.641098963389	0.209893649009	-0.210383202874
C	5.958089953729	2.377514053760	-0.396026480983
H	5.484949300164	3.231219619222	-0.886997624054
H	5.924109801369	2.542841550230	0.681824076061
O	7.386327377759	2.348849946782	-0.817996503363

O	-7.332420547509	-4.864621404507	0.501045199457
C	8.146152617436	3.490770831621	-0.600866291320
O	7.682178362193	4.486392488956	-0.101483704352
C	-8.092251318713	-6.006534863233	0.283896048324
O	-7.628286002472	-7.002144889697	-0.215517784785
C	9.601723667712	3.360431324171	-1.050905649685
H	9.845009851686	2.393257439901	-1.479731576657
C	10.568151916176	4.312140045070	-0.959798538736
H	10.360442645818	5.288775638286	-0.536276229639
H	11.570731939437	4.105870313719	-1.312727864806
C	-9.547816226959	-5.876203421307	0.733957641312
H	-9.791094681547	-4.909039750465	1.162810772319
C	-10.514247754238	-6.827907752711	0.642839622827
H	-10.306546037400	-7.804533407823	0.219291126325
H	-11.516822842277	-6.621644367613	0.995786425921

Azoalkane_TS-F2500

($E_F = -1374.83180495$ a.u.; $G_F = -1374.45071493$ a.u.)

0 1

N	-0.545630845887	-1.174753249532	-0.070646560893
N	0.599607028169	-1.341358711382	-0.246896902508
C	-1.573084969971	-2.892915410009	-0.135989265794
C	1.627172286117	0.377320127445	-0.181831596791
C	1.074757699089	1.075242868531	-1.397082957442
H	1.420989176167	0.612479090106	-2.324306896659
H	-0.017128026646	1.047169754239	-1.378193496404

H	1.364298611820	2.135017768226	-1.409614020174
C	1.161062670411	0.916023340070	1.146796867328
H	0.069138007199	0.932829839909	1.187039031944
H	1.541931322669	0.303241273906	1.966398210157
H	1.527146914844	1.940918841003	1.287130711120
C	-1.107881756404	-3.431057119636	-1.465189012396
H	-0.015990139411	-3.448344473787	-1.505995912664
H	-1.474536088749	-4.455684085649	-1.605945356690
H	-1.488877419255	-2.817605839740	-2.284232927944
C	-1.020204933376	-3.591715664206	1.078562163199
H	-1.309908009540	-4.651445657006	1.090542483968
H	0.071675170200	-3.563788353054	1.059174527816
H	-1.365937451579	-3.129489889023	2.006238093143
C	3.169661311480	0.132379094977	-0.141875522590
O	3.641839407449	-0.836700777039	0.422885231208
N	3.975315640624	1.156878488149	-0.653420119524
H	3.530337442969	1.846227995232	-1.240914215452
C	-3.115600068863	-2.647738527692	-0.174946282186
O	-3.587956958289	-1.677966957959	-0.738357167925
N	-3.921074656362	-3.672758168500	0.335840372267
H	-3.475839440614	-4.362798335307	0.922334733909
C	-5.412902501417	-3.628857150619	0.388350553913
H	-5.739702033105	-2.974169609194	-0.418642106019
H	-5.739481858483	-3.179965613626	1.331891175873
C	-6.078748349820	-5.035034773061	0.254154283899
H	-5.898788987449	-5.457062278730	-0.736091741290

H	-5.675606673420	-5.728009846945	0.996937282210
C	5.467174694684	1.113077788236	-0.705019267968
H	5.794352091624	0.663196098364	-1.647882349020
H	5.793571082132	0.459297715662	0.102873322607
C	6.132800290741	2.519467049062	-0.571958047546
H	5.730116795424	3.211566399872	-1.315804259159
H	5.952110445875	2.942592668441	0.417690464239
O	7.594080494581	2.423460457899	-0.782969448487
O	-7.539865878288	-4.939141382549	0.466320648037
C	8.316490589648	3.601350956860	-0.768079109687
O	7.795633412426	4.677944548418	-0.603288166153
C	-8.262440470933	-6.116913768771	0.450182611075
O	-7.741849999299	-7.193310212902	0.283310054323
C	9.807307131235	3.395007353651	-0.978172112097
H	10.102826974380	2.359099954699	-1.110136249642
C	10.742798509335	4.373634456896	-1.007609488773
H	10.469479835378	5.415063560474	-0.876882689010
H	11.786632906929	4.131266934118	-1.162721300273
C	-9.753060151634	-5.910714877392	0.661792506184
H	-10.048339796126	-4.874984041342	0.795637454501
C	-10.688650682481	-6.889269400005	0.690450494037
H	-10.415571533761	-7.930521213538	0.557853732654
H	-11.732327347017	-6.647019864199	0.846794904417

Azoalkane_R-F2500

($E_F = -1374.85245358$ a.u.; $G_F = -1374.46641589$ a.u.)

0 1

N	-0.582476312497	-1.231271843349	-0.058073752115
N	0.636505313839	-1.284309682563	-0.259367993232
C	-1.277656105480	-2.619685657109	-0.033198411302
C	1.331695299439	0.104098906869	-0.284203610720
C	0.855277229025	0.799420506228	-1.567379080836
H	1.167591458443	0.244637523632	-2.455302039205
H	-0.234486671113	0.856255716139	-1.556493988642
H	1.240477008331	1.819617779001	-1.639213254047
C	0.945377144617	0.898397611985	0.971495607117
H	-0.137694478049	1.020790620161	1.008659444626
H	1.270278155849	0.367346973499	1.869365895339
H	1.420106170686	1.881505238232	0.960968293122
C	-0.891214464951	-3.414105529428	-1.288781592356
H	0.191862055547	-3.536482612795	-1.325842196898
H	-1.365929226700	-4.397219380840	-1.278188202302
H	-1.216050379925	-2.883152126944	-2.186732076213
C	-0.801349937987	-3.314877802141	1.250087911528
H	-1.186552834186	-4.335069499752	1.321984764896
H	0.288414695659	-3.371716626727	1.239303719487
H	-1.113741213679	-2.760009145093	2.137929790544
C	2.914022841043	-0.095050545418	-0.247526299627
O	3.409226924351	-1.126015219493	0.161858889422
N	3.696293814860	1.008341364666	-0.601160855848
H	3.236124379693	1.759610479192	-1.092715011916
C	-2.859977317233	-2.420555868783	-0.070068203943

O	-3.355135514718	-1.389688475829	-0.479756172366
N	-3.642283776540	-3.523866503284	0.283733784808
H	-3.182171370178	-4.275015655681	0.775524141686
C	-5.131723740408	-3.486405192652	0.394406725372
H	-5.490174737892	-2.776156511789	-0.349538713325
H	-5.423403857422	-3.107518484322	1.379328533043
C	-5.804347052283	-4.879008476438	0.184486805435
H	-5.660957677441	-5.230773240175	-0.838631620280
H	-5.378604062374	-5.623199913283	0.862315538211
C	5.185717964901	0.970889089804	-0.712049443932
H	5.477255250640	0.592266092571	-1.697114891213
H	5.544260299615	0.260432529855	0.031652889042
C	5.858395883068	2.363423342010	-0.501845076156
H	5.432566800983	3.107808236825	-1.179406857274
H	5.715164106463	2.714910134946	0.521390521399
O	7.310704998161	2.280147726003	-0.771538008915
O	-7.256697564139	-4.795684955704	0.453942626055
C	8.038604515156	3.452462740011	-0.698998781883
O	7.528953787815	4.515633235818	-0.439519537254
C	-7.984563408070	-5.968035506197	0.381630438157
O	-7.474852513235	-7.031270822268	0.122532941440
C	9.519923427202	3.258129175192	-0.976842070656
H	9.805296694305	2.233550076054	-1.192765842234
C	10.458746113739	4.233971116079	-0.970310037080
H	10.195629299385	5.264156208553	-0.756185355471
H	11.495093266315	4.000601987787	-1.179831363051

C	-9.465928394922	-5.773651530598	0.659193416836
H	-9.751356111827	-4.749015115510	0.874776179285
C	-10.404729367809	-6.749515395209	0.652802329098
H	-10.141558382288	-7.779756970921	0.439014271685
H	-11.441112896941	-6.516107529199	0.862100833725

Azoalkane_TS-F2000

($E_F = -1374.55461051$ a.u.; $G_F = -1374.17203340$ a.u.)

0 1

N	-0.542598467715	-1.190953441085	-0.060471406217
N	0.596644090578	-1.324733414481	-0.257127280206
C	-1.536642908903	-2.943583225208	-0.187234472321
C	1.590681931934	0.427909577919	-0.130414157454
C	1.040602445757	1.137844901924	-1.338291642096
H	1.397006033089	0.692842132820	-2.270518925548
H	-0.050942870893	1.096974473878	-1.329485126266
H	1.318728446512	2.200972885236	-1.331040376108
C	1.088131252363	0.916517384229	1.202629330804
H	-0.004551118884	0.906623269282	1.224149450535
H	1.471695928194	0.290370161187	2.010132624573
H	1.425108757502	1.946565236083	1.376841088675
C	-1.034165199580	-3.432096310910	-1.520341469567
H	0.058516309356	-3.422228355516	-1.541910957927
H	-1.371177485860	-4.462121208977	-1.694622314916
H	-1.417750662767	-2.805873563101	-2.327777260952
C	-0.986503220750	-3.653608655992	1.020562888089

H	-1.264618493957	-4.716739194567	1.013242086138
H	0.105041462909	-3.612726449507	1.011710381012
H	-1.342869529111	-3.208681752153	1.952840742440
C	3.114313824373	0.172326556063	-0.067173356300
O	3.573018382514	-0.739353776548	0.599647012563
N	3.926967024492	1.119739630759	-0.684846839891
H	3.492215397012	1.761453331084	-1.330415767353
C	-3.060278670141	-2.687990749887	-0.250375394439
O	-3.519016253182	-1.776243390538	-0.917080692317
N	-3.872900419547	-3.635464222784	0.367247132587
H	-3.438111633177	-4.277249853237	1.012719422870
C	-5.355407538891	-3.585097289552	0.382717993756
H	-5.662839110949	-2.960297012108	-0.454973459996
H	-5.706759529593	-3.104967450681	1.301915143793
C	-6.002645800560	-4.992580665137	0.280701149000
H	-5.797013609345	-5.447947295209	-0.689922737060
H	-5.615417537193	-5.658621591914	1.056227149547
C	5.409475644849	1.069381876638	-0.700211967851
H	5.760895197201	0.589115860847	-1.619311917827
H	5.716857222331	0.444711383127	0.137594522188
C	6.056690879737	2.476887286426	-0.598362533045
H	5.669531011423	3.142798179563	-1.374032781948
H	5.850959968753	2.932407826374	0.372167850538
O	7.512746362488	2.366529721766	-0.772136016276
O	-7.458683390743	-4.882234334031	0.454636165287
C	8.231505488114	3.538897556160	-0.791172261802

O	7.711360098118	4.623531120589	-0.682202872054
C	-8.177459562674	-6.054595083451	0.473496122324
O	-7.657343333356	-7.139215708582	0.364234042670
C	9.715572625418	3.311401365701	-0.961674536590
H	10.011959635521	2.270996982663	-1.044210458729
C	10.640513588278	4.292254738918	-1.011378386506
H	10.352807452489	5.334703659983	-0.928541334449
H	11.690363740304	4.057527234605	-1.134771647518
C	-9.661504904183	-5.827109634078	0.644212138676
H	-9.957865878012	-4.786716277641	0.727009349575
C	-10.586456474812	-6.807959031817	0.693806232659
H	-10.298776361920	-7.850396662477	0.610708587862
H	-11.636289319505	-6.573239560590	0.817369108237

Azoalkane_R-F2000

($E_F = -1374.58252574$ a.u.; $G_F = -1374.19303677$ a.u.)

0 1

N	-0.571608357797	-1.251543851188	-0.007387611999
N	0.625653741876	-1.264145029930	-0.310227442877
C	-1.239741653735	-2.636689036825	-0.048954009347
C	1.293787070030	0.121000498294	-0.268660925891
C	0.819831463872	0.847345509017	-1.536630983410
H	1.141669311936	0.320761391074	-2.438098190145
H	-0.270549735135	0.893721670320	-1.531422620098
H	1.193957461048	1.873574545461	-1.574707114724
C	0.895834764768	0.884592618569	1.002970833920

H	-0.187028122655	1.005322429313	1.037568444239
H	1.216381847714	0.331289451981	1.888549042913
H	1.370658071833	1.867728311816	1.016423293200
C	-0.841789973967	-3.400281783252	-1.320585581829
H	0.241072831639	-3.521012351486	-1.355183308901
H	-1.316613794311	-4.383417241591	-1.334037595562
H	-1.162336786421	-2.846978867905	-2.206164001480
C	-0.765786015750	-3.363034076118	1.219016166928
H	-1.139912246067	-4.389263046029	1.257092462971
H	0.324595207558	-3.409410480477	1.213807664014
H	-1.087623640233	-2.836449774763	2.120483352033
C	2.861051081326	-0.083157379767	-0.208071453291
O	3.339810115252	-1.081191502681	0.296243728721
N	3.649261376864	0.977334557112	-0.639142188424
H	3.204529121133	1.687913952869	-1.199913858426
C	-2.807005784165	-2.432530301542	-0.109542351730
O	-3.285764453615	-1.434495528495	-0.613856336041
N	-3.595216285918	-3.493021918792	0.321528758563
H	-3.150483365229	-4.203602191889	0.882298678760
C	-5.078171552241	-3.445566816455	0.377803952946
H	-5.410301213207	-2.775251722827	-0.413974801805
H	-5.406818461563	-3.018653005093	1.331192444955
C	-5.727248773256	-4.845010718383	0.213925011969
H	-5.546784227580	-5.246719162789	-0.784992096990
H	-5.322878614831	-5.553269447230	0.942027387593
C	5.132217110509	0.929881583556	-0.695411731469

H	5.460868367373	0.502960745013	-1.648795865727
H	5.464345085909	0.259573037941	0.096373619115
C	5.781290601322	2.329328205780	-0.531541077548
H	5.376925266223	3.037579738138	-1.259653490352
H	5.600817313877	2.731045630343	0.467371166932
O	7.232119704588	2.226975957526	-0.747173301409
O	-7.178075932852	-4.742658667334	0.429570360590
C	7.953567747556	3.397617571000	-0.720313689128
O	7.439379789847	4.475391242936	-0.539266290428
C	-7.899526985485	-5.913297489524	0.402695319439
O	-7.385343497834	-6.991067958713	0.221622248684
C	9.432132738343	3.177084424952	-0.940317378732
H	9.722945544206	2.142159382788	-1.086808101854
C	10.358747792493	4.157414197587	-0.960106207568
H	10.076725280817	5.194400827090	-0.813571440352
H	11.404365592207	3.927672645508	-1.122598810124
C	-9.378089300551	-5.692766116562	0.622717416073
H	-9.668898238011	-4.657844288599	0.769230847072
C	-10.304706253825	-6.673094101469	0.642496638526
H	-10.022687315463	-7.710077628266	0.495939596219
H	-11.350321967367	-6.443354088549	0.805003160065

Azoalkane_TS-F1800

($E_F = -1374.44455675$ a.u.; $G_F = -1374.06170686$ a.u.)

0 1

N	-0.541639221722	-1.198501653775	-0.058045300040
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N	0.595687830074	-1.317357095131	-0.259091259097
C	-1.517890476617	-2.966972858774	-0.204425343809
C	1.571927992970	0.451623401572	-0.113221501289
C	1.021892323686	1.159134093675	-1.321924645578
H	1.381248108052	0.715194860605	-2.253602512770
H	-0.069485840113	1.113667632649	-1.315806671415
H	1.295929574140	2.223312681235	-1.314295382107
C	1.053805505294	0.924486952172	1.218657352645
H	-0.038866001497	0.900460286565	1.232772599613
H	1.440686933193	0.298410211968	2.024377806679
H	1.375322082138	1.958072486582	1.401640790775
C	-1.000822804068	-3.438926526507	-1.537062517224
H	0.091836368417	-3.415474871945	-1.551820184794
H	-1.323024730960	-4.472160815592	-1.720769244718
H	-1.387821139188	-2.811913581575	-2.342012343352
C	-0.967235625187	-3.675647594898	1.003326272033
H	-1.241306332538	-4.739809957126	0.994861779038
H	0.124139742089	-3.630203485494	0.996658603602
H	-1.326091458800	-3.232561998253	1.935599359094
C	3.088243441051	0.191103163252	-0.042702015671
O	3.542151808700	-0.700921291392	0.654848642746
N	3.903317554220	1.107453289629	-0.696825900536
H	3.470848577688	1.739038213362	-1.353634636453
C	-3.034259875721	-2.706193447686	-0.273650447199
O	-3.488517357212	-1.812913936659	-0.969206514816
N	-3.849000738325	-3.623640896878	0.379208322263

H	-3.416156268727	-4.256397928223	1.034595474490
C	-5.327673499743	-3.568707422728	0.389178497288
H	-5.631055426266	-2.944053529794	-0.450069293846
H	-5.682239245943	-3.088458477497	1.307136406043
C	-5.971071822886	-4.974042122391	0.284612197142
H	-5.762165007751	-5.429455617104	-0.685416618352
H	-5.586790191802	-5.640542208493	1.061357778686
C	5.382000254443	1.052695596083	-0.705647544628
H	5.737296586220	0.571202833632	-1.622676584445
H	5.684847443238	0.429258058051	0.134703542265
C	6.025154484289	2.458255750223	-0.602585032308
H	5.641361195265	3.123617629386	-1.380549328938
H	5.815475068489	2.915001808481	0.366657425846
O	7.478063466908	2.342279683193	-0.770470116101
O	-7.423832412119	-4.858130162722	0.453730736782
C	8.197376559984	3.511275316097	-0.793196939786
O	7.680137930797	4.598196194099	-0.690961876416
C	-8.143294363955	-6.027054532334	0.475176592484
O	-7.626286721139	-7.113866237493	0.370842273474
C	9.677449083604	3.275401468849	-0.958638325965
H	9.971911687030	2.234127119970	-1.035098804601
C	10.599490586000	4.256177435254	-1.010509159197
H	10.308341503013	5.298095482773	-0.933241426219
H	11.650512573963	4.024565272647	-1.130011655450
C	-9.623201278107	-5.791252906104	0.642112864732
H	-9.917460771405	-4.750073295497	0.720400403592

C	-10.545332681518	-6.771982275292	0.693203960689
H	-10.254388324085	-7.813804468323	0.614114630783
H	-11.596225732159	-6.540426554268	0.813882179217

Azoalkane_R-F1800

($E_F = -1374.47534590$ a.u.; $G_F = -1374.08598648$ a.u.)

0 1

N	-0.565840612791	-1.260924903577	0.012778128979
N	0.619871032725	-1.254623437133	-0.330181949205
C	-1.223858280482	-2.644144300870	-0.051103439237
C	1.277882704013	0.128600671435	-0.266325453176
C	0.806685460445	0.862499731573	-1.531484019348
H	1.132777207977	0.342959419210	-2.435463044599
H	-0.283863088515	0.905369499393	-1.529852993239
H	1.177446916636	1.890261520567	-1.560595942518
C	0.873890942779	0.884019496601	1.008352956325
H	-0.208666057385	1.006811778818	1.039257239199
H	1.189112434280	0.323676404456	1.891292509984
H	1.350735926918	1.866096662824	1.030314302527
C	-0.819952573545	-3.399481339207	-1.325857922234
H	0.262602247531	-3.522275951006	-1.356839110538
H	-1.296802645137	-4.381554893167	-1.347855212574
H	-1.135228503501	-2.839079209175	-2.208740849839
C	-0.752582086439	-3.378124294237	1.213977975149
H	-1.123338179064	-4.405889216525	1.243049079855
H	0.337966629046	-3.420987383053	1.212277415035

H	-1.078622121751	-2.858643273800	2.118009600465
C	2.839441664630	-0.078742764473	-0.197616700556
O	3.311687849963	-1.067043084311	0.332723629652
N	3.630075178356	0.966156411481	-0.651691027517
H	3.189626088513	1.666434500446	-1.228333546929
C	-2.785422571439	-2.436790888381	-0.119690132257
O	-3.257706122805	-1.448421077591	-0.649864510100
N	-3.576026070366	-3.481750927835	0.334298572348
H	-3.135535909922	-4.182112943118	0.910807762237
C	-5.055795202931	-3.430642213818	0.377599659081
H	-5.380931951856	-2.766592130591	-0.422335946428
H	-5.393123728063	-2.996767580310	1.324885176971
C	-5.698182797199	-4.829860259798	0.218517489348
H	-5.509807435443	-5.238584699255	-0.776208741017
H	-5.298768734480	-5.532882554396	0.954573241443
C	5.109848046457	0.915054631267	-0.694863432971
H	5.447259680322	0.481049205246	-1.642060041396
H	5.434924210088	0.251120622167	0.105193610979
C	5.752206796831	2.314303434148	-0.535926456460
H	5.352848072249	3.017216529849	-1.272116514296
H	5.563740163252	2.723166768954	0.458725600214
O	7.200821564195	2.206590932838	-0.740256820152
O	-7.146779178649	-4.722157914840	0.422988462292
C	7.921229423051	3.375113019380	-0.721661954954
O	7.407844577334	4.455838212752	-0.555123945705
C	-7.867204646646	-5.890667482352	0.404268040092

O	-7.353848640000	-6.971376466048	0.237508142976
C	9.396835615835	3.146474244817	-0.930956381320
H	9.687477043451	2.109924036873	-1.064713798064
C	10.319477112585	4.127751441972	-0.955385289121
H	10.032304601804	5.164970358729	-0.821040894873
H	11.367109828545	3.901192255387	-1.109328181915
C	-9.342790374300	-5.662037645296	0.613733950379
H	-9.633406383136	-4.625500391614	0.747694558697
C	-10.265443600402	-6.643306823755	0.638080175066
H	-9.978297018064	-7.680512402419	0.503534333099
H	-11.313060423477	-6.416754069810	0.792156668412

Azoalkane_TS-F1500

($E_F = -1374.28045955$ a.u.; $G_F = -1373.89788958$ a.u.)

0 1

N	-0.538690443887	-1.224234091742	-0.051264158253
N	0.595444984738	-1.312079753463	-0.262966621548
C	-1.477610244694	-3.007042055916	-0.245477176905
C	1.533675109513	0.496498049562	-0.076958925767
C	0.991293151112	1.191250304394	-1.295300709116
H	1.363368715904	0.744723643863	-2.220970643403
H	-0.099598484657	1.135643440593	-1.302197811373
H	1.256836790116	2.257726365708	-1.290563907733
C	0.970414889419	0.941964071194	1.244007403710
H	-0.120940879141	0.878654283082	1.234650717888
H	1.363938003030	0.326959304163	2.054483388805

H	1.248209056364	1.986440319859	1.437903247632
C	-0.946915555149	-3.438610109757	-1.585517843952
H	0.145362352830	-3.398424644174	-1.594374594174
H	-1.251427835652	-4.472465565211	-1.794407067455
H	-1.340896672312	-2.799181002191	-2.376811736374
C	-0.921886819635	-3.732785286562	0.949205017989
H	-1.195265969197	-4.796808092777	0.924854756967
H	0.169319974768	-3.684888541420	0.940313254752
H	-1.276767147958	-3.303923276736	1.889747367379
C	3.038626368707	0.237291333416	0.021706470588
O	3.484062865767	-0.592737532075	0.799411338867
N	3.860283012630	1.074495683657	-0.716130843088
H	3.435088001099	1.665478963575	-1.413789483227
C	-2.983837280612	-2.735507135168	-0.312007611352
O	-3.435059772463	-1.872247506883	-1.048349311652
N	-3.798085038608	-3.599405153603	0.402399988311
H	-3.365158385056	-4.217212236143	1.071496602778
C	-5.271003161951	-3.536005561989	0.411596106043
H	-5.571057217601	-2.904759486580	-0.423897112700
H	-5.624991618377	-3.062107596210	1.333105004621
C	-5.911383135758	-4.936579407855	0.295346177454
H	-5.701362021215	-5.385327940282	-0.677773896295
H	-5.529883916520	-5.609789906245	1.067917285325
C	5.333167707136	1.017455728944	-0.699888789156
H	5.703797026026	0.515478023416	-1.599727516857
H	5.621833836696	0.414907142074	0.160407895504

C	5.967002951588	2.423493662362	-0.618672048214
H	5.597282372603	3.069468388748	-1.419564260143
H	5.738364467326	2.903110005015	0.335329889790
O	7.417573758732	2.298315227849	-0.756133511828
O	-7.358703048882	-4.811561495673	0.462781085998
C	8.136301278175	3.462484580162	-0.804115379228
O	7.620744891504	4.553833597607	-0.746372425581
C	-8.080734195059	-5.974636386469	0.482100581472
O	-7.570120075923	-7.064641079415	0.375541159372
C	9.612889967738	3.212989400744	-0.935935736084
H	9.906838539168	2.169637953033	-0.972974958519
C	10.529905319902	4.193561285707	-1.003604537297
H	10.231374446058	5.235537147210	-0.965008462122
H	11.584381838472	3.965621979028	-1.097442977696
C	-9.553709639096	-5.725762200793	0.650191576929
H	-9.843258743898	-4.683557509506	0.730057546620
C	-10.472705620572	-6.705567072806	0.699949365364
H	-10.178552035684	-7.746346538124	0.618548243588
H	-11.524455802159	-6.478166547137	0.821635948218

Azoalkane_R-F1500

($E_F = -1374.31547436$ a.u.; $G_F = -1373.92454611$ a.u.)

0 1

N	-0.555083434582	-1.279577318758	0.044644672278
N	0.609963643246	-1.232257472658	-0.356811052036
C	-1.194549974850	-2.660115000820	-0.072753544020

C	1.249428738575	0.148280060073	-0.239411936004
C	0.781095499216	0.916013725478	-1.485471679517
H	1.117867465959	0.428339273968	-2.403245385681
H	-0.309778045989	0.947493661650	-1.491684178205
H	1.141374191349	1.948117611542	-1.475527954209
C	0.834904578263	0.868333700247	1.052376459829
H	-0.246883158808	0.996771926271	1.077702663317
H	1.139371728558	0.280483466192	1.920625795046
H	1.316943068799	1.846890753472	1.105558699210
C	-0.780025004044	-3.380169522011	-1.364541035332
H	0.301762784373	-3.508606984235	-1.389866533989
H	-1.262062910773	-4.358726897606	-1.417722692227
H	-1.084492052615	-2.792320140301	-2.232791021092
C	-0.726217771178	-3.427847464594	1.173307102373
H	-1.086497040517	-4.459951120959	1.163364389978
H	0.364655708488	-3.459327967107	1.179520091285
H	-1.062989879022	-2.940171792687	2.091080168420
C	2.802566324554	-0.062353600022	-0.156462062063
O	3.261470133270	-1.018016366564	0.443263727369
N	3.599666012159	0.939784243224	-0.675906282555
H	3.169514945658	1.601589726904	-1.303217494022
C	-2.747687123457	-2.449480122764	-0.155704687811
O	-3.206590143801	-1.493818119990	-0.755432415529
N	-3.544787722154	-3.451616773037	0.363740730845
H	-3.114637599867	-4.113421353924	0.991053654095
C	-5.019905796260	-3.397555984665	0.372967628948

H	-5.327372382013	-2.760484903482	-0.455385474699
H	-5.379538030947	-2.934636361856	1.298081961095
C	-5.648561493251	-4.800665574610	0.243653887075
H	-5.434277351605	-5.240810059057	-0.732441051437
H	-5.265722293356	-5.478331930537	1.011757510350
C	5.074784018789	0.885724278964	-0.685134265729
H	5.434415772077	0.422805901092	-1.610249284317
H	5.382251470200	0.248652426808	0.143217757400
C	5.703438877766	2.288833784737	-0.555819328141
H	5.320599342317	2.966500804928	-1.323922047291
H	5.489155177955	2.728977245108	0.420276053502
O	7.151413456104	2.172047234772	-0.721025429227
O	-7.096536101260	-4.683878411885	0.408859285594
C	7.868147394259	3.338629631979	-0.734250916000
O	7.352225009748	4.425693345713	-0.624304307147
C	-7.813269958256	-5.850461078980	0.422085467143
O	-7.297347360323	-6.937524845311	0.312140100760
C	9.342406389460	3.096521513177	-0.900368482141
H	9.636228442232	2.055819786187	-0.983667819298
C	10.257659040280	4.080074493405	-0.944601201292
H	9.959375023560	5.119392818475	-0.859949027728
H	11.310491969257	3.857192478276	-1.065104726457
C	-9.287529086849	-5.608352691267	0.588202081708
H	-9.581351236877	-4.567650742486	0.671500191966
C	-10.202781704438	-6.591905663078	0.632435377565
H	-9.904497566964	-7.631224123544	0.547784445171

H	-11.255614704047	-6.369023463939	0.752938150119
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Azoalkane_TS-F1000

($E_F = -1374.01007837$ a.u.; $G_F = -1373.62752923$ a.u.)

0 1

N	-0.537047256857	-1.246099201362	-0.045662033523
N	0.590974281696	-1.269483650121	-0.271848151052
C	-1.388163603791	-3.092711357979	-0.309586053511
C	1.441910035162	0.577460512521	-0.008978558314
C	0.891867531645	1.277722527184	-1.219887877050
H	1.261012642492	0.839482044184	-2.150798998092
H	-0.198468796370	1.213151902954	-1.225154582806
H	1.151095542050	2.345491571255	-1.208391298274
C	0.840246366766	0.961447662383	1.311848349966
H	-0.247086838077	0.850118764448	1.283928127607
H	1.250696477248	0.345321982389	2.112255126080
H	1.065857577399	2.012611793002	1.535205527445
C	-0.787940245574	-3.474955963122	-1.631593253863
H	0.299459002256	-3.364077065319	-1.604578071234
H	-1.014173397511	-4.525698631649	-1.856297467513
H	-1.198946002776	-2.857494233080	-2.430692224839
C	-0.836838331555	-3.794637610395	0.899771527684
H	-1.095894036329	-4.862435579765	0.886985142743
H	0.253494450367	-3.729886359211	0.904062918297
H	-1.205144434133	-3.357807505527	1.831673055757
C	2.931651834817	0.307397239682	0.093347214668

O	3.377105159332	-0.449041327028	0.945866958350
N	3.748693751211	1.022553850953	-0.757155299672
H	3.322773466462	1.585703066584	-1.476252132880
C	-2.878018151109	-2.822487834987	-0.409978684480
O	-3.324328822015	-2.064728586105	-1.260870530307
N	-3.694196730595	-3.538937481068	0.440263280490
H	-3.267539793635	-4.103302183066	1.157967045687
C	-5.157972270131	-3.465389015207	0.429372787585
H	-5.443992532430	-2.841631016644	-0.416330778452
H	-5.521133061206	-2.984218824573	1.343202189652
C	-5.791415023692	-4.861265587958	0.314345086356
H	-5.563266653801	-5.319941974333	-0.650316635316
H	-5.427298159159	-5.527831493299	1.101019317607
C	5.212463972761	0.949157934436	-0.744538911258
H	5.576684214923	0.465991986639	-1.656894774183
H	5.497640884075	0.327311448769	0.102858447280
C	5.845590688957	2.345372567022	-0.631921961676
H	5.482332684202	3.010107100471	-1.420540551794
H	5.616212255082	2.806198065592	0.331425284317
O	7.287246623582	2.202726011399	-0.767123283810
O	-7.232886162616	-4.718713401352	0.451618092756
C	8.013134693910	3.355881752391	-0.803987166864
O	7.510908145529	4.453309862999	-0.735182122671
C	-7.958934925244	-5.871824605489	0.486511033955
O	-7.456994103915	-6.969165744253	0.414346539644
C	9.477856307925	3.082321473323	-0.939945477987

H	9.761519972590	2.036841541283	-0.985684426844
C	10.392043696050	4.059638573343	-1.001068245113
H	10.091063165017	5.100500545235	-0.952744542007
H	11.447234925936	3.836347257746	-1.098998073410
C	-9.423435862639	-5.598342044951	0.624980139994
H	-9.706846049629	-4.552929631705	0.673691036687
C	-10.337729003329	-6.575639448256	0.684811328016
H	-10.037005095219	-7.616431283966	0.633505416630
H	-11.392754090702	-6.352401224350	0.784628558405

Azoalkane_R-F1000

($E_F = -1374.05136271$ a.u.; $G_F = -1373.66025679$ a.u.)

0 1

N	-0.522246857256	-1.323195630087	0.111420467273
N	0.576228115725	-1.192402329876	-0.428741578611
C	-1.134977169022	-2.696757344427	-0.057372956912
C	1.188957555654	0.181159333609	-0.259948442915
C	0.735433072023	0.959478607207	-1.505766134091
H	1.085665003363	0.481279448964	-2.423266901244
H	-0.355525164177	0.986315083519	-1.528495524925
H	1.090805480323	1.992894510138	-1.478704677055
C	0.752404229089	0.888650874885	1.030597339874
H	-0.327710579094	1.030724391019	1.037875990250
H	1.031185024319	0.287577157691	1.897833459650
H	1.244724568099	1.861120403536	1.103148885003
C	-0.698428481912	-3.404245532432	-1.347922045715

H	0.381686410556	-3.546317929787	-1.355205216527
H	-1.190748224492	-4.376715337343	-1.420473984658
H	-0.977213276404	-2.803169986772	-2.215155623537
C	-0.681448031175	-3.475079292287	1.188441283238
H	-1.036819875929	-4.508495384012	1.161378711113
H	0.409510322204	-3.501915037456	1.211166873780
H	-1.031677253677	-2.996882480469	2.105944380672
C	2.729365417990	-0.040938655373	-0.154908725138
O	3.169215069063	-0.969926821729	0.501153416608
N	3.535983130714	0.910735317867	-0.731739964406
H	3.116030695036	1.553695840705	-1.384590387102
C	-2.675385483098	-2.474658760582	-0.162406207847
O	-3.115237685806	-1.545667344202	-0.818462049648
N	-3.482000827890	-3.426335798527	0.414423502386
H	-3.062045200300	-4.069300426540	1.067267866582
C	-4.948593602051	-3.360395938290	0.399309934276
H	-5.239087921879	-2.720806214450	-0.433124167784
H	-5.322904021205	-2.899692676586	1.319750396034
C	-5.567278454305	-4.757980298845	0.254693071154
H	-5.334319338434	-5.196626804385	-0.718090506100
H	-5.201209740050	-5.438231863411	1.028947842967
C	5.002575889357	0.844796107649	-0.716617952914
H	5.376891624332	0.384081025721	-1.637050311966
H	5.293066235660	0.205217407443	0.115826008510
C	5.621258791686	2.242382787455	-0.572015770253
H	5.255197091521	2.922622913830	-1.346283804499

H	5.388290209907	2.681043147600	0.400759311234
O	7.063256239785	2.111185725592	-0.709389852276
O	-7.009274517717	-4.626784297754	0.392083137091
C	7.782339247946	3.269392119630	-0.729568308093
O	7.273368907756	4.362368193272	-0.643526904179
C	-7.728358795186	-5.784990171758	0.412243173170
O	-7.219390752996	-6.877965007262	0.326171552678
C	9.248186660156	3.005798662871	-0.871360142649
H	9.537240961077	1.962634740015	-0.933027961019
C	10.157132742943	3.988711983615	-0.919412219843
H	9.850860277641	5.027173740308	-0.855509886174
H	11.213292715682	3.772348355335	-1.022203757568
C	-9.194204327538	-5.521397965368	0.554057110394
H	-9.483256512241	-4.478235023320	0.615752372887
C	-10.103151242778	-6.504311136578	0.602096691544
H	-9.796880935369	-7.542771893387	0.538166828515
H	-11.159309772318	-6.287948377112	0.704905115037

Azoalkane_TS-F800

($E_F = -1373.90322434$ a.u.; $G_F = -1373.52157252$ a.u.)

0 1

N	-0.534315412513	-1.265880813352	-0.038251719703
N	0.588382636522	-1.249824884851	-0.279300993043
C	-1.332160881081	-3.136127760289	-0.339689116182
C	1.386135692665	0.620701945567	0.021860479357
C	0.835342493043	1.313751860826	-1.192603205371

H	1.202147690307	0.870139552476	-2.121974253865
H	-0.254878297610	1.248328147902	-1.197511889549
H	1.095624672207	2.381142905086	-1.187476051830
C	0.756875550276	0.978622838966	1.335549515318
H	-0.325936919253	0.831972794960	1.294088914110
H	1.178262955813	0.374050074893	2.138592197020
H	0.943909700001	2.036030361685	1.564894591709
C	-0.703491534802	-3.493589184366	-1.653800960285
H	0.379374722411	-3.347239925023	-1.612682606732
H	-0.890897965931	-4.550836739345	-1.883581600138
H	-1.125028761159	-2.888523603053	-2.456398769255
C	-0.780945817940	-3.829760789927	0.874253923901
H	-1.041199632810	-4.897156353469	0.868694425017
H	0.309275921309	-3.764315800684	0.878823997397
H	-1.147454807126	-3.386605793131	1.803958766809
C	2.870614174412	0.354193394778	0.133661584523
O	3.319572120454	-0.345878472889	1.032750369780
N	3.682508376385	0.990502596416	-0.778404287463
H	3.255571762314	1.525421752276	-1.517828901753
C	-2.816684393531	-2.869491193892	-0.450801362725
O	-3.265904138480	-2.168704077758	-1.349202669690
N	-3.628287950191	-3.506510404278	0.461029409226
H	-3.201114338582	-4.042004346903	1.199908546659
C	-5.088534352215	-3.425854500714	0.451445315605
H	-5.373376161490	-2.789818518275	-0.385275031412
H	-5.447354062642	-2.957642048498	1.373330104939

C	-5.724137223021	-4.816071756626	0.315589235205
H	-5.496631137451	-5.261222447442	-0.655647266062
H	-5.363326090306	-5.495239077806	1.092830018618
C	5.142752855368	0.909914623746	-0.768252969088
H	5.501916661626	0.440960291213	-1.689628320543
H	5.427336949940	0.274580321270	0.069089193707
C	5.778234035814	2.300277297536	-0.633312464098
H	5.417699340433	2.978768438680	-1.411274807009
H	5.550309118655	2.746233482709	0.337458392375
O	7.216188402011	2.149540892680	-0.770322482329
O	-7.162025755406	-4.665372550155	0.453314010985
C	7.946636365190	3.297312091640	-0.797283988761
O	7.451679489074	4.397429506518	-0.716664599459
C	-7.892531820334	-5.813122825129	0.479588212448
O	-7.397675845144	-6.913196613428	0.397804156237
C	9.406000527856	3.012845283716	-0.939579177934
H	9.683784412685	1.966433297567	-0.995437146313
C	10.320574326566	3.987707317347	-0.994504437847
H	10.020576839450	5.028309856759	-0.935698998287
H	11.375446888544	3.765061452593	-1.097651191376
C	-9.351816526305	-5.528692228379	0.622750802775
H	-9.629509058911	-4.482313965737	0.679636526096
C	-10.266428759352	-6.503543275465	0.677223318876
H	-9.966524236430	-7.544111168866	0.617386246987
H	-11.321241885908	-6.280922088009	0.781016377282

Azoalkane_R-F800

($E_F = -1373.94659685$ a.u.; $G_F = -1373.55543222$ a.u.)

0 1

N	-0.506268113185	-1.343017794726	0.135668679850
N	0.560308838229	-1.172614264387	-0.453188119512
C	-1.105492208561	-2.714965966241	-0.054816785292
C	1.159532871638	0.199333909867	-0.262702726455
C	0.711130428670	0.984967983788	-1.505722700781
H	1.066886351131	0.513547817832	-2.424531814952
H	-0.379786967028	1.008310333411	-1.534678122498
H	1.063133049329	2.019198664803	-1.468904574341
C	0.712143002924	0.896404591472	1.029358065158
H	-0.367648623380	1.041649303700	1.029069565576
H	0.981660065984	0.288189896595	1.894194462949
H	1.205853129141	1.867439012819	1.113040201001
C	-0.658103826419	-3.412035692385	-1.346878592471
H	0.421687813208	-3.557280209552	-1.346591498588
H	-1.151813884643	-4.383070138434	-1.430560820759
H	-0.927622039227	-2.803820449441	-2.211714243401
C	-0.657088137451	-3.500600796562	1.188202120818
H	-1.009090417148	-4.534831584115	1.151383651142
H	0.433829297348	-3.523942754056	1.217156323795
H	-1.012843252550	-3.029181441660	2.107011960392
C	2.695602516175	-0.026065286056	-0.148679520354
O	3.128195830186	-0.939146748397	0.534907907057
N	3.505578922459	0.898699563368	-0.756672532757

H	3.088224247471	1.533271494780	-1.419080012920
C	-2.641562024066	-2.489566826073	-0.168837833653
O	-3.074156337041	-1.576484138069	-0.852422946157
N	-3.451537509251	-3.414332997296	0.439154415691
H	-3.034181755991	-4.048906391069	1.101559807530
C	-4.914757276239	-3.343089318675	0.418230773335
H	-5.199780293770	-2.694394942365	-0.408937727567
H	-5.292004523433	-2.892000329159	1.342172968146
C	-5.531280993715	-4.736539699073	0.255621150242
H	-5.293936064022	-5.165311540187	-0.720601899396
H	-5.170530266797	-5.425590070315	1.024650164585
C	4.968798648991	0.827455949783	-0.735746206851
H	5.346047495036	0.376363397434	-1.659685881006
H	5.253820276909	0.178764876620	0.091425226550
C	5.585321999229	2.220906895776	-0.573140907551
H	5.224573248157	2.909953974290	-1.342173610270
H	5.347974600667	2.649682729115	0.403079654725
O	7.024463301661	2.083771857795	-0.704707250198
O	-6.970421983099	-4.599405070662	0.387191757225
C	7.745967548951	3.237908826074	-0.718096013487
O	7.241577458209	4.332886676173	-0.628309139756
C	-7.691926454945	-5.753541881931	0.400576199673
O	-7.187536847266	-6.848519266879	0.310782107915
C	9.207607180960	2.965430890493	-0.858510095036
H	9.493025872006	1.921615652040	-0.923459925306
C	10.115274745468	3.947302556070	-0.901832615855

H	9.807742016790	4.985166276358	-0.834434443199
H	11.171956806586	3.733061102750	-1.004143606453
C	-9.153565658163	-5.481064403700	0.540995610828
H	-9.438983928367	-4.437249455175	0.605951910878
C	-10.061233337334	-6.462936097452	0.584315193064
H	-9.753701038217	-7.500799526470	0.516910521832
H	-11.117915066366	-6.248694958883	0.686630165538

Azoalkane_TS-F600

($E_F = -1373.79738522$ a.u.; $G_F = -1373.41545887$ a.u.)

0 1

N	-0.529392916855	-1.293129361878	-0.025807391534
N	0.583486214742	-1.222632223642	-0.291401848392
C	-1.251661511993	-3.192254993784	-0.363841444737
C	1.305716504839	0.676557589903	0.046549775699
C	0.749031181715	1.351912344854	-1.175166334634
H	1.111977851123	0.896973129394	-2.100722157098
H	-0.340846287921	1.282175539519	-1.176598995967
H	1.007363554961	2.419500988737	-1.185236770428
C	0.645676145244	1.007069151382	1.350425165146
H	-0.429176391841	0.812990022335	1.295617442675
H	1.083448232755	0.423765961830	2.159970732983
H	0.781820042993	2.072143414695	1.579706337721
C	-0.591779217923	-3.522642914076	-1.667830432706
H	0.483091061954	-3.328635016580	-1.613112224739
H	-0.728012837787	-4.587680840406	-1.897233601538

H	-1.029604502864	-2.939209169354	-2.477255146989
C	-0.694856494482	-3.867764651818	0.857736666018
H	-0.953154667078	-4.935364019077	0.867682908559
H	0.395019600029	-3.798001574177	0.859085217117
H	-1.057739098801	-3.412960063056	1.783383635429
C	2.787031379492	0.425107487187	0.167638987160
O	3.248691457375	-0.187871208086	1.123702427377
N	3.585775563703	0.950974995550	-0.819626056592
H	3.154780834546	1.442826577937	-1.585693208370
C	-2.732987544241	-2.940756230765	-0.484739056785
O	-3.194729271876	-2.327536051729	-1.440608146417
N	-3.531639874421	-3.466842537662	0.502481108091
H	-3.100583720578	-3.958974025528	1.268333664388
C	-4.988392694988	-3.376727329222	0.499574797379
H	-5.274319140768	-2.703599744902	-0.307122835476
H	-5.336745923899	-2.949332354811	1.444314654450
C	-5.632573442026	-4.753334056209	0.303321429213
H	-5.414408753589	-5.153498636079	-0.689531017219
H	-5.272402657122	-5.470509455541	1.045521171550
C	5.042533296929	0.860927723851	-0.816505377705
H	5.391037856033	0.432640404475	-1.760791844432
H	5.328399655242	0.188587939091	-0.009126652033
C	5.686577679979	2.237769774328	-0.621488054655
H	5.326655074079	2.954140034861	-1.364588146586
H	5.468016124045	2.638981064381	0.370857709824
O	7.119462055322	2.077382463285	-0.774131741194

O	-7.065391676879	-4.593030438695	0.456696611729
C	7.858987562736	3.216813413218	-0.772521700537
O	7.377005928381	4.319218954009	-0.651893075210
C	-7.805007308239	-5.732401790899	0.453926483512
O	-7.323169391412	-6.834690749411	0.331620061981
C	9.310381537994	2.918839819533	-0.940637023236
H	9.577069239983	1.872105031609	-1.031142434202
C	10.229188117425	3.888119336240	-0.977586079457
H	9.935571492194	4.927979101333	-0.883837418804
H	11.281668511906	3.663926017754	-1.100449348340
C	-9.256297970519	-5.434526663665	0.623128400604
H	-9.522855458075	-4.387883539945	0.715123121050
C	-10.175165530244	-6.403779096651	0.659291706422
H	-9.881682056663	-7.443545953970	0.564052169142
H	-11.227566499218	-6.179654417618	0.782970545649

Azoalkane_R-F600

($E_F = -1373.84240219$ a.u.; $G_F = -1373.45196656$ a.u.)

0 1

N	-0.484419350514	-1.365653796109	0.164575285741
N	0.538619908620	-1.150210065828	-0.481932673944
C	-1.066739990701	-2.738941756490	-0.038038799065
C	1.120922196741	0.223090048569	-0.279293000645
C	0.671473839213	1.008862204712	-1.521620953916
H	1.028692062486	0.539455353321	-2.440855027445
H	-0.419518731121	1.027600533570	-1.552245382428

H	1.019296522334	2.044405007350	-1.482110199454
C	0.665135589339	0.914331739373	1.012336133180
H	-0.415168217274	1.057277520766	1.008337789631
H	0.932543391226	0.305283957238	1.876780996198
H	1.155265188901	1.887074672058	1.099630532933
C	-0.610368807262	-3.430551790429	-1.329260798597
H	0.469926417030	-3.573566148968	-1.324700576767
H	-1.100519952348	-4.403286456194	-1.416525103044
H	-0.877319643376	-2.821719458276	-2.193994769925
C	-0.617986865465	-3.524437152133	1.204710583354
H	-0.965972302406	-4.559928790324	1.165328720330
H	0.472988980253	-3.543358235264	1.235841702876
H	-0.975538553831	-3.054708378838	2.123649612456
C	2.654155314622	-0.002372920326	-0.160609982447
O	3.083313566379	-0.887316800416	0.561833303265
N	3.463657824396	0.881684358146	-0.820996544448
H	3.043513893241	1.504754560784	-1.492192797155
C	-2.599899056877	-2.513401122496	-0.157563058984
O	-3.028625357233	-1.628808608419	-0.880699442477
N	-3.409811280894	-3.397035178794	0.502881077219
H	-2.990102782718	-4.019661507795	1.174767474589
C	-4.869681825644	-3.321031630678	0.487386392702
H	-5.152735836133	-2.615839638315	-0.292642564713
H	-5.242760636888	-2.935644015614	1.441926354423
C	-5.488558042827	-4.696465600223	0.229192874731
H	-5.263248751888	-5.052568700811	-0.778715652343

H	-5.121686964460	-5.441026119867	0.941095372212
C	4.923535147065	0.805694799681	-0.806518242490
H	5.295978751975	0.421885004667	-1.761938071100
H	5.207066949329	0.099217182856	-0.027829576569
C	5.542650556564	2.180680558081	-0.546468315541
H	5.175100819600	2.926493666798	-1.256711696126
H	5.318313515084	2.535016704273	0.462279820592
O	6.976678035960	2.044849814182	-0.705400879263
O	-6.922737400080	-4.560382647467	0.386475871896
C	7.702313919158	3.193119241335	-0.668323554464
O	7.206838900379	4.284633382672	-0.510492400834
C	-7.648255562445	-5.708794075051	0.351299426421
O	-7.152539304358	-6.800642605235	0.196535070709
C	9.156299119204	2.917372703238	-0.849722822529
H	9.434413631010	1.877143728187	-0.974245656534
C	10.063989258418	3.897710938150	-0.858832021889
H	9.759092933642	4.930725443472	-0.731603429726
H	11.118461041917	3.689351718017	-0.991937804669
C	-9.102452786285	-5.432732740462	0.530493639616
H	-9.380783725532	-4.392230698772	0.652271542257
C	-10.010073860784	-6.413125847751	0.540899900418
H	-9.704956081922	-7.446417154173	0.416427065463
H	-11.064707251797	-6.204539272025	0.672363905499

Azoalkane_TS-F400

($E_F = -1373.69284982$ a.u.; $G_F = -1373.31167909$ a.u.)

0 1

N	-0.514686904353	-1.333765340646	0.008877065849
N	0.568743492094	-1.181932928391	-0.326512199735
C	-1.149379531534	-3.258169797749	-0.382722215859
C	1.203441086023	0.742464630381	0.065107126011
C	0.631435363925	1.404887628884	-1.156703779372
H	0.975531471064	0.935943211866	-2.082540776536
H	-0.458551284966	1.340932025960	-1.141944713463
H	0.897945076294	2.469776835664	-1.185176587318
C	0.523030533182	1.035916244068	1.365047016695
H	-0.538095825045	0.776204553908	1.308533566639
H	0.993442803038	0.484777793997	2.178323432403
H	0.591486338599	2.108377883788	1.589431288188
C	-0.468926770220	-3.551658360627	-1.682631672001
H	0.592196431161	-3.291940056864	-1.626092846991
H	-0.537370225711	-4.624127634645	-1.906984715809
H	-0.939315548809	-3.000546927600	-2.495940275374
C	-0.577416582740	-3.920562252464	0.839125602947
H	-0.843936959878	-4.985448316156	0.867621460613
H	0.512570921858	-3.856617130418	0.824398037953
H	-0.921536568958	-3.451587667276	1.764938867450
C	2.682592993113	0.506738190278	0.180030158580
O	3.169556210946	-0.010018587948	1.181005279612
N	3.455542551605	0.906728250904	-0.880706672217
H	3.015436388378	1.352903739683	-1.668784279363
C	-2.628526622802	-3.022441957847	-0.497700095208

O	-3.115454948136	-2.505715598642	-1.498707491054
N	-3.401512033088	-3.422396972621	0.563024006361
H	-2.961431321085	-3.868538439455	1.351134634089
C	-4.854749860000	-3.319874158674	0.573292231287
H	-5.144471505789	-2.609328949642	-0.199322962325
H	-5.188069783781	-2.935382645948	1.540725898242
C	-5.510116750464	-4.678260023815	0.315271068656
H	-5.289845059715	-5.036204407189	-0.693153601965
H	-5.162614461267	-5.430097937992	1.028320465957
C	4.908780021542	0.804204632039	-0.891026589247
H	5.242068061579	0.419812635372	-1.858514492807
H	5.198525899426	0.093575609637	-0.118492108190
C	5.564158768010	2.162565734184	-0.632882210737
H	5.216622123397	2.914486945255	-1.345835525911
H	5.343934188844	2.520399691692	0.375597571302
O	6.993050991768	1.987393250785	-0.783927868254
O	-6.939015099582	-4.503077214244	0.466226526895
C	7.745813203229	3.114599207936	-0.743090205166
O	7.279471477703	4.219587652438	-0.587701698295
C	-7.691772344403	-5.630285400005	0.425523555616
O	-7.225420812203	-6.735284311881	0.270333499721
C	9.190128828002	2.798689617847	-0.918431591357
H	9.443238030059	1.751706859800	-1.038773238252
C	10.116862991976	3.758645009439	-0.926999560437
H	9.832002725555	4.797852626003	-0.803468627752
H	11.167709352270	3.529675538562	-1.055449092055

C	-9.136096705493	-5.314363399873	0.600734261433
H	-9.389214427345	-4.267373807604	0.720899404406
C	-10.062828509394	-6.274316713610	0.609394943873
H	-9.777959412441	-7.313531404708	0.486040541703
H	-11.113681550007	-6.045338483756	0.737747545433

Azoalkane_R-F400

($E_F = -1373.73895359$ a.u.; $G_F = -1373.34844668$ a.u.)

0 1

N	-0.452061154280	-1.399774372495	0.198334098327
N	0.506128322907	-1.115945351884	-0.515915750021
C	-1.014413753425	-2.772544250791	-0.035832564643
C	1.068477798617	0.256828013443	-0.281751209562
C	0.606597465848	1.064775658860	-1.504406174183
H	0.953944454597	0.612460382952	-2.435939928052
H	-0.484703305541	1.081177969048	-1.525559109796
H	0.953506732659	2.099824056236	-1.447206941094
C	0.612391026865	0.916843803456	1.025053764653
H	-0.469704169204	1.047841821025	1.030049530103
H	0.892122597269	0.295740676071	1.876187907821
H	1.090892208635	1.894236076174	1.126558050091
C	-0.558292549100	-3.432581243002	-1.342614671987
H	0.523802387642	-3.563585633085	-1.347576681545
H	-1.036795813681	-4.409972412596	-1.444118355592
H	-0.837995729464	-2.811489506922	-2.193766202890
C	-0.552580134370	-3.580482016582	1.186846785408

H	-0.899501372248	-4.615526393247	1.129650506698
H	0.538719837888	-3.596899339026	1.208032671441
H	-0.899948592479	-3.128150034643	2.118364046065
C	2.601134683698	0.032348535066	-0.174360152216
O	3.036029761790	-0.812151984837	0.592523722019
N	3.402205218728	0.857654895550	-0.910079272738
H	2.973661654868	1.463391214185	-1.591306494839
C	-2.547065868692	-2.548052024876	-0.143274307853
O	-2.981928229643	-1.703563475769	-0.910189931743
N	-3.348167937790	-3.373331914976	0.592440820332
H	-2.919653209827	-3.979057946450	1.273695032997
C	-4.804989875901	-3.294282881657	0.588156858999
H	-5.090238327079	-2.547019281737	-0.150716422031
H	-5.169877641197	-2.963300032502	1.565446945660
C	-5.426022337754	-4.649953794846	0.254813810780
H	-5.197232000754	-4.952589056592	-0.769775307706
H	-5.066672929876	-5.432839840024	0.928099111778
C	4.859028236684	0.778612497209	-0.905852077451
H	5.223879024274	0.447692815530	-1.883177219384
H	5.144308295279	0.031303106053	-0.167036544241
C	5.480071014425	2.134261990229	-0.572445340452
H	5.120655225300	2.917199808651	-1.245637468161
H	5.251364048955	2.436813116109	0.452186677534
O	6.911329761243	1.994009519683	-0.729992334019
O	-6.857293469951	-4.509675827858	0.412221120630
C	7.642923828386	3.133279573469	-0.645223567634

O	7.155593889718	4.221617851915	-0.444727690801
C	-7.588879839094	-5.648966556851	0.327650688826
O	-7.101531784942	-6.737351354507	0.127467623326
C	9.091978191843	2.850856389574	-0.835738150744
H	9.363461384318	1.814181538707	-0.997662730272
C	10.001236637376	3.827038197904	-0.809123997889
H	9.698212253212	4.855335481629	-0.644671007463
H	11.055569468890	3.622197822452	-0.949014770132
C	-9.037954037049	-5.366498019585	0.517942400232
H	-9.309453747309	-4.329782522076	0.679593521612
C	-9.947210262489	-6.342688510415	0.491449001122
H	-9.644168262068	-7.371026735544	0.327269381029
H	-11.001558674415	-6.137815128756	0.631169694134

Azoalkane_TS-F200

($E_F = -1373.59029850$ a.u.; $G_F = -1373.21011810$ a.u.)

0 1

N	-0.465757714848	-1.418346922873	0.081632772147
N	0.519611916702	-1.097283825223	-0.399518991241
C	-0.959693480941	-3.360082103662	-0.426376000508
C	1.013686924899	0.844341933087	0.108697617582
C	0.413914540839	1.512209856398	-1.097724384260
H	0.717687063166	1.037837042746	-2.034991468860
H	-0.675910957379	1.466864330201	-1.051208291432
H	0.703476242834	2.569937201004	-1.138732782465
C	0.310668328142	1.054967376176	1.409745462172

H	-0.721887447880	0.698269214689	1.347342123788
H	0.828814682805	0.541396947980	2.217953676163
H	0.277751023571	2.125754328186	1.647978725340
C	-0.256560778253	-3.570877012686	-1.727330739748
H	0.775943185955	-3.214026552279	-1.664923211711
H	-0.223481128760	-4.641709196780	-1.965343496502
H	-0.774721641035	-3.057550008791	-2.535684418730
C	-0.359943048574	-4.027675142630	0.780211023040
H	-0.649508941272	-5.085390726133	0.821447809424
H	0.729882249078	-3.982325501866	0.733717392041
H	-0.663738837077	-3.553102761131	1.717369830892
C	2.496102456075	0.660860510482	0.208015845707
O	3.040810930649	0.362555832767	1.268917721491
N	3.216289283185	0.823781171146	-0.944207062778
H	2.747700487346	1.100591951081	-1.790314705214
C	-2.442124789793	-3.176810596242	-0.525821867718
O	-2.986868545194	-2.879191260363	-1.586912931499
N	-3.162313770552	-3.339161228977	0.626484215480
H	-2.693703696490	-3.615333964942	1.472802782446
C	-4.611605377124	-3.216316047819	0.655467411188
H	-4.911559328291	-2.484567782221	-0.094437232806
H	-4.919937986351	-2.853961423164	1.638231790190
C	-5.285059149952	-4.556214680105	0.365865035641
H	-5.049642807264	-4.898484913937	-0.644142822619
H	-4.966851632699	-5.324303027000	1.074950152539
C	4.665569255113	0.700824336739	-0.973303434767

H	4.973833644756	0.338711748514	-1.956184000780
H	4.965484202115	-0.031160852551	-0.223611385805
C	5.339140544440	2.040595082327	-0.683367295408
H	5.020948314871	2.808907236235	-1.392222384170
H	5.103810287161	2.382611767526	0.326751042562
O	6.764083565820	1.832561895412	-0.806560194319
O	-6.710024598574	-4.348251281872	0.488919875223
C	7.541236077142	2.937315889600	-0.720054334037
O	7.100252861646	4.050250077632	-0.547251649959
C	-7.487102191267	-5.453063045513	0.402532854563
O	-7.046038331841	-6.565991254340	0.229934178143
C	8.977643591410	2.585444213778	-0.871871726470
H	9.207403476280	1.535595302426	-1.011293042370
C	9.923250227683	3.523771652217	-0.837999417521
H	9.656709700810	4.565443955176	-0.696032633936
H	10.972047732246	3.276696421918	-0.948925179469
C	-8.923542286600	-5.101260422536	0.554197759612
H	-9.153375284700	-4.051410170259	0.693448006451
C	-9.869090402653	-6.039646689682	0.520399100272
H	-9.602477165565	-7.081318303380	0.378604435909
H	-10.917910560414	-5.792621404457	0.631215811999

Azoalkane_R-F200

($E_F = -1373.63654442$ a.u.; $G_F = -1373.24837690$ a.u.)

0 1

N	-0.385004335740	-1.447790552801	0.254694103017
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N	0.439041417672	-1.067908648554	-0.572342521607
C	-0.923154246488	-2.824185478250	0.007233246295
C	0.977193812711	0.308485322755	-0.324880749019
C	0.467274450885	1.130676991091	-1.517645928075
H	0.781212587039	0.692322495893	-2.467466933501
H	-0.624291509096	1.139907831441	-1.500417449461
H	0.810276234891	2.166880827165	-1.458112152426
C	0.550155466126	0.936401261874	1.005996782364
H	-0.534850057405	1.036073691354	1.049395972926
H	0.876010548776	0.314241848113	1.838760815498
H	1.002615738788	1.926727759139	1.103230637108
C	-0.496122270785	-3.452098358703	-1.323648079519
H	0.588882873818	-3.551770651965	-1.367053133749
H	-0.948582588600	-4.442424778151	-1.420882187327
H	-0.821981640257	-2.829936741735	-2.156408878367
C	-0.413224227905	-3.646377263425	1.199994119483
H	-0.756217278665	-4.682583942815	1.140458150690
H	0.678341634058	-3.655599356069	1.182761851335
H	-0.727163155115	-3.208028427215	2.149817751409
C	2.513971246065	0.094763905987	-0.270022364684
O	2.985617383191	-0.698804916978	0.529374913381
N	3.276351918425	0.850124630675	-1.108602766738
H	2.819961782181	1.453803106613	-1.772570318839
C	-2.459932239121	-2.610470487110	-0.047615243058
O	-2.931585609288	-1.816887213632	-0.846992907837
N	-3.222305342834	-3.365857409732	0.790948337335

H	-2.765908790521	-3.969542367218	1.454904948663
C	-4.675802782978	-3.287290246010	0.835885116792
H	-4.980293360802	-2.426799461122	0.242046325057
H	-5.005561183705	-3.130013831426	1.866334575001
C	-5.314294374090	-4.561768234383	0.290749659164
H	-5.102280555556	-4.688804968120	-0.773569618829
H	-4.955488662849	-5.448896546607	0.818804491158
C	4.729849474385	0.771547705065	-1.153531328852
H	5.059611995167	0.614262787784	-2.183979731991
H	5.034333036016	-0.088942372294	-0.559684866889
C	5.368344615688	2.046026774438	-0.608400004993
H	5.009547778042	2.933154690418	-1.136464752896
H	5.156323359117	2.173072634601	0.455918482814
O	6.792707344580	1.913374454106	-0.808727304356
O	-6.738655684999	-4.429127471879	0.491089221859
C	7.541893404382	3.013551207693	-0.559192316840
O	7.077026944652	4.063151029217	-0.178751762255
C	-7.487839501589	-5.529300315641	0.241536124689
O	-7.022972563222	-6.578886503765	-0.138932142447
C	8.979000106196	2.742064869752	-0.824192368971
H	9.230638173824	1.739276198416	-1.148885862992
C	9.899303863469	3.693426908339	-0.670263762949
H	9.611638584016	4.686863444996	-0.343813662722
H	10.948196307362	3.504481498680	-0.863687080314
C	-8.924944305817	-5.257828968319	0.506555372708
H	-9.176582393153	-4.255053221529	0.831279486631

C	-9.845246401391	-6.209188766893	0.352607222525
H	-9.557581147424	-7.202612044277	0.026125959658
H	-10.894137410803	-6.020254536325	0.546044710608