

# Mechanistic Investigation of the oxidation of hydrazides with application to the TB drug Isonaizid.

Ruth I. J. Amos,<sup>ac</sup> Brendon S. Gourlay,<sup>a</sup> Brian F. Yates,<sup>ac</sup> Carl H Schiesser<sup>bc</sup>, Trevor W. Lewis and Jason A. Smith,<sup>\*ac</sup>

Ruth I. J. Amos,<sup>a</sup> Carl H. Schiesser,<sup>bc</sup> Jason A. Smith<sup>a</sup> and Brian F. Yates.<sup>\*a</sup>

<sup>a</sup> School of Chemistry, University of Tasmania, Private Bag 75, Hobart, Tasmania 7001, Australia. Fax: 03 6226 2858; Tel: 03 6226 2167;

<sup>b</sup> School of Chemistry, The University of Melbourne, Victoria 3010, Australia.

<sup>c</sup> Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Victoria 3010, Australia.

E-mail: Brian.Yates@utas.edu.au

## Supporting Information

### Table of Contents

| Content   | Page number |
|---|-------------|
| Experimental details  | S2          |
| Computational details   | S2          |
| Supporting Information References                             | S4          |
| Bond Dissociation Benchmarking                                | S4          |
| Bond Dissociation Values                                      | S5          |
| Oxidation of Radical to Cation Values                         | S5          |
| Geometries, energies and energy corrections for all molecules | S6 – S35    |

NMR studies were carried out on a Varian Gemini Mercury Plus spectrometer at 293 K in CDCl<sub>3</sub> unless otherwise stated. <sup>1</sup>H NMR spectra were recorded at 300 MHz and were referenced to the residual <sup>1</sup>H resonance of the solvent. <sup>13</sup>C NMR spectra were recorded at 75 MHz and referenced to the resonance of the deuterated solvent. Isoniazid, benzhydrazide, periodic acid and TEMPO were purchased from Sigma-Aldrich and used as received. The manganese catalyst, [Mn<sup>IV</sup>-Mn<sup>IV</sup>(μ-O)<sub>3</sub>L<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub> (L=1,4,7-trimethyl-1,4,7-triazacyclononane) was available in the group and prepared by the method of Wieghardt.<sup>23</sup> All competitive trapping (section 3.2.2 and 3.2.3) experiments were performed in duplicate. Anhydrous magnesium sulphate was used for drying of solvent extracts and solvents removed under reduced pressure on a rotary evaporator. Mass Spectrometry was performed using a Finnigan LCQ ion trap mass spectrometer fitted with an electrospray ion source. The samples were infused directly using a syringe pump at 10 μL per minute. The nitrogen nebulising gas pressure was 413 kPa, the needle voltage 4 kV, and the capillary voltage 8 V. The MS/MS scans were selected interactively using an isolation width of 3 m/z units. Molecular ions and mass fragments are referenced in intensity relative to the most intense peak (given the value 100%).

## Computational details

All calculations were performed using the Gaussian 03<sup>1</sup> program.

### Bond dissociation benchmarking

B3LYP: Geometries were optimized and frequency calculations performed at B3LYP/6-31G(d), single point calculations on those geometries were performed at B3LYP/6-311+G(2d,2p).<sup>2-4</sup>

BHandHLYP: Geometries were optimized and frequency calculations performed at BHandHLYP/6-31G(d), single point calculations on those geometries were performed at BHandHLYP/6-311+G(2d,2p).<sup>3</sup>

QB3: All calculations performed at the CBS-QB3 level of theory.<sup>5</sup> Geometries were optimized and frequency calculations performed at B3LYP/CBS-B7.<sup>5</sup>

HF,<sup>6-8</sup> MP2,<sup>9-13</sup> MP4,<sup>14</sup> MPWB1K,<sup>15</sup> BMK<sup>16</sup>: Geometries were optimized and frequency calculations performed at B3LYP/CBS-B7. Single point calculations on those geometries were performed with a 6-311+G(2d,2p) basis set.

### Bond dissociation MPWB1K calculations

Geometries optimized and frequency calculations performed at MPWB1K/6-31G(d). Single point calculations on those geometries at MPWB1K/6-311+G(2d,2p).

### Oxidation of the radical to the cation

B3LYP: Geometries were optimized and frequency calculations performed at B3LYP/6-31G(d), single point calculations on those geometries were performed at B3LYP/6-311+G(2d,2p).

MPWB1K and CCSD(t)<sup>17</sup> single point calculations with a 6-311+G(2d,2p) basis set were performed on B3LYP optimized geometries.

Enthalpy corrections for MPWB1K and CCSD(t) were used from frequency calculations performed at B3LYP/6-31G(d).

CBS-QB3 calculations were performed separately.

The electrostatic effect of the bulk solvent was included according to the method of Fu *et al.*<sup>18</sup>

The ionization potentials were corrected by adding 0.28V as specified by Fu *et al.*<sup>18</sup>

The value for the normal hydrogen electrode is 4.28V<sup>19</sup>

## Supporting Information References

- (1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; J. R. Cheeseman; Montgomery Jr, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision D.01*; Gaussian, Inc., Wallingford CT, 2004.
- (2) Becke, A. D. *Physical Review A: Atomic, Molecular, and Optical Physics* **1988**, *38*, 3098-100.
- (3) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-52.
- (4) Lee, C.; Yang, W.; Parr, R. G. *Physical Review B: Condensed Matter and Materials Physics* **1988**, *37*, 785-9.
- (5) J. A. Montgomery, Jr., M. J. Frisch, J. W. Ochterski and G. A. Petersson, *J. Chem. Phys.*, 2000, **112**, 6532-6542.
- (6) C. C. J. Roothan, *Review of Modern Physics*, 1951, **23**, 69.
- (7) R. McWeeny and G. Diercksen, *J. Chem. Phys.*, 1968, **49**, 4852-4856.
- (8) J. A. Pople and R. K. Nesbet, *J. Chem. Phys.*, 1954, **22**, 571-572.
- (9) M. J. Frisch, M. Head-Gordon and J. A. Pople, *Chem. Phys. Lett.*, 1990, **166**, 281-289.
- (10) M. J. Frisch, M. Head-Gordon and J. A. Pople, *Chem. Phys. Lett.*, 1990, **166**, 275-280.
- (11) M. Head-Gordon and T. Head-Gordon, *Chem. Phys. Lett.*, 1994, **220**, 122-128.
- (12) M. Head-Gordon, J. A. Pople and M. J. Frisch, *Chem. Phys. Lett.*, 1988, **153**, 503-506.
- (13) S. Saebo and J. Almlöf, *Chem. Phys. Lett.*, 1989, **154**, 83-89.
- (14) R. Krishnan and J. A. Pople, *Int. J. Quantum Chem.*, 1978, **14**, 91-100.
- (15) Zhao, Y.; Truhlar, D.G. *J. Phys. Chem. A* **2004**, *108*, 6908-18
- (16) Boese, A.D; Martin, J. M. L. *J. Chem. Phys.* **2004**, *121*, 3405-16
- (17) Fu, Y.; Liu, L; Yu, H.; Wang, Y.; Guo, Q., *J. Am. Chem. Soc.* **2005**, *127*, 7227-34
- (18) J. A. Pople, M. Head-Gordon and K. Raghavachari, *J. Chem. Phys.*, 1987, **87**, 5968-5975.
- (19) Lewis, A.; Bumpus, J.A.; Truhlar, D. G.; Cramer, C. J. *J. Chem. Educ.* **2004**, *81*, 596-604

## Bond Dissociation Benchmarking Results

Table 1 Benchmarking of BDEs Enthalpies in kJ/mol

|                         | QB3  | B3LYP | BHandHLYP | MPWB1K | BMK  | HF   | MP2  | MP4  |
|-------------------------|------|-------|-----------|--------|------|------|------|------|
| Pyridyl                 | 56.1 | 58.6  | 74.2      | 58.5   | 58.8 | 27.2 | 57.8 | 56.7 |
| Phenyl                  | 57.6 | 60.4  | 50.0      | 60.5   | 64.3 | 29.3 | 59.3 | 58.3 |
| <i>p</i> -Methoxyphenyl | 59.8 | 61.1  | 45.4      | 61.0   | 68.0 | 30.8 | 59.2 | 57.7 |
| <i>m</i> -Nitrophenyl   | 54.1 | 62.1  | 45.7      | 55.7   | 59.4 | 25.0 | 56.1 | 55.2 |

## Bond Dissociation Calculated at MPWB1K

Table 2 BDEs (kJ/mol) for various functional groups calculated at MPWB1K

| Functional group | Pyridyl               | Phenyl                | <i>p</i> -Methoxyphenyl | <i>p</i> -Nitrophenyl | <i>p</i> -Chlorophenyl | <i>m</i> -Methoxyphenyl |                                 |
|------------------|-----------------------|-----------------------|-------------------------|-----------------------|------------------------|-------------------------|---------------------------------|
| BDE              | 58.5                  | 60.5                  | 61.0                    | 57.5                  | 59.5                   | 63.8                    |                                 |
| Functional group | <i>m</i> -Nitrophenyl | <i>m</i> -Bromophenyl | <i>m</i> -Methylphenyl  | Tolyl                 | <i>m</i> -Fluorophenyl | <i>p</i> - <b>co2et</b> | <i>p</i> -Trifluoromethylphenyl |
| BDE              | 55.7                  | 59.9                  | 60.4                    | 65.2                  | 59.6                   | 59.1                    | 58.7                            |

## Oxidation of the radical to the cation

|                                | IP eV | Corrected IP eV | E <sup>0</sup> V | V | E <sup>0</sup> vs NHE V |
|--------------------------------|-------|-----------------|------------------|---|-------------------------|
| <b>B3LYP</b>                   |       |                 |                  |   |                         |
| isoniazid                      | 7.00  | 7.28            | 4.78             |   | 0.50                    |
| benzhydrazide                  | 6.47  | 6.75            | 4.49             |   | 0.21                    |
| <i>p</i> -methoxybenzhydrazide | 6.04  | 6.32            | 4.28             |   | 0.00                    |
| <i>m</i> -nitrobenzhydrazide   | 7.04  | 7.32            | 4.74             |   | 0.46                    |
| <b>CBS-QB3</b>                 |       |                 |                  |   |                         |
| isoniazid                      | 6.94  | 7.22            | 4.70             |   | 0.42                    |
| benzhydrazide                  | 6.47  | 6.75            | 4.48             |   | 0.20                    |
| <i>p</i> -methoxybenzhydrazide | 6.38  | 6.38            | 4.34             |   | 0.06                    |
| <i>m</i> -nitrobenzhydrazide   | 7.13  | 7.41            | 4.82             |   | 0.54                    |
| <b>MPWB1K</b>                  |       |                 |                  |   |                         |
| isoniazid                      | 6.90  | 7.18            | 4.65             |   | 0.37                    |
| benzhydrazide                  | 6.38  | 6.66            | 4.39             |   | 0.10                    |

|                                |      |      |      |       |
|--------------------------------|------|------|------|-------|
| <i>p</i> -methoxybenzhydrazide | 5.96 | 6.24 | 4.20 | -0.08 |
| <i>m</i> -nitrobenzhydrazide   | 6.90 | 7.18 | 4.60 | 0.32  |
| <b>CCSD(t)</b>                 |      |      |      |       |
| isoniazid                      | 6.84 | 7.12 | 4.59 | 0.31  |
| benzhydrazide                  | 6.35 | 6.63 | 4.36 | 0.08  |
| <i>p</i> -methoxybenzhydrazide | 5.43 | 5.71 | 3.67 | -0.61 |
| <i>m</i> -nitrobenzhydrazide   | 6.29 | 6.57 | 3.99 | -0.29 |

## Geometries for all molecules

### Methane

#### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000000  |
| H | 0.631339  | 0.631339  | 0.631339  |
| H | -0.631339 | -0.631339 | 0.631339  |
| H | -0.631339 | 0.631339  | -0.631339 |
| H | 0.631339  | -0.631339 | -0.631339 |

E (au)= -40.536625

ZPVE correction (au)= 0.045214

#### BHandH

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000000  |
| H | 0.626165  | 0.626165  | 0.626165  |
| H | -0.626165 | -0.626165 | 0.626165  |
| H | -0.626165 | 0.626165  | -0.626165 |
| H | 0.626165  | -0.626165 | -0.626165 |

E (au)= -40.500325

ZPVE correction (au)= 0.045214

#### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000000  |
| H | 0.629729  | 0.629729  | 0.629729  |
| H | -0.629729 | -0.629729 | 0.629729  |
| H | -0.629729 | 0.629729  | -0.629729 |
| H | 0.629729  | -0.629729 | -0.629729 |

Zero point E (au)= -40.409999

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.044588

#### HF

E (au)= -40.211785

#### MP2

E (au)= -40.393458

#### MP4

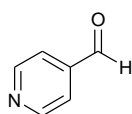
E (au)= -40.419229

#### BMK

E (au)= -40.491778

#### MPWB1K

E (au)= -40.495035



### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.749869 | 0.984890  | -0.000054 |
| C | -0.384796 | 1.277613  | -0.000022 |
| C | 0.524418  | 0.216644  | 0.000013  |
| C | 0.026114  | -1.091214 | 0.000024  |
| C | -1.354422 | -1.271511 | -0.000053 |
| H | -2.485524 | 1.787124  | -0.000023 |
| H | -0.039078 | 2.308653  | -0.000049 |
| H | 0.713000  | -1.931342 | 0.000155  |
| H | -1.779016 | -2.273582 | 0.000179  |
| C | 1.988877  | 0.475003  | 0.000114  |
| O | 2.834956  | -0.395378 | -0.000111 |
| H | 2.272346  | 1.550203  | 0.000294  |
| N | -2.237615 | -0.260940 | 0.000029  |

E (au)= -361.717234

ZPVE correction (au)= 0.098276

### BHandH

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.737718 | 0.976871  | -0.000026 |
| C | -0.382423 | 1.268273  | -0.000063 |
| C | 0.518643  | 0.215335  | -0.000055 |
| C | 0.026565  | -1.082896 | -0.000010 |
| C | -1.344015 | -1.262017 | 0.000012  |
| H | -2.468057 | 1.771340  | -0.000035 |
| H | -0.042281 | 2.291584  | -0.000093 |
| H | 0.706514  | -1.917056 | 0.000000  |
| H | -1.765360 | -2.255335 | 0.000064  |
| C | 1.976606  | 0.471838  | -0.000105 |
| O | 2.808448  | -0.392305 | 0.000162  |
| H | 2.264592  | 1.532994  | 0.000169  |
| N | -2.215563 | -0.258500 | 0.000012  |

E (au)= -361.486407

ZPVE correction (au)= 0.098276

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.746751  | 0.984560  | 0.000040  |
| C | 0.383001  | 1.274549  | 0.000042  |
| C | -0.523050 | 0.214666  | 0.000018  |
| C | -0.023894 | -1.089934 | -0.000007 |
| C | 1.354409  | -1.268932 | -0.000004 |
| H | 2.479960  | 1.786108  | 0.000061  |
| H | 0.037276  | 2.303358  | 0.000063  |
| H | -0.708586 | -1.929373 | -0.000027 |
| H | 1.779407  | -2.268478 | -0.000027 |
| C | -1.989091 | 0.471667  | 0.000022  |
| O | -2.830245 | -0.393716 | -0.000098 |
| H | -2.269931 | 1.546749  | -0.000067 |
| N | 2.233583  | -0.258300 | 0.000017  |

Zero point E (au)= -361.013390

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.097592

### HF

E (au)= -359.521101

### MP2

E (au)= -360.768243

**MP4**

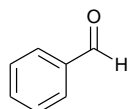
E (au)= -360.862711

**MPWB1K**

E (au)= -361.527605

**BMK**

E (au)= -361.489609



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.735786 | 1.060718  | 0.000166  |
| C | -0.361038 | 1.292088  | -0.000336 |
| C | 0.534004  | 0.214260  | -0.000521 |
| C | 0.045198  | -1.101122 | -0.000573 |
| C | -1.326436 | -1.331144 | 0.000045  |
| H | -2.430109 | 1.896291  | 0.000690  |
| H | 0.025263  | 2.309452  | -0.000342 |
| H | 0.758625  | -1.919655 | -0.000598 |
| H | -1.707930 | -2.348510 | 0.000424  |
| C | 1.992127  | 0.468649  | -0.000012 |
| O | 2.847640  | -0.395800 | 0.000521  |
| C | -2.216822 | -0.250739 | 0.000346  |
| H | -3.288215 | -0.433208 | 0.000588  |
| H | 2.273765  | 1.545770  | 0.000379  |

E (au)= -345.680870

ZPVE correction (au)= 0.110226

**BHandH**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.723442 | 1.053106  | 0.000179  |
| C | -0.357739 | 1.282725  | 0.000078  |
| C | 0.529059  | 0.213250  | -0.000031 |
| C | 0.045772  | -1.092570 | -0.000054 |
| C | -1.316191 | -1.321515 | 0.000049  |
| H | -2.412233 | 1.881866  | 0.000270  |
| H | 0.023845  | 2.292540  | 0.000097  |
| H | 0.752981  | -1.905005 | -0.000136 |
| H | -1.694704 | -2.330630 | 0.000038  |
| C | 1.980991  | 0.465127  | -0.000133 |
| O | 2.821970  | -0.393277 | -0.000236 |
| C | -2.199994 | -0.248646 | 0.000163  |
| H | -3.262772 | -0.430022 | 0.000242  |
| H | 2.266387  | 1.528611  | -0.000123 |

E (au)= -345.46984

ZPVE correction (au)= 0.114474

**QB3**



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.732338 | 1.059455  | 0.000184  |
| C | -0.359505 | 1.288919  | 0.000087  |
| C | 0.532830  | 0.212702  | -0.000046 |
| C | 0.043026  | -1.099645 | -0.000040 |
| C | -1.325901 | -1.327744 | 0.000045  |
| H | -2.424483 | 1.893548  | 0.000267  |
| H | 0.026195  | 2.303907  | 0.000091  |
| H | 0.754532  | -1.916962 | -0.000138 |
| H | -1.707829 | -2.342256 | 0.000022  |
| C | 1.992490  | 0.465469  | -0.000155 |
| O | 2.842673  | -0.394344 | -0.000225 |
| C | -2.213818 | -0.248450 | 0.000167  |
| H | -3.282938 | -0.429440 | 0.000238  |
| H | 2.272437  | 1.541716  | -0.000133 |

Zero point E (au)= -344.974798

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.109513

#### HF

E (au)= -343.528802

#### MP2

E (au)= -344.744114

#### MP4

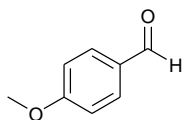
E (au)= -344.841808

#### MPWB1K

E (au)= -345.493877

#### BMK

E (au)= -345.450690



#### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.579549  | 1.466278  | 0.000009  |
| C | -0.805197 | 1.420015  | -0.000024 |
| C | -1.483004 | 0.189221  | -0.000016 |
| C | 0.652677  | -0.968244 | 0.000028  |
| H | 1.119769  | 2.407504  | -0.000022 |
| H | -1.376479 | 2.346163  | -0.000096 |
| C | -2.955509 | 0.148330  | -0.000045 |
| O | -3.626810 | -0.868399 | 0.000039  |
| H | 1.209512  | -1.898147 | -0.000012 |
| C | 1.318074  | 0.270140  | 0.000037  |
| H | -3.444824 | 1.148845  | -0.000171 |
| C | -0.736987 | -0.997342 | 0.000015  |
| H | -1.271092 | -1.942867 | 0.000025  |
| O | 2.667967  | 0.416271  | 0.000126  |
| C | 3.481464  | -0.750318 | -0.000101 |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 4.512206 | -0.392618 | -0.000469 |
| H | 3.307923 | -1.360106 | 0.895382  |
| H | 3.307324 | -1.360230 | -0.895367 |

E (au)= -460.244087

ZPVE correction (au)= 0.143132

### BHandH

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.576193 | 1.455392  | 0.000035  |
| C | 0.799141  | 1.409507  | 0.000048  |
| C | 1.470623  | 0.188213  | 0.000022  |
| C | -0.649017 | -0.959805 | -0.000036 |
| H | -1.112266 | 2.389017  | 0.000058  |
| H | 1.364480  | 2.329125  | 0.000082  |
| C | 2.936965  | 0.146027  | 0.000044  |
| O | 3.595090  | -0.861535 | -0.000117 |
| H | -1.200896 | -1.882589 | -0.000074 |
| C | -1.308601 | 0.268577  | -0.000007 |
| H | 3.427010  | 1.132737  | -0.000062 |
| C | 0.731922  | -0.988871 | -0.000021 |
| H | 1.260108  | -1.927807 | -0.000043 |
| O | -2.645789 | 0.408739  | -0.000026 |
| C | -3.453525 | -0.741691 | 0.000067  |
| H | -4.476613 | -0.388389 | 0.000138  |
| H | -3.282126 | -1.346929 | -0.887870 |
| H | -3.281983 | -1.346887 | 0.888005  |

E (au)= -459.9691

ZPVE correction (au)= 0.148742

### QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.576783 | 1.463128  | 0.000046  |
| C | 0.805293  | 1.415799  | 0.000077  |
| C | 1.481414  | 0.187026  | 0.000069  |
| C | -0.651402 | -0.965799 | -0.000018 |
| H | -1.116142 | 2.402167  | 0.000057  |
| H | 1.375432  | 2.339854  | 0.000115  |
| C | 2.954738  | 0.145463  | 0.000123  |
| O | 3.623368  | -0.864563 | -0.000237 |
| H | -1.206314 | -1.894024 | -0.000062 |
| C | -1.316060 | 0.270521  | -0.000002 |
| H | 3.440800  | 1.146396  | -0.000202 |
| C | 0.735708  | -0.996176 | 0.000018  |
| H | 1.268071  | -1.940250 | 0.000010  |
| O | -2.663625 | 0.416295  | -0.000040 |
| C | -3.483544 | -0.748390 | 0.000040  |
| H | -4.509503 | -0.385495 | 0.000094  |
| H | -3.313298 | -1.355990 | -0.894638 |
| H | -3.313184 | -1.355945 | 0.894728  |

Zero point E (au)= -459.336038

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.141923

### HF

E (au)= -457.446306

### MP2

E (au)= -459.033744

**MP4**

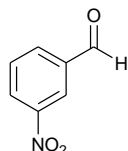
E (au)= -459.157989

**MPWB1K**

E (au)= -460.001839

**BMK**

E (au)= -459.952059



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.475006  | 2.042591  | -0.000076 |
| C | 1.591448  | 1.210745  | -0.000143 |
| C | 1.434210  | -0.184574 | 0.000017  |
| C | 0.154531  | -0.744830 | 0.000095  |
| C | -0.946185 | 0.106105  | -0.000007 |
| H | 0.596268  | 3.121416  | -0.000415 |
| H | 2.598736  | 1.615596  | -0.000272 |
| H | 0.004505  | -1.819102 | 0.000050  |
| C | 2.626161  | -1.071151 | 0.000159  |
| O | 3.772318  | -0.670381 | -0.000002 |
| C | -0.809051 | 1.492997  | -0.000007 |
| H | -1.696504 | 2.114105  | 0.000368  |
| H | 2.397623  | -2.158654 | 0.000603  |
| N | -2.299551 | -0.478511 | -0.000043 |
| O | -3.254429 | 0.296226  | 0.000330  |
| O | -2.387950 | -1.705231 | -0.000360 |

E (au)= -550.24712

ZPVE correction (au)= 0.112782

**BHandH**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.468046 | 2.026942  | 0.000148  |
| C | -1.576208 | 1.200330  | 0.000083  |
| C | -1.420147 | -0.184269 | 0.000026  |
| C | -0.151569 | -0.741503 | 0.000028  |
| C | 0.941857  | 0.103707  | 0.000093  |
| H | -0.588606 | 3.097006  | 0.000187  |
| H | -2.574994 | 1.603302  | 0.000079  |
| H | -0.002972 | -1.807260 | -0.000015 |
| C | -2.608546 | -1.063662 | -0.000034 |
| O | -3.738502 | -0.660264 | -0.000086 |
| C | 0.806528  | 1.480238  | 0.000154  |
| H | 1.686380  | 2.097306  | 0.000214  |
| H | -2.391162 | -2.141436 | -0.000106 |
| N | 2.279625  | -0.475371 | 0.000099  |
| O | 3.219348  | 0.285807  | -0.000213 |

O 2.365501 -1.682045 -0.000206

E (au)= -549.922228

ZPVE correction (au)= 0.117705

### QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.477258 | 2.040434  | 0.000137  |
| C | -1.591051 | 1.210056  | 0.000122  |
| C | -1.433670 | -0.182502 | 0.000048  |
| C | -0.156093 | -0.740963 | -0.000010 |
| C | 0.942203  | 0.108614  | -0.000002 |
| H | -0.598727 | 3.116861  | 0.000195  |
| H | -2.596599 | 1.613745  | 0.000170  |
| H | -0.003964 | -1.813025 | -0.000062 |
| C | -2.625659 | -1.071093 | 0.000043  |
| O | -3.766096 | -0.675579 | -0.000149 |
| C | 0.804973  | 1.492073  | 0.000068  |
| H | 1.691639  | 2.110890  | 0.000071  |
| H | -2.392702 | -2.156713 | -0.000246 |
| N | 2.303224  | -0.479229 | -0.000069 |
| O | 3.251141  | 0.292271  | -0.000091 |
| O | 2.389593  | -1.698801 | -0.000020 |

Zero point E (au)= -549.266482

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.111929

### HF

E (au)= -547.058205

### MP2

E (au)= -548.893255

### MP4

E (au)= -549.016931

### MPWB1K

E (au)= -549.973344

### BMK

E (au)= -549.9209857

### Methyl radical

#### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000555  |
| H | 0.000000  | 1.083310  | -0.001110 |
| H | 0.938174  | -0.541655 | -0.001110 |
| H | -0.938174 | -0.541655 | -0.001110 |

E (au)= -39.855963

ZPVE correction (au)= 0.029815

### BHandH

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000512  |
| H | 0.000000  | 1.074485  | -0.001025 |
| H | 0.930531  | -0.537242 | -0.001025 |
| H | -0.930531 | -0.537242 | -0.001025 |

E (au)= -39.825643

ZPVE correction (au)= 0.029815

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000526  |
| H | 0.000000  | 1.080395  | -0.001052 |
| H | 0.935649  | -0.540197 | -0.001052 |
| H | -0.935649 | -0.540197 | -0.001052 |

Zero point E (au)= -39.744794

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.029578

### HF

E (au)= -39.571586

### MP2

E (au)= -39.720368

### MP4

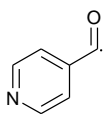
E (au)= -39.743807

### MPWB1K

E (au)= -39.816514

### BMK

E (au)= -39.812641



### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.725123  | -0.977972 | 0.000290  |
| C | 0.364262  | -1.289502 | -0.000015 |
| C | -0.554620 | -0.238001 | -0.000382 |
| C | -0.075523 | 1.079404  | -0.000257 |
| C | 1.303894  | 1.275002  | -0.000125 |
| H | 2.471159  | -1.770247 | 0.000304  |
| H | 0.021082  | -2.319404 | -0.000079 |
| H | -0.767745 | 1.915288  | -0.000192 |
| H | 1.716487  | 2.282222  | 0.000391  |
| C | -2.016641 | -0.530034 | -0.000596 |
| O | -2.912296 | 0.257243  | 0.000625  |
| N | 2.196918  | 0.274401  | 0.000156  |

E (au)= -361.061686

ZPVE correction (au)= 0.085734

Enthalpy correction (au)= 0.092988

S (J/molK)= 340.92

$\Delta G$  solv (kJ/mol)= -12.47

#### BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.713908  | -0.969773 | 0.000151  |
| C | 0.362987  | -1.280159 | -0.000027 |
| C | -0.547521 | -0.236463 | -0.000057 |
| C | -0.075253 | 1.070913  | -0.000019 |
| C | 1.293904  | 1.265933  | 0.000022  |
| H | 2.454786  | -1.754061 | 0.000191  |
| H | 0.026011  | -2.302592 | -0.000109 |
| H | -0.761299 | 1.900145  | -0.000036 |
| H | 1.703124  | 2.264304  | 0.000077  |
| C | -2.003453 | -0.522293 | -0.000219 |
| O | -2.889647 | 0.252155  | -0.000038 |
| N | 2.175304  | 0.272287  | 0.000154  |

E (au)= -360.846322

ZPVE correction (au)= 0.089344

#### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.722191  | -0.975429 | 0.000113  |
| C | 0.363328  | -1.287036 | -0.000008 |
| C | -0.553370 | -0.238008 | -0.000057 |
| C | -0.076546 | 1.077093  | -0.000016 |
| C | 1.300311  | 1.273957  | 0.000058  |
| H | 2.466962  | -1.765844 | 0.000153  |
| H | 0.020856  | -2.314936 | -0.000056 |
| H | -0.767776 | 1.911105  | -0.000044 |
| H | 1.711299  | 2.279442  | 0.000099  |
| C | -2.016268 | -0.525793 | -0.000182 |
| O | -2.908628 | 0.251056  | -0.000104 |
| N | 2.190492  | 0.274789  | 0.000133  |

Zero point E (au)= -360.369541

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.085216

Enthalpy corrected E(au)= -360.362244

S (J/molK)= 340.92

$\Delta G$  solv (kJ/mol)= -12.34

#### HF

E (au)= -358.898830

#### MP2

E (au)= -360.118475

**MP4**

E (au)= -360.211674

**CCSD(t)**

E (au)= -360.200461

Enthalpy correction (au)= 0.092467

S (J/molK)= 340.92

$\Delta G$  solv (kJ/mol)= -12.34

**MPWB1K**

E (au)= -360.873794

ZPVE correction (au)= 0.085734

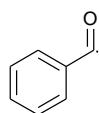
Enthalpy correction (au)= 0.092988

S (J/molK)= 340.92

$\Delta G$  solv (kJ/mol)= -12.34

**BMK**

E (au)= -360.836855



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.711575 | -1.053979 | -0.000030 |
| C | -0.340426 | -1.304642 | 0.000012  |
| C | 0.565111  | -0.236031 | -0.000022 |
| C | 0.094785  | 1.089041  | -0.000007 |
| C | -1.274598 | 1.334271  | 0.000029  |
| H | -2.416551 | -1.880364 | 0.000067  |
| H | 0.043608  | -2.320761 | -0.000007 |
| H | 0.813544  | 1.903112  | -0.000014 |
| H | -1.644537 | 2.356006  | 0.000000  |
| C | 2.019024  | -0.522520 | 0.000038  |
| O | 2.924005  | 0.258171  | -0.000017 |
| C | -2.176132 | 0.263485  | -0.000002 |
| H | -3.245235 | 0.458889  | -0.000031 |

E (au)= -345.026130

ZPVE correction (au)= 0.097791

Enthalpy correction (au)= 0.092988

S (J/molK)= 339.32

$\Delta G$  solv (kJ/mol)= -6.23416

### BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.700081 | -1.046439 | 0.000009  |
| C | -0.338198 | -1.295155 | 0.000008  |
| C | 0.559068  | -0.234334 | 0.000003  |
| C | 0.094428  | 1.080441  | -0.000005 |
| C | -1.265238 | 1.324752  | -0.000008 |
| H | -2.399703 | -1.865713 | 0.000007  |
| H | 0.040765  | -2.303730 | 0.000013  |
| H | 0.807326  | 1.887838  | -0.000009 |
| H | -1.632009 | 2.338050  | -0.000010 |
| C | 2.006962  | -0.514149 | 0.000001  |
| O | 2.902813  | 0.253454  | -0.000006 |
| C | -2.160027 | 0.261570  | 0.000000  |
| H | -3.220364 | 0.455801  | 0.000002  |

E (au)= -344.81712

ZPVE correction (au)= 0.101627

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.708478 | -1.052151 | 0.000002  |
| C | -0.339756 | -1.302338 | 0.000012  |
| C | 0.563252  | -0.235502 | 0.000000  |
| C | 0.093647  | 1.086796  | -0.000007 |
| C | -1.272959 | 1.331115  | -0.000001 |
| H | -2.411704 | -1.876653 | 0.000008  |
| H | 0.044219  | -2.315892 | 0.000018  |
| H | 0.810436  | 1.899485  | -0.000012 |
| H | -1.642158 | 2.350414  | -0.000005 |
| C | 2.017928  | -0.516117 | 0.000004  |
| O | 2.919052  | 0.255110  | -0.000009 |
| C | -2.172628 | 0.262306  | 0.000000  |
| H | -3.239244 | 0.457111  | -0.000001 |

Zero point E (au)= -344.331537

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.097262

Enthalpy corrected E (au)= -344.324215

S (J/molK)= 339.32

$\Delta G$  solv (kJ/mol)= -5.77

### HF

E (au)= -342.907581

ZPVE correction (au)= 0.097262



**MP2**

E (au)= -344.094846

ZPVE correction (au)= 0.097262

**MP4**

E (au)= -344.191411

ZPVE correction (au)= 0.097262

**CCSD(t)**

E (au)= -344.181994

Enthalpy correction (au)= 0.104534

S (J/molK)= 340.92

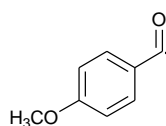
$\Delta G$  solv (kcal/mol)= -12.34

**BMK**

E (au)= -344.798692

**MPWB1K**

E (au)= -344.840918



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.543884  | 1.468728  | -0.000165 |
| C | -0.840540 | 1.432115  | 0.000225  |
| C | -1.522857 | 0.203425  | -0.000107 |
| C | 0.606435  | -0.967238 | -0.000296 |
| H | 1.089115  | 2.406956  | -0.000112 |
| H | -1.415455 | 2.353762  | 0.000515  |
| C | -2.995186 | 0.186123  | 0.000278  |
| O | -3.729260 | -0.759936 | 0.000177  |
| H | 1.159211  | -1.899708 | -0.000271 |
| C | 1.276580  | 0.268709  | -0.000372 |
| C | -0.783614 | -0.990748 | -0.000323 |
| H | -1.315922 | -1.937495 | -0.000548 |
| O | 2.626002  | 0.408226  | -0.000257 |
| C | 3.435710  | -0.761476 | 0.000561  |
| H | 4.467522  | -0.407135 | 0.001085  |
| H | 3.259000  | -1.370090 | 0.896126  |
| H | 3.260116  | -1.370438 | -0.894960 |

E (au)= -459.589673

ZPVE correction (au)= 0.130782

Enthalpy correction (au)= 0.140549

S (J/molK)= 390.94

$\Delta G$  solv (kcal/mol)= -10.5018

#### BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.541390  | 1.458301  | 0.000076  |
| C | -0.833392 | 1.422463  | 0.000011  |
| C | -1.509175 | 0.202940  | -0.000088 |
| C | 0.603321  | -0.958968 | -0.000064 |
| H | 1.083236  | 2.388461  | 0.000157  |
| H | -1.401934 | 2.337904  | 0.000042  |
| C | -2.975321 | 0.179871  | -0.000154 |
| O | -3.701025 | -0.752554 | -0.000235 |
| H | 1.150647  | -1.884481 | -0.000108 |
| C | 1.267715  | 0.266867  | 0.000041  |
| C | -0.777962 | -0.981564 | -0.000126 |
| H | -1.305656 | -1.920954 | -0.000210 |
| O | 2.604148  | 0.400184  | 0.000089  |
| C | 3.408114  | -0.753734 | 0.000325  |
| H | 4.432160  | -0.403675 | 0.000535  |
| H | 3.234015  | -1.357629 | 0.888448  |
| H | 3.234416  | -1.357717 | -0.887817 |

E (au)= -459.31671

ZPVE correction (au)= 0.135947

#### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.541228  | 1.466034  | 0.000088  |
| C | -0.840269 | 1.429677  | -0.000010 |
| C | -1.520630 | 0.203091  | -0.000089 |
| C | 0.604368  | -0.964629 | -0.000038 |
| H | 1.086223  | 2.401683  | 0.000163  |
| H | -1.414886 | 2.348791  | 0.000005  |
| C | -2.992342 | 0.179777  | -0.000164 |
| O | -3.724364 | -0.756411 | -0.000273 |
| H | 1.154461  | -1.895859 | -0.000091 |
| C | 1.274142  | 0.268811  | 0.000096  |
| C | -0.783125 | -0.988371 | -0.000121 |
| H | -1.314217 | -1.933240 | -0.000215 |
| O | 2.621100  | 0.407616  | 0.000101  |
| C | 3.436940  | -0.760401 | 0.000308  |
| H | 4.464057  | -0.401054 | 0.000507  |
| H | 3.264110  | -1.366915 | 0.895142  |
| H | 3.264487  | -1.366980 | -0.894556 |

Zero point E (au)= -458.693595

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.129751

Enthalpy correction (au)= -458.683740

S (J/molK)= 390.94

$\Delta G$  solv (kcal/mol)= -10.33

**HF**

E (au)= -456.820834

**MP2**

E (au)= -458.386189

**MP4**

E (au)= -458.507550

**MPWB1K**

E (au)= -459.349150

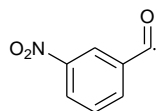
**CCSD(t)**

E (au)= -458.498647

Enthalpy correction (au)= 0.139538

S (J/molK)= 390.94

$\Delta G$  solv (kcal/mol)= -10.33



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.315000  | 2.240336  | -0.000057 |
| C | 1.536617  | 1.566032  | 0.000020  |
| C | 1.569593  | 0.165451  | 0.000072  |
| C | 0.376242  | -0.571627 | 0.000096  |
| C | -0.824714 | 0.124351  | 0.000029  |
| H | 0.288682  | 3.325390  | -0.000144 |
| H | 2.474878  | 2.112811  | 0.000014  |
| H | 0.390078  | -1.654930 | 0.000122  |
| C | 2.884349  | -0.528962 | 0.000062  |
| O | 3.088000  | -1.703935 | -0.000105 |
| C | -0.877867 | 1.519833  | -0.000039 |
| H | -1.842565 | 2.012490  | -0.000009 |
| N | -2.091486 | -0.634933 | 0.000005  |
| O | -3.138635 | 0.009781  | 0.000006  |
| O | -2.017613 | -1.861311 | -0.000042 |

E (au)= -550.24712

ZPVE correction (au)= 0.112782

Enthalpy correction (au)= 0.110048

S (J/molK)= 399.72

$\Delta G$  solv (kcal/mol)= -17.9912

#### BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.304690 | 2.224286  | 0.000045  |
| C | -1.518768 | 1.556198  | 0.000019  |
| C | -1.553787 | 0.167085  | 0.000001  |
| C | -0.372628 | -0.568085 | 0.000010  |
| C | 0.821107  | 0.120609  | 0.000030  |
| H | -0.276740 | 3.300492  | 0.000060  |
| H | -2.447423 | 2.102326  | 0.000010  |
| H | -0.389387 | -1.642842 | -0.000002 |
| C | -2.860699 | -0.525814 | -0.000031 |
| O | -3.067108 | -1.684571 | -0.000039 |
| C | 0.877292  | 1.505817  | 0.000051  |
| H | 1.834876  | 1.993601  | 0.000070  |
| N | 2.071189  | -0.633016 | 0.000029  |
| O | 3.102933  | -0.001623 | -0.000059 |
| O | 1.995849  | -1.839186 | -0.000039 |

E (au)= -549.267763

ZPVE correction (au)= 0.104793

#### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.320993 | 2.236774  | 0.000044  |
| C | -1.539085 | 1.561501  | 0.000025  |
| C | -1.568231 | 0.164064  | -0.000006 |
| C | -0.375571 | -0.569193 | -0.000017 |
| C | 0.821262  | 0.127560  | -0.000002 |
| H | -0.297135 | 3.319467  | 0.000069  |
| H | -2.476818 | 2.104678  | 0.000032  |
| H | -0.384824 | -1.650692 | -0.000038 |
| C | -2.878849 | -0.537951 | -0.000028 |
| O | -3.083611 | -1.703304 | -0.000033 |
| C | 0.871149  | 1.520123  | 0.000028  |
| H | 1.833869  | 2.012311  | 0.000037  |
| N | 2.096240  | -0.633833 | -0.000020 |
| O | 3.135086  | 0.010339  | -0.000002 |
| O | 2.022668  | -1.852812 | 0.000007  |

Zero point E (au)= -548.621869

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.099572

Enthalpy corrected E (au)= -548.611825

S (J/molK)= 399.72

$\Delta G$  solv (kJ/mol)= -17.24

#### HF

E (au)= -546.430366

#### MP2

E (au)= -548.244346

#### MP4

E (au)= -548.365363

**MPWB1K**

E (au)= -549.318462

**CCSD(t)**

E (au)= -548.344925

Enthalpy correction (au)= 0.109397

S (J/molK)= 399.72

$\Delta G$  solv (kJ/mol)= -17.24

**Methyl cation**

**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000068  |
| H | 0.000000  | 1.094991  | -0.000136 |
| H | -0.948290 | -0.547496 | -0.000136 |
| H | 0.948290  | -0.547496 | -0.000136 |

E (au)= -39.493472

ZPVE correction (au)= 0.031596

**BHandH**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000023  |
| H | 0.000000  | 1.084768  | -0.000047 |
| H | -0.939437 | -0.542384 | -0.000047 |
| H | 0.939437  | -0.542384 | -0.000047 |

E (au)= -39.471411

ZPVE correction (au)= 0.031596

**CBS-QB3**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.000000  | 0.000000  | 0.000005  |
| H | 0.000000  | 1.093498  | -0.000115 |
| H | -0.946997 | -0.546749 | -0.000115 |
| H | 0.946997  | -0.546749 | -0.000115 |

Zero point E (au)= -39.384653

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.031172

**MPWB1K**

E (au)= -39.459980

**BMK**

E (au)= -39.457880

**HF**

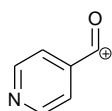
E (au)= -39.245950

**MP2**

E (au)= -39.364941

**MP4**

E (au)= -39.388045



**B3LYP**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.542988 | 1.158332  | 0.000284  |
| C | -0.151879 | 1.235966  | 0.000038  |
| C | 0.540431  | 0.000162  | -0.000027 |
| C | -0.151605 | -1.235783 | -0.000038 |
| C | -1.542668 | -1.158592 | -0.000122 |
| H | -2.140195 | 2.066279  | 0.000115  |
| H | 0.367689  | 2.188030  | -0.000024 |
| H | 0.368428  | -2.187600 | -0.000045 |
| H | -2.139698 | -2.066635 | 0.000067  |
| C | 1.934029  | 0.000194  | -0.000090 |
| O | 3.067651  | -0.000069 | -0.000141 |
| N | -2.215622 | -0.000171 | 0.000107  |

E (au)= -360.805619

ZPVE correction (au)= 0.087028

Enthalpy correction (au)= 0.094081

S (J/molK)= 330.83

$\Delta G$  solv (kJ/mol)= -256.94

**CBS-QB3**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.538483  | -1.156438 | 0.000094  |
| C | 0.150153  | -1.232677 | 0.000014  |
| C | -0.540491 | -0.000008 | -0.000031 |
| C | 0.150132  | 1.232668  | 0.000003  |
| C | 1.538469  | 1.156446  | 0.000082  |
| H | 2.134474  | -2.062858 | 0.000132  |
| H | -0.368063 | -2.182978 | -0.000011 |
| H | -0.368091 | 2.182965  | -0.000031 |
| H | 2.134439  | 2.062881  | 0.000113  |
| C | -1.930360 | -0.000011 | -0.000110 |
| O | -3.053885 | 0.000003  | -0.000175 |

N 2.208572 0.000013 0.000127

Zero point E (au)= -360.114101

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.086626

Enthalpy corrected E (au)= -360.107028

S (J/molK)= 330.83

$\Delta G$  solv (kJ/mol)= -258.91

#### HF

E (au)= -358.657151

#### MP2

E (au)= -359.874896

#### MP4

E (au)= -359.965629

#### MPWB1K

E (au)= -360.621418

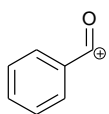
#### CCSD(t)

E (au)= -359.950341

Enthalpy correction (au)= 0.093653

S (J/molK)= 330.83

$\Delta G$  solv (kJ/mol)= -258.91



#### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.515414  | 1.225236  | 0.000004  |
| C | 0.132136  | 1.248204  | 0.000005  |
| C | -0.554766 | 0.000280  | 0.000000  |
| C | 0.131730  | -1.247645 | -0.000010 |
| C | 1.514987  | -1.225749 | -0.000005 |
| H | 2.067469  | 2.159126  | 0.000009  |
| H | -0.418714 | 2.182866  | 0.000013  |
| H | -0.419723 | -2.182011 | -0.000015 |
| H | 2.066539  | -2.159895 | -0.000008 |
| C | -1.937095 | 0.000347  | 0.000001  |
| O | -3.074577 | -0.000236 | 0.000002  |
| C | 2.200080  | -0.000348 | 0.000001  |
| H | 3.286127  | -0.000147 | 0.000007  |

E (au)= -344.790067

ZPVE correction (au)= 0.099508

Enthalpy correction (au)= 0.106639

S (J/molK)= 331.65

$\Delta G$  solv (kJ/mol)= -226.438

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.512573  | 1.222388  | 0.000007  |
| C | 0.132186  | 1.244776  | 0.000006  |
| C | -0.553824 | 0.000215  | 0.000000  |
| C | 0.131773  | -1.244570 | -0.000007 |
| C | 1.512175  | -1.222662 | -0.000006 |
| H | 2.063563  | 2.154263  | 0.000012  |
| H | -0.416966 | 2.177834  | 0.000011  |
| H | -0.417690 | -2.177448 | -0.000012 |
| H | 2.062832  | -2.154732 | -0.000009 |
| C | -1.932554 | 0.000346  | 0.000000  |
| O | -3.059981 | 0.000279  | 0.000000  |
| C | 2.195829  | -0.000254 | 0.000001  |
| H | 3.279692  | -0.000407 | 0.000002  |

Zero point E (au)= -344.093523

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.099083

Enthalpy corrected E (au)= -344.086374

S (J/molK)= 340.92

$\Delta G$  solv (kJ/mol)= -12.34

### HF

E (au)= -342.687588

### MP2

E (au)= -343.868435

### MP4

E (au)= -343.963198

### MPWB1K

E (au)= -344.608200

### CCSD(t)

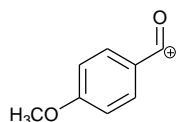
E (au)= -343.950244

Enthalpy correction (au)= 0.106183



S (J/molK)= 331.65

$\Delta G$  solv (kcal/mol)= -226.94



### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.446593 | 1.421470  | 0.000344  |
| C | 0.915026  | 1.296703  | 0.000411  |
| C | 1.490086  | -0.017035 | 0.001102  |
| C | -0.706211 | -1.034370 | 0.001213  |
| H | -0.921856 | 2.396280  | 0.000084  |
| H | 1.553101  | 2.173959  | 0.000060  |
| C | 2.851286  | -0.164070 | -0.000551 |
| O | 3.987440  | -0.288143 | -0.001931 |
| H | -1.334102 | -1.916610 | 0.002114  |
| C | -1.279553 | 0.266463  | 0.000318  |
| C | 0.659357  | -1.179559 | 0.001506  |
| H | 1.105748  | -2.168587 | 0.002672  |
| O | -2.572853 | 0.510405  | 0.000904  |
| C | -3.541441 | -0.564494 | -0.002239 |
| H | -4.509815 | -0.067941 | -0.011841 |
| H | -3.423860 | -1.176821 | -0.900462 |
| H | -3.437660 | -1.169019 | 0.902966  |

E (au)= -459.369225

ZPVE correction (au)= 0.132468

Enthalpy correction (au)= 0.142195

S (J/molK)= 385.43

$\Delta G$  solv (kJ/mol)= -209.116

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.442071  | 1.418089  | -0.000061 |
| C | -0.915877 | 1.292110  | 0.000021  |
| C | -1.489411 | -0.019112 | 0.000034  |
| C | 0.703042  | -1.031847 | -0.000219 |
| H | 0.916354  | 2.390979  | -0.000056 |
| H | -1.552869 | 2.167483  | 0.000129  |
| C | -2.846932 | -0.165546 | 0.000088  |
| O | -3.973441 | -0.285751 | 0.000138  |
| H | 1.329322  | -1.912571 | -0.000446 |
| C | 1.276155  | 0.266530  | -0.000091 |
| C | -0.659379 | -1.177942 | -0.000149 |
| H | -1.103073 | -2.165744 | -0.000243 |
| O | 2.565687  | 0.510126  | -0.000247 |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 3.540594 | -0.561939 | 0.000369  |
| H | 4.503723 | -0.060871 | 0.001079  |
| H | 3.432879 | -1.168266 | 0.901150  |
| H | 3.434123 | -1.168075 | -0.900696 |

Zero point E (au)= -458.469200

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.131600

Enthalpy corrected E(au)= -458.459414

S (J/molK)= 385.43

$\Delta G$  solv (kJ/mol)= -209.33

#### HF

E (au)= -456.620348

#### MP2

E (au)= -458.171075

#### MP4

E (au)= -458.293658

#### MPWB1K

E (au)= -459.131714

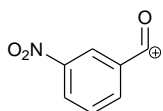
#### CCSD(t)

E (au)= -458.300823

Enthalpy correction (au)= 0.141319

S (J/molK)= 385.43

$\Delta G$  solv (kJ/mol)= -209.33



#### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.385201 | 2.162085  | 0.000046  |
| C | -1.570448 | 1.444259  | 0.000183  |
| C | -1.495189 | 0.021792  | 0.000006  |
| C | -0.259414 | -0.676327 | -0.000330 |
| C | 0.883949  | 0.095424  | 0.000034  |
| H | -0.412275 | 3.246593  | 0.000126  |
| H | -2.532047 | 1.946935  | 0.000129  |
| H | -0.191613 | -1.758873 | -0.000072 |
| C | -2.670416 | -0.716625 | -0.000059 |
| O | -3.631802 | -1.320796 | -0.000055 |
| C | 0.846753  | 1.492660  | 0.000021  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 1.784689 | 2.038698  | -0.000016 |
| N | 2.202033 | -0.599384 | 0.000375  |
| O | 3.191842 | 0.116188  | -0.000288 |
| O | 2.169561 | -1.822551 | 0.000069  |

E (au)= -549.33478

ZPVE correction (au)= 0.101596

Enthalpy correction (au)= 0.111213

S (J/molK)= 390.94

$\Delta G$  solv (kJ/mol)= -269.491

### CBS-QB3

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.394462 | 2.156854  | 0.000049  |
| C | -1.574396 | 1.436342  | 0.000031  |
| C | -1.495648 | 0.017458  | -0.000018 |
| C | -0.259908 | -0.674505 | -0.000043 |
| C | 0.878835  | 0.098945  | -0.000005 |
| H | -0.425116 | 3.239026  | 0.000080  |
| H | -2.535542 | 1.935378  | 0.000036  |
| H | -0.186472 | -1.755045 | -0.000068 |
| C | -2.665912 | -0.721990 | -0.000035 |
| O | -3.617680 | -1.322395 | -0.000014 |
| C | 0.837211  | 1.492692  | 0.000037  |
| H | 1.772795  | 2.039548  | 0.000062  |
| N | 2.206979  | -0.596156 | -0.000017 |
| O | 3.187420  | 0.119154  | 0.000040  |
| O | 2.176656  | -1.811832 | -0.000039 |

Zero point E (au)= -548.365584

Includes B3LYP/CBS-B7 ZPVE correction (au)= 0.101015

Enthalpy corrected E (au)= -548.349813

S (J/molK)= 390.94

$\Delta G$  solv (kcal/mol)= -269.28

### HF

E (au)= -546.194078

### MP2

E (au)= -547.997598

### MP4

E (au)= -548.118916

### MPWB1K

E (au)= -549.065983

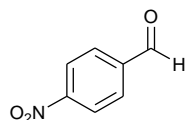
### CCSD(t)

E (au)= -548.114889

Enthalpy correction (au)= 0.110643

S (J/molK)= 390.94

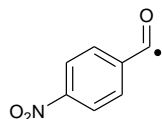
$\Delta G$  solv (kcal/mol)= -269.28



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.473899  | 1.280234  | 0.000148  |
| C | -0.914875 | 1.376775  | 0.000110  |
| C | -1.705054 | 0.220079  | 0.000056  |
| C | -1.101063 | -1.046788 | 0.000024  |
| C | 0.283279  | -1.159263 | 0.000044  |
| H | 1.111715  | 2.155210  | 0.000288  |
| H | -1.389438 | 2.355010  | 0.000151  |
| H | -1.735829 | -1.926989 | 0.000044  |
| C | -3.187037 | 0.336840  | -0.000099 |
| O | -3.945339 | -0.611238 | -0.000097 |
| C | 1.046337  | 0.010102  | 0.000047  |
| H | 0.780908  | -2.121085 | 0.000028  |
| H | -3.572830 | 1.379261  | -0.000138 |
| N | 2.518647  | -0.102797 | -0.000032 |
| O | 3.168992  | 0.940892  | -0.000246 |
| O | 3.001601  | -1.233366 | 0.000076  |

E (au)= -549.9723805

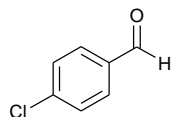
ZPVE correction (au)= 0.112667



|   |           |           |          |
|---|-----------|-----------|----------|
| C | 1.280086  | 0.454039  | 0.000000 |
| C | 1.403196  | -0.932652 | 0.000000 |
| C | 0.258518  | -1.739499 | 0.000000 |
| C | -1.022291 | -1.160026 | 0.000000 |
| C | -1.156977 | 0.222987  | 0.000000 |
| H | 2.143451  | 1.107435  | 0.000000 |
| H | 2.382635  | -1.400736 | 0.000000 |
| H | -1.895819 | -1.804196 | 0.000000 |
| C | 0.419844  | -3.219452 | 0.000000 |
| O | -0.442055 | -4.043808 | 0.000000 |
| C | 0.000000  | 1.003613  | 0.000000 |
| H | -2.126981 | 0.704874  | 0.000000 |
| N | -0.139292 | 2.475437  | 0.000000 |
| O | 0.892630  | 3.143114  | 0.000000 |
| O | -1.278388 | 2.937007  | 0.000000 |

E (au)= -549.3181748

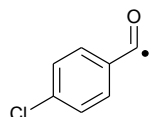
ZPVE correction (au)= 0.100111



|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.748730 | 1.259663  | -0.000010 |
| C  | 0.640305  | 1.363369  | -0.000002 |
| C  | 1.441373  | 0.214939  | 0.000076  |
| C  | 0.838255  | -1.052110 | 0.000094  |
| C  | -0.545735 | -1.171689 | 0.000077  |
| H  | -1.377240 | 2.143482  | -0.000014 |
| H  | 1.106873  | 2.346046  | -0.000039 |
| H  | 1.475051  | -1.931411 | 0.000139  |
| C  | 2.916248  | 0.339269  | 0.000023  |
| O  | 3.687766  | -0.600441 | -0.000178 |
| C  | -1.326657 | -0.010670 | 0.000024  |
| H  | -1.023784 | -2.145389 | 0.000049  |
| Cl | -3.074518 | -0.155992 | -0.000049 |
| H  | 3.293434  | 1.386040  | 0.000430  |

E (au)= -805.1725207

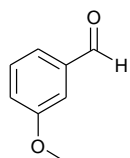
ZPVE correction (au)= 0.100529



|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.713893  | 1.263458  | 0.000113  |
| C  | -0.673858 | 1.377822  | -0.000091 |
| C  | -1.479108 | 0.232137  | 0.000319  |
| C  | -0.884844 | -1.041991 | 0.000133  |
| C  | 0.499226  | -1.167490 | -0.000035 |
| H  | 1.347940  | 2.143321  | 0.000285  |
| H  | -1.144674 | 2.356511  | -0.000128 |
| H  | -1.520409 | -1.922368 | 0.000177  |
| C  | -2.952323 | 0.382440  | -0.000207 |
| O  | -3.779058 | -0.480263 | -0.000085 |
| C  | 1.285049  | -0.010273 | 0.000051  |
| H  | 0.972189  | -2.143813 | 0.000001  |
| Cl | 3.031129  | -0.165187 | -0.000080 |

E (au)= -804.5191749

ZPVE correction (au)= 0.088092

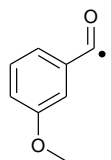


|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.442515 | 0.032226  | 0.378261  |
| C | 0.948596  | 0.118641  | 0.512133  |
| C | 1.585889  | 1.347528  | 0.293948  |
| C | 0.840230  | 2.473892  | -0.053431 |
| C | -0.556001 | 2.390027  | -0.188486 |
| C | -1.181947 | 1.170937  | 0.028676  |
| H | -0.958246 | -0.907241 | 0.542013  |
| H | 2.666189  | 1.402679  | 0.400664  |
| H | -1.112382 | 3.280968  | -0.459556 |
| H | -2.260748 | 1.086716  | -0.071109 |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 1.539036 | 3.760890  | -0.278432 |
| O | 0.991046 | 4.802394  | -0.583877 |
| H | 2.643240 | 3.717196  | -0.145785 |
| O | 1.765645 | -0.920421 | 0.846916  |
| C | 1.178259 | -2.191567 | 1.080393  |
| H | 0.663096 | -2.568141 | 0.186900  |
| H | 2.003880 | -2.860430 | 1.329069  |
| H | 0.471014 | -2.161060 | 1.919646  |

E (au)= -459.9989795

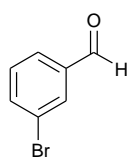
ZPVE correction (au)= 0.143022



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.475554 | 0.059965  | 0.471704  |
| C | 0.922736  | 0.148246  | 0.386641  |
| C | 1.516841  | 1.358009  | 0.011808  |
| C | 0.714076  | 2.467583  | -0.274490 |
| C | -0.683604 | 2.382994  | -0.190553 |
| C | -1.266227 | 1.176819  | 0.182712  |
| H | -0.953982 | -0.868959 | 0.760647  |
| H | 2.597474  | 1.428836  | -0.054715 |
| H | -1.285809 | 3.256967  | -0.417418 |
| H | -2.346943 | 1.091791  | 0.253337  |
| C | 1.334882  | 3.755134  | -0.672841 |
| O | 2.495863  | 4.008831  | -0.795813 |
| O | 1.780047  | -0.878489 | 0.646904  |
| C | 1.237161  | -2.133002 | 1.031439  |
| H | 0.592893  | -2.551254 | 0.246920  |
| H | 2.092580  | -2.792830 | 1.184931  |
| H | 0.666320  | -2.056091 | 1.966175  |

E (au)= -459.3472336

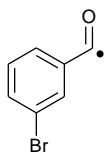
ZPVE correction (au)= 0.13052



|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.566205 | 0.236248  | 0.000078  |
| C  | 0.477690  | -0.684007 | 0.000275  |
| C  | 1.798420  | -0.218978 | 0.000210  |
| C  | 2.063594  | 1.158091  | 0.000078  |
| C  | 1.008000  | 2.063498  | 0.000037  |
| C  | -0.314964 | 1.607975  | 0.000004  |
| H  | 0.270313  | -1.750236 | 0.000276  |
| H  | 3.097417  | 1.488189  | -0.000054 |
| H  | 1.202463  | 3.132179  | -0.000121 |
| H  | -1.142224 | 2.309690  | -0.000126 |
| C  | 2.914245  | -1.196578 | 0.000107  |
| O  | 4.091144  | -0.894674 | -0.000386 |
| H  | 2.598072  | -2.262918 | 0.000610  |
| Br | -2.372568 | -0.387343 | -0.000064 |

E (au)= -2919.367031

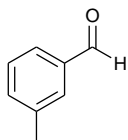
ZPVE correction (au)= 0.100135



|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.453013 | 0.300135  | 0.000092  |
| C  | 0.657241  | -0.532901 | 0.000688  |
| C  | 1.937783  | 0.047069  | 0.000294  |
| C  | 2.090488  | 1.437863  | -0.000284 |
| C  | 0.961686  | 2.256141  | 0.000295  |
| C  | -0.314559 | 1.691342  | 0.000068  |
| H  | 0.554688  | -1.612475 | 0.001240  |
| H  | 3.090600  | 1.860292  | -0.001140 |
| H  | 1.068119  | 3.336904  | -0.000038 |
| H  | -1.198057 | 2.320629  | -0.000394 |
| C  | 3.145630  | -0.815704 | -0.000391 |
| O  | 3.197344  | -2.008111 | -0.000081 |
| Br | -2.207018 | -0.461261 | -0.000103 |

E (au)= -2918.713799

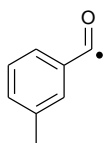
ZPVE correction (au)= 0.087662



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.376564  | -0.499101 | -0.000110 |
| C | 0.011116  | -0.779339 | -0.000078 |
| C | -0.939022 | 0.253861  | 0.000050  |
| C | -0.521523 | 1.588903  | 0.000136  |
| C | 0.841593  | 1.884448  | 0.000001  |
| C | 1.776125  | 0.849726  | -0.000162 |
| H | -0.347571 | -1.805032 | -0.000203 |
| H | -1.261051 | 2.386837  | 0.000221  |
| H | 1.177247  | 2.917835  | -0.000048 |
| H | 2.837746  | 1.088414  | -0.000352 |
| C | -2.384325 | -0.064294 | 0.000045  |
| O | -2.849600 | -1.188309 | -0.000088 |
| H | -3.053055 | 0.825834  | 0.000188  |
| C | 2.406272  | -1.605066 | 0.000134  |
| H | 3.054888  | -1.546308 | 0.882915  |
| H | 1.931300  | -2.590558 | -0.000740 |
| H | 3.056499  | -1.545372 | -0.881365 |

E (au)= -384.7982028

ZPVE correction (au)= 0.137739

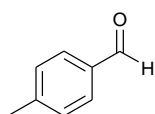


|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.331668  | -0.512020 | -0.000091 |
| C | -0.037269 | -0.777745 | -0.000074 |
| C | -0.974379 | 0.270934  | 0.000013  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.544331 | 1.601696  | 0.000068  |
| C | 0.822413  | 1.878446  | 0.000011  |
| C | 1.744570  | 0.832356  | -0.000082 |
| H | -0.401824 | -1.801525 | -0.000145 |
| H | -1.281559 | 2.399149  | 0.000117  |
| H | 1.171038  | 2.907372  | 0.000006  |
| H | 2.808843  | 1.058766  | -0.000165 |
| C | -2.427394 | -0.018187 | 0.000058  |
| O | -2.968086 | -1.084425 | -0.000033 |
| C | 2.349161  | -1.629494 | 0.000083  |
| H | 2.997190  | -1.578445 | 0.883651  |
| H | 1.863913  | -2.610012 | -0.002213 |
| H | 3.000454  | -1.575825 | -0.880901 |

E (au)= -384.145246

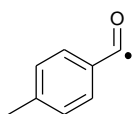
ZPVE correction (au)= 0.125342



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.755208 | -0.064247 | -0.000079 |
| C | -0.917784 | -1.195372 | -0.000090 |
| C | 0.463221  | -1.062608 | -0.000035 |
| C | 1.047478  | 0.214663  | 0.000005  |
| C | 0.223262  | 1.345328  | -0.000020 |
| C | -1.163473 | 1.205262  | -0.000072 |
| H | 1.114909  | -1.931203 | -0.000053 |
| H | 0.671286  | 2.337095  | -0.000027 |
| H | -1.795968 | 2.089565  | -0.000121 |
| C | 2.517040  | 0.368584  | 0.000043  |
| O | 3.313294  | -0.551726 | 0.000055  |
| H | 2.870934  | 1.424347  | 0.000068  |
| H | -1.364152 | -2.187397 | -0.000156 |
| C | -3.256015 | -0.226624 | 0.000112  |
| H | -3.594508 | -0.782755 | 0.883086  |
| H | -3.765677 | 0.741535  | -0.002369 |
| H | -3.594309 | -0.787284 | -0.880043 |

E (au)= -384.7990357

ZPVE correction (au)= 0.137702

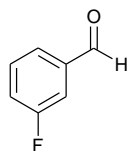


|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.713481 | -0.067495 | -0.000768 |
| C | -0.869100 | -1.193061 | -0.000841 |
| C | 0.511397  | -1.050991 | -0.000304 |
| C | 1.083867  | 0.234561  | 0.000083  |
| C | 0.253208  | 1.360420  | -0.000152 |
| C | -1.131672 | 1.206948  | -0.000674 |
| H | 1.164605  | -1.918670 | -0.000452 |
| H | 0.703258  | 2.349175  | -0.000188 |
| H | -1.771475 | 2.085795  | -0.001088 |
| C | 2.551483  | 0.414497  | 0.000448  |
| O | 3.399750  | -0.428670 | 0.000499  |
| H | -1.308183 | -2.188459 | -0.001457 |
| C | -3.212930 | -0.241113 | 0.001023  |
| H | -3.547609 | -0.781003 | 0.895484  |
| H | -3.729648 | 0.722884  | -0.021924 |



H -3.545585 -0.822957 -0.867260  
E (au)= -384.1479025

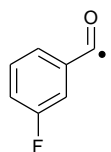
ZPVE correction (au)= 0.125282



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.547839  | -0.394868 | -0.000325 |
| C | 0.295315  | -0.993245 | 0.000092  |
| C | -0.840685 | -0.174081 | 0.000068  |
| C | -0.707274 | 1.222424  | 0.000052  |
| C | 0.560995  | 1.795569  | 0.000146  |
| C | 1.702731  | 0.987539  | -0.000175 |
| H | 0.211981  | -2.076483 | 0.000130  |
| H | -1.606249 | 1.829983  | 0.000078  |
| H | 0.672205  | 2.875970  | 0.000169  |
| H | 2.702049  | 1.410596  | -0.000091 |
| C | -2.186416 | -0.797339 | -0.000089 |
| O | -3.232175 | -0.178443 | -0.000037 |
| F | 2.647211  | -1.175404 | 0.000135  |
| H | -2.182524 | -1.909891 | 0.000182  |

E (au)= -444.738588

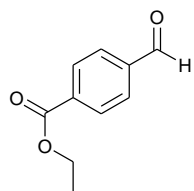
ZPVE correction (au)= 0.101933



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.291205 | -0.620410 | 0.000051  |
| C | 0.078895  | -0.824160 | -0.000099 |
| C | 0.918064  | 0.303100  | 0.000100  |
| C | 0.378721  | 1.595148  | 0.000089  |
| C | -1.005665 | 1.767435  | -0.000157 |
| C | -1.850630 | 0.657045  | 0.000095  |
| H | 0.494207  | -1.826179 | 0.000046  |
| H | 1.050166  | 2.448019  | -0.000036 |
| H | -1.432182 | 2.765998  | -0.000055 |
| H | -2.930787 | 0.761969  | 0.000228  |
| C | 2.392780  | 0.136047  | -0.000127 |
| O | 3.016539  | -0.882089 | 0.000060  |
| F | -2.115498 | -1.686479 | -0.000041 |

E (au)= -444.085295

ZPVE correction (au)= 0.089503

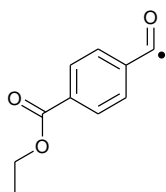


|   |          |           |           |
|---|----------|-----------|-----------|
| C | 0.371485 | -0.854410 | -0.000261 |
|---|----------|-----------|-----------|

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.743632  | -1.069953 | -0.000201 |
| C | 2.626439  | 0.020709  | 0.000053  |
| C | 2.121736  | 1.327949  | 0.000182  |
| C | 0.748172  | 1.547278  | 0.000094  |
| C | -0.131818 | 0.457027  | -0.000145 |
| H | -0.318437 | -1.690444 | -0.000372 |
| H | 2.157389  | -2.073580 | -0.000254 |
| H | 2.810177  | 2.170273  | 0.000439  |
| H | 0.334729  | 2.550128  | 0.000270  |
| C | 4.092037  | -0.204463 | 0.000051  |
| O | 4.621426  | -1.298652 | 0.000070  |
| H | 4.704222  | 0.724438  | 0.000140  |
| C | -1.598033 | 0.750241  | -0.000127 |
| O | -2.067327 | 1.871536  | -0.000347 |
| O | -2.347357 | -0.371533 | 0.000213  |
| C | -3.780941 | -0.173267 | 0.000285  |
| C | -4.431190 | -1.543417 | 0.000009  |
| H | -4.052580 | 0.413720  | -0.882793 |
| H | -4.052538 | 0.413354  | 0.883633  |
| H | -5.521164 | -1.435189 | 0.000027  |
| H | -4.142417 | -2.114652 | -0.888096 |
| H | -4.142437 | -2.115021 | 0.887879  |

E (au)= -361.885202

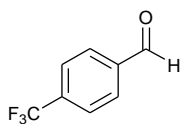
ZPVE correction (au)= 0.112128



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.416097 | -0.853604 | -0.000055 |
| C | -1.788783 | -1.069125 | -0.000056 |
| C | -2.668943 | 0.026931  | 0.000014  |
| C | -2.166076 | 1.334349  | 0.000085  |
| C | -0.791798 | 1.549210  | 0.000086  |
| C | 0.086463  | 0.457612  | 0.000013  |
| H | 0.273399  | -1.690180 | -0.000097 |
| H | -2.197659 | -2.074918 | -0.000108 |
| H | -2.861209 | 2.168698  | 0.000139  |
| H | -0.376679 | 2.551299  | 0.000132  |
| C | -4.139106 | -0.182648 | -0.000002 |
| O | -4.730822 | -1.220059 | -0.000016 |
| C | 1.554181  | 0.748813  | -0.000020 |
| O | 2.023582  | 1.869690  | -0.000077 |
| O | 2.301175  | -0.373865 | -0.000003 |
| C | 3.735731  | -0.178059 | -0.000116 |
| C | 4.383423  | -1.549268 | 0.000152  |
| H | 4.007704  | 0.408548  | 0.883047  |
| H | 4.007615  | 0.408146  | -0.883577 |
| H | 5.473548  | -1.442694 | -0.000269 |
| H | 4.094227  | -2.119851 | 0.888542  |
| H | 4.093611  | -2.120446 | -0.887656 |

E (au)= -361.249842

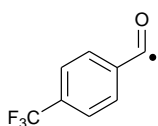
ZPVE correction (au)= 0.085734



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.713791  | 0.036780  | -0.038701 |
| C | 0.103612  | 1.293612  | -0.027661 |
| C | -1.286455 | 1.380196  | -0.010093 |
| C | -2.066158 | 0.217718  | -0.003067 |
| C | -1.445839 | -1.040312 | -0.015870 |
| C | -0.060009 | -1.131194 | -0.033628 |
| H | 0.712070  | 2.191465  | -0.039174 |
| H | -1.770889 | 2.353960  | -0.004679 |
| H | -2.069402 | -1.928743 | -0.014402 |
| H | 0.428187  | -2.099932 | -0.051148 |
| C | 2.217115  | -0.069223 | 0.002341  |
| F | 2.658569  | -1.163949 | -0.653904 |
| F | 2.668802  | -0.161619 | 1.273733  |
| F | 2.813289  | 1.007947  | -0.552516 |
| C | -3.546436 | 0.319802  | 0.014322  |
| H | -3.940408 | 1.359906  | 0.023123  |
| O | -4.300402 | -0.632792 | 0.019326  |

E (au)= -682.551575

ZPVE correction (au)= 0.114905



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.672185  | 0.039408  | -0.038454 |
| C | 0.068670  | 1.299684  | -0.027288 |
| C | -1.320553 | 1.395966  | -0.009266 |
| C | -2.103032 | 0.235691  | -0.002545 |
| C | -1.491363 | -1.029241 | -0.015723 |
| C | -0.105298 | -1.125532 | -0.033530 |
| H | 0.682166  | 2.194028  | -0.039099 |
| H | -1.810028 | 2.365166  | -0.002922 |
| H | -2.113846 | -1.918600 | -0.014623 |
| H | 0.378629  | -2.096535 | -0.051138 |
| C | 2.175895  | -0.073560 | 0.002090  |
| F | 2.610583  | -1.177132 | -0.643100 |
| F | 2.626442  | -0.154932 | 1.274305  |
| F | 2.775620  | 0.994733  | -0.564245 |
| C | -3.583388 | 0.361995  | 0.015950  |
| O | -4.391179 | -0.516817 | 0.019716  |

E (au)= -681.897897

ZPVE correction (au)= 0.102442