

# **Theoretical mechanistic insights on the thermal and acid-catalyzed rearrangements of *N*-methyl-*N*-nitroanilines**

Shi Cheng, Chongjie Su, Tian Chen, and Jiaxi Xu\*

*State Key Laboratory of Chemical Resource Engineering, Department of Organic Chemistry, College of Chemistry, Beijing University of Chemical Technology, Beijing 100029, China. E-mail: jxxu@mail.buct.edu.cn.*

## **Electronic Supporting Information**

### **Contents**

|                                                                           |            |
|---------------------------------------------------------------------------|------------|
| <b>1. Details of Calculations .....</b>                                   | <b>S2</b>  |
| <b>2. Coordinates of All Stationary Points.....</b>                       | <b>S4</b>  |
| <b>3. Source Data of Distances of Key Bonds in Transition States.....</b> | <b>S37</b> |
| <b>4. Computed Energies and Charges .....</b>                             | <b>S40</b> |

## 1. Details of Calculations

All calculations were performed with the Gaussian 09,<sup>1</sup> ORCA 5.0.3,<sup>2</sup> and Multiwfn<sup>3</sup> programs. Density functional theory (DFT) calculations using the B3LYP-D3(BJ) theoretical method were used to locate all the stationary points involved.<sup>18</sup> Structural optimizations were obtained at the B3LYP-D3(BJ)/def2-tzvp level under the PCM solution model which computed by a self-consistent reaction field (SCRF) in Gaussian 09, while frequency calculations are under the same level and the substrates, intermediates, and products were characterized by no imaginary vibrational mode, but transition states characterized by only one.<sup>5</sup> Intrinsic reaction coordinate (IRC) calculations for typical transition states were performed, helping to confirm the transition states.<sup>6</sup> The single point energies ( $E_{\text{gas}}$ ) can be obtained at a high level DLPNO-CCSD(T)/cc-pVTZ by using the ORCA 5.0.3 program,<sup>7</sup> and the ORCA 5.0.3 input files are created by the Multiwfn<sup>3</sup> program. The contribution of vibration to entropy was calculated using a quasi-rigid-rotor-harmonic-oscillator (quasi-RRHO) approximation, which uses the Grimme method implemented<sup>8</sup> in the Shermo program,<sup>9</sup> switching to a free rotor description of vibrational modes below 100 cm<sup>-1</sup>. The relative Gibbs free energies were corrected with quasi-RRHO and the scale factor of 0.985 was employed for ZPE.<sup>10</sup> We described the solvation free energies under M05-2X/6-31G\* with the SMD model.<sup>11</sup>  $G_{\text{SMD}}$  and  $G_{\text{gas}}$  were obtained using the Gaussian 09 program and combined for  $G_{\text{solv}}$ . After calculations of above all, the Gibbs free energies in solution were computed in this formula according to Junming Ho's work:<sup>12</sup>

$$\begin{aligned}\Delta G_{\text{solv}} &= G_{\text{gas}} + G_{\text{solv}} + RT\ln(RT/p) \\ G_{\text{gas}} &= E_{\text{gas}} + \Delta G_{\text{corr}} \\ G_{\text{solv}} &= G_{\text{SMD}} - G_{\text{gas}}(\text{M05-2X/6-31G*})\end{aligned}$$

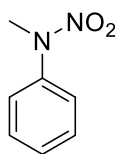
All wavefunctions analysis including atomic charges described by the atomic dipole moment corrected Hirshfeld (ADCH) method<sup>13</sup> and Mulliken Population analysis<sup>3</sup> are calculated using the Multiwfn<sup>3</sup> program. All presented structures were visualized by CYLview20 programs.<sup>14</sup>

## References

- 1 Gaussian 09, Revision B.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford, CT, 2009.

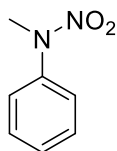
- 2 (a) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73–78. (b) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2017, **8**, e1327. (c) F. Neese, F. Wennmohs, U. Becker and C. Riplinger, *J. Chem. Phys.*, 2020, **152**, 224108. (d) T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007–1023.
- 3 (a) T. Lu and F. W. Chen, *J. Comput. Chem.*, 2012, **33**, 580. (b) T. Lu, *J. Chem. Phys.*, 2024, **161**, 082503.
- 4 (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785–789. (c) S. Grimme, J. Antony, S. Ehrlich and K. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104. (d) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.
- 5 (a) S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117–129. (b) S. Miertuš and J. Tomasi, *Chem. Phys.*, 1982, **65**, 239–245. (c) J. L. Pascual-Ahuir, E. Silla and I. Tuñón, *J. Comp. Chem.*, 1994, **15**, 1127–1138. (d) F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057–1065.
- 6 (a) K. J. Fukui, *Phys. Chem.*, 1970, **74**, 4161–4163. (b) K. Ishida, K. Morokuma and A. Komornicki, *J. Chem. Phys.*, 1977, **66**, 2153–2156.
- 7 (a) Y. Guo, C. Riplinger, U. Becker, D. E. Liakos, Y. Minenkov, L. Cavallo and F. Neese, *J. Chem. Phys.*, 2018, **148**, 011101. (b) J. Thom and H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007–1023.
- 8 G. Stefan, *Chem-Eur J.*, 2012, **18**, 9955–9984.
- 9 T. Lu and Q. X. Chen, *Comput. Theor. Chem.*, 2021, **1200**, 113249.
- 10 J. L. Bao, J. Zheng, I. M. Alecu, B. J. Lynch, Y. Zhao and D. G. Truhlar, Database of Frequency Scale Factors for Electronic Model Chemistries (Version 3 Beta 2). <https://comp.chem.umn.edu/freqscale/version3b2.htm>.
- 11 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.
- 12 J. Ho, A. Klamt and M. L. Coote, *J. Phys. Chem. A*, 2010, **114**, 13442–13444.
- 13 T. Lu and F. W. Chen, *J. Theor. Comput. Chem.*, 2012, **11**, 163–183.
- 14 C. Y. Legault, CYLview20, Université de Sherbrooke, 2020 (<http://www.cylview.org>).

## 2. Coordinates of All Stationary Points



**1a (Thermal)**

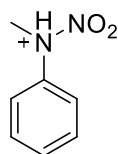
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.00081000  | 0.30558300  | 1.13094600  |
| C | 2.37330700  | 0.09550400  | 1.18435600  |
| C | 3.07957100  | -0.19366900 | 0.02330500  |
| C | 2.41226800  | -0.26561000 | -1.19561000 |
| C | 1.04440300  | -0.04319700 | -1.25815200 |
| C | 0.34166900  | 0.23747800  | -0.09151500 |
| N | -1.05855700 | 0.51160500  | -0.14421200 |
| C | -1.63286700 | 1.73153300  | 0.40578600  |
| N | -1.92715600 | -0.49835600 | -0.45066200 |
| O | -3.12276400 | -0.23951300 | -0.35342400 |
| O | -1.46037500 | -1.57172100 | -0.80879800 |
| H | 0.44297900  | 0.51782800  | 2.03326400  |
| H | 2.88651100  | 0.14943100  | 2.13523700  |
| H | 4.14736000  | -0.36261300 | 0.06675400  |
| H | 2.95935300  | -0.48898800 | -2.10183700 |
| H | 0.51768400  | -0.09350100 | -2.20040500 |
| H | -0.81629700 | 2.43640400  | 0.53016500  |
| H | -2.36662700 | 2.14248800  | -0.28411400 |
| H | -2.11711600 | 1.55173700  | 1.36689500  |



**1a (Acid)**

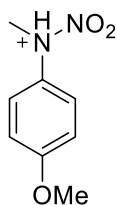
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.07549400 | 1.07766900  | -0.59847500 |
| C | -2.45186700 | 0.92673500  | -0.71457400 |
| C | -3.08914900 | -0.14594000 | -0.10338400 |
| C | -2.34839200 | -1.06594400 | 0.63216400  |
| C | -0.97591800 | -0.91345700 | 0.76387100  |
| C | -0.34242900 | 0.15742400  | 0.14280500  |
| N | 1.06249800  | 0.35340900  | 0.30382000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.62122700  | 1.61172200  | 0.77798000  |
| N | 1.93223600  | -0.53105900 | -0.27316200 |
| O | 3.12274700  | -0.23916900 | -0.22080200 |
| O | 1.47118900  | -1.54415500 | -0.78154300 |
| H | -0.57183700 | 1.90321900  | -1.08343600 |
| H | -3.02223600 | 1.64330400  | -1.29049900 |
| H | -4.16016900 | -0.26579600 | -0.19905800 |
| H | -2.84148900 | -1.90155900 | 1.11076900  |
| H | -0.39257500 | -1.62086000 | 1.33569800  |
| H | 0.81286500  | 2.15485600  | 1.25833900  |
| H | 2.41087100  | 1.41980300  | 1.50095200  |
| H | 2.03200600  | 2.20537100  | -0.04032600 |



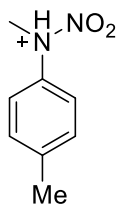
**1aH**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.14974400 | -0.48191600 | -1.22687700 |
| C | -2.47491900 | -0.74253400 | -0.92936900 |
| C | -3.03932100 | -0.22214800 | 0.23157000  |
| C | -2.27866100 | 0.56105700  | 1.09795100  |
| C | -0.95374600 | 0.83351300  | 0.81188700  |
| C | -0.39683200 | 0.31668200  | -0.36076500 |
| N | 0.95702300  | 0.54065900  | -0.68377300 |
| C | 1.64025100  | 1.79408300  | -0.31197300 |
| N | 1.98521200  | -0.84870100 | 0.10265300  |
| O | 3.14119300  | -0.64370400 | 0.02021300  |
| O | 1.28151800  | -1.67711000 | 0.54012900  |
| H | -0.70020700 | -0.88527400 | -2.12622200 |
| H | -3.06687800 | -1.34990200 | -1.59900400 |
| H | -4.07499000 | -0.42785200 | 0.46456800  |
| H | -2.72182600 | 0.95882000  | 1.99985100  |
| H | -0.37032300 | 1.43769700  | 1.49013900  |
| H | 1.14797400  | 2.61703300  | -0.82826700 |
| H | 1.59131400  | 1.94481100  | 0.76121100  |
| H | 2.67531200  | 1.72502900  | -0.63160700 |
| H | 1.14583700  | 0.30652800  | -1.65743200 |



**1bH**

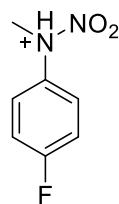
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.04645700  | -0.65215200 | 1.15437000  |
| C | 2.36249700  | -0.93931000 | 0.87922500  |
| C | 3.01386300  | -0.25621400 | -0.16266500 |
| C | 2.31398300  | 0.71116700  | -0.91386500 |
| C | 1.00414400  | 0.99351900  | -0.63630000 |
| C | 0.35487500  | 0.32131500  | 0.41688100  |
| N | -0.98013300 | 0.54194400  | 0.71329700  |
| C | -1.65594500 | 1.81939800  | 0.43597100  |
| N | -2.02906600 | -0.77728500 | -0.32526500 |
| O | -3.20208500 | -0.64189100 | -0.25137300 |
| O | -1.29274400 | -1.51588100 | -0.87350900 |
| H | 0.54058400  | -1.17881900 | 1.95426700  |
| H | 2.87951500  | -1.68403300 | 1.46336000  |
| H | 2.83664100  | 1.21915800  | -1.71158100 |
| H | 0.48563300  | 1.73312300  | -1.22746500 |
| H | -1.23711700 | 2.58713600  | 1.08564900  |
| H | -1.51876800 | 2.09799400  | -0.60340900 |
| H | -2.71436300 | 1.69619200  | 0.64503900  |
| H | -1.24264100 | 0.16861000  | 1.62201200  |
| O | 4.27810600  | -0.45243000 | -0.51245000 |
| C | 5.07238700  | -1.42210000 | 0.18787300  |
| H | 6.05075200  | -1.38447600 | -0.27902900 |
| H | 5.15286400  | -1.15936400 | 1.24310500  |
| H | 4.64421100  | -2.41834400 | 0.07445100  |



**1cH**

|   |            |             |            |
|---|------------|-------------|------------|
| C | 1.11305600 | -0.65541100 | 1.08063200 |
|---|------------|-------------|------------|

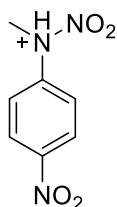
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.43271300  | -0.89326100 | 0.76130300  |
| C | 3.06180200  | -0.18626100 | -0.27023600 |
| C | 2.32008000  | 0.77638100  | -0.96931000 |
| C | 0.99897500  | 1.02842600  | -0.66489200 |
| C | 0.39185600  | 0.31565300  | 0.37529100  |
| N | -0.95763400 | 0.49875900  | 0.70258900  |
| C | -1.64972100 | 1.78142000  | 0.48071900  |
| N | -1.97016100 | -0.79535200 | -0.30930300 |
| O | -3.13514900 | -0.66876500 | -0.18041400 |
| O | -1.24019200 | -1.50690700 | -0.89065100 |
| H | 0.63689900  | -1.21414300 | 1.87681800  |
| H | 2.98816900  | -1.63734300 | 1.31574900  |
| H | 2.79288400  | 1.33472500  | -1.76602300 |
| H | 0.45448600  | 1.77267300  | -1.22632700 |
| H | -1.21129000 | 2.53097100  | 1.13846700  |
| H | -1.54786600 | 2.08854600  | -0.55448900 |
| H | -2.69956900 | 1.64898800  | 0.72523500  |
| H | -1.17849600 | 0.12211000  | 1.62297800  |
| C | 4.48333200  | -0.47133100 | -0.63841000 |
| H | 4.51864400  | -1.24264300 | -1.41373400 |
| H | 4.97651900  | 0.41398300  | -1.03776500 |
| H | 5.05015200  | -0.83999800 | 0.21540900  |



**1dH**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.11394000  | -0.66735000 | 1.07978400  |
| C | 2.43092000  | -0.92127700 | 0.75995700  |
| C | 3.00556200  | -0.20591200 | -0.28256700 |
| C | 2.30679000  | 0.75127700  | -1.00984500 |
| C | 0.99049400  | 1.00413500  | -0.68528500 |
| C | 0.39420200  | 0.30164900  | 0.36895300  |
| N | -0.95603700 | 0.49223900  | 0.70152900  |
| C | -1.63273900 | 1.78685400  | 0.49420100  |
| N | -1.97804100 | -0.77856900 | -0.31411000 |

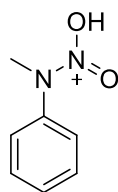
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.13853700 | -0.63561500 | -0.17776000 |
| O | -1.25615500 | -1.49172700 | -0.90152900 |
| H | 0.64076500  | -1.21725500 | 1.88325700  |
| H | 3.01278900  | -1.65687300 | 1.29582200  |
| H | 2.79884100  | 1.27792000  | -1.81467000 |
| H | 0.44069800  | 1.74168400  | -1.24981800 |
| H | -1.17368700 | 2.52659700  | 1.14909400  |
| H | -1.54123900 | 2.09655600  | -0.54135700 |
| H | -2.68104900 | 1.66844000  | 0.75199400  |
| H | -1.17461600 | 0.11516000  | 1.62269800  |
| F | 4.27411300  | -0.44620900 | -0.59979600 |



**1eH**

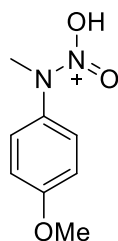
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.12102900  | -0.65005100 | 1.09631200  |
| C | 2.44702300  | -0.88678200 | 0.78429000  |
| C | 3.01013100  | -0.18951200 | -0.27228200 |
| C | 2.29914400  | 0.73500000  | -1.02391900 |
| C | 0.97337800  | 0.97223400  | -0.71258000 |
| C | 0.39397200  | 0.28209800  | 0.35358700  |
| N | -0.97171200 | 0.46208200  | 0.68133200  |
| C | -1.62721800 | 1.77609500  | 0.52915900  |
| N | -1.97730200 | -0.75345200 | -0.35854000 |
| O | -3.12597800 | -0.52917800 | -0.28177400 |
| O | -1.26532400 | -1.51498400 | -0.88770200 |
| H | 0.65808600  | -1.17925300 | 1.91939100  |
| H | 3.03871200  | -1.59595700 | 1.34187600  |
| H | 2.78315900  | 1.25222400  | -1.83764500 |
| H | 0.41105800  | 1.68412600  | -1.29682500 |
| H | -1.14672700 | 2.47848100  | 1.20877800  |
| H | -1.53636700 | 2.12256300  | -0.49453200 |
| H | -2.67473300 | 1.66845500  | 0.79385000  |
| H | -1.18201100 | 0.05849200  | 1.59363000  |
| N | 4.43004600  | -0.44405400 | -0.61616600 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 4.89483100 | 0.17876900  | -1.55295000 |
| O | 5.02830000 | -1.25855700 | 0.06202100  |



**1aH'**

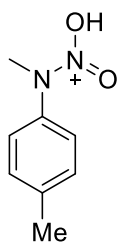
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.01766500 | 0.11663500  | -1.21744000 |
| C | -2.39299200 | -0.07231600 | -1.20766300 |
| C | -3.07601100 | -0.16732600 | 0.00000200  |
| C | -2.39298900 | -0.07229800 | 1.20766400  |
| C | -1.01766300 | 0.11665300  | 1.21743600  |
| C | -0.35845400 | 0.20211100  | -0.00000400 |
| N | 1.06926400  | 0.44410000  | -0.00000700 |
| C | 1.65690000  | 1.79171000  | -0.00001800 |
| N | 1.91150200  | -0.53925900 | 0.00000300  |
| O | 3.10150000  | -0.42173500 | 0.00000700  |
| O | 1.32488300  | -1.75692700 | 0.00001900  |
| H | -0.47195700 | 0.19415200  | -2.14770800 |
| H | -2.92814900 | -0.14472900 | -2.14404100 |
| H | -4.14723700 | -0.31463200 | 0.00000400  |
| H | -2.92814400 | -0.14469900 | 2.14404400  |
| H | -0.47195200 | 0.19418300  | 2.14770100  |
| H | 0.82481000  | 2.48566200  | -0.00002300 |
| H | 2.27075200  | 1.92244000  | 0.89037100  |
| H | 2.27075200  | 1.92242700  | -0.89040800 |
| H | 2.07414100  | -2.38749900 | 0.00002900  |



**1bH'**

|   |            |            |            |
|---|------------|------------|------------|
| C | 0.08584200 | 0.33418000 | 1.20840400 |
|---|------------|------------|------------|

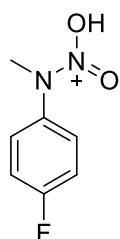
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.44948900  | 0.23888700  | 1.36152900  |
| C | 2.27913000  | 0.03451200  | 0.24716100  |
| C | 1.71547200  | -0.06418900 | -1.03076000 |
| C | 0.34326300  | 0.03672700  | -1.18513900 |
| C | -0.46257800 | 0.22505100  | -0.07027300 |
| N | -1.87409000 | 0.37498000  | -0.27462000 |
| C | -2.45044800 | 1.42005100  | -1.13679400 |
| N | -2.74350200 | -0.39072700 | 0.30774100  |
| O | -3.93470100 | -0.25696100 | 0.23092400  |
| O | -2.20089300 | -1.38785100 | 1.04707700  |
| H | -0.54629600 | 0.50085400  | 2.06931600  |
| H | 1.90487800  | 0.32816600  | 2.33750300  |
| H | 2.33224800  | -0.22278100 | -1.90116900 |
| H | -0.09389700 | -0.04669300 | -2.17109500 |
| H | -1.61580600 | 1.95634900  | -1.57037500 |
| H | -3.06829900 | 0.96232100  | -1.90710100 |
| H | -3.05863000 | 2.09006900  | -0.53004600 |
| H | -2.97655400 | -1.88613000 | 1.37495700  |
| O | 3.58928600  | -0.04730100 | 0.50416600  |
| C | 4.50321100  | -0.24987400 | -0.57770200 |
| H | 4.44731000  | 0.57467400  | -1.29036100 |
| H | 5.48940500  | -0.27742900 | -0.12542900 |
| H | 4.30277500  | -1.19675500 | -1.08211200 |



**1cH'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.56074100 | -0.52392100 | -1.05131100 |
| C | -1.93716600 | -0.65498700 | -1.00122300 |
| C | -2.69047200 | -0.03656600 | 0.00208700  |
| C | -2.02304800 | 0.73098000  | 0.95836100  |
| C | -0.64488200 | 0.87811600  | 0.92725200  |
| C | 0.06932300  | 0.23885500  | -0.07589600 |
| N | 1.49453200  | 0.44709600  | -0.13082300 |

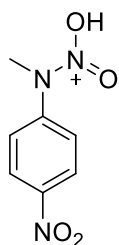
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.09759200  | 1.76820300  | -0.36906200 |
| N | 2.33559700  | -0.52544700 | 0.02566900  |
| O | 3.52673400  | -0.41916200 | -0.05587400 |
| O | 1.75737800  | -1.71858500 | 0.29577600  |
| H | 0.01010600  | -0.99756100 | -1.83777000 |
| H | -2.43785800 | -1.24155800 | -1.76024800 |
| H | -2.58734300 | 1.22070200  | 1.74052700  |
| H | -0.13595100 | 1.47263300  | 1.67386600  |
| H | 1.27506600  | 2.46709300  | -0.45848400 |
| H | 2.74807400  | 2.03082800  | 0.46371700  |
| H | 2.67651200  | 1.73939500  | -1.29148900 |
| H | 2.51358600  | -2.32700200 | 0.42337500  |
| C | -4.17955000 | -0.21007600 | 0.05108700  |
| H | -4.64494900 | 0.52118800  | 0.70970300  |
| H | -4.61916800 | -0.11442500 | -0.94224900 |
| H | -4.43298800 | -1.20597200 | 0.42319400  |



**1dH'**

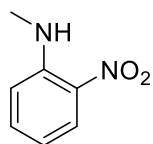
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.03796100  | 0.13587400  | 1.21667600  |
| C | 2.40759900  | -0.07443200 | 1.21682000  |
| C | 3.06397400  | -0.17734100 | -0.00000200 |
| C | 2.40760300  | -0.07439100 | -1.21682200 |
| C | 1.03796400  | 0.13591500  | -1.21667600 |
| C | 0.37607300  | 0.23175500  | 0.00000100  |
| N | -1.04425400 | 0.49549600  | 0.00000200  |
| C | -1.61298100 | 1.85196500  | 0.00000700  |
| N | -1.90353000 | -0.47515900 | -0.00000200 |
| O | -3.09032700 | -0.33564000 | 0.00000600  |
| O | -1.33973800 | -1.70300900 | 0.00000200  |
| H | 0.49690600  | 0.22216500  | 2.14871200  |
| H | 2.96383400  | -0.15809800 | 2.13920400  |
| H | 2.96384000  | -0.15802700 | -2.13920800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.49691300  | 0.22223600  | -2.14871100 |
| H | -0.77131200 | 2.53410400  | 0.00001500  |
| H | -2.22480300 | 1.99177200  | -0.89029100 |
| H | -2.22481100 | 1.99176200  | 0.89030200  |
| H | -2.10175800 | -2.31879200 | 0.00000500  |
| F | 4.38450000  | -0.38169900 | -0.00000300 |



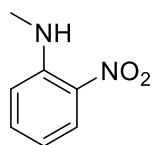
**1eH'**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.04708400  | 1.21546300  | -0.07901800 |
| C | -1.33345200 | 1.19545700  | -0.20136200 |
| C | -2.00525900 | 0.00875000  | 0.04480300  |
| C | -1.35656200 | -1.16082400 | 0.40665200  |
| C | 0.02477300  | -1.14533000 | 0.52553300  |
| C | 0.69747800  | 0.04249700  | 0.27740000  |
| N | 2.13258300  | 0.06959600  | 0.45952400  |
| C | 2.76746600  | 0.23739300  | 1.77603800  |
| N | 2.93727500  | -0.02715000 | -0.55239200 |
| O | 4.12820300  | 0.01476800  | -0.48159500 |
| O | 2.30423500  | -0.18954300 | -1.73382000 |
| H | 0.60317300  | 2.12523400  | -0.25530900 |
| H | -1.88460000 | 2.08072000  | -0.47830900 |
| H | -1.92441300 | -2.06005800 | 0.58867000  |
| H | 0.56380900  | -2.04085200 | 0.80113100  |
| H | 1.96381200  | 0.23773300  | 2.50297500  |
| H | 3.45601000  | -0.58608000 | 1.95666700  |
| H | 3.30793300  | 1.18328000  | 1.79861000  |
| H | 3.02555500  | -0.25378400 | -2.39356800 |
| N | -3.48270600 | -0.00909700 | -0.08193200 |
| O | -4.02380100 | 1.02206200  | -0.43693900 |
| O | -4.05169100 | -1.05344300 | 0.17779200  |



**2a (Thermal)**

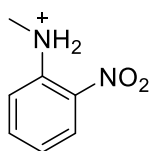
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.37460900  | -0.87909200 | -0.18402800 |
| C | 2.74651400  | -0.89398200 | 0.09719200  |
| C | 3.41832800  | 0.30195400  | 0.17531700  |
| C | 2.75239300  | 1.51761500  | -0.02103300 |
| C | 1.35513100  | 1.55677600  | -0.30863900 |
| C | 0.69962800  | 0.30225600  | -0.38052900 |
| H | 0.82859400  | -1.81162700 | -0.24947900 |
| H | 3.26980400  | -1.82670800 | 0.25036800  |
| H | 4.47488500  | 0.33705100  | 0.38959000  |
| H | -0.35758100 | 0.28047500  | -0.59559400 |
| N | 0.66491900  | 2.69692700  | -0.50621200 |
| H | 1.19915000  | 3.54856800  | -0.43916300 |
| C | -0.74897900 | 2.75400100  | -0.79811100 |
| H | -1.03030400 | 3.79839000  | -0.90734900 |
| H | -0.99309100 | 2.23339400  | -1.72830300 |
| H | -1.34788100 | 2.31933400  | 0.00703700  |
| N | 3.54562500  | 2.71387600  | 0.08190100  |
| O | 4.74265300  | 2.61680300  | 0.33143200  |
| O | 2.99823400  | 3.81595700  | -0.08458200 |



**2a (Acid)**

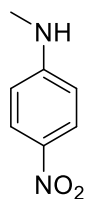
|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.37469700 | -0.87929300 | -0.18400100 |
| C | 2.74644000 | -0.89408000 | 0.09718200  |
| C | 3.41818400 | 0.30203800  | 0.17528500  |
| C | 2.75220600 | 1.51744800  | -0.02106200 |
| C | 1.35507900 | 1.55654400  | -0.30863700 |
| C | 0.69963400 | 0.30212300  | -0.38052100 |
| H | 0.82869500 | -1.81184700 | -0.24944800 |
| H | 3.26985700 | -1.82673400 | 0.25038000  |
| H | 4.47475000 | 0.33744600  | 0.38954400  |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.35758700 | 0.28028100 | -0.59558600 |
| N | 0.66494400  | 2.69696100 | -0.50620900 |
| H | 1.19961000  | 3.54836900 | -0.43905900 |
| C | -0.74880400 | 2.75412700 | -0.79808100 |
| H | -1.03016900 | 3.79853500 | -0.90732800 |
| H | -0.99311000 | 2.23359500 | -1.72832300 |
| H | -1.34790300 | 2.31953500 | 0.00702800  |
| N | 3.54569100  | 2.71417100 | 0.08189900  |
| O | 4.74241100  | 2.61679800 | 0.33138400  |
| O | 2.99800300  | 3.81595100 | -0.08463200 |



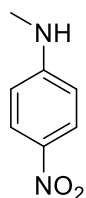
**2aH**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.68367800 | -0.34955400 | 0.16908400  |
| C | -2.42636800 | 1.01425600  | 0.20481100  |
| C | -1.12875600 | 1.48039200  | 0.06608900  |
| C | -0.08679200 | 0.58020400  | -0.11138600 |
| C | -0.34769200 | -0.79392900 | -0.15314000 |
| C | -1.64274000 | -1.25299000 | -0.01238800 |
| H | -3.69349500 | -0.71834100 | 0.28065200  |
| H | -3.23393600 | 1.71849500  | 0.34389400  |
| H | -0.90568400 | 2.53576800  | 0.09726600  |
| H | -1.84639600 | -2.31509900 | -0.04611700 |
| N | 0.72592900  | -1.77205800 | -0.37152800 |
| H | 1.61108200  | -1.23371400 | -0.26311600 |
| N | 1.27137400  | 1.13717200  | -0.23623800 |
| O | 1.39841100  | 2.33493600  | -0.27169900 |
| O | 2.22574500  | 0.34718600  | -0.29329400 |
| H | 0.69163800  | -2.48983400 | 0.35436300  |
| C | 0.70599400  | -2.41662400 | -1.73093600 |
| H | 1.54935600  | -3.09870200 | -1.79124300 |
| H | -0.23011000 | -2.95159400 | -1.85323400 |
| H | 0.79530600  | -1.63126700 | -2.47544600 |



**3a (Thermal)**

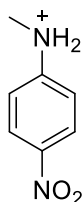
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.11629900 | -0.98639500 | 0.21106700  |
| C | 0.26494000  | -1.07899700 | 0.02719000  |
| C | 1.00816100  | 0.04215100  | -0.32948400 |
| C | 0.38149200  | 1.25798100  | -0.50441700 |
| C | -1.01277600 | 1.37635400  | -0.32428400 |
| C | -1.74452300 | 0.22234500  | 0.03792500  |
| H | -1.67515200 | -1.86730100 | 0.48759900  |
| H | 2.07464600  | -0.05209500 | -0.46645400 |
| H | 0.96826900  | 2.12094800  | -0.78113000 |
| H | -2.81526300 | 0.29892700  | 0.17941300  |
| N | 0.92714500  | -2.34946500 | 0.20889300  |
| O | 0.24502200  | -3.32286500 | 0.52401200  |
| O | 2.14395100  | -2.40417500 | 0.04099300  |
| N | -1.65521400 | 2.55874700  | -0.48952300 |
| H | -2.64920400 | 2.57092200  | -0.34522100 |
| C | -1.00980300 | 3.79858000  | -0.85786100 |
| H | -0.51724900 | 3.72264900  | -1.83136800 |
| H | -1.76535500 | 4.57802100  | -0.91767500 |
| H | -0.26373300 | 4.09994600  | -0.11715300 |



**3a (Acid)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.11615600 | -0.98644100 | 0.21105600  |
| C | 0.26488800  | -1.07889300 | 0.02717400  |
| C | 1.00807800  | 0.04203300  | -0.32944600 |
| C | 0.38129800  | 1.25798100  | -0.50438800 |
| C | -1.01277400 | 1.37626900  | -0.32426600 |
| C | -1.74442900 | 0.22242500  | 0.03789400  |

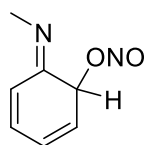
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.67474900 | -1.86752200 | 0.48758800  |
| H | 2.07455800  | -0.05247300 | -0.46635800 |
| H | 0.96809300  | 2.12095100  | -0.78110400 |
| H | -2.81520300 | 0.29891500  | 0.17940600  |
| N | 0.92739800  | -2.34994800 | 0.20896100  |
| O | 0.24495800  | -3.32281500 | 0.52401100  |
| O | 2.14394800  | -2.40409600 | 0.04097600  |
| N | -1.65542200 | 2.55901600  | -0.48955200 |
| H | -2.64934700 | 2.57109200  | -0.34523700 |
| C | -1.00988100 | 3.79863200  | -0.85786100 |
| H | -0.51726100 | 3.72275100  | -1.83138800 |
| H | -1.76519700 | 4.57835100  | -0.91777200 |
| H | -0.26374400 | 4.10004800  | -0.11717500 |



**3aH**

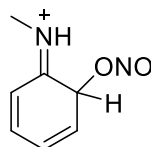
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.49076800  | 1.20536100  | -0.05563800 |
| C | 1.18896900  | 0.00814700  | -0.03762500 |
| C | 0.56313900  | -1.21841700 | -0.16553200 |
| C | -0.81686000 | -1.25686400 | -0.32135000 |
| C | -1.51338100 | -0.06226500 | -0.33869900 |
| C | -0.88525600 | 1.16801400  | -0.20864600 |
| H | 1.01752900  | 2.14116800  | 0.04886900  |
| H | 1.14466800  | -2.12703300 | -0.14403600 |
| H | -1.30952800 | -2.21120600 | -0.41991900 |
| H | -1.45029100 | 2.09128800  | -0.22689300 |
| N | 2.66102100  | 0.04467900  | 0.12577600  |
| O | 3.18299000  | 1.13995200  | 0.22771600  |
| O | 3.24651100  | -1.02251500 | 0.14569400  |
| N | -2.99034400 | -0.04294500 | -0.52261100 |
| H | -3.38348400 | 0.61096000  | 0.15893000  |
| C | -3.72683500 | -1.34539200 | -0.39955400 |
| H | -3.52529300 | -1.76592500 | 0.58028500  |
| H | -4.78533700 | -1.13323600 | -0.51236900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.39692200 | -2.01355900 | -1.18751600 |
| H | -3.19685300 | 0.35905200  | -1.44167200 |



**INT1**

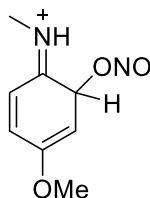
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.86202100 | -0.08668000 | 0.28025400  |
| C | -1.29194800 | 1.07713800  | -0.48533900 |
| C | -0.53421700 | 2.18784500  | -0.52215800 |
| C | 0.74438700  | 2.27085200  | 0.16483900  |
| C | 1.27732600  | 1.20629300  | 0.77186200  |
| C | 0.58622700  | -0.11856900 | 0.73642900  |
| N | -1.57247500 | -1.08996500 | 0.62039100  |
| C | -2.95228000 | -1.19494600 | 0.18296500  |
| H | -2.25264500 | 1.05559100  | -0.97865900 |
| H | -0.88289800 | 3.06122400  | -1.05905500 |
| H | 1.26258600  | 3.22120100  | 0.17245000  |
| H | 2.23436500  | 1.25852700  | 1.27262400  |
| H | 0.64733000  | -0.63412800 | 1.69273600  |
| H | -3.59009500 | -0.52997600 | 0.77433300  |
| H | -3.09483800 | -0.94783900 | -0.87349300 |
| H | -3.29553500 | -2.21505000 | 0.34705000  |
| O | 1.26686500  | -0.97613300 | -0.26080400 |
| N | 2.36841800  | -1.69977900 | 0.16476900  |
| O | 2.69751600  | -1.52806200 | 1.28355300  |



**INT1H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.16832000 | -1.57120000 | 0.01279400  |
| C | -0.83656200 | -1.64633600 | 0.13048700  |
| C | 0.00996400  | -0.43364000 | -0.07980900 |
| C | -0.72284300 | 0.87867200  | 0.01983400  |
| C | -2.12353400 | 0.88327700  | -0.21547800 |

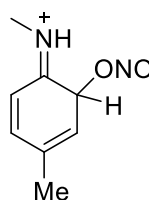
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.80058200 | -0.29691100 | -0.21342200 |
| H | -2.78570500 | -2.45428000 | 0.09302100  |
| H | -0.31578600 | -2.58046800 | 0.29048900  |
| H | -2.65320100 | 1.81960000  | -0.30242700 |
| H | -3.87543100 | -0.27654600 | -0.34070700 |
| N | -0.02980900 | 1.94975000  | 0.28370700  |
| H | 0.29251800  | -0.48933500 | -1.15457500 |
| O | 1.18369700  | -0.40924700 | 0.69607900  |
| N | 2.48821800  | -0.71399700 | -0.05458100 |
| O | 2.35204100  | -0.94158000 | -1.16750700 |
| C | -0.54744300 | 3.31611200  | 0.33128000  |
| H | -0.95492600 | 3.59903400  | -0.63822600 |
| H | -1.32068300 | 3.40164900  | 1.09377500  |
| H | 0.27488600  | 3.97879600  | 0.57960500  |
| H | 0.94129400  | 1.80642000  | 0.53452200  |



**INT1Hb**

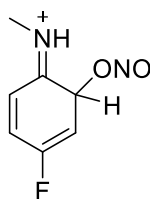
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.74527300  | 2.40719100  | 0.13507300  |
| C | -0.44417900 | 1.78887100  | 0.26588500  |
| C | -0.56251100 | 0.33137700  | -0.04142000 |
| C | 0.73329300  | -0.43271200 | -0.06314200 |
| C | 1.93340800  | 0.28939500  | -0.31190300 |
| C | 1.92411100  | 1.63995200  | -0.20880700 |
| H | -1.36264300 | 2.30976800  | 0.48584300  |
| H | 2.85694000  | -0.23921300 | -0.49136900 |
| H | 2.84192900  | 2.19829500  | -0.34344800 |
| N | 0.69381000  | -1.72082600 | 0.11848900  |
| H | -0.91144600 | 0.27349800  | -1.09332800 |
| O | -1.50009100 | -0.34395800 | 0.77540100  |
| N | -2.85453200 | -0.63101100 | 0.14324200  |
| O | -2.97058300 | -0.24997500 | -0.93199800 |
| C | 1.83208100  | -2.63638700 | 0.04880600  |
| H | 2.27590000  | -2.61219900 | -0.94552500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.58132300  | -2.36579100 | 0.79189300  |
| H | 1.47162400  | -3.63898500 | 0.25404900  |
| H | -0.20330700 | -2.10506100 | 0.39137100  |
| O | 1.00175800  | 3.71500200  | 0.29201700  |
| C | -0.08940400 | 4.56756400  | 0.64795200  |
| H | 0.32934500  | 5.56463400  | 0.73668200  |
| H | -0.85549600 | 4.55309500  | -0.13029200 |
| H | -0.52111100 | 4.25800900  | 1.60198700  |



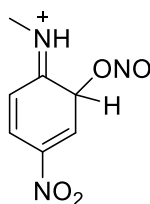
**INT1Hc**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.85569100  | 2.45497500  | 0.12216200  |
| C | -0.33561600 | 1.85118900  | 0.25657200  |
| C | -0.51248100 | 0.39612400  | -0.02736000 |
| C | 0.75555400  | -0.41011200 | -0.05394600 |
| C | 1.97268100  | 0.27611100  | -0.30259300 |
| C | 1.99999300  | 1.63215500  | -0.21465000 |
| H | -1.23756400 | 2.40090200  | 0.49076000  |
| H | 2.88179200  | -0.28021800 | -0.47366800 |
| H | 2.94942300  | 2.13373600  | -0.36052500 |
| N | 0.67116700  | -1.69831900 | 0.12132700  |
| H | -0.87194600 | 0.35642500  | -1.07787500 |
| O | -1.46994300 | -0.23065700 | 0.80152700  |
| N | -2.82823600 | -0.49573500 | 0.17253000  |
| O | -2.92764200 | -0.14399100 | -0.91449200 |
| C | 1.78090200  | -2.64708300 | 0.04857200  |
| H | 2.22174700  | -2.63731700 | -0.94736900 |
| H | 2.54122700  | -2.39741300 | 0.78754500  |
| H | 1.39250900  | -3.63846500 | 0.25686900  |
| H | -0.23849500 | -2.05531600 | 0.38966600  |
| C | 1.06360700  | 3.92697400  | 0.31271200  |
| H | 1.78444000  | 4.11228800  | 1.11192700  |
| H | 1.46436400  | 4.38030100  | -0.59650900 |
| H | 0.13188300  | 4.42827700  | 0.56615300  |



**INT1Hd**

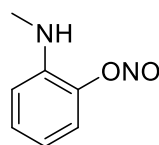
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.84890100  | 2.39641800  | 0.10616800  |
| C | -0.35307900 | 1.84013300  | 0.26121200  |
| C | -0.51554300 | 0.38149100  | -0.02090500 |
| C | 0.76583600  | -0.41350300 | -0.05687600 |
| C | 1.98776100  | 0.27333700  | -0.31199000 |
| C | 2.01743600  | 1.62627300  | -0.22562200 |
| H | -1.23630200 | 2.41703500  | 0.49503400  |
| H | 2.89662300  | -0.28229000 | -0.48394200 |
| H | 2.94701500  | 2.16316300  | -0.36501000 |
| N | 0.68914500  | -1.69926000 | 0.12119700  |
| H | -0.87843200 | 0.33580500  | -1.07039700 |
| O | -1.45316400 | -0.25656400 | 0.81281000  |
| N | -2.85902700 | -0.44543800 | 0.20884600  |
| O | -2.97442800 | -0.03590900 | -0.85158500 |
| C | 1.79718200  | -2.65051100 | 0.04191400  |
| H | 2.28376300  | -2.58190600 | -0.92950000 |
| H | 2.52102600  | -2.45287400 | 0.83174500  |
| H | 1.39246900  | -3.64900000 | 0.16784100  |
| H | -0.21796800 | -2.05631100 | 0.40050400  |
| F | 1.04044500  | 3.70918600  | 0.26267000  |



**INT1He**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.87469500  | 2.40712100  | 0.10839600  |
| C | -0.32679200 | 1.85689500  | 0.29362000  |
| C | -0.51452700 | 0.40452100  | 0.00530600  |
| C | 0.76453000  | -0.39733600 | -0.05127300 |
| C | 1.98465700  | 0.28197700  | -0.34067600 |

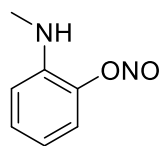
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.03100500  | 1.63359200  | -0.25937500 |
| H | -1.19135900 | 2.44354600  | 0.57060100  |
| H | 2.88479400  | -0.28108000 | -0.53541300 |
| H | 2.95911700  | 2.16183700  | -0.42367500 |
| N | 0.67778300  | -1.67736900 | 0.14277300  |
| H | -0.87621700 | 0.39635200  | -1.04974900 |
| O | -1.45937300 | -0.22248500 | 0.82313800  |
| N | -2.84495700 | -0.52934200 | 0.13953100  |
| O | -2.91408000 | -0.18590700 | -0.94199800 |
| C | 1.77008800  | -2.64707300 | 0.05482500  |
| H | 2.24622700  | -2.58874000 | -0.92199600 |
| H | 2.50453800  | -2.45813800 | 0.83674100  |
| H | 1.34978300  | -3.63802900 | 0.18912900  |
| H | -0.23091100 | -2.01662900 | 0.44089500  |
| N | 1.04593400  | 3.86564200  | 0.30635900  |
| O | 2.16732000  | 4.31033000  | 0.14014500  |
| O | 0.06199500  | 4.50633900  | 0.61794600  |



**INT2 (Thermal)**

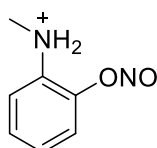
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.05694100 | -2.44918100 | -0.14434200 |
| C | -1.66970900 | -2.52377900 | -0.09250500 |
| C | -0.91741000 | -1.38428900 | 0.13999300  |
| C | -1.52529100 | -0.12011800 | 0.30227500  |
| C | -2.92497100 | -0.06519100 | 0.25667200  |
| C | -3.67148600 | -1.21481900 | 0.03126900  |
| H | -3.64524300 | -3.33976000 | -0.31646300 |
| H | -1.15289500 | -3.46659500 | -0.21691500 |
| H | -3.42921800 | 0.88048300  | 0.39396100  |
| H | -4.75101900 | -1.14074800 | -0.00179000 |
| N | -0.73283400 | 0.98793300  | 0.47396100  |
| H | 0.20871900  | 0.78414900  | 0.76650400  |
| C | -1.27665800 | 2.25865600  | 0.90038800  |
| H | -0.45601200 | 2.96027800  | 1.03486000  |
| H | -1.94536300 | 2.66805000  | 0.14037000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.83399600 | 2.18799400  | 1.84257200  |
| O | 0.45268200  | -1.45530700 | 0.21593800  |
| N | 1.17410600  | -1.32552400 | -1.15296200 |
| O | 0.46104300  | -1.23926200 | -2.04710500 |



**INT2 (Acid)**

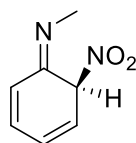
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.23912000 | 2.53757000  | -0.02472000 |
| C | 0.76058400  | 1.66900300  | -0.44757000 |
| C | 0.52420300  | 0.30531200  | -0.50063300 |
| C | -0.71528400 | -0.24370600 | -0.10557800 |
| C | -1.71454800 | 0.64726300  | 0.30863600  |
| C | -1.47084900 | 2.01422400  | 0.35070500  |
| H | -0.05838000 | 3.60298500  | 0.00807100  |
| H | 1.73090500  | 2.03667200  | -0.75540600 |
| H | -2.68284600 | 0.26826000  | 0.60219300  |
| H | -2.26112100 | 2.67777300  | 0.67802000  |
| N | -0.88072200 | -1.60677300 | -0.12306400 |
| H | -0.21290500 | -2.09875400 | -0.69367800 |
| C | -2.18290300 | -2.22092800 | 0.01530200  |
| H | -2.07364100 | -3.29728700 | -0.10042200 |
| H | -2.59639700 | -2.03186400 | 1.00813300  |
| H | -2.90425400 | -1.86090800 | -0.72864000 |
| O | 1.50003600  | -0.55640200 | -0.94000400 |
| N | 2.47014400  | -1.04027900 | 0.17164800  |
| O | 2.27021800  | -0.57089200 | 1.19884600  |



**INT2H**

|   |             |            |            |
|---|-------------|------------|------------|
| C | 0.31003300  | 2.42970700 | 0.04229100 |
| C | -0.58187700 | 1.50963800 | 0.57823200 |
| C | -0.34890200 | 0.14197600 | 0.41860500 |

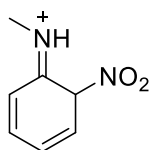
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.79541200  | -0.25153500 | -0.28848900 |
| C | 1.69597200  | 0.65268500  | -0.80999200 |
| C | 1.44084400  | 2.01095800  | -0.65039900 |
| H | 0.12300000  | 3.48662900  | 0.17329300  |
| H | -1.44681300 | 1.83664700  | 1.13762800  |
| H | 2.58135700  | 0.31507200  | -1.33362400 |
| H | 2.12941900  | 2.73616000  | -1.05956100 |
| N | 1.02024500  | -1.70041700 | -0.38589800 |
| H | 0.12293100  | -2.13783600 | -0.14175600 |
| C | 2.07637700  | -2.22924800 | 0.54731900  |
| H | 2.13507300  | -3.30760300 | 0.42619900  |
| H | 3.02240100  | -1.76085700 | 0.29702900  |
| H | 1.78080000  | -1.96995700 | 1.55879500  |
| O | -1.15886500 | -0.81250000 | 0.89758900  |
| N | -2.73847100 | -0.78749300 | 0.19914500  |
| O | -2.89883300 | 0.07845400  | -0.49051900 |
| H | 1.24589400  | -1.96185500 | -1.34703200 |



**INT3**

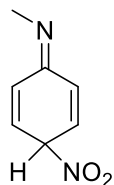
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.76220100 | -0.07327400 | 0.34858100  |
| C | -1.33449200 | 1.11407100  | -0.26759000 |
| C | -0.62588600 | 2.24235400  | -0.42863400 |
| C | 0.75523900  | 2.33814800  | 0.01431600  |
| C | 1.39115500  | 1.30063100  | 0.56179500  |
| C | 0.70983100  | -0.01980700 | 0.74552900  |
| N | -1.51575500 | -1.08615200 | 0.53764300  |
| N | 1.52288700  | -1.04548700 | -0.07973100 |
| O | 2.50334100  | -1.51903800 | 0.46322000  |
| O | 1.16057900  | -1.27635300 | -1.21498600 |
| H | -2.36605100 | 1.03441500  | -0.58196900 |
| H | -1.07960400 | 3.10968800  | -0.88961700 |
| H | 1.26959500  | 3.28379500  | -0.09891000 |
| H | 2.41842800  | 1.36631600  | 0.89406300  |
| H | 0.84605000  | -0.37145200 | 1.76783400  |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.00983500 | -2.30304300 | 1.12672500 |
| H | -0.64326800 | -2.96242900 | 0.33317500 |
| H | -0.19371400 | -2.16360000 | 1.84539400 |
| H | -1.82830500 | -2.82149400 | 1.62445500 |



**INT3H**

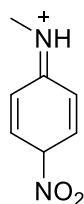
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.76102800 | 0.22676700  | 0.16555600  |
| C | -1.01781500 | 1.56055700  | -0.24838900 |
| C | -0.01012500 | 2.46937600  | -0.29127600 |
| C | 1.35011400  | 2.15407300  | 0.06706100  |
| C | 1.67750000  | 0.91781200  | 0.45231900  |
| C | 0.64647200  | -0.14420400 | 0.59812900  |
| N | -1.69495100 | -0.68093400 | 0.22262000  |
| C | -3.09928300 | -0.48733000 | -0.13569500 |
| N | 1.10101200  | -1.45220200 | -0.10822900 |
| O | 0.39936500  | -2.42967500 | 0.08486500  |
| O | 2.10688100  | -1.41109100 | -0.76672700 |
| H | -2.01723400 | 1.83755900  | -0.54587700 |
| H | -0.23087900 | 3.47556900  | -0.62315800 |
| H | 2.09999100  | 2.92934500  | 0.00465400  |
| H | 2.69075200  | 0.64503300  | 0.70793900  |
| H | 0.60147600  | -0.44576300 | 1.65012500  |
| H | -1.40222100 | -1.62012900 | 0.47658900  |
| H | -3.54619500 | 0.27219800  | 0.50434800  |
| H | -3.18818700 | -0.18780600 | -1.17930100 |
| H | -3.61490900 | -1.43022200 | 0.01260300  |



**INT4**

|   |             |            |            |
|---|-------------|------------|------------|
| C | -8.20522100 | 0.52034100 | 0.11923900 |
|---|-------------|------------|------------|

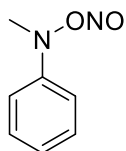
|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -8.87620900  | 1.50957700  | -0.47088200 |
| C | -10.20328200 | 1.30398700  | -1.11301600 |
| C | -10.76362900 | -0.07429100 | -0.96604700 |
| C | -10.08432500 | -1.04338700 | -0.35564500 |
| C | -8.75335000  | -0.83883100 | 0.22330300  |
| N | -8.18939700  | -1.84574400 | 0.77957100  |
| C | -6.87533200  | -1.72309800 | 1.37923400  |
| N | -11.24656600 | 2.29554200  | -0.53498900 |
| O | -12.26339000 | 2.44180100  | -1.18623800 |
| O | -10.99837500 | 2.84003200  | 0.52165900  |
| H | -7.23514700  | 0.72317300  | 0.54919100  |
| H | -8.45915400  | 2.50691900  | -0.52065200 |
| H | -10.17982100 | 1.59220000  | -2.16752200 |
| H | -11.74187600 | -0.24784900 | -1.39382400 |
| H | -10.49094400 | -2.04250200 | -0.26975100 |
| H | -6.17424000  | -1.11752800 | 0.79679600  |
| H | -6.95578600  | -1.28054500 | 2.37779700  |
| H | -6.45110500  | -2.71918400 | 1.49761800  |



**INT4H**

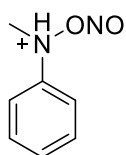
|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -8.21582300  | 0.51425900  | 0.14398000  |
| C | -8.90467600  | 1.52176400  | -0.40417800 |
| C | -10.21283200 | 1.30947800  | -1.06932500 |
| C | -10.76457500 | -0.06757200 | -0.97802800 |
| C | -10.07336700 | -1.06213600 | -0.41495000 |
| C | -8.77375700  | -0.81724100 | 0.16968600  |
| N | -8.13627200  | -1.80855000 | 0.73383900  |
| C | -6.82876100  | -1.75021800 | 1.38904200  |
| N | -11.28105900 | 2.30595300  | -0.53753600 |
| O | -12.34706400 | 2.28368600  | -1.10699800 |
| O | -10.96314100 | 3.01145500  | 0.39360100  |
| H | -7.25003300  | 0.69254200  | 0.59138100  |
| H | -8.50549800  | 2.52622200  | -0.40110500 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | -10.13305000 | 1.58967300  | -2.12706900 |
| H | -11.74563300 | -0.23230700 | -1.40172200 |
| H | -10.47814700 | -2.06520100 | -0.37272800 |
| H | -8.59687300  | -2.70993300 | 0.73307700  |
| H | -6.07858500  | -1.36469400 | 0.70123400  |
| H | -6.87687000  | -1.11860100 | 2.27528700  |
| H | -6.55678400  | -2.75858300 | 1.68251100  |



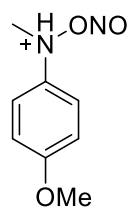
**INT5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.33442500  | -1.17531200 | 0.27302900  |
| C | 2.66772300  | -0.80325600 | 0.38590300  |
| C | 3.06980000  | 0.50031700  | 0.12548100  |
| C | 2.11197700  | 1.43484000  | -0.25421200 |
| C | 0.77590900  | 1.08237500  | -0.36743800 |
| C | 0.36972800  | -0.23009200 | -0.09736100 |
| N | -0.98297900 | -0.58751900 | -0.16017400 |
| C | -1.40414600 | -1.97534900 | -0.22722900 |
| H | 1.05257400  | -2.19745300 | 0.47601800  |
| H | 3.39719700  | -1.54882300 | 0.67588000  |
| H | 4.11015400  | 0.78290300  | 0.21246800  |
| H | 2.40570100  | 2.45451700  | -0.46907400 |
| H | 0.04623200  | 1.81593500  | -0.67394900 |
| H | -1.10704400 | -2.49640900 | 0.68176400  |
| H | -2.48850200 | -1.99010400 | -0.29158500 |
| H | -0.98482700 | -2.49487400 | -1.09602500 |
| O | -1.77101800 | 0.24939900  | -0.89225200 |
| N | -2.69376300 | 1.12254600  | 0.08751600  |
| O | -2.51565700 | 0.86732800  | 1.18502500  |



**INT5H**

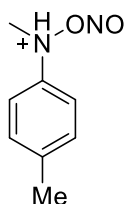
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.05028600  | -0.46409800 | 1.18581600  |
| C | 2.39493100  | -0.70017500 | 0.92732800  |
| C | 2.97759100  | -0.19476900 | -0.22793500 |
| C | 2.22415500  | 0.54858600  | -1.13234800 |
| C | 0.88205500  | 0.79901600  | -0.88690100 |
| C | 0.32747300  | 0.28608800  | 0.27459200  |
| N | -1.09429700 | 0.54115100  | 0.56963200  |
| C | -1.46597900 | 1.98553800  | 0.72124700  |
| H | 0.58763300  | -0.85897400 | 2.08196200  |
| H | 2.97966400  | -1.27997900 | 1.62737200  |
| H | 4.02340600  | -0.38268200 | -0.42791700 |
| H | 2.68109300  | 0.93386900  | -2.03286300 |
| H | 0.28920200  | 1.36444400  | -1.59200000 |
| H | -0.82820600 | 2.40285000  | 1.49620800  |
| H | -1.29477400 | 2.47816400  | -0.22889100 |
| H | -2.51413500 | 2.03234700  | 1.00027000  |
| H | -1.31504000 | 0.05901500  | 1.45574400  |
| O | -1.92771400 | -0.03783000 | -0.42167700 |
| N | -2.81145500 | -1.25203400 | 0.14368500  |
| O | -2.65607100 | -1.44994500 | 1.24715200  |



**INT5Hb**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.90462800  | -1.06295600 | 0.73330300  |
| C | 2.24299700  | -1.38182600 | 0.55623200  |
| C | 3.07275200  | -0.50902600 | -0.15543800 |
| C | 2.54507300  | 0.67951500  | -0.68712900 |
| C | 1.21889500  | 0.99844300  | -0.50469800 |
| C | 0.41312000  | 0.12159500  | 0.21507300  |
| N | -0.99998300 | 0.44104800  | 0.42322200  |
| C | -1.28315800 | 1.73759400  | 1.11710600  |
| H | 0.26324700  | -1.74347700 | 1.28064800  |
| H | 2.62382600  | -2.30233100 | 0.96937400  |
| H | 3.20078600  | 1.33374100  | -1.24374800 |

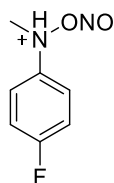
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.81719000  | 1.90575200  | -0.93303200 |
| H | -0.78028200 | 1.70404400  | 2.08006900  |
| H | -0.89420100 | 2.54387500  | 0.50602400  |
| H | -2.35920700 | 1.82462400  | 1.23421300  |
| H | -1.41485200 | -0.31930300 | 0.98440400  |
| O | -1.70791000 | 0.44084000  | -0.82130900 |
| N | -2.81401400 | -0.67481500 | -0.90091200 |
| O | -2.90259100 | -1.30215400 | 0.04330200  |
| O | 4.37441300  | -0.71943300 | -0.38498400 |
| C | 4.98858300  | -1.91216500 | 0.11063100  |
| H | 6.02826600  | -1.85386000 | -0.19542200 |
| H | 4.92781100  | -1.95648900 | 1.19953300  |
| H | 4.52485900  | -2.79756200 | -0.32811000 |



**INT5Hc**

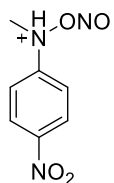
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.98991600  | -1.01245300 | 0.73739500  |
| C | 2.33285900  | -1.28457000 | 0.51975600  |
| C | 3.12393300  | -0.43315900 | -0.25270200 |
| C | 2.53008800  | 0.70079600  | -0.81685100 |
| C | 1.19336400  | 0.99480300  | -0.60822900 |
| C | 0.44736700  | 0.13108400  | 0.17773000  |
| N | -0.97135500 | 0.42279700  | 0.43044500  |
| C | -1.24819900 | 1.74194000  | 1.08598600  |
| H | 0.38724600  | -1.68672100 | 1.33382900  |
| H | 2.76841500  | -2.17397600 | 0.95496800  |
| H | 3.12401700  | 1.36316500  | -1.43226000 |
| H | 0.74772400  | 1.86679100  | -1.06557100 |
| H | -0.67733300 | 1.76892800  | 2.01034000  |
| H | -0.92834300 | 2.52892000  | 0.41282400  |
| H | -2.31543600 | 1.80315200  | 1.27463500  |
| H | -1.33709000 | -0.32110000 | 1.04561000  |
| O | -1.72410900 | 0.35295300  | -0.77626100 |
| N | -2.78602500 | -0.83643300 | -0.78301800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.80548700 | -1.43693500 | 0.17804200  |
| C | 4.58322100  | -0.71436500 | -0.45698000 |
| H | 4.79457500  | -1.78101200 | -0.39481100 |
| H | 4.92714300  | -0.34472300 | -1.42234000 |
| H | 5.17452400  | -0.21510300 | 0.31524000  |



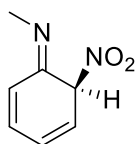
**INT5Hd**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97653600  | -1.04640100 | 0.68365300  |
| C | 2.31961400  | -1.32524700 | 0.47901600  |
| C | 3.08293800  | -0.41311100 | -0.23070100 |
| C | 2.55570400  | 0.76228300  | -0.74763600 |
| C | 1.21646900  | 1.04161700  | -0.53819200 |
| C | 0.45330200  | 0.13399700  | 0.18179900  |
| N | -0.96793300 | 0.42157500  | 0.42420600  |
| C | -1.24685600 | 1.69921100  | 1.15917000  |
| H | 0.35888300  | -1.74848800 | 1.22959700  |
| H | 2.77046100  | -2.23093900 | 0.85780400  |
| H | 3.18941800  | 1.43826100  | -1.30305100 |
| H | 0.78287800  | 1.94355700  | -0.94549500 |
| H | -0.69236800 | 1.66261500  | 2.09314400  |
| H | -0.91130800 | 2.52518200  | 0.54269600  |
| H | -2.31691000 | 1.75537200  | 1.33246400  |
| H | -1.35181400 | -0.35506300 | 0.98604100  |
| O | -1.69327000 | 0.43413600  | -0.79756100 |
| N | -2.77031800 | -0.75674700 | -0.90005800 |
| O | -2.81001300 | -1.41314000 | 0.02015200  |
| F | 4.37668400  | -0.67582700 | -0.43000100 |



**INT5He**

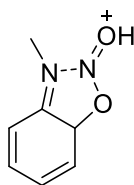
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.00129500  | -0.96861000 | 0.80365700  |
| C | 2.34489500  | -1.23266500 | 0.57651200  |
| C | 3.05301700  | -0.38902000 | -0.26183300 |
| C | 2.47628300  | 0.70765800  | -0.88469700 |
| C | 1.13641300  | 0.97636600  | -0.65711700 |
| C | 0.43263200  | 0.13110700  | 0.18472000  |
| N | -0.99128700 | 0.42473300  | 0.45393600  |
| C | -1.21404800 | 1.60730800  | 1.35556500  |
| H | 0.42603600  | -1.61654200 | 1.45222200  |
| H | 2.83545300  | -2.07768300 | 1.03397700  |
| H | 3.06894600  | 1.33246200  | -1.53463800 |
| H | 0.65404000  | 1.81325600  | -1.14063400 |
| H | -0.67316300 | 1.41836900  | 2.27919100  |
| H | -0.82345800 | 2.48481600  | 0.85205200  |
| H | -2.28233600 | 1.69458900  | 1.52761500  |
| H | -1.40096400 | -0.40670000 | 0.90973200  |
| O | -1.70091200 | 0.63565100  | -0.74395600 |
| N | -2.65487900 | -0.64163700 | -1.14270200 |
| O | -2.62611500 | -1.47280400 | -0.38479300 |
| N | 4.48686200  | -0.67393800 | -0.50873400 |
| O | 4.96241100  | -1.65275000 | 0.03721500  |
| O | 5.08847500  | 0.09099600  | -1.23984300 |



**INT6**

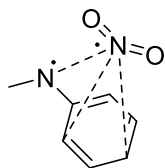
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.84604500 | -0.08713400 | 0.25885100  |
| C | -1.31938600 | 1.10640900  | -0.43071600 |
| C | -0.56774000 | 2.21946500  | -0.47269200 |
| C | 0.74821300  | 2.28276200  | 0.14453200  |
| C | 1.31232300  | 1.20815100  | 0.70041100  |
| C | 0.60976000  | -0.11457600 | 0.68961000  |
| N | -1.52728800 | -1.12078100 | 0.56185500  |
| C | -2.91710500 | -1.22220100 | 0.15331600  |
| N | 1.41817700  | -1.01719800 | -0.27606400 |
| O | 2.42915900  | -1.51714400 | 0.17909000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.02238200  | -1.13470300 | -1.41776000 |
| H | -2.30398600 | 1.09447500  | -0.87449300 |
| H | -0.94421900 | 3.10870200  | -0.96204300 |
| H | 1.26924900  | 3.23133700  | 0.14869700  |
| H | 2.29545700  | 1.24190900  | 1.14921000  |
| H | 0.70399900  | -0.63176500 | 1.64088000  |
| H | -3.53326000 | -0.46476600 | 0.64820400  |
| H | -3.03914300 | -1.10259300 | -0.92769700 |
| H | -3.29612200 | -2.20283500 | 0.43383700  |



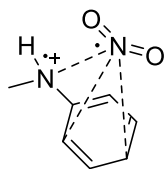
**INT6H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.04877200  | -1.13370200 | -0.64554600 |
| C | 2.35832200  | -1.37843300 | -0.79189900 |
| C | 3.28706400  | -0.21322500 | -0.81353000 |
| C | 2.75832200  | 1.00381800  | -0.13710300 |
| C | 1.36891700  | 1.26991100  | -0.11818000 |
| C | 0.55919700  | 0.20340000  | -0.36845900 |
| O | 4.54939700  | -0.40945600 | -0.17872800 |
| N | 4.99432200  | 0.84403800  | 0.33185700  |
| O | 5.81108000  | 1.48193200  | -0.59393200 |
| N | 3.75136000  | 1.60337600  | 0.44100200  |
| C | 3.81436000  | 2.81873500  | 1.23406000  |
| H | 0.32703100  | -1.93370600 | -0.72659800 |
| H | 2.75827000  | -2.35536400 | -1.02377200 |
| H | 3.40705800  | 0.03555500  | -1.88607100 |
| H | 0.97574300  | 2.22330400  | 0.20031500  |
| H | -0.51211400 | 0.34051100  | -0.29446700 |
| H | 5.37374100  | 1.51540600  | -1.46574600 |
| H | 4.50486000  | 3.51546700  | 0.76301200  |
| H | 2.82060300  | 3.25258800  | 1.28537700  |
| H | 4.17116600  | 2.56261500  | 2.22974700  |



**INT7**

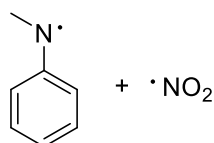
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.94234300 | 0.82688300  | -0.75599600 |
| C | -1.80901200 | -0.16361000 | -1.16560800 |
| C | -2.16736300 | -1.19931100 | -0.29956800 |
| C | -1.64040700 | -1.24354500 | 0.99366300  |
| C | -0.78039200 | -0.25828500 | 1.42366800  |
| C | -0.41697600 | 0.83186600  | 0.57478200  |
| N | 0.39668500  | 1.75186800  | 1.09183900  |
| C | 0.81962800  | 2.84755600  | 0.25433200  |
| N | 1.30627500  | -1.14475500 | -0.64536400 |
| O | 2.35704200  | -0.59772500 | -0.48498900 |
| O | 1.00932500  | -2.17785700 | -1.16745200 |
| H | -0.67338100 | 1.61818100  | -1.44045800 |
| H | -2.20715000 | -0.14566700 | -2.17189700 |
| H | -2.84399100 | -1.97353300 | -0.63550600 |
| H | -1.90614400 | -2.05654200 | 1.65637300  |
| H | -0.36269600 | -0.26740500 | 2.42132900  |
| H | -0.02834600 | 3.43254300  | -0.12264400 |
| H | 1.46276500  | 3.51042000  | 0.83044800  |
| H | 1.38452800  | 2.49430200  | -0.61710500 |



**INT7H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.53483400  | -1.31518500 | -0.00000300 |
| C | 1.86913400  | -1.00679100 | 0.00000100  |
| C | 2.27989700  | 0.33429200  | 0.00000600  |
| C | 1.33417400  | 1.37281100  | 0.00000100  |
| C | -0.00718000 | 1.09271100  | -0.00000500 |
| C | -0.43417600 | -0.26625200 | -0.00000300 |
| N | -1.72816900 | -0.58974700 | 0.00000100  |

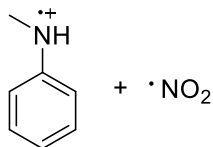
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.84761800 | 0.33652400  | 0.00000200  |
| H | 0.19792000  | -2.34317600 | -0.00001000 |
| H | 2.60649600  | -1.79666400 | -0.00000500 |
| H | 3.33448200  | 0.57198800  | 0.00000800  |
| H | 1.66802800  | 2.40061500  | -0.00000200 |
| H | -0.73512000 | 1.88934900  | -0.00001600 |
| H | -2.81448500 | 0.96727200  | 0.88834500  |
| H | -2.81445400 | 0.96731600  | -0.88830700 |
| H | -3.76571200 | -0.24049700 | -0.00002400 |
| H | -1.95436400 | -1.57662500 | 0.00000900  |
| N | 0.00000000  | 0.32112400  | 0.00000000  |
| O | 1.09696300  | -0.14049200 | 0.00000000  |
| O | -1.09696300 | -0.14049100 | 0.00000000  |



**Radicals (Thermal)**

|                       |             |             |             |
|-----------------------|-------------|-------------|-------------|
| C                     | -1.15722700 | 0.92564800  | -0.74766100 |
| C                     | -2.14211500 | 0.04802400  | -1.15192500 |
| C                     | -2.47406900 | -1.06116900 | -0.36978800 |
| C                     | -1.80425000 | -1.28832400 | 0.83556200  |
| C                     | -0.81833900 | -0.42145100 | 1.25341500  |
| C                     | -0.45860000 | 0.71725500  | 0.47730300  |
| N                     | 0.51443900  | 1.50188700  | 0.96977500  |
| C                     | 0.90347700  | 2.66330200  | 0.20950900  |
| H                     | -0.91546200 | 1.77731100  | -1.36678000 |
| H                     | -2.66359900 | 0.22016600  | -2.08501700 |
| H                     | -3.24831100 | -1.74210500 | -0.69774100 |
| H                     | -2.06122600 | -2.14748100 | 1.44160700  |
| H                     | -0.28647600 | -0.57698300 | 2.18246400  |
| H                     | 0.06716700  | 3.35928900  | 0.06454800  |
| H                     | 1.69646000  | 3.18956600  | 0.73863900  |
| H                     | 1.27518100  | 2.39642300  | -0.78820600 |
| <b>NO<sub>2</sub></b> |             |             |             |
| N                     | 1.87388400  | -1.21030500 | -0.41820500 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 2.23889800 | -0.44830600 | -1.25673700 |
| O | 2.41821800 | -1.81736400 | 0.44908200  |

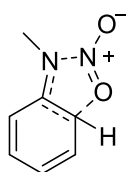


#### Cationic radical and NO<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.53581600  | -1.31484000 | 0.00057200  |
| C | 1.86981100  | -1.00819200 | -0.00114700 |
| C | 2.28157600  | 0.33342800  | -0.00316800 |
| C | 1.33617300  | 1.37346200  | -0.00268600 |
| C | -0.00494800 | 1.09428700  | -0.00010200 |
| C | -0.43344000 | -0.26475500 | 0.00067500  |
| N | -1.72865900 | -0.58856800 | 0.00106400  |
| C | -2.85307800 | 0.33496300  | -0.00140300 |
| H | 0.20067400  | -2.34400100 | 0.00224300  |
| H | 2.60695300  | -1.79844200 | -0.00098500 |
| H | 3.33653800  | 0.57013700  | -0.00488100 |
| H | 1.67176600  | 2.40079400  | -0.00440100 |
| H | -0.73163000 | 1.89256100  | 0.00043000  |
| H | -2.79768500 | 1.00102500  | 0.85932100  |
| H | -2.85248900 | 0.92850200  | -0.91633000 |
| H | -3.77017200 | -0.24271300 | 0.05034600  |
| H | -1.95197900 | -1.57581900 | -0.00513700 |

#### NO<sub>2</sub>

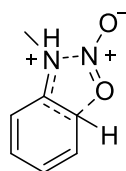
|   |            |             |             |
|---|------------|-------------|-------------|
| N | 0.00000000 | 0.00000000  | 0.32100200  |
| O | 0.00000000 | 1.09732900  | -0.14043100 |
| O | 0.00000000 | -1.09732900 | -0.14043100 |



#### TS1

|   |            |            |             |
|---|------------|------------|-------------|
| C | 0.25250100 | 0.75129500 | 0.39006600  |
| C | 1.11328200 | 1.16817900 | -0.69581200 |
| C | 2.23681400 | 0.46496900 | -0.97427900 |

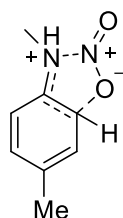
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.58003400  | -0.70471100 | -0.22289500 |
| C | 1.77638200  | -1.17090600 | 0.77401000  |
| C | 0.55845400  | -0.50745200 | 1.04431000  |
| N | -0.83540400 | 1.32540400  | 0.80563500  |
| C | -1.38850200 | 2.47616900  | 0.14528800  |
| N | -1.82342400 | -0.95371900 | -0.20059600 |
| O | -2.77323800 | -1.45377100 | -0.77567100 |
| O | -0.77020200 | -1.63333600 | -0.08023800 |
| H | 0.88350700  | 2.06639700  | -1.24820800 |
| H | 2.90309600  | 0.79221300  | -1.76129300 |
| H | 3.50763400  | -1.21361800 | -0.45170500 |
| H | 2.04095400  | -2.05482300 | 1.33657000  |
| H | -0.00909700 | -0.73554500 | 1.93227400  |
| H | -1.19567600 | 3.35014700  | 0.77720000  |
| H | -1.02048300 | 2.67476200  | -0.86314400 |
| H | -2.47166600 | 2.35263100  | 0.11325100  |



#### TS1H

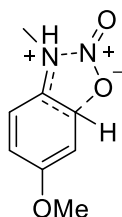
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.58251400  | -0.58661500 | 0.98471000  |
| C | 1.84904400  | -1.15956100 | 0.72305200  |
| C | 2.65593200  | -0.58369600 | -0.20666600 |
| C | 2.26960900  | 0.62415600  | -0.88743900 |
| C | 1.10564000  | 1.25963500  | -0.60488800 |
| C | 0.24582100  | 0.69906500  | 0.38474400  |
| N | -0.92240700 | 1.20917900  | 0.69858200  |
| C | -1.54253300 | 2.38765700  | 0.09878000  |
| N | -1.78732500 | -1.09460000 | -0.15016400 |
| O | -2.73306800 | -1.57112200 | -0.71334900 |
| O | -0.63617800 | -1.58710800 | -0.26020300 |
| H | 0.02337100  | -0.90822600 | 1.85136800  |
| H | 2.13779500  | -2.06008800 | 1.24400600  |
| H | 3.61787100  | -1.02043000 | -0.43775800 |
| H | 2.94030700  | 1.03786800  | -1.62761200 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 0.83980200  | 2.18175600 | -1.09786900 |
| H | -1.03294700 | 3.28713600 | 0.44710700  |
| H | -1.48777900 | 2.33063900 | -0.98537200 |
| H | -2.58103900 | 2.41763500 | 0.41058700  |
| H | -1.43728600 | 0.76932400 | 1.45016400  |



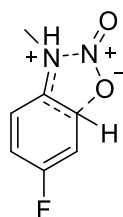
**TS1Hc**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.56435600  | -0.60122300 | 0.99343800  |
| C | 1.80942900  | -1.20462600 | 0.74749700  |
| C | 2.65653600  | -0.67766400 | -0.18774500 |
| C | 2.28078100  | 0.54247500  | -0.87999900 |
| C | 1.14093500  | 1.21481000  | -0.60608600 |
| C | 0.26166100  | 0.69187100  | 0.39095400  |
| N | -0.87805100 | 1.25229800  | 0.70833000  |
| C | -1.45598700 | 2.44613100  | 0.09569100  |
| N | -1.83709900 | -1.03444600 | -0.15762000 |
| O | -2.77787100 | -1.49888800 | -0.74253500 |
| O | -0.68399700 | -1.53344500 | -0.29437000 |
| H | -0.01791300 | -0.91292100 | 1.84834200  |
| H | 2.06618200  | -2.10911700 | 1.27914000  |
| H | 2.95982100  | 0.92892900  | -1.62895100 |
| H | 0.90294400  | 2.13870300  | -1.11058600 |
| H | -0.90826700 | 3.33093300  | 0.42214200  |
| H | -1.41638500 | 2.36631300  | -0.98791200 |
| H | -2.48946700 | 2.52250000  | 0.41578400  |
| H | -1.41797900 | 0.82363600  | 1.44896100  |
| C | 3.96461200  | -1.29848900 | -0.52173800 |
| H | 3.98034400  | -1.57994400 | -1.57926800 |
| H | 4.77516100  | -0.57751900 | -0.38282400 |
| H | 4.16400800  | -2.18105000 | 0.08053800  |



**TS1Hb**

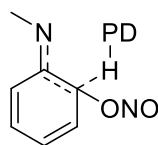
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.47924300  | -0.60148500 | 1.03293900  |
| C | 1.71518400  | -1.21734700 | 0.87060300  |
| C | 2.58536000  | -0.71090400 | -0.07487700 |
| C | 2.25865000  | 0.49362600  | -0.82408100 |
| C | 1.12120000  | 1.17444500  | -0.59970700 |
| C | 0.20419600  | 0.68228300  | 0.39042900  |
| N | -0.90633900 | 1.29724600  | 0.68878000  |
| C | -1.41839300 | 2.51867900  | 0.06708200  |
| N | -1.93145800 | -1.06703200 | -0.14665800 |
| O | -2.82920100 | -1.59295500 | -0.75021200 |
| O | -0.74046300 | -1.49986500 | -0.32327200 |
| H | -0.14999300 | -0.89379900 | 1.86023400  |
| H | 1.94017600  | -2.10783900 | 1.43406000  |
| H | 2.97895700  | 0.82367800  | -1.55970100 |
| H | 0.89889800  | 2.07849100  | -1.14497900 |
| H | -0.71528800 | 3.33612100  | 0.21877200  |
| H | -1.57522000 | 2.35889300  | -0.99834400 |
| H | -2.36394400 | 2.76416700  | 0.53798700  |
| H | -1.50872900 | 0.85562400  | 1.37248800  |
| O | 3.75317100  | -1.21203300 | -0.39126800 |
| C | 4.21476900  | -2.42477300 | 0.24266900  |
| H | 5.18069000  | -2.62999600 | -0.20403900 |
| H | 4.31715300  | -2.26515900 | 1.31525100  |
| H | 3.51752500  | -3.23570400 | 0.03523600  |



**TS1Hd**

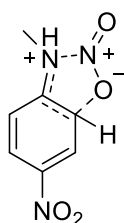
|   |            |             |            |
|---|------------|-------------|------------|
| C | 0.56574600 | -0.60109600 | 0.98418600 |
|---|------------|-------------|------------|

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 1.81295300  | -1.20587500 | 0.74656800  | H | 0.01479600  | -0.88133600 | 1.87246900  |
| C | 2.61391300  | -0.64311400 | -0.19538300 | H | 2.09757800  | -2.11254500 | 1.24078400  |
| C | 2.28020500  | 0.56244200  | -0.90712400 | H | 2.98269200  | 0.93354800  | -1.64000200 |
| C | 1.13568900  | 1.22280500  | -0.62758700 | H | 0.91397100  | 2.16192700  | -1.10511700 |
| C | 0.26371500  | 0.69385500  | 0.37809700  | H | -0.99246300 | 3.32879500  | 0.48102300  |
| N | -0.87384700 | 1.25390300  | 0.69967800  | H | -1.36724500 | 2.40139900  | -0.99484300 |
| C | -1.45904700 | 2.44603700  | 0.08939200  | H | -2.53379600 | 2.45452900  | 0.34223500  |
| N | -1.83031800 | -1.04547200 | -0.12532100 | H | -1.39956000 | 0.84479200  | 1.46636900  |
| O | -2.77153000 | -1.52228700 | -0.69440400 | N | 3.91023500  | -1.29807100 | -0.52515800 |
| O | -0.67323700 | -1.54421700 | -0.26531100 | O | 4.23931700  | -2.24211600 | 0.16298600  |
| H | -0.00141000 | -0.89834500 | 1.85392800  | O | 4.53660600  | -0.83187400 | -1.45835700 |
| H | 2.10390500  | -2.10690100 | 1.26461400  |   |             |             |             |
| H | 2.97830600  | 0.92497600  | -1.64890500 |   |             |             |             |
| H | 0.89158300  | 2.14544900  | -1.13130600 |   |             |             |             |
| H | -0.92859100 | 3.33404000  | 0.43582700  |   |             |             |             |
| H | -1.40145000 | 2.37722300  | -0.99375000 |   |             |             |             |
| H | -2.49830000 | 2.50428500  | 0.39438700  |   |             |             |             |
| H | -1.40550000 | 0.83152200  | 1.45039900  |   |             |             |             |
| F | 3.77964100  | -1.18349100 | -0.48743200 |   |             |             |             |



TS2

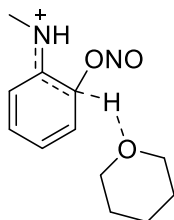
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.80391000  | 0.19094400  | -0.21309200 |
| C | 2.16116800  | 1.24223100  | 0.72553700  |
| C | 1.76521700  | 1.21311800  | 2.02400500  |
| C | 1.00256400  | 0.13131400  | 2.56375900  |
| C | 0.66967800  | -0.91097400 | 1.76189300  |
| C | 0.91087200  | -0.85776600 | 0.34384200  |
| N | 2.08065700  | 0.16002400  | -1.47541100 |
| C | 2.85890500  | 1.24513500  | -2.03819200 |
| H | 2.79786500  | 2.04410100  | 0.38071400  |
| H | 2.06402300  | 2.01830300  | 2.68531900  |
| H | 0.73646700  | 0.12974000  | 3.61180000  |
| H | 0.15529200  | -1.77166300 | 2.16516500  |
| H | -0.21669700 | -0.34431400 | -0.27713100 |
| H | 2.36354200  | 2.22153200  | -1.93109800 |
| H | 3.85354700  | 1.33865100  | -1.58385100 |
| H | 3.00208400  | 1.06518900  | -3.10386800 |
| O | 1.15033200  | -2.11782600 | -0.31291600 |
| N | 0.14849400  | -3.04742300 | -0.40561700 |
| O | -0.88538100 | -2.75022900 | 0.10318800  |
| H | -0.53677300 | 0.07056800  | -2.04007500 |
| C | -1.05396300 | 1.70098800  | -0.89930800 |



TS1He

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.55740500  | -0.59037500 | 0.98438900  |
| C | 1.81259900  | -1.20780300 | 0.72671500  |
| C | 2.61235700  | -0.64539500 | -0.20618200 |
| C | 2.28841000  | 0.56416400  | -0.90061800 |
| C | 1.14652900  | 1.23248100  | -0.60927100 |
| C | 0.27092600  | 0.70655200  | 0.38585100  |
| N | -0.88585800 | 1.24783900  | 0.69284500  |
| C | -1.47981600 | 2.43597200  | 0.08510900  |
| N | -1.78728300 | -1.02803400 | -0.15200000 |
| O | -2.74257300 | -1.46783000 | -0.72068600 |
| O | -0.65883500 | -1.57962400 | -0.21387000 |

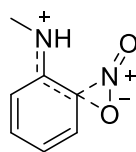
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.71647100 | 1.97428500  | 0.44367500  |
| H | -1.59406200 | 2.21235600  | -1.70359100 |
| H | -0.02385800 | 2.05217400  | -0.90651100 |
| H | -1.75483400 | 3.05309500  | 0.60449500  |
| H | -1.09453300 | 1.55395700  | 1.23777300  |
| N | -1.03896400 | 0.25073100  | -1.17487100 |
| C | -2.38518000 | -0.35139700 | -1.19180400 |
| C | -3.07114800 | -0.12428300 | 0.14880400  |
| H | -2.27828000 | -1.41351000 | -1.40107100 |
| H | -2.97100500 | 0.09858600  | -2.00135200 |
| H | -4.07728300 | -0.54485500 | 0.10704300  |
| H | -2.52445700 | -0.67225600 | 0.91987700  |
| C | -3.11731600 | 1.36333500  | 0.50081700  |
| H | -3.55029800 | 1.50333800  | 1.49281600  |
| H | -3.77107500 | 1.88453100  | -0.20693300 |



**TS2H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.20108000  | 0.73414000  | -2.46227200 |
| C | 1.22948600  | 1.46588800  | -1.31370100 |
| C | 1.36125400  | 0.79999100  | -0.04508700 |
| C | 1.82969700  | -0.57128100 | -0.01538100 |
| C | 1.76283200  | -1.29802000 | -1.22891500 |
| C | 1.45197800  | -0.65664200 | -2.40137100 |
| H | 1.02085700  | 1.21064100  | -3.41470900 |
| H | 1.07443900  | 2.53517800  | -1.32001700 |
| H | 2.02671100  | -2.34475900 | -1.23868500 |
| H | 1.43520300  | -1.23153900 | -3.31808700 |
| N | 2.23223300  | -1.10336600 | 1.13463900  |
| H | 0.03489000  | 0.43601900  | 0.07086300  |
| O | 1.75902700  | 1.52574600  | 1.09188900  |
| N | 0.81964400  | 2.50918100  | 1.67587200  |
| O | -0.16451000 | 2.64581100  | 1.08460900  |

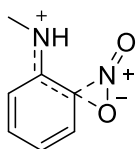
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.62721400  | -2.49156100 | 1.31619000  |
| H | 1.80941100  | -3.16592100 | 1.05797500  |
| H | 3.49833800  | -2.73924700 | 0.70756000  |
| H | 2.88110300  | -2.63843500 | 2.36170800  |
| H | 2.34980200  | -0.46737400 | 1.90853400  |
| C | -1.41215100 | -1.35305100 | 0.40238700  |
| C | -2.11856800 | 0.67044200  | -0.72328800 |
| C | -3.53107600 | 0.38457900  | -0.26343700 |
| C | -2.85059500 | -1.57293300 | 0.82169600  |
| H | -1.90044400 | 1.73501100  | -0.73594700 |
| H | -1.19452400 | -1.84703700 | -0.54568800 |
| H | -0.71309000 | -1.67974400 | 1.16864600  |
| H | -3.72473700 | 0.89041900  | 0.68960500  |
| H | -4.23909200 | 0.74818700  | -1.00670000 |
| H | -3.02369900 | -1.13127100 | 1.81029300  |
| H | -3.05795500 | -2.64111100 | 0.87104700  |
| H | -1.92000700 | 0.23135700  | -1.70220400 |
| O | -1.19360300 | 0.07816800  | 0.23800400  |
| O | -3.73837800 | -1.01330200 | -0.13074800 |



**TS3 (Thermal)**

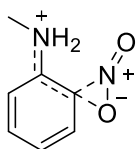
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.25043900  | 2.50734400  | 0.00492100  |
| C | -0.78941300 | 1.62800100  | 0.27700100  |
| C | -0.51356600 | 0.27265700  | 0.24591600  |
| C | 0.76863000  | -0.27215600 | 0.04368600  |
| C | 1.78958800  | 0.64683400  | -0.22379800 |
| C | 1.52812100  | 2.01196800  | -0.24360700 |
| H | 0.05609000  | 3.57029100  | -0.02363500 |
| H | -1.80113300 | 1.96867300  | 0.43965600  |
| H | 2.79318400  | 0.28674200  | -0.39836300 |
| H | 2.33822400  | 2.69780000  | -0.45220400 |
| N | 0.92548400  | -1.62301700 | 0.08865300  |
| H | 0.23216900  | -2.12022800 | 0.62219900  |
| C | 2.21619800  | -2.25980100 | -0.05997000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.07878200  | -3.33726900 | -0.00963900 |
| H | 2.65173100  | -2.01627600 | -1.03030600 |
| H | 2.92255200  | -1.95946400 | 0.72197800  |
| O | -1.54292500 | -0.67429100 | 1.36688000  |
| N | -1.76850000 | -0.75669600 | 0.06207400  |
| O | -2.88853800 | -0.62773800 | -0.37204600 |



**TS3 (Acid)**

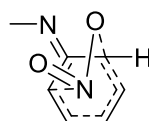
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.02797600  | 2.52979900  | 0.03262100  |
| C | -0.95411500 | 1.55646500  | 0.16293300  |
| C | -0.56292700 | 0.23138500  | 0.09371300  |
| C | 0.77369600  | -0.19719600 | -0.01207700 |
| C | 1.73314500  | 0.81358400  | -0.13769400 |
| C | 1.36005900  | 2.15263000  | -0.11726500 |
| H | -0.25229200 | 3.57377600  | 0.03667400  |
| H | -2.00158000 | 1.80568700  | 0.24536900  |
| H | 2.77526900  | 0.54493700  | -0.23345800 |
| H | 2.12477100  | 2.91138700  | -0.21548500 |
| N | 1.03941700  | -1.53200200 | -0.01677300 |
| H | 0.34559300  | -2.11066500 | 0.42635700  |
| C | 2.38765200  | -2.05407000 | -0.07094300 |
| H | 2.33842800  | -3.14026800 | -0.08437200 |
| H | 2.88763300  | -1.72406200 | -0.98292700 |
| H | 2.99189100  | -1.74104900 | 0.78791000  |
| O | -1.60503400 | -0.85609100 | 1.06499900  |
| N | -1.70523600 | -0.88307800 | -0.25766200 |
| O | -2.78833400 | -0.82117300 | -0.78834900 |



**TS3H**

|   |             |            |            |
|---|-------------|------------|------------|
| C | -0.56139800 | 2.48786200 | 0.05853500 |
|---|-------------|------------|------------|

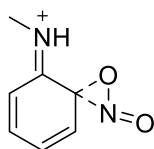
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.32280800 | 1.32239400  | 0.12408600  |
| C | -0.64157700 | 0.12614900  | 0.08771400  |
| C | 0.74393700  | 0.04437700  | 0.02525700  |
| C | 1.48277700  | 1.20723400  | -0.03534900 |
| C | 0.82259600  | 2.43549400  | -0.02019300 |
| H | -1.06950500 | 3.44196800  | 0.07591500  |
| H | -2.40088400 | 1.34679900  | 0.17846100  |
| H | 2.56036200  | 1.17571200  | -0.09335000 |
| H | 1.40078000  | 3.34649500  | -0.06687000 |
| N | 1.32988700  | -1.30225400 | 0.03363200  |
| H | 1.04050900  | -1.76919000 | 0.90067700  |
| C | 2.81895600  | -1.40749300 | -0.10817200 |
| H | 3.07323600  | -2.46294500 | -0.09908900 |
| H | 3.11298800  | -0.95511600 | -1.05000300 |
| H | 3.28562600  | -0.90164700 | 0.73063700  |
| O | -1.42802000 | -1.22312700 | 0.97536700  |
| N | -1.53705000 | -1.25621100 | -0.33719800 |
| O | -2.55223900 | -1.55539000 | -0.87239300 |
| H | 0.88470700  | -1.84274300 | -0.71883800 |



**TS4**

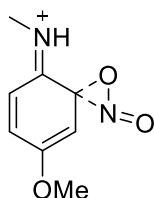
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.78670300  | -1.49057300 | 0.01980900  |
| C | 0.85693500  | -1.62234400 | -1.02971900 |
| C | -0.39930300 | -1.10157800 | -0.91767800 |
| C | -0.81575600 | -0.48118400 | 0.32455200  |
| C | 0.21481700  | -0.23901700 | 1.32194200  |
| C | 1.47906800  | -0.76838100 | 1.16713200  |
| H | 2.77171300  | -1.92382500 | -0.09057000 |
| H | 1.15422200  | -2.12888800 | -1.93797900 |
| H | -0.09036300 | 0.27234300  | 2.22211700  |
| H | 2.22674000  | -0.62017200 | 1.93310200  |
| N | -2.01626300 | -0.11500700 | 0.65138100  |
| O | 0.15497600  | 2.03379500  | 0.15590500  |
| N | 0.87784000  | 1.76461700  | -0.80311500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.06419000  | 1.52162400  | -0.66453300 |
| H | -1.10125800 | -1.20523500 | -1.72973000 |
| C | -3.13472700 | -0.26242600 | -0.23054300 |
| H | -3.52288900 | 0.74172200  | -0.43235500 |
| H | -2.95281400 | -0.77193900 | -1.17820600 |
| H | -3.92891400 | -0.78262200 | 0.31264300  |



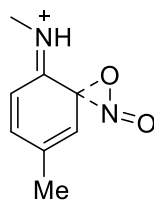
**TS4'H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.22078100  | -1.13198700 | -0.03785700 |
| C | 1.31259800  | -1.43221900 | -1.07176000 |
| C | -0.02991500 | -1.21223100 | -0.91636700 |
| C | -0.51260700 | -0.70787300 | 0.32723300  |
| C | 0.43314100  | -0.33704200 | 1.35104100  |
| C | 1.77821700  | -0.56431000 | 1.15293500  |
| H | 3.27337700  | -1.33339000 | -0.17921700 |
| H | 1.68274700  | -1.84315700 | -2.00056600 |
| H | 0.06400200  | 0.03871000  | 2.29522400  |
| H | 2.48348700  | -0.31209700 | 1.93170900  |
| N | -1.80951500 | -0.55689500 | 0.56622700  |
| O | -0.61780300 | 2.01896600  | 0.49542100  |
| N | -0.04378500 | 2.13683800  | -0.53877200 |
| O | 1.09831400  | 2.20037000  | -0.83610100 |
| H | -0.72222400 | -1.45275600 | -1.70828800 |
| C | -2.88499800 | -0.80472300 | -0.37735900 |
| H | -2.78571200 | -0.14155000 | -1.24086900 |
| H | -2.86815900 | -1.84014100 | -0.71789500 |
| H | -3.82929300 | -0.60700100 | 0.11887300  |
| H | -2.07250600 | -0.18058800 | 1.46708900  |



**TS4'Hb**

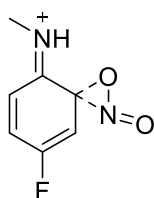
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.71783100  | -0.53282200 | -0.15748800 |
| C | 0.83743400  | -1.05203400 | -1.15623800 |
| C | -0.49262200 | -1.15675100 | -0.92346600 |
| C | -1.02136400 | -0.76382900 | 0.34980000  |
| C | -0.12761900 | -0.19231400 | 1.33291400  |
| C | 1.21064200  | -0.10348400 | 1.08797900  |
| H | 1.26831600  | -1.34365400 | -2.10349100 |
| H | -0.53300600 | 0.10199000  | 2.29059100  |
| H | 1.86565300  | 0.30596400  | 1.84067500  |
| N | -2.29544700 | -0.91070600 | 0.64915300  |
| O | -1.78421200 | 1.81795700  | 0.49553900  |
| N | -1.32741000 | 2.05355700  | -0.61076600 |
| O | -0.19143000 | 2.41798000  | -0.82024300 |
| H | -1.15115400 | -1.54673300 | -1.68379800 |
| C | -3.33818900 | -1.39959800 | -0.23893900 |
| H | -3.49786000 | -0.68816300 | -1.05267000 |
| H | -3.06570700 | -2.36876100 | -0.65310500 |
| H | -4.25477100 | -1.50025000 | 0.33298200  |
| H | -2.59850400 | -0.54908900 | 1.54407600  |
| O | 2.97830800  | -0.48430400 | -0.50555400 |
| C | 3.98177500  | 0.04623700  | 0.38895100  |
| H | 4.91750400  | -0.04925600 | -0.14962400 |
| H | 3.77116900  | 1.09322900  | 0.60102300  |
| H | 4.00970100  | -0.54072700 | 1.30561800  |



**TS4'Hc**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.10310000  | -0.46736600 | 0.04033000  |
| C | 1.30690900  | -0.94946400 | -1.03128400 |
| C | -0.04296000 | -1.10665300 | -0.91239100 |
| C | -0.67607300 | -0.80550600 | 0.33149800  |
| C | 0.11985200  | -0.26229000 | 1.40355100  |
| C | 1.47460100  | -0.11998500 | 1.24450200  |
| H | 1.78916200  | -1.19477800 | -1.96816100 |

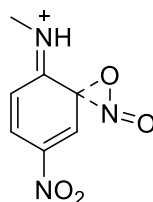
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.35683000 | -0.03941800 | 2.34829900  |
| H | 2.06804300  | 0.26568400  | 2.06203900  |
| N | -1.97228200 | -0.99747800 | 0.52192000  |
| O | -1.50307600 | 1.76116300  | 0.53751700  |
| N | -1.01639000 | 2.05529100  | -0.51490400 |
| O | 0.06781000  | 2.45212500  | -0.79785800 |
| H | -0.62774200 | -1.48312100 | -1.73743300 |
| C | -2.92514900 | -1.43949000 | -0.48094900 |
| H | -3.00492800 | -0.69100500 | -1.27459600 |
| H | -2.61488800 | -2.38901700 | -0.91586600 |
| H | -3.89330100 | -1.56184400 | -0.00625100 |
| H | -2.34968900 | -0.72382100 | 1.41917800  |
| C | 3.56616000  | -0.28779000 | -0.14110800 |
| H | 3.99623900  | -1.08631300 | -0.74664700 |
| H | 3.74827800  | 0.64962700  | -0.68243900 |
| H | 4.08984400  | -0.22572900 | 0.81059700  |



**TS4'He**

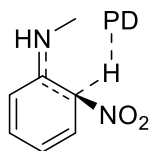
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.10577700  | -0.42349800 | 0.02225800  |
| C | 1.35967100  | -0.93409800 | -1.05484000 |
| C | 0.01342700  | -1.10637100 | -0.91205500 |
| C | -0.61092700 | -0.79367900 | 0.33614400  |
| C | 0.17901700  | -0.21076800 | 1.39367500  |
| C | 1.53104800  | -0.04776300 | 1.23287100  |
| H | 1.86756400  | -1.17548100 | -1.97779100 |
| H | -0.29629900 | 0.02224300  | 2.33609000  |
| H | 2.14982500  | 0.36096200  | 2.01838600  |
| N | -1.90047000 | -1.01057800 | 0.54219200  |
| O | -1.51058000 | 1.74007100  | 0.53659300  |
| N | -1.05556100 | 2.01887400  | -0.53781400 |
| O | 0.02211500  | 2.44530700  | -0.82646900 |
| H | -0.57538700 | -1.50231300 | -1.72468400 |
| C | -2.85149700 | -1.50303100 | -0.43892600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.98132200 | -0.76382100 | -1.23518800 |
| H | -2.50531800 | -2.44022400 | -0.87305400 |
| H | -3.80312000 | -1.66631300 | 0.05602000  |
| H | -2.27705000 | -0.72356000 | 1.43620000  |
| F | 3.40688300  | -0.28192700 | -0.13582000 |



**TS4'He**

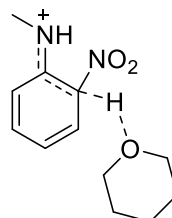
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.41954600  | -0.43496900 | 0.15409600  |
| C | 0.71975000  | -1.26266800 | -0.74086000 |
| C | -0.63912800 | -1.36811000 | -0.64756100 |
| C | -1.32927100 | -0.66259200 | 0.38024800  |
| C | -0.59019100 | 0.23825300  | 1.23526000  |
| C | 0.78443700  | 0.32399000  | 1.11955500  |
| H | 1.27146900  | -1.80670800 | -1.49247200 |
| H | -1.10407500 | 0.74563000  | 2.03942000  |
| H | 1.35893700  | 0.96369800  | 1.77150000  |
| N | -2.63089600 | -0.80958400 | 0.57943500  |
| O | -2.07777300 | 2.05214300  | -0.11940800 |
| N | -1.12733800 | 2.15125700  | -0.88085000 |
| O | 0.07536900  | 2.38034600  | -0.79874800 |
| H | -1.18193700 | -2.00514900 | -1.32817400 |
| C | -3.52071200 | -1.68116800 | -0.17188600 |
| H | -3.54036300 | -1.38639000 | -1.22261900 |
| H | -3.19027300 | -2.71801500 | -0.09682700 |
| H | -4.51875100 | -1.59008800 | 0.24340300  |
| H | -3.04986700 | -0.26782800 | 1.32466900  |
| N | 2.88624400  | -0.35585900 | 0.04102600  |
| O | 3.42725000  | -1.14757600 | -0.71097500 |
| O | 3.44917900  | 0.49605300  | 0.70547000  |



**TS5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.31461500 | 0.63417500  | -0.10065200 |
| C | -1.20534300 | 1.16011400  | -1.12637200 |
| C | -1.97144500 | 0.37357200  | -1.90929800 |
| C | -1.98935400 | -1.05788300 | -1.74822000 |
| C | -1.24083600 | -1.63345400 | -0.79065800 |
| C | -0.30698800 | -0.85546200 | 0.02953700  |
| N | 0.46427600  | 1.47910900  | 0.48275700  |
| C | 1.44391900  | 1.07495100  | 1.45492600  |
| H | -1.21449900 | 2.23721600  | -1.22809500 |
| H | -2.60834500 | 0.82209000  | -2.66164600 |
| H | -2.63719500 | -1.65990900 | -2.37093500 |
| H | -1.28175100 | -2.69802900 | -0.60429000 |
| H | 0.90576100  | -1.27242900 | -0.47909300 |
| H | 1.03348800  | 1.13168300  | 2.46764800  |
| H | 1.81978100  | 0.05208700  | 1.33044200  |
| H | 2.29283900  | 1.75969200  | 1.40138100  |
| N | -0.22375900 | -1.43285800 | 1.37966100  |
| O | -0.50716700 | -0.75206500 | 2.35370400  |
| O | 0.14397700  | -2.61067500 | 1.45662800  |
| C | 3.23454400  | -1.03992000 | -0.90889300 |
| C | 3.07126600  | 0.19539600  | -1.78328200 |
| C | 2.71768300  | -0.19300200 | -3.21992800 |
| C | 1.49590400  | -1.11256200 | -3.24838300 |
| C | 1.69364900  | -2.32014500 | -2.34217500 |
| H | 2.52803000  | 0.70166300  | -3.81484100 |
| H | 2.28753600  | 0.83172100  | -1.36553400 |
| H | 3.99860000  | 0.76991400  | -1.75496100 |
| H | 4.08814800  | -1.63638600 | -1.24906900 |
| H | 3.40879500  | -0.77046000 | 0.13127100  |
| H | 0.60913000  | -0.56335900 | -2.92450000 |
| H | 1.29809600  | -1.46400400 | -4.26244200 |
| H | 0.79136600  | -2.92771000 | -2.29201900 |
| H | 2.50884900  | -2.94991300 | -2.71425200 |

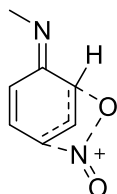
|   |            |             |             |
|---|------------|-------------|-------------|
| H | 2.10493400 | -2.67637100 | -0.35147400 |
| H | 3.56962200 | -0.70554800 | -3.67913700 |
| N | 2.01476000 | -1.87421500 | -0.96812400 |



**TS5H**

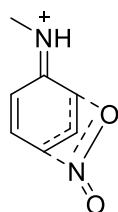
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.88299300  | 0.27534000  | -0.47030500 |
| C | 2.30039700  | 1.62411500  | -0.28151400 |
| C | 2.11926900  | 2.26364400  | 0.90878700  |
| C | 1.50759900  | 1.63078500  | 2.02596800  |
| C | 1.06404200  | 0.36057100  | 1.90484400  |
| C | 1.08952600  | -0.31515800 | 0.61934000  |
| N | 2.12986300  | -0.36175500 | -1.59802300 |
| C | 2.83180300  | 0.19967800  | -2.74444300 |
| N | 0.97555300  | -1.80035000 | 0.70973000  |
| O | 1.13562300  | -2.45467400 | -0.31898700 |
| O | 0.66083700  | -2.28183000 | 1.77603900  |
| H | 2.81561700  | 2.12395700  | -1.08685700 |
| H | 2.48096400  | 3.27814900  | 1.01421700  |
| H | 1.42832700  | 2.15425400  | 2.96729000  |
| H | 0.62237400  | -0.17178300 | 2.73295400  |
| H | -0.13737400 | -0.05737500 | 0.17226000  |
| H | 1.84114100  | -1.33158900 | -1.63045800 |
| H | 2.29148300  | 1.05648200  | -3.14790500 |
| H | 3.84293800  | 0.50587100  | -2.47532600 |
| H | 2.89078600  | -0.56908300 | -3.50870400 |
| C | -1.97009700 | 1.33532200  | 0.12918200  |
| C | -2.18922700 | -1.07479400 | -0.02348500 |
| C | -3.53904700 | -0.86762400 | -0.67307500 |
| C | -3.32991500 | 1.45441400  | -0.52561000 |
| H | -1.66812900 | -1.93256700 | -0.44220200 |
| H | -2.05320200 | 1.31561000  | 1.21750900  |
| H | -1.30269100 | 2.13408400  | -0.18587400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.43081100 | -0.84410300 | -1.76390100 |
| H | -4.20251600 | -1.68777800 | -0.40249700 |
| H | -3.21498000 | 1.54920500  | -1.61203500 |
| H | -3.83993800 | 2.33920200  | -0.14670800 |
| H | -2.27968900 | -1.17472800 | 1.05966100  |
| O | -1.34646500 | 0.08859100  | -0.30705100 |
| O | -4.13724700 | 0.33283700  | -0.21228100 |



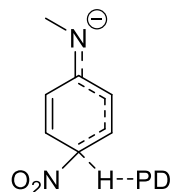
**TS6**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.24657000  | 1.78371100  | -0.01599000 |
| C | 0.97724500  | 1.21817200  | 1.20292300  |
| C | -0.05915200 | 0.29345600  | 1.27694300  |
| C | -1.07490600 | 0.21119000  | 0.22796200  |
| C | -0.77632400 | 0.89563500  | -1.02091700 |
| C | 0.35668300  | 1.62092200  | -1.13141900 |
| H | 2.12368600  | 2.40438800  | -0.14297500 |
| H | 1.65387700  | 1.34690300  | 2.03525800  |
| H | -1.45594600 | 0.81969300  | -1.85516100 |
| H | 0.60240600  | 2.11262400  | -2.06300000 |
| N | -2.12599400 | -0.47597100 | 0.52178500  |
| H | -0.28195400 | -0.23735400 | 2.18982200  |
| O | 1.01337800  | -1.41064000 | 0.42963000  |
| N | 1.94828800  | -0.96469800 | -0.27697500 |
| O | 2.64629400  | -1.74740400 | -0.90068600 |
| C | -3.19751400 | -0.68345800 | -0.41245300 |
| H | -3.09810900 | -0.20086500 | -1.38640700 |
| H | -3.30437500 | -1.76224900 | -0.55904200 |
| H | -4.12634700 | -0.35055300 | 0.05875600  |



**TS6H**

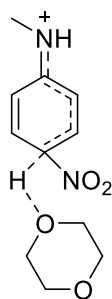
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.78605900  | 2.42127100  | -0.08761000 |
| C | -0.42348400 | 1.80099800  | -0.06653000 |
| C | -0.43547000 | 0.42125500  | 0.19999900  |
| C | 0.77475400  | -0.37819000 | -0.03745300 |
| C | 2.02081200  | 0.30075400  | -0.16126300 |
| C | 2.01692600  | 1.65431000  | -0.11203600 |
| H | 0.85467800  | 3.49929600  | -0.13377400 |
| H | -1.34924500 | 2.35618600  | -0.06021500 |
| H | 2.94158000  | -0.25378000 | -0.25149200 |
| H | 2.95347800  | 2.19417100  | -0.14238900 |
| N | 0.66220100  | -1.68128600 | -0.04151300 |
| H | -1.37535500 | -0.10849400 | 0.27111900  |
| O | -0.08809700 | 0.34902500  | 2.15851300  |
| N | 0.64024200  | 1.34054700  | 2.46687900  |
| O | 0.96462000  | 1.52330000  | 3.60449900  |
| C | 1.76185200  | -2.63630900 | -0.16034100 |
| H | 2.26562500  | -2.51135000 | -1.11820700 |
| H | 2.47363800  | -2.48894300 | 0.65090700  |
| H | 1.34879900  | -3.63717100 | -0.09922700 |
| H | -0.26621000 | -2.07135800 | 0.06480800  |



**TS7**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.03371200  | -0.96860400 | -1.14702700 |
| C | -1.18312500 | -0.40452500 | -1.18005100 |
| C | -1.60407600 | 0.55449000  | -0.15287300 |
| C | -0.52739200 | 1.12552000  | 0.66940200  |
| C | 0.68535000  | 0.55757900  | 0.69275000  |

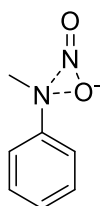
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.04466100  | -0.57216900 | -0.16299300 |
| N | 2.20911600  | -1.10407800 | -0.01616300 |
| C | 2.58862800  | -2.21994500 | -0.86602700 |
| N | -2.64420800 | 1.50020200  | -0.57378100 |
| O | -2.79794800 | 2.52890700  | 0.08117200  |
| O | -3.38655500 | 1.17959100  | -1.50010300 |
| H | 0.28536600  | -1.72086800 | -1.88026400 |
| H | -1.91264200 | -0.69587900 | -1.92160100 |
| H | -2.23976800 | -0.16425300 | 0.66552300  |
| H | -0.76987000 | 1.96066200  | 1.30943200  |
| H | 1.45831500  | 0.92903000  | 1.35315700  |
| H | 1.87490600  | -3.05021800 | -0.81653800 |
| H | 2.67467400  | -1.92316600 | -1.91781200 |
| H | 3.56114500  | -2.59416600 | -0.54802600 |
| C | -3.92854900 | -1.89749500 | 1.11822300  |
| C | -5.11744200 | -0.98362400 | 0.85011400  |
| C | -5.51717500 | -0.21782800 | 2.11204600  |
| C | -4.31724500 | 0.52732000  | 2.69807700  |
| C | -3.14705800 | -0.41968500 | 2.92994400  |
| H | -6.32507200 | 0.48149900  | 1.88977300  |
| H | -4.86121600 | -0.27963200 | 0.05365500  |
| H | -5.95003200 | -1.58732300 | 0.48468900  |
| H | -4.22050900 | -2.69205500 | 1.81534900  |
| H | -3.58195800 | -2.37119500 | 0.19944000  |
| H | -4.00809900 | 1.32610800  | 2.01839300  |
| H | -4.58120000 | 0.99999600  | 3.64572500  |
| H | -2.26109800 | 0.12291100  | 3.26039800  |
| H | -3.40579100 | -1.14603200 | 3.70967300  |
| H | -2.01677000 | -1.74767300 | 1.84910000  |
| H | -5.90199800 | -0.92330800 | 2.85591000  |
| N | -2.80432200 | -1.12930200 | 1.68390600  |



**TS7H**

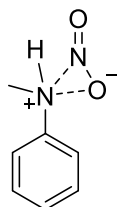
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.31144700  | -0.28752500 | -0.95739700 |
| C | 1.25237900  | 0.52797700  | -1.18567200 |
| C | 0.57040900  | 1.16559500  | -0.09061300 |
| C | 1.21512700  | 1.15803000  | 1.19869500  |
| C | 2.27147300  | 0.34526900  | 1.42466100  |
| C | 2.84183600  | -0.42722500 | 0.36275300  |
| N | 3.86613400  | -1.22793400 | 0.61780800  |
| C | 4.57023600  | -2.04995300 | -0.35728300 |
| N | -0.25429700 | 2.36260200  | -0.42633200 |
| O | -0.53765800 | 3.12174100  | 0.48226900  |
| O | -0.64442500 | 2.46238800  | -1.57672300 |
| H | 2.77843100  | -0.80406300 | -1.78191400 |
| H | 0.86753800  | 0.67507600  | -2.18432700 |
| H | -0.43153200 | 0.30794900  | 0.10227300  |
| H | 0.80172400  | 1.77215600  | 1.98489300  |
| H | 2.72030000  | 0.29258900  | 2.40808000  |
| H | 4.19839900  | -1.26083500 | 1.56939600  |
| H | 3.89229100  | -2.76814900 | -0.81950500 |
| H | 5.02415500  | -1.43194600 | -1.13220500 |
| H | 5.35505400  | -2.59300300 | 0.16035100  |
| C | -1.83611400 | -1.12821300 | -1.00121600 |
| C | -2.57999600 | 0.11369100  | 0.93880600  |
| C | -3.62821300 | -0.95298200 | 1.16913400  |
| C | -2.91000900 | -2.15387700 | -0.70642300 |
| H | -2.19344800 | 0.51294100  | 1.87363200  |
| H | -2.20124400 | -0.35290500 | -1.67729100 |
| H | -0.93634000 | -1.58802100 | -1.40395700 |
| H | -3.24160800 | -1.71540800 | 1.85592800  |
| H | -4.51794500 | -0.50218300 | 1.60641600  |
| H | -2.49888900 | -2.95842000 | -0.08480500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.27426300 | -2.58021000 | -1.64015100 |
| H | -2.96436300 | 0.92011900  | 0.31207700  |
| O | -1.44193200 | -0.49866500 | 0.25495500  |
| O | -4.01536000 | -1.54723500 | -0.05924200 |



**TS8**

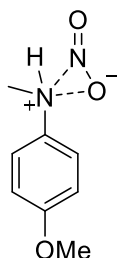
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.91451200  | -0.76491000 | 0.96420900  |
| C | 2.12874700  | -1.28226700 | 0.57907700  |
| C | 2.91036900  | -0.59559500 | -0.35142300 |
| C | 2.47378000  | 0.62196900  | -0.89846500 |
| C | 1.26308400  | 1.15207100  | -0.53451200 |
| C | 0.44016800  | 0.47453800  | 0.42483200  |
| N | -0.72841700 | 0.90003200  | 0.88011700  |
| C | -1.27666700 | 2.13822600  | 0.39519000  |
| H | 0.27078400  | -1.27362200 | 1.66607000  |
| H | 2.47558400  | -2.22114700 | 0.98834100  |
| H | 3.86304300  | -1.00566500 | -0.65978500 |
| H | 3.09899700  | 1.13825700  | -1.61465000 |
| H | 0.93082800  | 2.08646500  | -0.96179300 |
| H | -0.64462000 | 2.97566700  | 0.72037400  |
| H | -1.34276000 | 2.18204500  | -0.69642200 |
| H | -2.27172400 | 2.27073000  | 0.80975600  |
| O | -1.85316200 | -1.74850400 | 0.10368300  |
| N | -2.22434700 | -0.96711400 | -0.74753100 |
| O | -3.08856500 | -0.12477800 | -0.60009500 |



**TS8H**

|   |            |             |            |
|---|------------|-------------|------------|
| C | 1.07600500 | -1.12378900 | 0.66809100 |
|---|------------|-------------|------------|

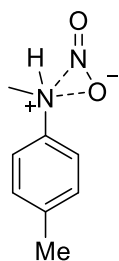
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.35387100  | -1.40319100 | 0.25405500  |
| C | 3.10018500  | -0.42878400 | -0.41903200 |
| C | 2.55583800  | 0.84038300  | -0.66961500 |
| C | 1.28049700  | 1.14421500  | -0.26383300 |
| C | 0.51794000  | 0.16339000  | 0.42327700  |
| N | -0.73654600 | 0.41557600  | 0.84227400  |
| C | -1.38833700 | 1.71822400  | 0.82382600  |
| H | 0.48125200  | -1.87038100 | 1.17842200  |
| H | 2.78127000  | -2.37799600 | 0.44054900  |
| H | 4.10275700  | -0.65628200 | -0.75358900 |
| H | 3.14583700  | 1.58372700  | -1.18681100 |
| H | 0.86296600  | 2.12069400  | -0.45733300 |
| H | -0.80876500 | 2.43693800  | 1.40721100  |
| H | -1.48744600 | 2.08612600  | -0.19668100 |
| H | -2.37761400 | 1.61165000  | 1.25646800  |
| H | -1.16493900 | -0.29426200 | 1.42089700  |
| O | -1.71570100 | -1.85113200 | -0.75056100 |
| N | -2.25123500 | -0.92096000 | -1.24481700 |
| O | -3.17104800 | -0.22866500 | -0.98042800 |



**TS8Hb**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.96723100 | -0.82262700 | -0.96569800 |
| C | -2.18862800 | -1.31030000 | -0.60801200 |
| C | -2.98273900 | -0.58702800 | 0.31464000  |
| C | -2.51245700 | 0.64635400  | 0.85061000  |
| C | -1.29709300 | 1.13588500  | 0.49347900  |
| C | -0.48757600 | 0.41497700  | -0.43476000 |
| N | 0.71525000  | 0.85480400  | -0.80197400 |
| C | 1.31386500  | 2.12973800  | -0.42779800 |
| H | -0.34184000 | -1.37418700 | -1.65398400 |
| H | -2.53482200 | -2.24649700 | -1.01716000 |

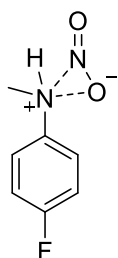
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.14821400 | 1.17080200  | 1.54974400  |
| H | -0.94508100 | 2.06658100  | 0.91185600  |
| H | 0.66307200  | 2.95104400  | -0.73064200 |
| H | 1.48154700  | 2.17603000  | 0.64754500  |
| H | 2.26878900  | 2.21635500  | -0.93431700 |
| H | 1.21395000  | 0.30327500  | -1.48765300 |
| O | 1.83915400  | -1.71877100 | -0.09186000 |
| N | 2.35203300  | -0.95126900 | 0.67954400  |
| O | 3.30776500  | -0.24347600 | 0.53293300  |
| O | -4.15949700 | -0.97326600 | 0.74473300  |
| C | -4.74760800 | -2.21271500 | 0.29487500  |
| H | -4.11047300 | -3.04996400 | 0.57678600  |
| H | -5.70067600 | -2.27517200 | 0.80731900  |
| H | -4.89850300 | -2.18393600 | -0.78323700 |



**TS8Hc**

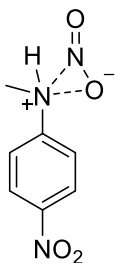
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.05756200 | -0.81707500 | -0.90941700 |
| C | -2.29389300 | -1.25238800 | -0.51775800 |
| C | -3.05693200 | -0.52585800 | 0.41683000  |
| C | -2.51916100 | 0.67342800  | 0.94523900  |
| C | -1.28763500 | 1.13143600  | 0.57146200  |
| C | -0.52861800 | 0.39708000  | -0.38191100 |
| N | 0.67756100  | 0.81248400  | -0.79186400 |
| C | 1.30110800  | 2.08453900  | -0.45270300 |
| H | -0.47036000 | -1.38550500 | -1.61811500 |
| H | -2.69198300 | -2.17184300 | -0.92432200 |
| H | -3.10244600 | 1.23682500  | 1.66132200  |
| H | -0.89816400 | 2.04829000  | 0.98747700  |
| H | 0.67174400  | 2.91162400  | -0.78639100 |
| H | 1.45574000  | 2.16202300  | 0.62259900  |
| H | 2.26307200  | 2.13644200  | -0.95108900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.10636100  | 0.28268200  | -1.53877400 |
| O | 1.89937700  | -1.76643700 | -0.09515700 |
| N | 2.42175200  | -0.98947400 | 0.64035800  |
| O | 3.30683800  | -0.20778700 | 0.50596600  |
| C | -4.39276300 | -1.00099900 | 0.85952200  |
| H | -4.36629300 | -1.25670300 | 1.92445200  |
| H | -5.13670100 | -0.20620800 | 0.75729200  |
| H | -4.72258000 | -1.87439000 | 0.30236600  |



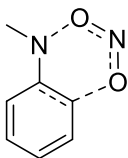
**TS8Hd**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.06768200 | -0.82620000 | -0.90987200 |
| C | -2.30466400 | -1.26048300 | -0.51786800 |
| C | -3.01656300 | -0.49316400 | 0.40822200  |
| C | -2.51849200 | 0.69981500  | 0.94740400  |
| C | -1.28216000 | 1.13959000  | 0.55656400  |
| C | -0.53350900 | 0.38945000  | -0.39160900 |
| N | 0.67916900  | 0.79392900  | -0.80665900 |
| C | 1.29828400  | 2.07521900  | -0.49354200 |
| H | -0.48634800 | -1.40199400 | -1.61712300 |
| H | -2.73459500 | -2.17600400 | -0.89787900 |
| H | -3.11702100 | 1.24964000  | 1.65937400  |
| H | -0.88564800 | 2.05748800  | 0.96243200  |
| H | 0.66756700  | 2.89358900  | -0.84636500 |
| H | 1.45106700  | 2.17744500  | 0.58011400  |
| H | 2.26117300  | 2.11961600  | -0.99102600 |
| H | 1.09536100  | 0.26346500  | -1.56011700 |
| O | 1.87263100  | -1.75995400 | 0.00974000  |
| N | 2.41559300  | -0.96501400 | 0.70173300  |
| O | 3.29508900  | -0.18697100 | 0.55063200  |
| F | -4.20751000 | -0.91031400 | 0.79665800  |



**TS8He**

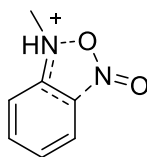
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.01284000  | -0.55993700 | 1.17821600  |
| C | 1.34013000  | -0.79942400 | 0.92308100  |
| C | 2.01673100  | 0.04434200  | 0.04462900  |
| C | 1.39623600  | 1.12695400  | -0.57825500 |
| C | 0.06940300  | 1.37719800  | -0.32462400 |
| C | -0.64437200 | 0.53965000  | 0.56665100  |
| N | -1.95462900 | 0.75067900  | 0.83740300  |
| C | -2.70025000 | 1.94603700  | 0.46153800  |
| H | -0.53972500 | -1.20767100 | 1.84604400  |
| H | 1.86202400  | -1.62492600 | 1.38188100  |
| H | 1.96547600  | 1.75265800  | -1.24816600 |
| H | -0.41709500 | 2.21671700  | -0.79644100 |
| H | -2.25264800 | 2.83195000  | 0.91830200  |
| H | -2.70951600 | 2.07321500  | -0.61975200 |
| H | -3.72122800 | 1.83708300  | 0.81258100  |
| H | -2.33696500 | 0.21515300  | 1.60538100  |
| O | -2.54750400 | -1.93990500 | -0.27834500 |
| N | -3.15511100 | -1.23249600 | -0.97907000 |
| O | -4.11091000 | -0.56423700 | -1.00823000 |
| N | 3.43890000  | -0.21796600 | -0.23986500 |
| O | 3.95432400  | -1.16775600 | 0.32405000  |
| O | 3.99943900  | 0.53317600  | -1.01942800 |



**TS9**

|   |            |             |            |
|---|------------|-------------|------------|
| C | 0.76832600 | -0.29930200 | 1.18535300 |
| C | 2.07427300 | -0.65582600 | 0.88966200 |

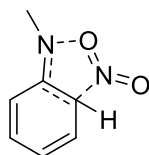
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.68409700  | -0.10903100 | -0.22345900 |
| C | 2.00968300  | 0.80560600  | -1.06582300 |
| C | 0.72986700  | 1.18367100  | -0.78692100 |
| C | 0.07795700  | 0.67333600  | 0.38633700  |
| N | -1.13639100 | 0.95665200  | 0.79569000  |
| C | -1.99338900 | 1.86029700  | 0.09417100  |
| H | 0.24788800  | -0.68027200 | 2.04909700  |
| H | 2.59777000  | -1.37142600 | 1.50691400  |
| H | 3.70141000  | -0.38853100 | -0.46613900 |
| H | 2.51988700  | 1.20044800  | -1.93353500 |
| H | 0.21857400  | 1.88588100  | -1.42699400 |
| H | -1.98124000 | 2.80080400  | 0.65968900  |
| H | -1.74367700 | 2.05656400  | -0.94888100 |
| H | -3.00835100 | 1.47063600  | 0.16251600  |
| O | -2.18667500 | -0.94952500 | -0.19373000 |
| N | -1.31839900 | -1.61981700 | -0.81134000 |
| O | -0.38061300 | -2.04261700 | -0.08411400 |



**TS9H**

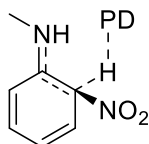
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.77335100  | -0.48875200 | 1.21393100  |
| C | 2.01892100  | -1.02053100 | 0.97041400  |
| C | 2.75777300  | -0.56889800 | -0.12407700 |
| C | 2.25424500  | 0.41553800  | -0.98163400 |
| C | 1.01336900  | 0.96287100  | -0.75305100 |
| C | 0.27591100  | 0.52464800  | 0.36596100  |
| N | -0.97625800 | 1.00895400  | 0.63063100  |
| C | -1.46456800 | 2.31641300  | 0.17298300  |
| N | -1.56738300 | -1.05277700 | -0.66448300 |
| O | -2.19709600 | -1.87299200 | -1.25363500 |
| O | -2.26102900 | -0.04874900 | -0.17690000 |
| H | 0.17488500  | -0.83260000 | 2.04829000  |
| H | 2.41771900  | -1.78782600 | 1.61774300  |
| H | 3.73416800  | -0.99205400 | -0.31791600 |
| H | 2.83917900  | 0.74302300  | -1.82903600 |

|   |             |            |             |   |             |             |             |
|---|-------------|------------|-------------|---|-------------|-------------|-------------|
| H | 0.62022700  | 1.71663900 | -1.41760500 | C | -0.86551400 | 2.73974900  | 1.05555600  |
| H | -0.87577500 | 3.08768100 | 0.66969500  | C | -0.85678500 | 2.75187600  | -0.38005600 |
| H | -1.36220900 | 2.39100200 | -0.90344500 | C | -1.04335900 | 1.59804000  | -1.05526700 |
| H | -2.50946200 | 2.39694000 | 0.45321600  | C | -1.10650700 | 0.32510900  | -0.35979100 |
| H | -1.31920900 | 0.76321700 | 1.55659300  | N | -1.22286200 | -0.83834800 | 1.72660200  |



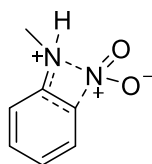
**TS10**

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.32407000  | 0.65213600  | 0.37173000  | H | -1.09109300 | 1.65038700  | 2.84596000  |
| C | 1.08369400  | 1.05316400  | -0.75877300 | H | -0.76209100 | 3.68227400  | 1.58042100  |
| C | 2.27109900  | 0.42280100  | -1.04439900 | H | -0.74831700 | 3.68857300  | -0.90898500 |
| C | 2.71417600  | -0.64704200 | -0.25260100 | H | -1.10775300 | 1.57748700  | -2.13480700 |
| C | 1.97086100  | -1.08019300 | 0.83511400  | H | 0.09778400  | -0.23505800 | -0.57058100 |
| C | 0.78447300  | -0.43783200 | 1.15063900  | H | -0.24109000 | -0.45122600 | 3.57101100  |
| N | -0.85951400 | 1.16844700  | 0.75006600  | H | -2.00333300 | -0.32980100 | 3.64096800  |
| C | -1.42603900 | 2.28673000  | 0.04690000  | H | -1.23426400 | -1.91121100 | 3.50518300  |
| N | -1.52837200 | -1.26602700 | -0.10568200 | N | -1.92278800 | -0.65907900 | -1.10673800 |
| O | -2.08719500 | -2.25588000 | -0.54414900 | O | -2.91518600 | -1.15004700 | -0.60686600 |
| O | -2.14707300 | -0.18107500 | -0.06671900 | O | -1.52287200 | -0.93229800 | -2.24401800 |
| H | 0.74642700  | 1.87103300  | -1.37762800 | C | 1.87226100  | -1.48830500 | 0.36276600  |
| H | 2.86598100  | 0.74576700  | -1.88821300 | C | 2.38956300  | -0.35526200 | 1.23776800  |
| H | 3.64760300  | -1.13752800 | -0.49652000 | C | 3.32802000  | 0.56376900  | 0.45520900  |
| H | 2.31555100  | -1.91019800 | 1.43612200  | C | 2.64443500  | 1.07344600  | -0.81399100 |
| H | 0.19617900  | -0.72515300 | 2.00914800  | C | 2.12349000  | -0.08220300 | -1.65885600 |
| H | -0.97338600 | 3.19040200  | 0.47022700  | H | 3.64014500  | 1.40389200  | 1.07791300  |
| H | -1.27522100 | 2.28471700  | -1.03459300 | H | 1.54189400  | 0.22021000  | 1.61612200  |
| H | -2.49185500 | 2.32193500  | 0.26314800  | H | 2.89749200  | -0.78399200 | 2.10334800  |
|   |             |             |             | H | 2.69967600  | -2.14584700 | 0.07084600  |
|   |             |             |             | H | 1.12223900  | -2.07770000 | 0.88624600  |
|   |             |             |             | H | 1.80955300  | 1.72641200  | -0.54756600 |
|   |             |             |             | H | 3.33473800  | 1.66616700  | -1.41679900 |
|   |             |             |             | H | 1.55026900  | 0.27717900  | -2.51349700 |
|   |             |             |             | H | 2.95962600  | -0.67982300 | -2.03896500 |
|   |             |             |             | H | 0.86938000  | -1.69555700 | -1.43036100 |
|   |             |             |             | H | 4.23598000  | 0.01401500  | 0.18487000  |
|   |             |             |             | N | 1.23304000  | -0.94238800 | -0.85505100 |



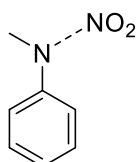
**TS11**

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.18077000 | 0.30011000 | 1.12948000 |
| C | -1.03867600 | 1.60156800 | 1.76809400 |



**TS11H**

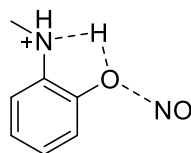
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.60486200 | -0.23303000 | -1.23686000 |
| C | -1.91898100 | -0.63995700 | -0.98616600 |
| C | -2.63017600 | -0.09960400 | 0.07225500  |
| C | -2.03097500 | 0.88974800  | 0.84890000  |
| C | -0.72319200 | 1.31905200  | 0.60513900  |
| C | 0.00643300  | 0.75253300  | -0.43081400 |
| N | 1.38312200  | 0.94236300  | -0.55759000 |
| C | 2.07432200  | 1.99331800  | 0.17526700  |
| N | 1.10423800  | -1.45947900 | 0.25779000  |
| O | 1.69290900  | -2.01802500 | -0.55124000 |
| O | 0.72000100  | -1.28661300 | 1.31960400  |
| H | -0.07699700 | -0.62938700 | -2.09480100 |
| H | -2.37497200 | -1.37595900 | -1.63433100 |
| H | -3.64086100 | -0.42006100 | 0.27889100  |
| H | -2.58178900 | 1.33674700  | 1.66578000  |
| H | -0.28349300 | 2.06850800  | 1.24553900  |
| H | 1.66435700  | 2.98461200  | -0.03896600 |
| H | 2.00277400  | 1.81169500  | 1.24796500  |
| H | 3.12365300  | 1.97679500  | -0.10657600 |
| H | 1.73737600  | 0.79205900  | -1.49289400 |



**TS12**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.76681200 | -0.03990200 | 0.39841900  |
| C | -1.25596800 | 1.10768000  | -0.30967000 |
| C | -0.48582600 | 2.23984400  | -0.43602800 |
| C | 0.80044600  | 2.31363100  | 0.12257600  |
| C | 1.30106200  | 1.22420400  | 0.81979700  |
| C | 0.54647900  | 0.06717800  | 0.95602600  |

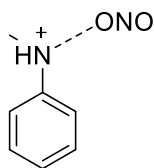
|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.38508300 | -1.21444700 | 0.51140200  |
| C | -2.69063400 | -1.35014100 | -0.05207800 |
| N | 0.12544700  | -2.21373500 | -1.33162100 |
| O | 1.05127900  | -1.80121400 | -0.75705800 |
| O | -0.82205200 | -2.38554500 | -1.99827700 |
| H | -2.24085200 | 1.08309400  | -0.75313900 |
| H | -0.87842700 | 3.09182200  | -0.97835200 |
| H | 1.38702100  | 3.21652800  | 0.01764800  |
| H | 2.28482700  | 1.27485900  | 1.26991400  |
| H | 0.90143000  | -0.75811200 | 1.55656400  |
| H | -3.37385300 | -0.52618800 | 0.18909100  |
| H | -2.64411500 | -1.40203100 | -1.15910900 |
| H | -3.14414700 | -2.28182000 | 0.28875900  |



**TS12H**

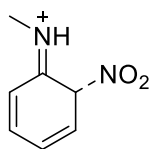
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.10944300 | -2.28384900 | 0.20703000  |
| C | 0.15349300  | -1.71936900 | 0.34997800  |
| C | 0.26627800  | -0.35321800 | 0.14418800  |
| C | -0.83812100 | 0.44236000  | -0.19262300 |
| C | -2.08759000 | -0.12420300 | -0.32309900 |
| C | -2.21347200 | -1.50132500 | -0.12603800 |
| H | -1.23621800 | -3.34644700 | 0.36098000  |
| H | 1.01547500  | -2.31292000 | 0.62127800  |
| H | -2.95001100 | 0.47999900  | -0.57094200 |
| H | -3.18458100 | -1.96533600 | -0.22789000 |
| N | -0.44634500 | 1.82399300  | -0.31484800 |
| H | 0.94549500  | 1.33701800  | -0.02618100 |
| C | -1.02114100 | 2.73644600  | 0.69906500  |
| H | -0.61020200 | 3.73185200  | 0.54555900  |
| H | -2.10875600 | 2.77755900  | 0.63234300  |
| H | -0.74002200 | 2.38237900  | 1.68862400  |
| O | 1.41977500  | 0.36408400  | 0.23995600  |
| N | 2.69023500  | -0.17898200 | -1.20598100 |
| O | 3.71119600  | 0.01224900  | -0.86678000 |

H -0.61956900 2.18000100 -1.24985600



**TS13H**

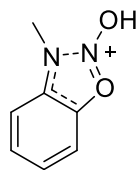
C 0.97660300 -1.12986900 0.56441500  
 C 2.30097100 -1.41973100 0.30042400  
 C 3.12618300 -0.44502300 -0.25738600  
 C 2.63002100 0.82415000 -0.55226700  
 C 1.30737100 1.13165600 -0.29615900  
 C 0.49150800 0.15141400 0.27676200  
 N -0.85805500 0.41794900 0.57021200  
 C -1.31438700 1.78007600 0.91302600  
 H 0.32405500 -1.88008800 0.99391000  
 H 2.69230800 -2.40147700 0.52542200  
 H 4.16180800 -0.67583200 -0.46626000  
 H 3.27790700 1.57242500 -0.98589300  
 H 0.92353400 2.11222200 -0.53331800  
 H -0.74441000 2.10714700 1.78201200  
 H -1.14391300 2.44581200 0.07439400  
 H -2.37282900 1.73599600 1.14727800  
 H -1.26952400 -0.28753200 1.18617700  
 O -1.79202200 0.05689400 -0.84722800  
 N -2.75142600 -0.80447900 -0.69410700  
 O -2.96504800 -1.27377100 0.36943800



**TS14H**

C -0.74245500 0.27032100 0.46246600  
 C -0.85425700 1.38274700 -0.42365700  
 C 0.19552400 2.24801500 -0.54183900  
 C 1.39165300 2.06156700 0.19385600  
 C 1.53800700 0.97292300 1.03094800

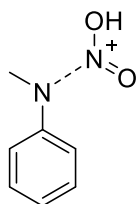
C 0.51510800 0.04081300 1.12562200  
 N -1.73602400 -0.58138400 0.66639300  
 C -3.02090500 -0.58005600 -0.02112500  
 N 0.86509900 -1.14001600 -0.93173100  
 O 0.19461400 -2.11768800 -0.98679600  
 O 1.75996800 -0.69142200 -1.55762300  
 H -1.77020000 1.54926800 -0.96955600  
 H 0.11152300 3.09912700 -1.20322400  
 H 2.19408700 2.77809900 0.08855900  
 H 2.45685100 0.81521400 1.57684000  
 H 0.60445700 -0.81350500 1.78389400  
 H -1.57346000 -1.32976900 1.32618400  
 H -3.55863600 0.34776700 0.17262900  
 H -2.87364200 -0.69903500 -1.09505800  
 H -3.60658000 -1.41406600 0.35137700



**TS15H**

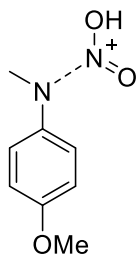
C 2.84496800 -0.45308700 -0.19214900  
 C 1.86123100 -1.40836100 -0.17469100  
 C 0.54769700 -1.03849800 0.15511800  
 C 0.22931200 0.36660700 0.27238300  
 C 1.26595400 1.30763600 0.42541200  
 C 2.54284600 0.89467800 0.13803400  
 O -1.33398800 -1.17832500 -1.01260500  
 N -1.85384200 -0.39276100 -0.20019000  
 O -2.20816600 -0.93064900 1.05658400  
 N -1.03920300 0.74148400 0.01644400  
 C -1.56351200 2.03306100 -0.39492200  
 H 3.87223500 -0.73352200 -0.37664100  
 H 2.09953200 -2.45610300 -0.28804600  
 H -0.06579300 -1.76464900 0.67604500  
 H 1.04161400 2.34499400 0.62111300  
 H 3.33918600 1.62690900 0.13192800

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.57813000 | -1.81012400 | 0.85529900  |
| H | -2.02825500 | 2.54852600  | 0.44461400  |
| H | -0.74932000 | 2.62933600  | -0.79859900 |
| H | -2.30924300 | 1.85367300  | -1.16821700 |



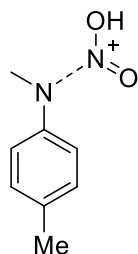
**TS16H**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.01710800 | -0.25999900 | 0.08452300  |
| C | 0.09219300  | -0.38870400 | 1.45173800  |
| C | 1.29886000  | -0.07480300 | 2.07712800  |
| C | 2.39965300  | 0.37265600  | 1.33875300  |
| C | 2.30507400  | 0.50579500  | -0.02801200 |
| C | 1.08414500  | 0.20103500  | -0.67259200 |
| N | 0.85645800  | 0.37813300  | -2.00838200 |
| C | 1.68118200  | 1.26684900  | -2.80021900 |
| N | 1.01551100  | -1.21032300 | -2.92335500 |
| O | 0.90546500  | -1.28878600 | -4.08421200 |
| O | 0.68671500  | -2.24701300 | -2.14261300 |
| H | -0.94070700 | -0.48356600 | -0.43049600 |
| H | -0.75146200 | -0.72558900 | 2.03712600  |
| H | 1.38661000  | -0.17827500 | 3.15050500  |
| H | 3.32604400  | 0.60861200  | 1.84301000  |
| H | 3.15915700  | 0.84230500  | -0.59661200 |
| H | 1.35606300  | 2.27208700  | -2.51833600 |
| H | 2.75363900  | 1.18025400  | -2.62890900 |
| H | 1.44862700  | 1.12749300  | -3.85238700 |
| H | 0.39707400  | -2.98001600 | -2.72967600 |



**TS16Hb**

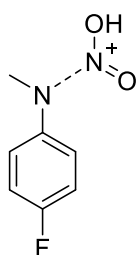
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.02188100 | -0.34703100 | -0.00900100 |
| C | 0.00906500  | -0.46814800 | 1.35456700  |
| C | 1.17585500  | -0.09324100 | 2.05312100  |
| C | 2.29762000  | 0.40542300  | 1.34906000  |
| C | 2.26020200  | 0.52148600  | -0.00961400 |
| C | 1.08963700  | 0.15706800  | -0.72504400 |
| N | 0.94440400  | 0.31370300  | -2.06673000 |
| C | 1.78211300  | 1.23793300  | -2.81740900 |
| N | 1.02458700  | -1.14891300 | -2.97792400 |
| O | 0.78701400  | -1.17069300 | -4.12995400 |
| O | 0.67053600  | -2.20602600 | -2.20794900 |
| H | -0.91175500 | -0.61756900 | -0.55941100 |
| H | -0.85674400 | -0.83651600 | 1.88188100  |
| H | 3.17553500  | 0.68184400  | 1.91554900  |
| H | 3.12661900  | 0.89677000  | -0.53359800 |
| H | 1.49186400  | 2.23608600  | -2.48907300 |
| H | 2.85120200  | 1.10284600  | -2.65465100 |
| H | 1.55182000  | 1.14369600  | -3.87450400 |
| H | 0.27612000  | -2.86734800 | -2.81417000 |
| O | 1.31498500  | -0.17073200 | 3.36358600  |
| C | 0.24169800  | -0.66879300 | 4.18240200  |
| H | 0.61619800  | -0.62868400 | 5.19942200  |
| H | -0.63776200 | -0.03294500 | 4.08248300  |
| H | 0.00488500  | -1.69750700 | 3.91145400  |



**TS16Hc**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.00381200 | -0.29462900 | 0.05880800  |
| C | 0.09936300  | -0.41612800 | 1.42419300  |
| C | 1.29371200  | -0.09026900 | 2.08304100  |
| C | 2.38921900  | 0.36607300  | 1.32335000  |
| C | 2.30357900  | 0.49424800  | -0.03937000 |
| C | 1.09188700  | 0.17730900  | -0.69796700 |

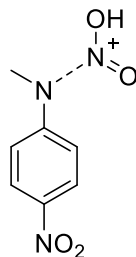
|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.87961400  | 0.34934100  | -2.03389300 |
| C | 1.69359100  | 1.26203900  | -2.81440000 |
| N | 1.01392300  | -1.18837400 | -2.95208700 |
| O | 0.86479800  | -1.24297700 | -4.11228600 |
| O | 0.66617200  | -2.23208700 | -2.18081600 |
| H | -0.92414600 | -0.53379400 | -0.45561000 |
| H | -0.74817100 | -0.76122700 | 2.00061000  |
| H | 3.31411500  | 0.61268500  | 1.82789300  |
| H | 3.16049700  | 0.83614500  | -0.60061800 |
| H | 1.35520200  | 2.26002000  | -2.52742000 |
| H | 2.76586900  | 1.18515100  | -2.63751200 |
| H | 1.47220100  | 1.12468400  | -3.86896600 |
| H | 0.33984300  | -2.93826800 | -2.77990800 |
| C | 1.41573900  | -0.21481400 | 3.56454400  |
| H | 1.59044000  | 0.76814700  | 4.01064400  |
| H | 2.27614400  | -0.83443900 | 3.82736200  |
| H | 0.52202800  | -0.64355200 | 4.01166100  |



**TS16Hd**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.01457400 | -0.26692500 | 0.08596700  |
| C | 0.08269400  | -0.39357400 | 1.45021700  |
| C | 1.29646000  | -0.07084100 | 2.05225000  |
| C | 2.41057500  | 0.37325200  | 1.33734500  |
| C | 2.30793200  | 0.49801200  | -0.02589100 |
| C | 1.08695400  | 0.19334200  | -0.67368900 |
| N | 0.86740300  | 0.36229000  | -2.00921800 |
| C | 1.68064200  | 1.26583500  | -2.79909400 |
| N | 1.01970600  | -1.19962200 | -2.91767100 |
| O | 0.89550400  | -1.27239300 | -4.07795100 |
| O | 0.68708900  | -2.23692200 | -2.13602700 |
| H | -0.93834200 | -0.49440200 | -0.42686900 |
| H | -0.74724400 | -0.72521200 | 2.05730300  |

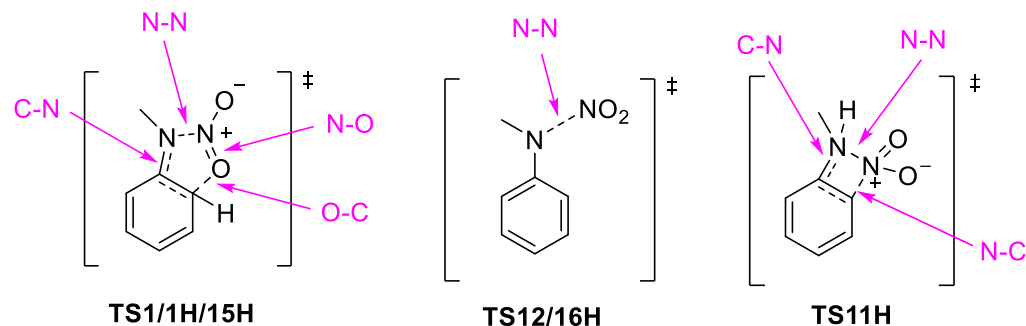
|   |            |             |             |
|---|------------|-------------|-------------|
| H | 3.32496800 | 0.60260700  | 1.86525200  |
| H | 3.16411800 | 0.83036800  | -0.59340600 |
| H | 1.33549600 | 2.26585900  | -2.52545000 |
| H | 2.75314100 | 1.19746000  | -2.61981300 |
| H | 1.46064700 | 1.11588800  | -3.85229800 |
| H | 0.39103700 | -2.96559200 | -2.72489700 |
| F | 1.40214000 | -0.19002100 | 3.36656100  |



**TS16He**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.02725700 | -0.23738600 | 0.09981500  |
| C | 0.08992500  | -0.38458400 | 1.46574900  |
| C | 1.31102200  | -0.08260800 | 2.05207000  |
| C | 2.41773200  | 0.36020300  | 1.33278600  |
| C | 2.30154000  | 0.50809500  | -0.03070500 |
| C | 1.06985700  | 0.22257500  | -0.66246800 |
| N | 0.82097000  | 0.42091100  | -1.99316500 |
| C | 1.65802400  | 1.28345100  | -2.78755900 |
| N | 1.01783600  | -1.24449500 | -2.92660100 |
| O | 1.02503100  | -1.33194600 | -4.08899600 |
| O | 0.62265600  | -2.27115900 | -2.17116800 |
| H | -0.95881200 | -0.44814800 | -0.40532200 |
| H | -0.73466900 | -0.71889000 | 2.07591100  |
| H | 3.34069900  | 0.57315900  | 1.84923700  |
| H | 3.15386600  | 0.84176600  | -0.60246300 |
| H | 1.30480000  | 2.29314600  | -2.54727700 |
| H | 2.72696700  | 1.22646500  | -2.58613600 |
| H | 1.44963300  | 1.11674600  | -3.84133900 |
| H | 0.38986500  | -3.01761400 | -2.76890000 |
| N | 1.44788800  | -0.24181300 | 3.52538200  |
| O | 0.46325500  | -0.61268500 | 4.13511300  |
| O | 2.53514300  | 0.00990400  | 4.00941300  |

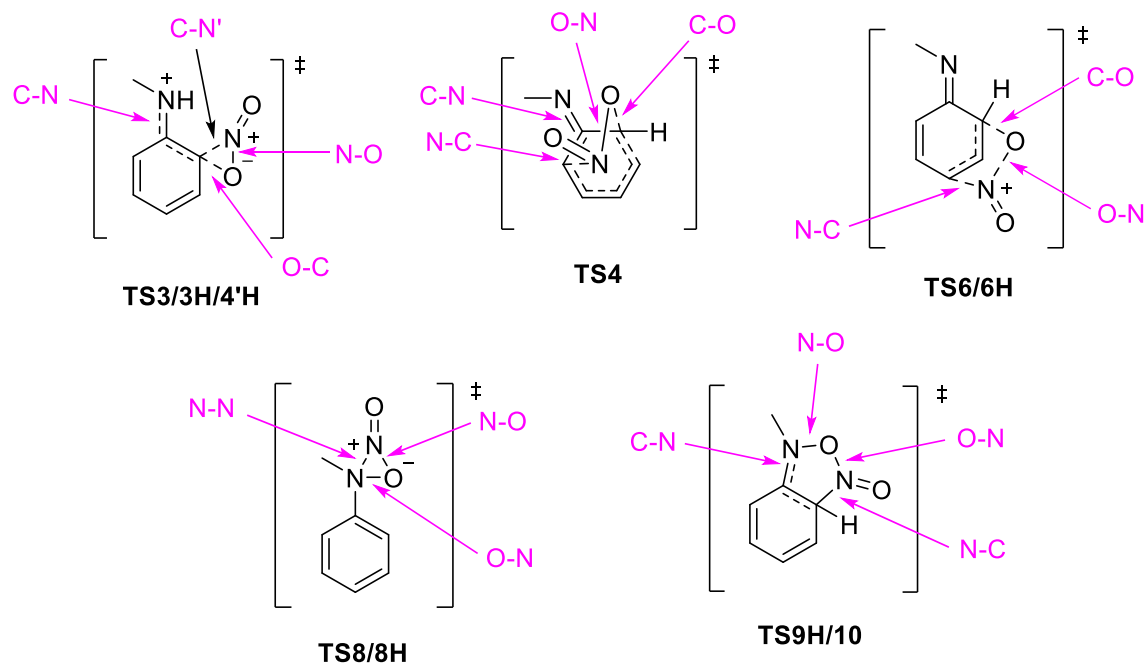
### 3. Source Data of Distances of Key Bonds in Transition States



**Figure S1.** Schematic diagrams on names of the key bonds

**Table S1.** Distances of key bonds in transition states. Different types of transition states have different meanings in **Table S1**. The figures of transition states are shown in **Figure S1**, which figure out names of bonds (Note that bonds in Å).

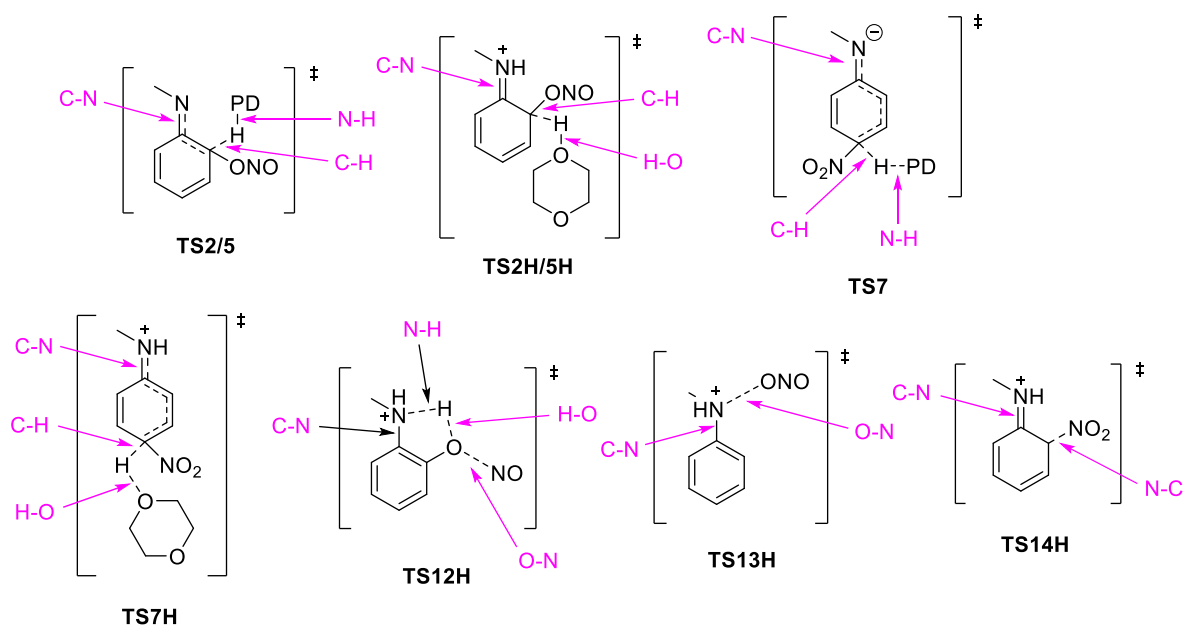
| Structure | C-N  | N-N  | N-O  | O-C  | N-C  |
|-----------|------|------|------|------|------|
| TS1       | 1.30 | 2.68 | 1.26 | 2.07 | -    |
| TS1Hb     | 1.30 | 2.71 | 1.28 | 2.03 | -    |
| TS1Hc     | 1.30 | 2.63 | 1.26 | 2.02 | -    |
| TS1Hd     | 1.30 | 2.62 | 1.27 | 2.00 | -    |
| TS1He     | 1.31 | 2.59 | 1.26 | 1.97 | -    |
| TS11H     | 1.40 | 2.55 | -    | -    | 2.58 |
| TS12      | -    | 2.58 | -    | -    | -    |
| TS15H     | 1.35 | 1.41 | 1.24 | 2.22 | -    |
| TS16H     | -    | 1.84 | -    | -    | -    |
| TS16Hb    | -    | 1.73 | -    | -    | -    |
| TS16Hc    | -    | 1.80 | -    | -    | -    |
| TS16Hd    | -    | 1.81 | -    | -    | -    |
| TS16He    | -    | 1.92 | -    | -    | -    |



**Figure S2.** Schematic diagrams on names of the key bonds

**Table S2.** Distances of key bonds in transition states. Different types of transition states have different meanings in **Table S2**. The figures of transition states are shown in **Figure S2**, which figure out names of bonds (Note that bonds in Å).

| Structure | C-N  | C-N' | N-O  | O-C  | C-O  | O-N  | N-C  | N-O' | N-N  |
|-----------|------|------|------|------|------|------|------|------|------|
| TS3       | 1.36 | 1.63 | 1.33 | 1.79 | -    | -    | -    | -    | -    |
| TS3H      | 1.47 | 1.70 | 1.32 | 1.80 | -    | -    | -    | -    | -    |
| TS4       | 1.30 | -    | -    | -    | 2.56 | 1.23 | 3.14 | -    | -    |
| TS4'H     | 1.33 | 3.15 | 1.19 | 2.72 | -    | -    | -    | -    | -    |
| TS4'Hb    | 1.32 | 3.20 | 1.22 | 2.74 | -    | -    | -    | -    | -    |
| TS4'Hc    | 1.32 | 3.22 | 1.20 | 2.73 | -    | -    | -    | -    | -    |
| TS4'Hd    | 1.32 | 3.20 | 1.20 | 2.72 | -    | -    | -    | -    | -    |
| TS4'He    | 1.32 | 2.90 | 1.22 | 2.71 | -    | -    | -    | -    | -    |
| TS6       | -    | -    | -    | -    | 2.18 | 1.25 | 2.85 | -    | -    |
| TS6H      | -    | -    | -    | -    | 1.99 | 1.27 | 2.78 | -    | -    |
| TS8       | -    | -    | 1.22 | -    | -    | 2.89 | -    | -    | 2.89 |
| TS8H      | -    | -    | 1.18 | -    | -    | 2.94 | -    | -    | 2.90 |
| TS8Hb     | -    | -    | 1.20 | -    | -    | 2.90 | -    | -    | 2.85 |
| TS8Hc     | -    | -    | 1.19 | -    | -    | 2.94 | -    | -    | 2.89 |
| TS8Hd     | -    | -    | 1.19 | -    | -    | 2.93 | -    | -    | 2.90 |
| TS8He     | -    | -    | 1.17 | -    | -    | 2.97 | -    | -    | 2.95 |
| TS9H      | 1.37 | -    | 1.85 | -    | -    | 1.31 | 3.05 | -    | -    |
| TS10      | 1.35 | -    | 2.04 | -    | -    | 1.25 | 2.76 | -    | -    |



**Figure S3.** Schematic diagrams on names of the key bonds

**Table S3.** Distances of key bonds in transition states. Different types of transition states have different meanings in **Table S3**. The figures of transition states are shown in **Figure S3**, which figure out names of bonds (Note that bonds in Å).

| Structure | C–N  | N–H  | C–H  | H–O  | O–N  | N–C  |
|-----------|------|------|------|------|------|------|
| TS2       | 1.44 | 1.36 | 1.39 | -    | -    | -    |
| TS2H      | 1.41 | 1.29 | 1.38 | -    | -    | -    |
| TS5       | 1.47 | 1.35 | 1.38 | -    | -    | -    |
| TS5H      | 1.49 | -    | 1.33 | 1.31 | -    | -    |
| TS7       | 1.29 | 1.51 | 1.26 | -    | -    | -    |
| TS7H      | 1.32 | -    | 1.33 | 1.30 | -    | -    |
| TS12H     | 1.44 | 1.50 | -    | 1.11 | 2.00 | -    |
| TS13H     | 1.41 | -    | -    | -    | 1.74 | -    |
| TS14H     | 1.32 | -    | -    | 1.29 | -    | 2.40 |

#### 4. Computed Energies and Charges

**Table S4.** Electronic energies ( $E_{\text{gas}}$  in Hartree), thermal corrections to Gibbs free energies ( $\Delta G_{\text{correction}}$  in Hartree), Electronic energies under M052X/6-31G\* without SMD model ( $G_{\text{gas}}$  in Hartree), Electronic energies under M052X/6-31G\* with SMD model ( $G_{\text{SMD}}$  in Hartree), solvation free energies ( $G_{\text{solv}} = G_{\text{SMD}} - G_{\text{gas}}$  in Hartree) Gibbs free energies about molecules converts from the gas-phase standard state to the solution-phase standard state of 1M  $RT\ln(RT/p)$  in kcal/mol, free energies in solution ( $\Delta G_{\text{solv}}$  in kcal/mol,  $\Delta G_{\text{solv}} = G_{\text{gas}} + G_{\text{solv}} + RT\ln(RT/p) = E_{\text{gas}} + \Delta G_{\text{correction}} + G_{\text{solv}} + RT\ln(RT/p)$ ). Relative energies ( $\Delta G$ ) at **373.15 K** are reported in kcal/mol.

| Structure             | $E_{\text{gas}}$ | $\Delta G_{\text{correction}}$ | $G_{\text{gas}}$ | $G_{\text{SMD}}$ | $RT\ln(RT/p)$ | $G_{\text{solv}}$ | $\Delta G_{\text{solv}}$ | $\Delta G$   |
|-----------------------|------------------|--------------------------------|------------------|------------------|---------------|-------------------|--------------------------|--------------|
| <b>1a</b>             | -530.5092311     | 0.098312                       | -531.3186828     | -531.3312723     | 2.55          | -0.0125895        | -332843.5061             | <b>0</b>     |
| <b>2a</b>             | -530.5352312     | 0.099356                       | -531.3446925     | -531.3561118     | 2.55          | -0.0114193        | -332858.4317             | <b>-14.9</b> |
| <b>3a</b>             | -530.5351554     | 0.097831                       | -531.344118      | -531.3581334     | 2.55          | -0.0140154        | -332860.97               | <b>-17.5</b> |
| <b>INT1</b>           | -530.4845545     | 0.094266                       | -531.2821284     | -531.2907129     | 2.55          | -0.0085845        | -332828.0466             | <b>15.5</b>  |
| <b>INT2</b>           | -530.5335519     | 0.095357                       | -531.3345571     | -531.3427691     | 2.55          | -0.008212         | -332857.8749             | <b>-14.4</b> |
| <b>INT3</b>           | -530.4876803     | 0.097172                       | -531.2857748     | -531.2975739     | 2.55          | -0.0117991        | -332830.2021             | <b>13.3</b>  |
| <b>INT4</b>           | -530.4898576     | 0.096243                       | -531.2882091     | -531.3004267     | 2.55          | -0.0122176        | -332832.414              | <b>11.1</b>  |
| <b>INT5</b>           | -530.4820271     | 0.094922                       | -531.2820607     | -531.291002      | 2.55          | -0.0089413        | -332826.273              | <b>17.2</b>  |
| <b>INT6</b>           | -530.4864836     | 0.096482                       | -531.2842765     | -531.2963102     | 2.55          | -0.0120337        | -332830.0312             | <b>28.4</b>  |
| <b>INT7</b>           | -530.4398337     | 0.0884314                      | -531.2540788     | -531.2638041     | 2.55          | -0.0097253        | -332804.3612             | <b>39.1</b>  |
| <b>TS1</b>            | -530.4261707     | 0.092499                       | -531.2239211     | -531.2383882     | 2.55          | -0.0144671        | -332796.2108             | <b>47.3</b>  |
| <b>TS2</b>            | -781.9180195     | 0.23863                        | -783.1338012     | -783.1488618     | 2.55          | -0.0150606        | -490518.5345             | <b>40.2</b>  |
| <b>TS3</b>            | -530.433041      | 0.094415                       | -531.2319384     | -531.2433626     | 2.55          | -0.0114242        | -332797.4103             | <b>46.1</b>  |
| <b>TS4</b>            | -530.3986836     | 0.090735                       | -531.2080059     | -531.2225738     | 2.55          | -0.0145679        | -332780.1326             | <b>63.4</b>  |
| <b>TS5</b>            | -781.9256016     | 0.242158                       | -783.1434935     | -783.1624748     | 2.55          | -0.0189813        | -490523.5384             | <b>35.2</b>  |
| <b>TS6</b>            | -530.4218016     | 0.092349                       | -531.2194313     | -531.2343224     | 2.55          | -0.0148911        | -332793.8289             | <b>49.7</b>  |
| <b>TS7</b>            | -781.9393513     | 0.240161                       | -783.1538842     | -783.1726834     | 2.55          | -0.0187992        | -490533.3054             | <b>25.4</b>  |
| <b>TS8</b>            | -530.376865      | 0.089853                       | -531.1951143     | -531.2092261     | 2.55          | -0.0141118        | -332766.7082             | <b>76.8</b>  |
| <b>TS9</b>            | -530.4011266     | 0.091500                       | -531.2028819     | -531.2204505     | 2.55          | -0.0175686        | -332783.068              | <b>60.4</b>  |
| <b>TS10</b>           | -530.431648      | 0.093446                       | -531.2281711     | -531.2416589     | 2.55          | -0.0134878        | -332798.439              | <b>60</b>    |
| <b>TS11</b>           | -781.9269745     | 0.240237                       | -783.142195      | -783.1608922     | 2.55          | -0.0186972        | -490525.4273             | <b>33.3</b>  |
| <b>TS12</b>           | -530.3736666     | 0.092485                       | -531.1588616     | -531.1685349     | 2.55          | -0.0096733        | -332760.2644             | <b>83.2</b>  |
| <b>piperidineH</b>    | -251.8303193     | 0.134446                       | -252.2410869     | -252.30619       | 2.55          | -0.0651031        | -157979.9803             | <b>0</b>     |
| <b>piperidine</b>     | -251.4505025     | 0.118528                       | -251.8611824     | -251.8682165     | 2.55          | -0.0070341        | -157715.1914             | <b>0</b>     |
| <b>NO<sub>2</sub></b> | -204.7965696     | -0.0216908                     | -205.0322163     | -205.0324386     | 2.55          | -0.0002223        | -128523.0961             | <b>19.7</b>  |
| <b>Radical</b>        | -325.655256      | 0.0870068                      | -326.2161692     | -326.2256143     | 2.55          | -0.0094451        | -204300.709              |              |

**Table S5.** Electronic energies ( $E_{\text{gas}}$  in Hartree), thermal corrections to Gibbs free energies ( $\Delta G_{\text{correction}}$  in Hartree), Electronic energies under M052X/6-31G\* without SMD model ( $G_{\text{gas}}$  in Hartree), Electronic energies under M052X/6-31G\* with SMD model ( $G_{\text{SMD}}$  in Hartree), solvation free energies ( $G_{\text{solv}} = G_{\text{SMD}} - G_{\text{gas}}$  in Hartree), Gibbs free energies about molecules converts from the gas-phase standard state to the solution-phase standard state of 1M  $RT\ln(RT/p)$  in kcal/mol (for 1,4-Dioxane is 11.74 mol/L because 1,4-Dioxane is the solvent), free energies in solution ( $\Delta G_{\text{solv}}$  in kcal/mol,  $\Delta G_{\text{solv}} = G_{\text{gas}} + G_{\text{solv}} + RT\ln(RT/p) = E_{\text{gas}} + \Delta G_{\text{correction}} + G_{\text{solv}} + RT\ln(RT/p)$ ). Relative energies ( $\Delta G$ ) at **313.15 K** are reported in kcal/mol.

| Structure       | $E_{\text{gas}}$ | $\Delta G_{\text{correction}}$ | $G_{\text{gas}}$ | $G_{\text{SMD}}$ | $RT\ln(RT/p)$ | $G_{\text{solv}}$ | $\Delta G_{\text{solv}}$ | $\Delta G$   |
|-----------------|------------------|--------------------------------|------------------|------------------|---------------|-------------------|--------------------------|--------------|
| <b>1aH</b>      | -530.8418072     | 0.119926                       | -531.6366805     | -531.6890451     | 2.02          | -0.05236          | -333064                  | <b>0</b>     |
| <b>1aH'</b>     | -530.8462763     | 0.119893                       | -531.6471656     | -531.6961915     | 2.02          | -0.04903          | -333065                  | <b>-0.7</b>  |
| <b>1a</b>       | -530.5092767     | 0.107768                       | -531.3187335     | -531.3266889     | 2.02          | -0.00796          | -332835                  | <b>0</b>     |
| <b>2aH</b>      | -530.8902045     | 0.123477                       | -531.6910522     | -531.747527      | 2.02          | -0.05647          | -333095                  | <b>-30.7</b> |
| <b>2a</b>       | -530.535252      | 0.108802                       | -531.3447074     | -531.3516383     | 2.02          | -0.00693          | -332850                  | <b>-14.1</b> |
| <b>3aH</b>      | -530.8784494     | 0.123221                       | -531.6796182     | -531.7458825     | 2.02          | -0.06626          | -333094                  | <b>-29.6</b> |
| <b>3a</b>       | -530.5351914     | 0.107389                       | -531.3441471     | -531.3534644     | 2.02          | -0.00932          | -332853                  | <b>-16.4</b> |
| <b>dioxaneH</b> | -307.4899493     | 0.102273                       | -307.9269003     | -307.9847279     | 2.02          | -0.05783          | -192923                  | <b>0</b>     |
| <b>dioxane</b>  | -307.1706635     | 0.090819                       | -307.6123842     | -307.6172303     | 3.56          | -0.00485          | -192695                  | <b>0</b>     |
| <b>INT1H</b>    | -530.8699827     | 0.11789                        | -531.6672707     | -531.7154122     | 2.02          | -0.04814          | -333080                  | <b>-16.3</b> |
| <b>INT2H</b>    | -530.8986271     | 0.119633                       | -531.6930063     | -531.7442542     | 2.02          | -0.05125          | -333099                  | <b>-35.1</b> |
| <b>INT3H</b>    | -530.8596557     | 0.121251                       | -531.6605674     | -531.7148449     | 2.02          | -0.05428          | -333076                  | <b>-11.6</b> |
| <b>INT4H</b>    | -530.8643572     | 0.120612                       | -531.6642987     | -531.7221258     | 2.02          | -0.05783          | -333081                  | <b>-17.1</b> |
| <b>INT5H</b>    | -530.8360521     | 0.119635                       | -531.6292921     | -531.6780587     | 2.02          | -0.04877          | -333058                  | <b>5.7</b>   |
| <b>INT6H</b>    | -530.8133844     | 0.119567                       | -531.6134948     | -531.6673721     | 2.02          | -0.05388          | -333047                  | <b>16.7</b>  |
| <b>INT7H</b>    | -530.8269824     | 0.1141567                      | -531.638037      | -531.6888949     | 2.02          | -0.0508579        | -333057.4991             | <b>6.6</b>   |
| <b>TS1H</b>     | -530.7988543     | 0.117169                       | -531.5926723     | -531.6492024     | 2.02          | -0.05653          | -333042                  | <b>22.6</b>  |
| <b>TS2H</b>     | -838.0440177     | 0.226647                       | -839.2881485     | -839.3345472     | 2.02          | -0.0464           | -525766                  | <b>-6.6</b>  |
| <b>TS3H</b>     | -530.7825466     | 0.118918                       | -531.5772437     | -531.6361035     | 2.02          | -0.05886          | -333032                  | <b>32.5</b>  |
| <b>TS4'H</b>    | -530.8119425     | 0.11628                        | -531.5868886     | -531.6372058     | 2.02          | -0.05032          | -333046                  | <b>17.7</b>  |
| <b>TS5H</b>     | -838.0440947     | 0.231076                       | -839.2902988     | -839.3477489     | 2.02          | -0.05745          | -525770                  | <b>-10.8</b> |
| <b>TS6H</b>     | -530.8000556     | 0.116646                       | -531.5944864     | -531.6509513     | 2.02          | -0.05646          | -333043                  | <b>21.6</b>  |
| <b>TS7H</b>     | -838.0450068     | 0.229944                       | -839.2922426     | -839.3449898     | 2.02          | -0.05275          | -525768                  | <b>-9.1</b>  |
| <b>TS8H</b>     | -530.8055862     | 0.114602                       | -531.5715179     | -531.6198337     | 2.02          | -0.04832          | -333042                  | <b>21.9</b>  |
| <b>TS9H</b>     | -530.798972      | 0.117296                       | -531.5879958     | -531.643603      | 2.02          | -0.05561          | -333041                  | <b>23.2</b>  |
| <b>TS11H</b>    | -530.7914886     | 0.11652                        | -531.5805897     | -531.6269202     | 2.02          | -0.04633          | -333031                  | <b>33.2</b>  |
| <b>TS12H</b>    | -530.8693715     | 0.113799                       | -531.6594662     | -531.7043031     | 2.02          | -0.04484          | -333081                  | <b>-16.4</b> |
| <b>TS13H</b>    | -530.8160491     | 0.118409                       | -531.6114047     | -531.6615928     | 2.02          | -0.05019          | -333048                  | <b>16.6</b>  |
| <b>TS14H</b>    | -530.8353082     | 0.117497                       | -531.6343354     | -531.6850335     | 2.02          | -0.0507           | -333061                  | <b>3.6</b>   |
| <b>TS15H</b>    | -530.7551676     | 0.116571                       | -531.5476037     | -531.5966298     | 2.02          | -0.04903          | -333010                  | <b>55.1</b>  |
| <b>TS16H</b>    | -530.7960457     | 0.116365                       | -531.5928697     | -531.6395406     | 2.02          | -0.04667          | -333034                  | <b>30.8</b>  |
| <b>INT2</b>     | -530.5335555     | 0.105137                       | -531.3345624     | -531.3386731     | 2.02          | -0.00411          | -332850                  | <b>-13.5</b> |

|                         |              |          |              |              |      |          |         |             |
|-------------------------|--------------|----------|--------------|--------------|------|----------|---------|-------------|
| <b>TS3</b>              | -530.4330767 | 0.104058 | -531.2319787 | -531.238983  | 2.02 | -0.007   | -332789 | <b>47.8</b> |
| <b>NO<sub>2</sub></b>   | -204.7965704 | -0.01609 | -205.0322161 | -205.031477  | 2.02 | 0.000739 | -128520 | <b>-9.0</b> |
| <b>Cationic radical</b> | -326.0377126 | 0.10995  | -326.6008075 | -326.6529932 | 2.02 | -0.05219 | -204554 |             |

**Table S6.** Electronic energies ( $E_{\text{gas}}$  in Hartree), thermal corrections to Gibbs free energies ( $\Delta G_{\text{correction}}$  in Hartree), Electronic energies under M052X/6-31G\* without SMD model ( $G_{\text{gas}}$  in Hartree), Electronic energies under M052X/6-31G\* with SMD model ( $G_{\text{SMD}}$  in Hartree), solvation free energies ( $G_{\text{solv}} = G_{\text{SMD}} - G_{\text{gas}}$  in Hartree), Gibbs free energies about molecules converts from the gas-phase standard state to the solution-phase standard state of 1M  $RT\ln(RT/p)$  in kcal/mol, free energies in solution ( $\Delta G_{\text{solv}}$  in kcal/mol,  $\Delta G_{\text{solv}} = G_{\text{gas}} + G_{\text{solv}} + RT\ln(RT/p) = E_{\text{gas}} + \Delta G_{\text{correction}} + G_{\text{solv}} + RT\ln(RT/p)$ ). Relative energies ( $\Delta G$ ) at **313.15 K** are reported in kcal/mol.

| Structure     | $E_{\text{gas}}$ | $\Delta G_{\text{correction}}$ | $G_{\text{gas}}$ | $G_{\text{SMD}}$ | $RT\ln(RT/p)$ | $G_{\text{solv}}$ | $\Delta G_{\text{solv}}$ | $\Delta G$  |
|---------------|------------------|--------------------------------|------------------|------------------|---------------|-------------------|--------------------------|-------------|
| <b>1bH</b>    | -645.2007447     | 0.149143                       | -646.151         | -646.201         | 2.02          | -0.05             | -404805.6869             | <b>0</b>    |
| <b>1bH'</b>   | -645.2031343     | 0.148905                       | -646.16          | -646.207         | 2.02          | -0.04754          | -404805.789              | <b>0</b>    |
| <b>1cH</b>    | -570.0881473     | 0.144566                       | -570.951         | -571.002         | 2.02          | -0.05104          | -357675.3053             | <b>0</b>    |
| <b>1cH'</b>   | -570.0913863     | 0.145245                       | -570.961         | -571.009         | 2.02          | -0.04828          | -357675.1768             | <b>0</b>    |
| <b>1dH</b>    | -629.9687932     | 0.110778                       | -630.86          | -630.913         | 2.02          | -0.05262          | -395273.202              | <b>0</b>    |
| <b>1dH'</b>   | -629.9727558     | 0.110171                       | -630.871         | -630.921         | 2.02          | -0.04961          | -395274.1785             | <b>0</b>    |
| <b>1eH</b>    | -735.0528344     | 0.119217                       | -736.092         | -736.151         | 2.02          | -0.05837          | -461212.8051             | <b>0</b>    |
| <b>1eH'</b>   | -735.0579214     | 0.119366                       | -736.104         | -736.159         | 2.02          | -0.05528          | -461213.9623             | <b>0</b>    |
| <b>TS1Hb</b>  | -645.1702988     | 0.144366                       | -646.12          | -646.175         | 2.02          | -0.05508          | -404792.7634             | <b>12.9</b> |
| <b>TS1Hc</b>  | -570.0491506     | 0.141531                       | -570.911         | -570.967         | 2.02          | -0.05559          | -357655.5946             | <b>19.7</b> |
| <b>TS1Hd</b>  | -629.9272437     | 0.107426                       | -630.818         | -630.875         | 2.02          | -0.05703          | -395252.0025             | <b>21.2</b> |
| <b>TS1He</b>  | -735.0062089     | 0.114336                       | -736.044         | -736.104         | 2.02          | -0.06032          | -461187.8332             | <b>25.0</b> |
| <b>TS8Hb</b>  | -645.1717685     | 0.143688                       | -646.097         | -646.147         | 2.02          | -0.04926          | -404790.4612             | <b>15.2</b> |
| <b>TS8Hc</b>  | -570.0591742     | 0.138843                       | -570.889         | -570.937         | 2.02          | -0.04818          | -357658.92               | <b>16.4</b> |
| <b>TS8Hd</b>  | -629.9356382     | 0.105433                       | -630.798         | -630.847         | 2.02          | -0.04873          | -395253.3122             | <b>19.9</b> |
| <b>TS8He</b>  | -735.0054032     | 0.112506                       | -736.027         | -736.081         | 2.02          | -0.05335          | -461184.1002             | <b>28.7</b> |
| <b>TS16Hb</b> | -645.1619022     | 0.145702                       | -646.116         | -646.16          | 2.02          | -0.04451          | -404780.0241             | <b>25.8</b> |
| <b>TS16Hc</b> | -570.0441922     | 0.141243                       | -570.91          | -570.956         | 2.02          | -0.04559          | -357646.3886             | <b>28.8</b> |
| <b>TS16Hd</b> | -629.9253982     | 0.107688                       | -630.821         | -630.867         | 2.02          | -0.04667          | -395244.1763             | <b>30.0</b> |
| <b>TS16He</b> | -735.0035384     | 0.114384                       | -736.045         | -736.097         | 2.02          | -0.05176          | -461180.7511             | <b>33.2</b> |