

Article

# Mechanistic Insight into the Degradation of Nitrosamines in Aqueous-phase UV or UV-based Advanced Oxidation System: Quantum Mechanical Calculations

Supplemental Materials

Daisuke Minakata <sup>1, \*</sup> and Erica Coscarelli<sup>1</sup>

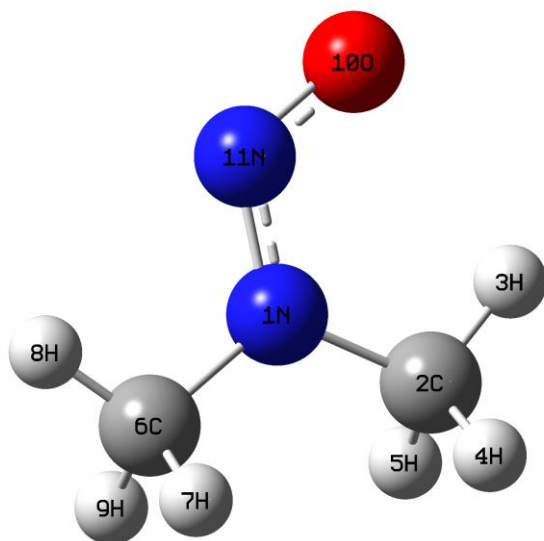
<sup>1</sup> Department of Civil and Environmental Engineering, Michigan Technological University, 1400 Townsend Drive, Houghton, MI, 49931; mkhare@mtu.edu

\* Correspondence: dminakat@mtu.edu; Tel.: +1-906-487-1830

Academic Editor: name

Received: date; Accepted: date; Published: date

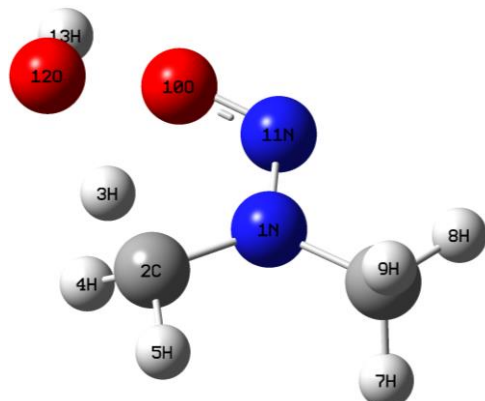
26 Pathway 1-1

27  $(\text{CH}_3)_2\text{NNO}$ 

28

| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4568287 |             |              |
| 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0876413 | 108.7050894 |              |
| 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0937024 | 109.4491937 | 120.3865004  |
| 5   | No        | Show    | 5   | H      | 2  | 1  | 3  | 1.0937082 | 109.4557860 | -120.3875549 |
| 6   | No        | Show    | 6   | C      | 1  | 2  | 3  | 1.4524329 | 119.3236651 | -179.9498121 |
| 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.0941437 | 110.0995030 | 59.9314814   |
| 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0900064 | 108.4145188 | 179.9962015  |
| 9   | No        | Show    | 9   | H      | 6  | 1  | 2  | 1.0941440 | 110.1008003 | -59.9373046  |
| 10  | No        | Show    | 10  | O      | 1  | 6  | 2  | 2.1732633 | 147.3486737 | 179.9851117  |
| 11  | No        | Show    | 11  | N      | 10 | 1  | 6  | 1.2400000 | 32.6670507  | 0.0222369    |

41 TS1

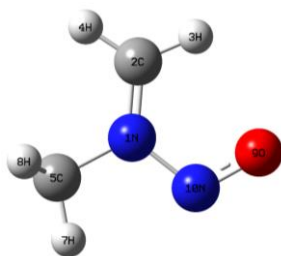


42

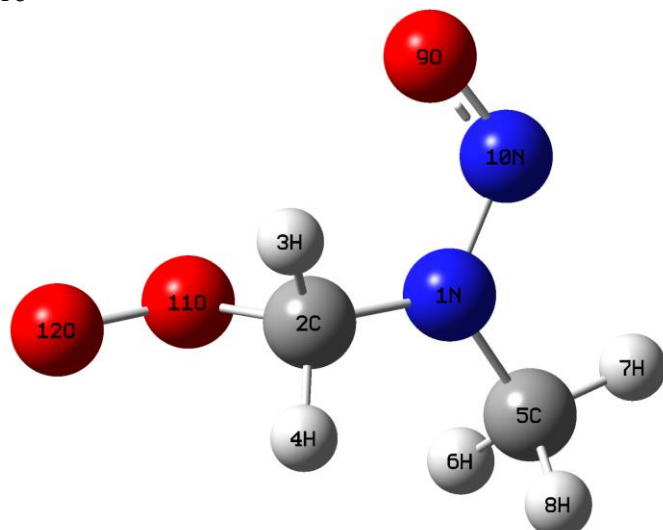
| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4298033 |             |              |
| 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.1660733 | 109.4228963 |              |
| 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0909529 | 111.5359651 | 115.6655653  |
| 5   | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0884771 | 110.1028677 | 126.1736837  |
| 6   | No        | Show    | 6   | C      | 1  | 2  | 5  | 1.4562684 | 121.5805093 | -9.4138368   |
| 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.0922003 | 109.8916567 | 60.9850784   |
| 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0896006 | 108.0781735 | -178.9372843 |
| 9   | No        | Show    | 9   | H      | 6  | 1  | 2  | 1.0935028 | 109.8863769 | -59.1590961  |
| 10  | No        | Show    | 10  | O      | 1  | 2  | 6  | 2.1550014 | 89.6243717  | -173.6728086 |

70 TS285 TS3

— — — — —

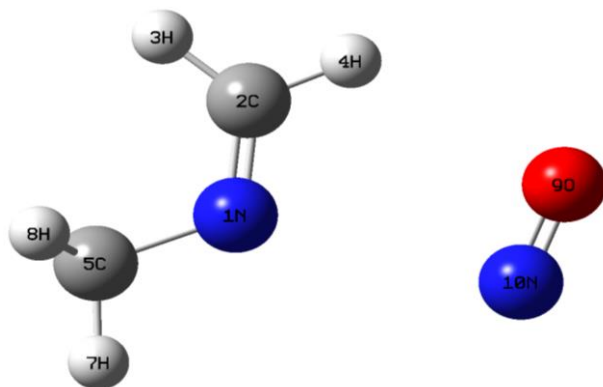


| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 2   | No        | Show    | 2   | C      | 1  |    |    | 1.3161424 |             |              |
| 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0798367 | 117.9071895 |              |
| 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0800741 | 118.7380394 | 179.9887752  |
| 5   | No        | Show    | 5   | C      | 1  | 2  | 3  | 1.4621912 | 122.5540303 | -179.9975377 |
| 6   | No        | Show    | 6   | H      | 5  | 1  | 2  | 1.0913285 | 109.7549479 | 60.4428595   |
| 7   | No        | Show    | 7   | H      | 5  | 1  | 2  | 1.0891590 | 107.6137062 | -179.8475651 |
| 8   | No        | Show    | 8   | H      | 5  | 1  | 2  | 1.0913067 | 109.7485366 | -60.1370326  |
| 9   | No        | Show    | 9   | O      | 1  | 2  | 5  | 2.2021350 | 92.0916085  | 179.9890536  |
| 10  | No        | Show    | 10  | N      | 9  | 1  | 2  | 1.2493087 | 35.8841163  | -179.9990601 |

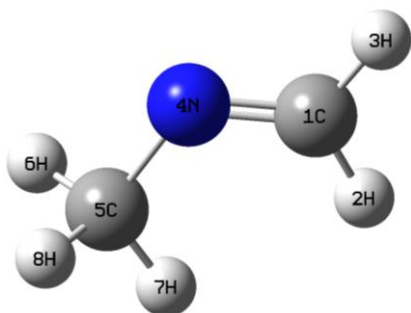


| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4260258 |             |              |
| 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0882082 | 110.8830670 |              |
| 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0884305 | 110.4654214 | -125.5621054 |
| 5   | No        | Show    | 5   | C      | 1  | 2  | 3  | 1.4583876 | 121.1483516 | 154.6717579  |
| 6   | No        | Show    | 6   | H      | 5  | 1  | 2  | 1.0930170 | 110.0919261 | 60.1862469   |
| 7   | No        | Show    | 7   | H      | 5  | 1  | 2  | 1.0897246 | 107.9208956 | 179.7810278  |
| 8   | No        | Show    | 8   | H      | 5  | 1  | 2  | 1.0925006 | 110.1281321 | -60.4348911  |
| 9   | No        | Show    | 9   | O      | 1  | 2  | 5  | 2.1682276 | 90.9000330  | 174.4682854  |
| 10  | No        | Show    | 10  | N      | 9  | 1  | 2  | 1.2257030 | 33.7529491  | 179.9490209  |
| 11  | No        | Show    | 11  | O      | 2  | 1  | 10 | 1.4776556 | 108.0580106 | 86.4243309   |
| 12  | No        | Show    | 12  | O      | 11 | 2  | 1  | 1.3083348 | 110.5660529 | 178.4111096  |

TS4



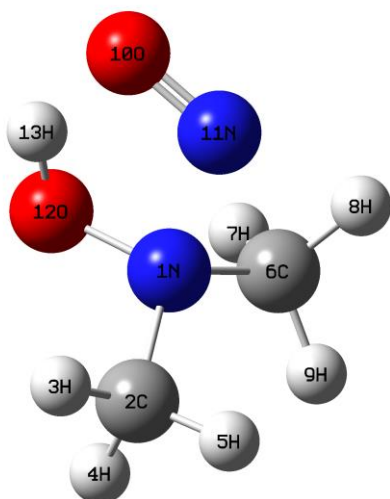
| 115 | 116 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 117 |     | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 118 |     | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.2683431 |             |              |
| 119 |     | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0966224 | 123.9880427 |              |
| 120 |     | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0909702 | 119.3942047 | -180.0000000 |
| 121 |     | 5   | No        | Show    | 5   | C      | 1  | 2  | 4  | 1.4662881 | 117.0043990 | 179.9990560  |
| 122 |     | 6   | No        | Show    | 6   | H      | 5  | 1  | 2  | 1.0949899 | 111.0980455 | 60.2380318   |
| 123 |     | 7   | No        | Show    | 7   | H      | 5  | 1  | 2  | 1.0917995 | 109.8235214 | 179.9932588  |
| 124 |     | 8   | No        | Show    | 8   | H      | 5  | 1  | 2  | 1.0949896 | 111.0967873 | -60.2532126  |
| 125 |     | 9   | No        | Show    | 9   | O      | 2  | 1  | 5  | 3.2212727 | 79.0735081  | 179.9986043  |
| 126 |     | 10  | No        | Show    | 10  | N      | 9  | 2  | 1  | 1.1544162 | 85.2225352  | 0.0043929    |
| 127 |     | P4  |           |         |     |        |    |    |    |           |             |              |



| 128 | 129 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 130 |     | 1   | No        | Show    | 1   | C      |    |    |    |           |             |              |
| 131 |     | 2   | No        | Show    | 2   | H      | 1  |    |    | 1.0968350 |             |              |
| 132 |     | 3   | No        | Show    | 3   | H      | 1  | 2  |    | 1.0898435 | 116.8631844 |              |
| 133 |     | 4   | No        | Show    | 4   | N      | 1  | 3  | 2  | 1.2715121 | 119.4976807 | -179.9378284 |
| 134 |     | 5   | No        | Show    | 5   | C      | 4  | 1  | 3  | 1.4548237 | 116.4847970 | -179.9912735 |
| 135 |     | 6   | No        | Show    | 6   | H      | 5  | 4  | 1  | 1.0947055 | 109.2434968 | -121.8552085 |
| 136 |     | 7   | No        | Show    | 7   | H      | 5  | 4  | 1  | 1.0978746 | 113.6840652 | 0.0102200    |
| 137 |     | 8   | No        | Show    | 8   | H      | 5  | 4  | 1  | 1.0946601 | 109.2546109 | 121.8927213  |

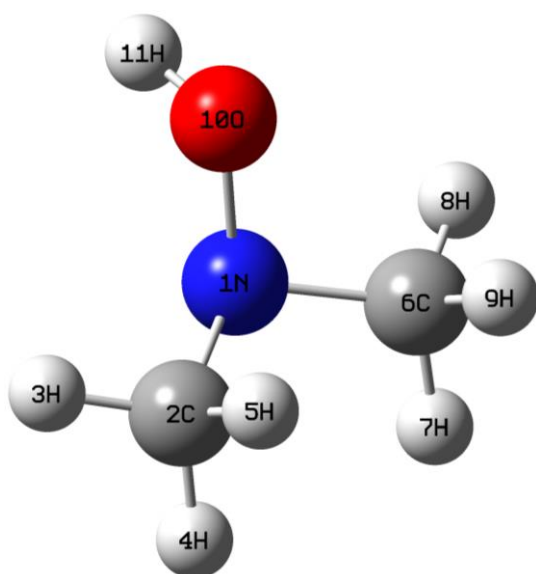
139 Pathway 1-2

140 TS5



141

| 142 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 143 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 144 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4569985 |             |              |
| 145 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0914789 | 108.9222629 |              |
| 146 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0975779 | 111.3827540 | 121.0480784  |
| 147 | 5   | No        | Show    | 5   | H      | 2  | 1  | 3  | 1.0924138 | 108.3773128 | -118.6913298 |
| 148 | 6   | No        | Show    | 6   | C      | 1  | 2  | 3  | 1.4693886 | 115.9300548 | 175.8026202  |
| 149 | 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.0908424 | 109.1200646 | 121.6449344  |
| 150 | 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0938829 | 109.7604942 | -118.6918474 |
| 151 | 9   | No        | Show    | 9   | H      | 6  | 1  | 2  | 1.0927972 | 110.4540806 | 1.7982376    |
| 152 | 10  | No        | Show    | 10  | O      | 1  | 2  | 6  | 2.6316959 | 116.9659899 | -150.1144784 |
| 153 | 11  | No        | Show    | 11  | N      | 10 | 1  | 2  | 1.1929329 | 50.7696593  | 78.0715557   |
| 154 | 12  | No        | Show    | 12  | O      | 1  | 2  | 6  | 1.3983760 | 109.9974639 | 127.3055187  |
| 155 | 13  | No        | Show    | 13  | H      | 12 | 1  | 2  | 0.9839695 | 103.7954009 | 112.3702310  |
| 156 | P5  |           |         |     |        |    |    |    |           |             |              |

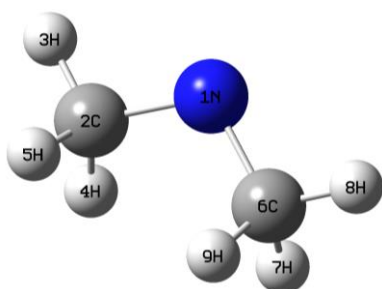


157

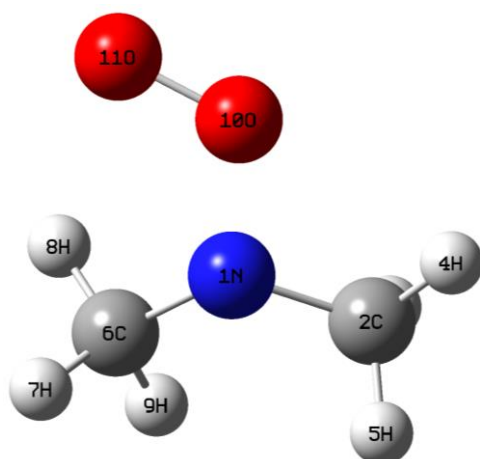
| 158 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 159 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 160 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4601490 |             |              |
| 161 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0921199 | 109.6344162 |              |
| 162 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0933223 | 108.4902188 | 118.3758424  |
| 163 | 5   | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.1006068 | 112.4573725 | 120.3206899  |
| 164 | 6   | No        | Show    | 6   | C      | 1  | 2  | 3  | 1.4602495 | 110.4708477 | 177.6829790  |
| 165 | 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.0932969 | 108.5133527 | 63.9250683   |
| 166 | 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0921144 | 109.6145982 | -177.6754574 |
| 167 | 9   | No        | Show    | 9   | H      | 6  | 1  | 2  | 1.1006085 | 112.4450152 | -56.4027286  |
| 168 | 10  | No        | Show    | 10  | O      | 1  | 2  | 6  | 1.4576323 | 105.3096817 | -113.1788977 |
| 169 | 11  | No        | Show    | 11  | H      | 10 | 1  | 2  | 0.9650138 | 103.4132598 | -121.4607138 |

TS6

P6

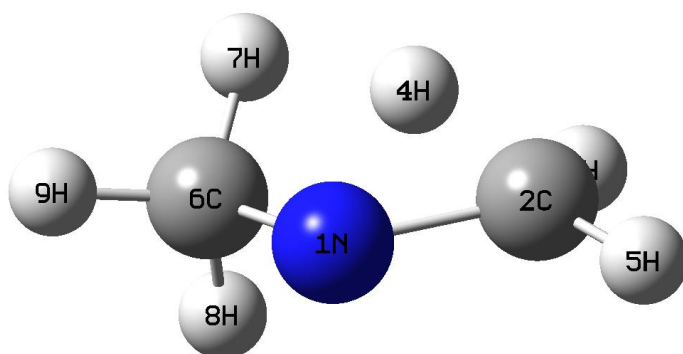


|     |     |           |         |     |        |    |    |    |           |             |              |  |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|--|
| 173 |     |           |         |     |        |    |    |    |           |             |              |  |
| 174 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |  |
| 175 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |  |
| 176 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4399579 |             |              |  |
| 177 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0922830 | 110.9335532 |              |  |
| 178 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.1004971 | 111.8662577 | 121.8097228  |  |
| 179 | 5   | No        | Show    | 5   | H      | 2  | 1  | 3  | 1.1012208 | 110.6487485 | -120.1778077 |  |
| 180 | 6   | No        | Show    | 6   | C      | 1  | 2  | 3  | 1.4399579 | 110.6968204 | -174.9022460 |  |
| 181 | 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.1012208 | 110.6487485 | 64.9199463   |  |
| 182 | 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0922830 | 110.9335532 | -174.9022460 |  |
| 183 | 9   | No        | Show    | 9   | H      | 6  | 1  | 2  | 1.1004971 | 111.8662577 | -53.0925232  |  |
| 184 | TS7 |           |         |     |        |    |    |    |           |             |              |  |



185

| 186 | Row | Highlight | Display | Tag | Symbol | NA | NB        | NC        | Bond        | Angle       | Dihedral     |
|-----|-----|-----------|---------|-----|--------|----|-----------|-----------|-------------|-------------|--------------|
| 187 | 1   | No        | Show    | 1   | N      |    |           |           |             |             |              |
| 188 | 2   | No        | Show    | 2   | C      | 1  | 1.4601651 |           |             |             |              |
| 189 | 3   | No        | Show    | 3   | H      | 2  | 1         | 1.0968539 | 112.7808185 |             |              |
| 190 | 4   | No        | Show    | 4   | H      | 2  | 1         | 3         | 1.0914807   | 109.2367340 | 122.5086927  |
| 191 | 5   | No        | Show    | 5   | H      | 2  | 1         | 4         | 1.0916196   | 107.3501883 | 117.2808560  |
| 192 | 6   | No        | Show    | 6   | C      | 1  | 2         | 4         | 1.4663259   | 114.5264627 | 172.6627217  |
| 193 | 7   | No        | Show    | 7   | H      | 6  | 1         | 2         | 1.0922071   | 110.3049893 | 123.4210007  |
| 194 | 8   | No        | Show    | 8   | H      | 6  | 1         | 2         | 1.0917787   | 109.4691362 | -117.8519399 |
| 195 | 9   | No        | Show    | 9   | H      | 6  | 1         | 2         | 1.0927559   | 110.2356221 | 2.4662359    |
| 196 | 10  | No        | Show    | 10  | O      | 1  | 2         | 6         | 1.4793148   | 103.1516951 | -120.6554929 |
| 197 | 11  | No        | Show    | 11  | O      | 10 | 1         | 2         | 1.2896223   | 114.6925236 | 162.0244429  |
| 198 | TS8 |           |         |     |        |    |           |           |             |             |              |

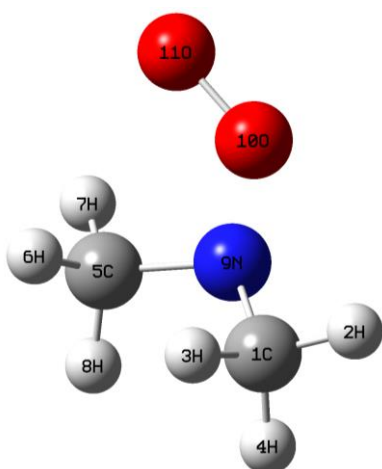


199

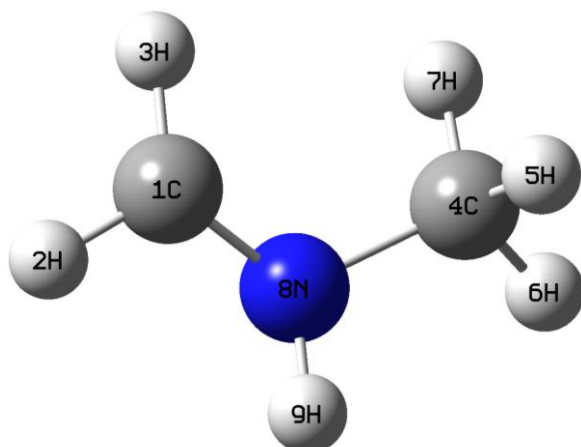
| 200 | Row | Highlight | Display | Tag | Symbol | NA | NB        | NC        | Bond        | Angle       | Dihedral     |
|-----|-----|-----------|---------|-----|--------|----|-----------|-----------|-------------|-------------|--------------|
| 201 | 1   | No        | Show    | 1   | N      |    |           |           |             |             |              |
| 202 | 2   | No        | Show    | 2   | C      | 1  | 1.4451364 |           |             |             |              |
| 203 | 3   | No        | Show    | 3   | H      | 2  | 1         | 1.0877322 | 120.3124602 |             |              |
| 204 | 4   | No        | Show    | 4   | H      | 1  | 2         | 3         | 1.2241581   | 57.1431930  | -110.6350017 |
| 205 | 5   | No        | Show    | 5   | H      | 2  | 1         | 4         | 1.0846293   | 115.4220957 | 95.1725145   |
| 206 | 6   | No        | Show    | 6   | C      | 1  | 2         | 5         | 1.4620514   | 110.7719858 | -165.9813146 |
| 207 | 7   | No        | Show    | 7   | H      | 6  | 1         | 2         | 1.0978134   | 113.0921219 | -43.3215830  |
| 208 | 8   | No        | Show    | 8   | H      | 6  | 1         | 2         | 1.0977636   | 109.6126957 | 76.3564551   |



209 9 No Show 9 H 6 1 2 1.0922577 110.0836425 -164.7087497  
 210 P7

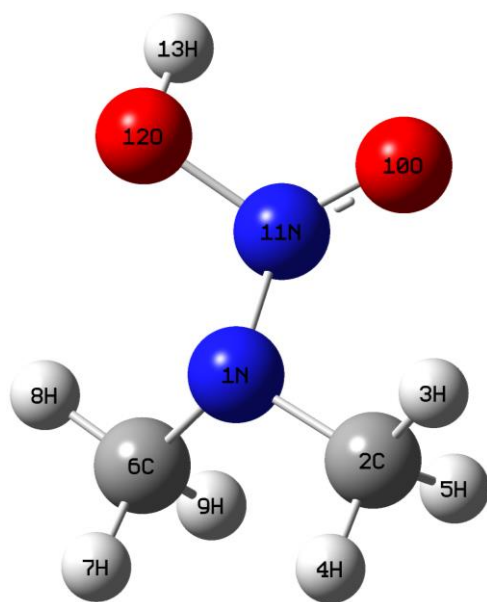


211  
 212 Row Highlight Display Tag Symbol NA NB NC Bond Angle Dihedral  
 213 1 No Show 1 C  
 214 2 No Show 2 H 1 1.0914194  
 215 3 No Show 3 H 1 2 1.0971352 109.6696262  
 216 4 No Show 4 H 1 2 3 1.0913491 108.4491644 -119.4818390  
 217 5 No Show 5 C 1 4 2 2.4420018 95.2369285 149.0911215  
 218 6 No Show 6 H 5 1 4 1.0975448 93.6161955 117.9810016  
 219 7 No Show 7 H 5 1 4 1.0891663 143.7237458 -111.0337953  
 220 8 No Show 8 H 5 1 4 1.0919141 88.2109414 8.8141912  
 221 9 No Show 9 N 5 1 4 1.4533789 33.2302644 -114.8108959  
 222 10 No Show 10 O 9 5 1 1.4813762 110.4343568 -115.3564094  
 223 11 No Show 11 O 10 9 5 1.2917186 115.1509932 -21.6557791  
 224 P8



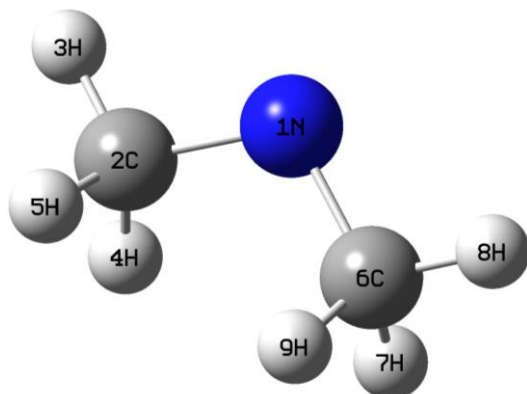
225  
 226 Row Highlight Display Tag Symbol NA NB NC Bond Angle Dihedral  
 227 1 No Show 1 C  
 228 2 No Show 2 H 1 1.0853877  
 229 3 No Show 3 H 1 2 1.0866627 118.0786662





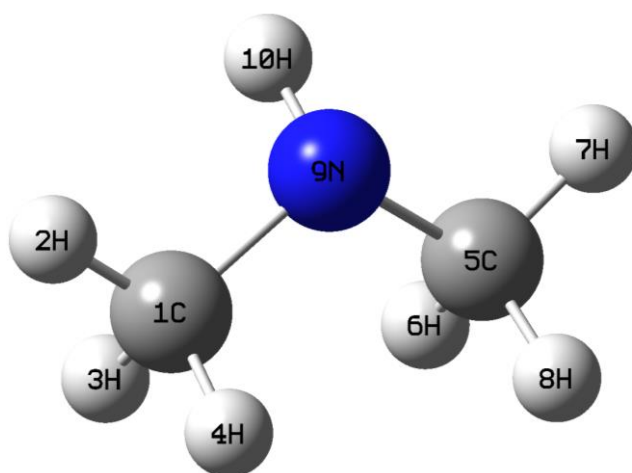
254

| 255 | Row | Highlight | Display | Tag | Symbol | NA | NB        | NC        | Bond        | Angle       | Dihedral     |
|-----|-----|-----------|---------|-----|--------|----|-----------|-----------|-------------|-------------|--------------|
| 256 | 1   | No        | Show    | 1   | N      |    |           |           |             |             |              |
| 257 | 2   | No        | Show    | 2   | C      | 1  | 1.4635942 |           |             |             |              |
| 258 | 3   | No        | Show    | 3   | H      | 2  | 1         | 1.0891337 | 110.1167791 |             |              |
| 259 | 4   | No        | Show    | 4   | H      | 2  | 1         | 3         | 1.0908062   | 106.7271340 | 118.2954113  |
| 260 | 5   | No        | Show    | 5   | H      | 2  | 1         | 4         | 1.0977723   | 112.5962273 | 119.3614203  |
| 261 | 6   | No        | Show    | 6   | C      | 1  | 2         | 3         | 1.4700875   | 112.4762731 | -175.1557087 |
| 262 | 7   | No        | Show    | 7   | H      | 6  | 1         | 2         | 1.0909071   | 107.8623692 | 64.2651032   |
| 263 | 8   | No        | Show    | 8   | H      | 6  | 1         | 2         | 1.0889918   | 109.5455174 | -177.5170281 |
| 264 | 9   | No        | Show    | 9   | H      | 6  | 1         | 2         | 1.0975324   | 112.0170387 | -55.7861895  |
| 265 | 10  | No        | Show    | 10  | O      | 1  | 2         | 6         | 2.3153311   | 85.5526209  | -135.4458246 |
| 266 | 11  | No        | Show    | 11  | N      | 10 | 1         | 2         | 1.2495681   | 32.2559248  | 153.1312055  |
| 267 | 12  | No        | Show    | 12  | O      | 11 | 10        | 1         | 1.4409188   | 116.2207248 | 130.1236851  |
| 268 | 13  | No        | Show    | 13  | H      | 12 | 11        | 10        | 0.9709238   | 102.1697911 | 51.8057450   |
| 269 | P10 |           |         |     |        |    |           |           |             |             |              |

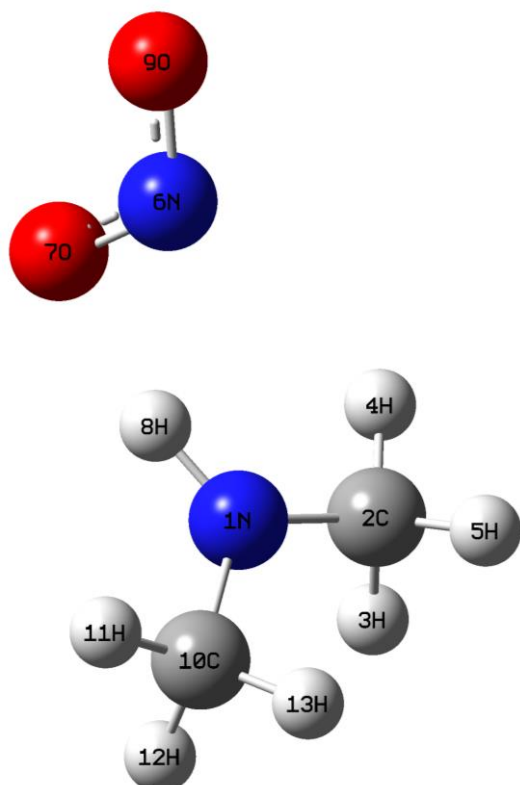


270

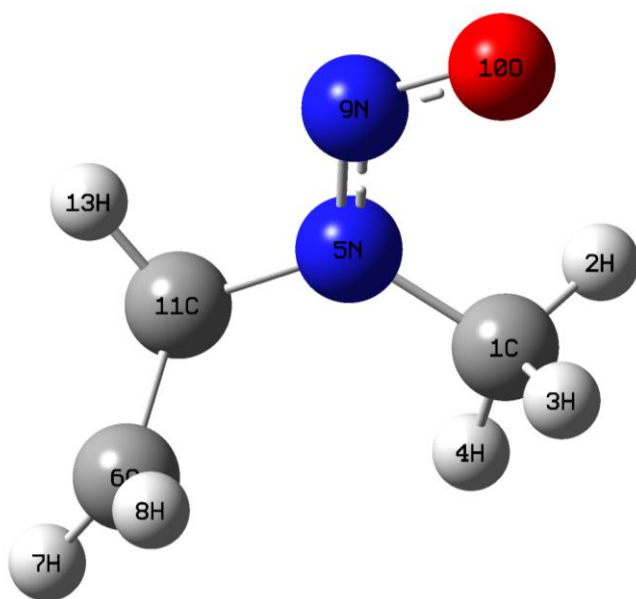
| 271 | Row | Highlight | Display | Tag | Symbol | NA | NB        | NC | Bond | Angle | Dihedral |
|-----|-----|-----------|---------|-----|--------|----|-----------|----|------|-------|----------|
| 272 | 1   | No        | Show    | 1   | N      |    |           |    |      |       |          |
| 273 | 2   | No        | Show    | 2   | C      | 1  | 1.4399579 |    |      |       |          |

[illegible]

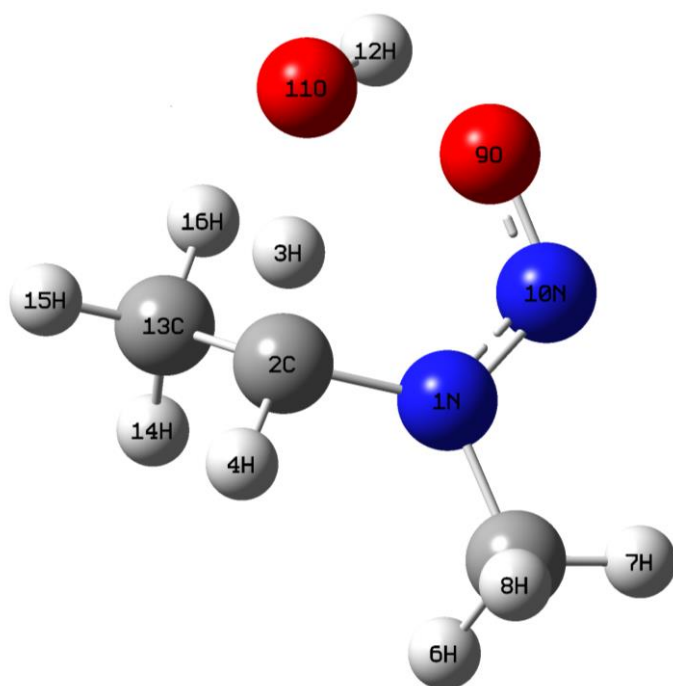
|     |      |           |         |     |        |    |    |    |           |             |              |  |  |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|--|--|
| 282 |      |           |         |     |        |    |    |    |           |             |              |  |  |
| 283 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |  |  |
| 284 | 1    | No        | Show    | 1   | C      |    |    |    |           |             |              |  |  |
| 285 | 2    | No        | Show    | 2   | H      | 1  |    |    | 1.0936924 |             |              |  |  |
| 286 | 3    | No        | Show    | 3   | H      | 1  | 2  |    | 1.1032237 | 108.0525516 |              |  |  |
| 287 | 4    | No        | Show    | 4   | H      | 1  | 2  | 3  | 1.0956165 | 107.7824685 | -115.6537590 |  |  |
| 288 | 5    | No        | Show    | 5   | C      | 1  | 2  | 4  | 2.4095480 | 144.3105390 | -123.7171349 |  |  |
| 289 | 6    | No        | Show    | 6   | H      | 5  | 1  | 2  | 1.1032237 | 91.7710014  | -125.0635832 |  |  |
| 290 | 7    | No        | Show    | 7   | H      | 5  | 1  | 2  | 1.0936924 | 144.3105390 | 0.0000000    |  |  |
| 291 | 8    | No        | Show    | 8   | H      | 5  | 1  | 2  | 1.0956165 | 93.4580976  | 127.4868983  |  |  |
| 292 | 9    | No        | Show    | 9   | N      | 5  | 1  | 2  | 1.4614110 | 34.4732072  | 6.8271493    |  |  |
| 293 | 10   | No        | Show    | 10  | H      | 9  | 5  | 1  | 1.0167389 | 107.0839348 | -116.5911491 |  |  |
| 294 | TS11 |           |         |     |        |    |    |    |           |             |              |  |  |

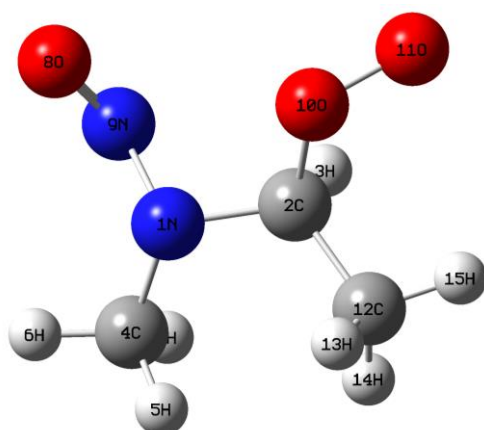


|     |              |           |         |     |        |    |    |           |             |             |              |  |
|-----|--------------|-----------|---------|-----|--------|----|----|-----------|-------------|-------------|--------------|--|
| 295 |              |           |         |     |        |    |    |           |             |             |              |  |
| 296 | Row          | Highlight | Display | Tag | Symbol | NA | NB | NC        | Bond        | Angle       | Dihedral     |  |
| 297 | 1            | No        | Show    | 1   | N      |    |    |           |             |             |              |  |
| 298 | 2            | No        | Show    | 2   | C      | 1  |    | 1.4318095 |             |             |              |  |
| 299 | 3            | No        | Show    | 3   | H      | 2  | 1  | 1.0990542 | 109.8184278 |             |              |  |
| 300 | 4            | No        | Show    | 4   | H      | 2  | 1  | 3         | 1.0888511   | 109.8739958 | 121.4017611  |  |
| 301 | 5            | No        | Show    | 5   | H      | 2  | 1  | 4         | 1.0977322   | 109.7175653 | 121.3114068  |  |
| 302 | 6            | No        | Show    | 6   | N      | 1  | 2  | 4         | 2.8277076   | 108.1400296 | -30.3676204  |  |
| 303 | 7            | No        | Show    | 7   | O      | 6  | 1  | 2         | 1.2665598   | 70.9499890  | 110.7622207  |  |
| 304 | 8            | No        | Show    | 8   | H      | 1  | 2  | 6         | 1.0494585   | 118.8004486 | 35.7799502   |  |
| 305 | 9            | No        | Show    | 9   | O      | 6  | 1  | 2         | 1.2339902   | 171.3425683 | -55.3196328  |  |
| 306 | 10           | No        | Show    | 10  | C      | 1  | 2  | 6         | 1.4321576   | 120.6996395 | -153.7766169 |  |
| 307 | 11           | No        | Show    | 11  | H      | 10 | 1  | 2         | 1.0895569   | 109.8636772 | 169.7214270  |  |
| 308 | 12           | No        | Show    | 12  | H      | 10 | 1  | 2         | 1.1012890   | 109.5188781 | -70.3416221  |  |
| 309 | 13           | No        | Show    | 13  | H      | 10 | 1  | 2         | 1.0952168   | 110.0655853 | 47.2926346   |  |
| 310 | Pathway 2-1  |           |         |     |        |    |    |           |             |             |              |  |
| 311 | CH3CH2NNOCH3 |           |         |     |        |    |    |           |             |             |              |  |



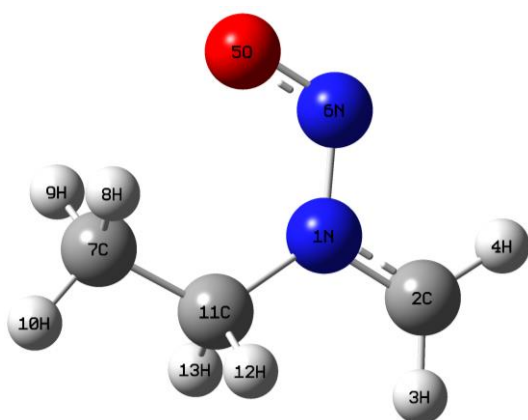
|     |      |                   |      |    |   |     |        |    |           |             |              |       |          |
|-----|------|-------------------|------|----|---|-----|--------|----|-----------|-------------|--------------|-------|----------|
| 312 |      |                   |      |    |   |     |        |    |           |             |              |       |          |
| 313 | Row  | Highlight Display |      |    |   | Tag | Symbol | NA | NB        | NC          | Bond         | Angle | Dihedral |
| 314 | 1    | No                | Show | 1  | C |     |        |    |           |             |              |       |          |
| 315 | 2    | No                | Show | 2  | H | 1   |        |    | 1.0930419 |             |              |       |          |
| 316 | 3    | No                | Show | 3  | H | 1   | 2      |    | 1.0938291 | 108.3762702 |              |       |          |
| 317 | 4    | No                | Show | 4  | H | 1   | 2      | 3  | 1.0886719 | 110.1149353 | -120.1508015 |       |          |
| 318 | 5    | No                | Show | 5  | N | 1   | 4      | 3  | 1.4583877 | 108.3087268 | -120.7743019 |       |          |
| 319 | 6    | No                | Show | 6  | C | 5   | 1      | 4  | 2.4619382 | 102.3754974 | 35.7210646   |       |          |
| 320 | 7    | No                | Show | 7  | H | 6   | 5      | 1  | 1.0828968 | 144.7153651 | -75.7663084  |       |          |
| 321 | 8    | No                | Show | 8  | H | 6   | 5      | 1  | 1.0841443 | 94.0441635  | 85.0323235   |       |          |
| 322 | 9    | No                | Show | 9  | N | 5   | 1      | 6  | 1.3083450 | 121.1636750 | 149.0287177  |       |          |
| 323 | 10   | No                | Show | 10 | O | 9   | 5      | 1  | 1.2428842 | 114.9221064 | -0.0939093   |       |          |
| 324 | 11   | No                | Show | 11 | C | 5   | 1      | 9  | 1.4664845 | 121.7931482 | -179.0951293 |       |          |
| 325 | 12   | No                | Show | 12 | H | 11  | 5      | 1  | 1.0955196 | 108.6460740 | -61.5558315  |       |          |
| 326 | 13   | No                | Show | 13 | H | 11  | 5      | 1  | 1.0993087 | 105.0860072 | -175.7751436 |       |          |
| 327 | TS12 |                   |      |    |   |     |        |    |           |             |              |       |          |

[illegible]



347

| 348 | Row  | Highlight | Display | Tag | Symbol | NA | NB        | NC        | Bond        | Angle       | Dihedral     |
|-----|------|-----------|---------|-----|--------|----|-----------|-----------|-------------|-------------|--------------|
| 349 | 1    | No        | Show    | 1   | N      |    |           |           |             |             |              |
| 350 | 2    | No        | Show    | 2   | C      | 1  | 1.4483591 |           |             |             |              |
| 351 | 3    | No        | Show    | 3   | H      | 2  | 1         | 1.0973252 | 113.0493102 |             |              |
| 352 | 4    | No        | Show    | 4   | C      | 1  | 2         | 3         | 1.4766563   | 112.3522086 | 76.4717803   |
| 353 | 5    | No        | Show    | 5   | H      | 4  | 1         | 2         | 1.0901335   | 108.6793598 | 70.4622551   |
| 354 | 6    | No        | Show    | 6   | H      | 4  | 1         | 2         | 1.0917089   | 108.3841510 | -172.4532360 |
| 355 | 7    | No        | Show    | 7   | H      | 4  | 1         | 2         | 1.0973760   | 113.2566787 | -51.2864462  |
| 356 | 8    | No        | Show    | 8   | O      | 1  | 2         | 4         | 2.2489493   | 116.0443459 | -138.8454849 |
| 357 | 9    | No        | Show    | 9   | N      | 8  | 1         | 2         | 1.1770599   | 39.2450088  | 69.8560307   |
| 358 | 10   | No        | Show    | 10  | O      | 2  | 1         | 4         | 1.4885359   | 102.8410054 | -171.1558779 |
| 359 | 11   | No        | Show    | 11  | O      | 10 | 2         | 1         | 1.3089050   | 111.6684114 | -159.0434874 |
| 360 | 12   | No        | Show    | 12  | C      | 2  | 1         | 4         | 1.5132180   | 115.0974438 | -53.2096540  |
| 361 | 13   | No        | Show    | 13  | H      | 12 | 2         | 1         | 1.0926569   | 111.3490728 | -48.4342762  |
| 362 | 14   | No        | Show    | 14  | H      | 12 | 2         | 1         | 1.0917530   | 110.4190229 | 73.4098661   |
| 363 | 15   | No        | Show    | 15  | H      | 12 | 2         | 1         | 1.0925069   | 108.0939636 | -168.4990405 |
| 364 | TS14 |           |         |     |        |    |           |           |             |             |              |

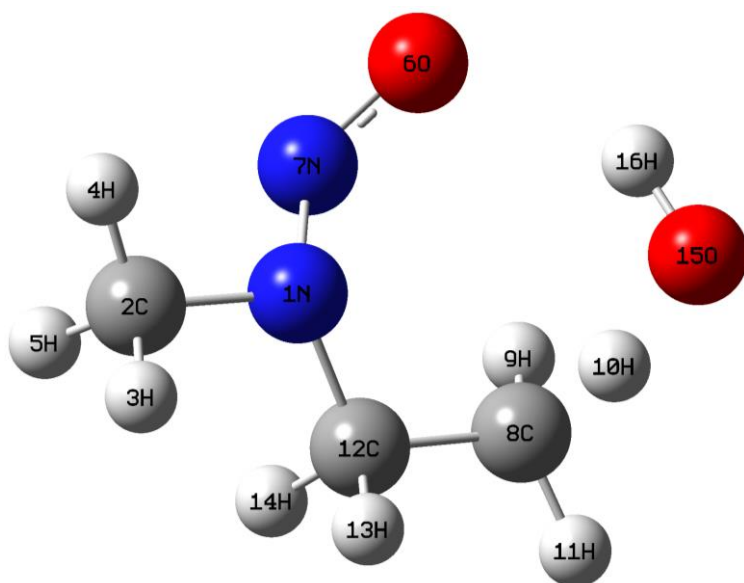


365

| 366 | Row | Highlight | Display | Tag | Symbol | NA | NB        | NC        | Bond        | Angle | Dihedral |
|-----|-----|-----------|---------|-----|--------|----|-----------|-----------|-------------|-------|----------|
| 367 | 1   | No        | Show    | 1   | N      |    |           |           |             |       |          |
| 368 | 2   | No        | Show    | 2   | C      | 1  | 1.3335576 |           |             |       |          |
| 369 | 3   | No        | Show    | 3   | H      | 2  | 1         | 1.0787447 | 118.9218232 |       |          |

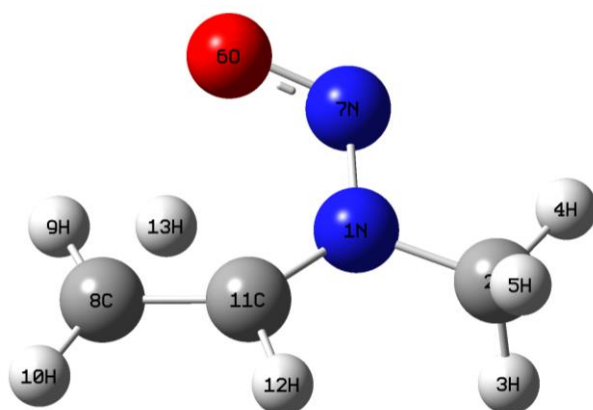






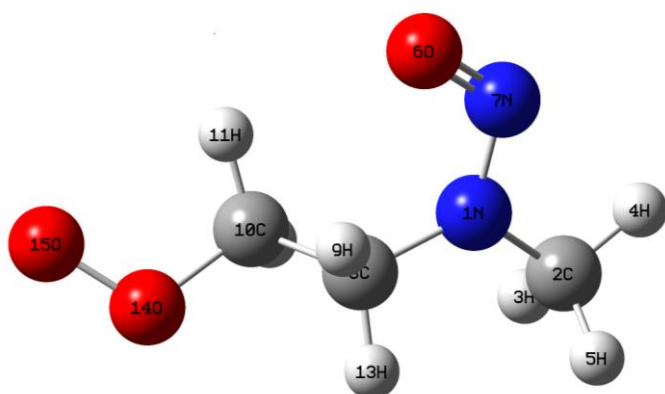
399

| 400 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 401 | 1    | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 402 | 2    | No        | Show    | 2   | C      | 1  |    |    | 1.4649917 |             |              |
| 403 | 3    | No        | Show    | 3   | H      | 2  | 1  |    | 1.0920570 | 107.6504330 |              |
| 404 | 4    | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0906767 | 109.1561140 | 118.6358429  |
| 405 | 5    | No        | Show    | 5   | H      | 2  | 1  | 3  | 1.0961524 | 112.1879422 | -119.7010663 |
| 406 | 6    | No        | Show    | 6   | O      | 1  | 2  | 4  | 2.3488200 | 127.4194101 | -30.6376704  |
| 407 | 7    | No        | Show    | 7   | N      | 6  | 1  | 2  | 1.2430704 | 28.9445771  | -58.5528574  |
| 408 | 8    | No        | Show    | 8   | C      | 1  | 7  | 6  | 2.4975521 | 89.1271663  | -72.9402128  |
| 409 | 9    | No        | Show    | 9   | H      | 8  | 1  | 7  | 1.0915134 | 97.5634396  | -14.2283576  |
| 410 | 10   | No        | Show    | 10  | H      | 8  | 1  | 7  | 1.1955920 | 87.9772386  | 90.6337019   |
| 411 | 11   | No        | Show    | 11  | H      | 8  | 1  | 7  | 1.0920982 | 143.4884676 | -156.3848999 |
| 412 | 12   | No        | Show    | 12  | C      | 1  | 7  | 6  | 1.4777646 | 113.4424544 | -96.7190806  |
| 413 | 13   | No        | Show    | 13  | H      | 12 | 1  | 7  | 1.0939578 | 105.3876482 | 168.6923925  |
| 414 | 14   | No        | Show    | 14  | H      | 12 | 1  | 7  | 1.1007244 | 109.9115365 | -76.1316161  |
| 415 | 15   | No        | Show    | 15  | O      | 8  | 1  | 7  | 2.5589287 | 82.5868282  | 84.9708770   |
| 416 | 16   | No        | Show    | 16  | H      | 15 | 8  | 1  | 0.9747580 | 88.6905015  | -53.1669150  |
| 417 | TS17 |           |         |     |        |    |    |    |           |             |              |



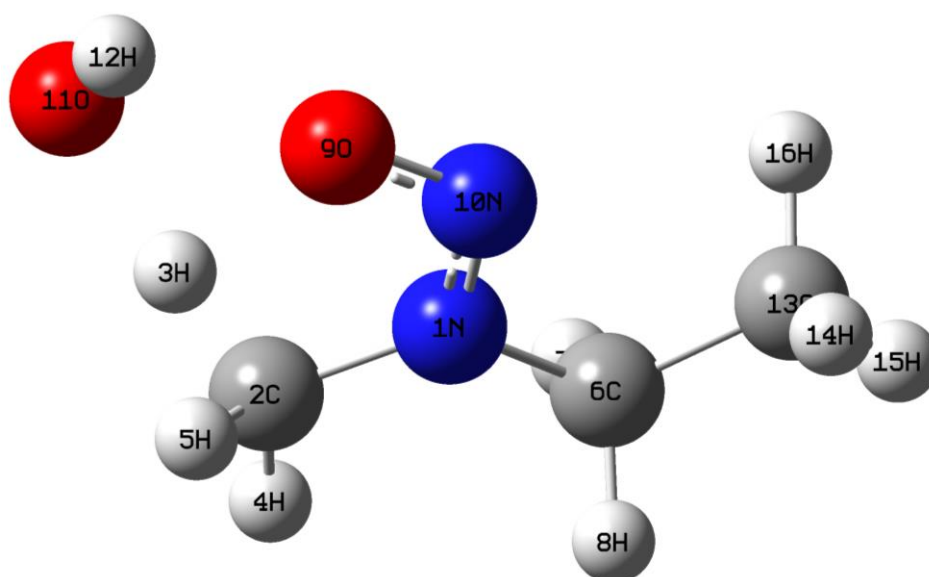
418

| 419 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond                  | Angle        | Dihedral |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------------------|--------------|----------|
| 420 | 1    | No        | Show    | 1   | N      |    |    |    |                       |              |          |
| 421 | 2    | No        | Show    | 2   | C      | 1  |    |    | 1.4620341             |              |          |
| 422 | 3    | No        | Show    | 3   | H      | 2  | 1  |    | 1.0921752 110.6263818 |              |          |
| 423 | 4    | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0892566 107.4461271 | 119.8394657  |          |
| 424 | 5    | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0930933 110.3486376 | 119.0260063  |          |
| 425 | 6    | No        | Show    | 6   | O      | 1  | 2  | 4  | 2.1879719 145.6948058 | -13.1882701  |          |
| 426 | 7    | No        | Show    | 7   | N      | 6  | 1  | 2  | 1.2622427 34.3913082  | 16.9278121   |          |
| 427 | 8    | No        | Show    | 8   | C      | 1  | 7  | 6  | 2.5673660 102.5932002 | 15.6016741   |          |
| 428 | 9    | No        | Show    | 9   | H      | 8  | 1  | 7  | 1.0751875 98.2384183  | 13.1331261   |          |
| 429 | 10   | No        | Show    | 10  | H      | 8  | 1  | 7  | 1.0814570 139.8367340 | -170.4765698 |          |
| 430 | 11   | No        | Show    | 11  | C      | 1  | 7  | 6  | 1.3833155 126.2189791 | 2.2081798    |          |
| 431 | 12   | No        | Show    | 12  | H      | 11 | 1  | 7  | 1.0831741 112.9048078 | -168.8789150 |          |
| 432 | 13   | No        | Show    | 13  | H      | 11 | 1  | 7  | 1.2523589 115.7584993 | -41.9325129  |          |
| 433 | TS18 |           |         |     |        |    |    |    |                       |              |          |



| 434 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond                  | Angle        | Dihedral |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------------------|--------------|----------|
| 435 | 1   | No        | Show    | 1   | N      |    |    |    |                       |              |          |
| 436 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4485433             |              |          |
| 437 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0958596 111.2226087 |              |          |
| 438 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0908621 107.3450035 | 119.3820956  |          |
| 439 | 5   | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0958514 111.0185778 | 119.5540348  |          |
| 440 | 6   | No        | Show    | 6   | O      | 1  | 2  | 4  | 2.1578147 147.5529145 | -0.6884636   |          |
| 441 | 7   | No        | Show    | 7   | N      | 6  | 1  | 2  | 1.2201443 34.3246045  | -0.8915772   |          |
| 442 | 8   | No        | Show    | 8   | C      | 1  | 7  | 6  | 1.4560585 121.0502111 | -2.6925460   |          |
| 443 | 9   | No        | Show    | 9   | H      | 8  | 1  | 7  | 1.0930302 108.0761032 | -38.5029839  |          |
| 444 | 10  | No        | Show    | 10  | C      | 8  | 1  | 7  | 1.5308759 111.7388457 | 81.7523387   |          |
| 445 | 11  | No        | Show    | 11  | H      | 10 | 8  | 1  | 1.0888184 112.0444544 | -70.5035867  |          |
| 446 | 12  | No        | Show    | 12  | H      | 10 | 8  | 1  | 1.0954829 111.4428384 | 53.7530160   |          |
| 447 | 13  | No        | Show    | 13  | H      | 8  | 1  | 7  | 1.0928014 108.1724623 | -156.9199235 |          |
| 448 | 14  | No        | Show    | 14  | O      | 10 | 8  | 1  | 1.4529866 107.3743870 | 170.9059452  |          |
| 449 | 15  | No        | Show    | 15  | O      | 14 | 10 | 8  | 1.3144352 112.3778313 | 133.6034651  |          |

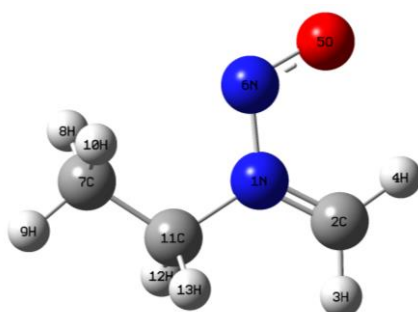
451 TS19



452

| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral    |
|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|-------------|
| 1   | No        | Show    | 1   | N      |    |    |    |           |             |             |
| 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4300719 |             |             |
| 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.1695185 | 109.3662399 |             |
| 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0883004 | 110.2416976 | 118.1157555 |
| 5   | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0910063 | 111.7369802 | 126.3781161 |
| 6   | No        | Show    | 6   | C      | 1  | 2  | 4  | 1.4729949 | 120.1463783 | 6.2702978   |
| 7   | No        | Show    | 7   | H      | 6  | 1  | 2  | 1.0950168 | 106.9829757 | 55.4421572  |
| 8   | No        | Show    | 8   | H      | 6  | 1  | 2  | 1.0942843 | 106.9387884 | -59.0723147 |
| 9   | No        | Show    | 9   | O      | 1  | 2  | 6  | 2.1546848 | 89.2940418  | 176.1419648 |
| 10  | No        | Show    | 10  | N      | 9  | 1  | 2  | 1.2439177 | 33.6406092  | 179.9664902 |
| 11  | No        | Show    | 11  | O      | 2  | 1  | 10 | 2.5969230 | 105.4639763 | 53.3652019  |
| 12  | No        | Show    | 12  | H      | 11 | 2  | 1  | 0.9754838 | 85.4743703  | -53.7095488 |
| 13  | No        | Show    | 13  | C      | 6  | 1  | 10 | 1.5183748 | 114.1599288 | 1.9295061   |
| 14  | No        | Show    | 14  | H      | 13 | 6  | 1  | 1.0924477 | 111.7942732 | 60.4346536  |
| 15  | No        | Show    | 15  | H      | 13 | 6  | 1  | 1.0936271 | 107.7447353 | 179.3590583 |
| 16  | No        | Show    | 16  | H      | 13 | 6  | 1  | 1.0924374 | 111.8564822 | -61.6231326 |

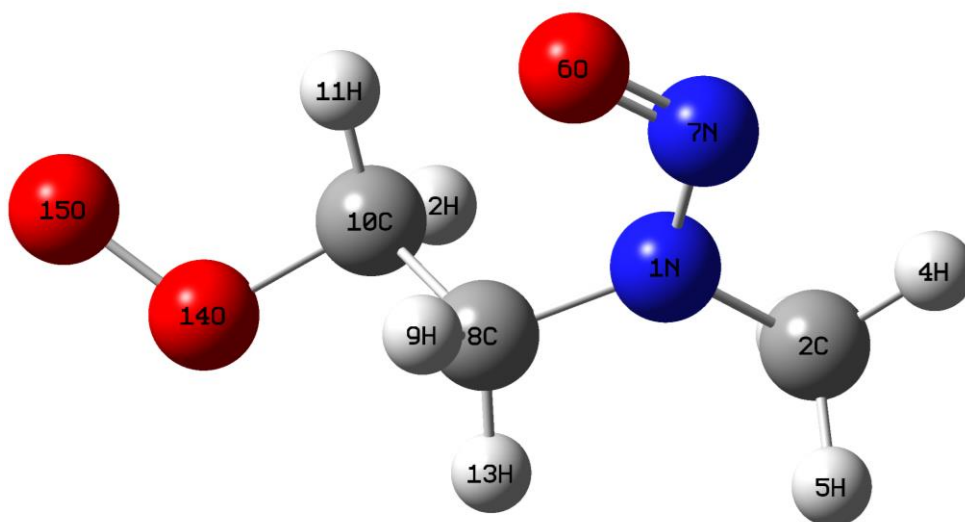
470 TS20



471

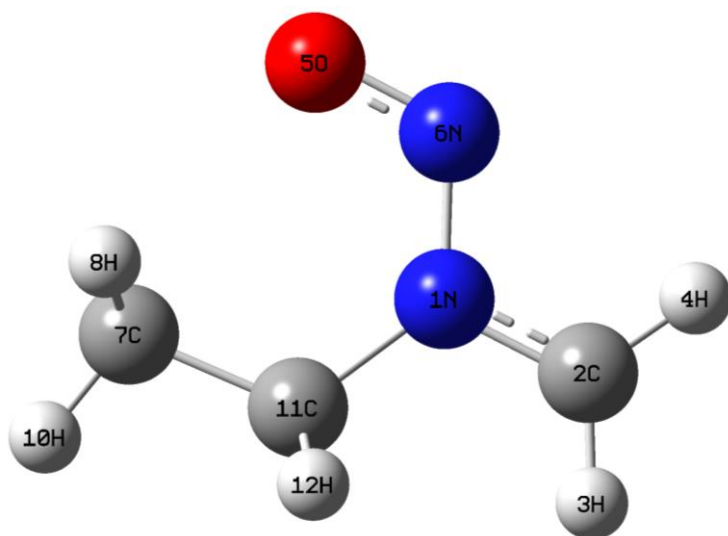
| Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral |
|-----|-----------|---------|-----|--------|----|----|----|------|-------|----------|
|-----|-----------|---------|-----|--------|----|----|----|------|-------|----------|

|     |      |    |      |    |   |    |   |   |           |             |              |  |
|-----|------|----|------|----|---|----|---|---|-----------|-------------|--------------|--|
| 473 | 1    | No | Show | 1  | N |    |   |   |           |             |              |  |
| 474 | 2    | No | Show | 2  | C | 1  |   |   | 1.3198271 |             |              |  |
| 475 | 3    | No | Show | 3  | H | 2  | 1 |   | 1.0798681 | 118.7371622 |              |  |
| 476 | 4    | No | Show | 4  | H | 2  | 1 | 3 | 1.0790779 | 118.2110887 | 180.0000000  |  |
| 477 | 5    | No | Show | 5  | O | 1  | 2 | 4 | 2.1971428 | 91.4999655  | -0.0007252   |  |
| 478 | 6    | No | Show | 6  | N | 5  | 1 | 2 | 1.2517924 | 35.6601502  | 180.0000000  |  |
| 479 | 7    | No | Show | 7  | C | 1  | 2 | 6 | 2.5261853 | 153.6887383 | -179.9793137 |  |
| 480 | 8    | No | Show | 8  | H | 7  | 1 | 2 | 1.0917744 | 94.5373085  | -125.4108780 |  |
| 481 | 9    | No | Show | 9  | H | 7  | 1 | 2 | 1.0940138 | 139.6542106 | -0.0298870   |  |
| 482 | 10   | No | Show | 10 | H | 7  | 1 | 2 | 1.0917770 | 94.5334992  | 125.3453983  |  |
| 483 | 11   | No | Show | 11 | C | 1  | 2 | 6 | 1.4833324 | 120.5270406 | 179.9976292  |  |
| 484 | 12   | No | Show | 12 | H | 11 | 1 | 2 | 1.0927890 | 106.6121220 | -57.4280026  |  |
| 485 | 13   | No | Show | 13 | H | 11 | 1 | 2 | 1.0927880 | 106.6106493 | 57.3920450   |  |
| 486 | TS21 |    |      |    |   |    |   |   |           |             |              |  |

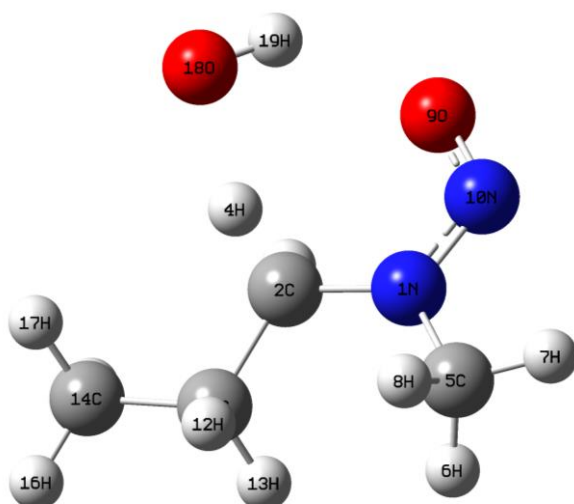


|     |     |           |         |     |        |    |    |    |           |             |              |  |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|--|
| 487 |     |           |         |     |        |    |    |    |           |             |              |  |
| 488 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |  |
| 489 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |  |
| 490 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4485433 |             |              |  |
| 491 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0958596 | 111.2226087 |              |  |
| 492 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0908621 | 107.3450035 | 119.3820956  |  |
| 493 | 5   | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0958514 | 111.0185778 | 119.5540348  |  |
| 494 | 6   | No        | Show    | 6   | O      | 1  | 2  | 4  | 2.1578147 | 147.5529145 | -0.6884636   |  |
| 495 | 7   | No        | Show    | 7   | N      | 6  | 1  | 2  | 1.2201443 | 34.3246045  | -0.8915772   |  |
| 496 | 8   | No        | Show    | 8   | C      | 1  | 7  | 6  | 1.4560585 | 121.0502111 | -2.6925460   |  |
| 497 | 9   | No        | Show    | 9   | H      | 8  | 1  | 7  | 1.0930302 | 108.0761032 | -38.5029839  |  |
| 498 | 10  | No        | Show    | 10  | C      | 8  | 1  | 7  | 1.5308759 | 111.7388457 | 81.7523387   |  |
| 499 | 11  | No        | Show    | 11  | H      | 10 | 8  | 1  | 1.0888184 | 112.0444544 | -70.5035867  |  |
| 500 | 12  | No        | Show    | 12  | H      | 10 | 8  | 1  | 1.0954829 | 111.4428384 | 53.7530160   |  |
| 501 | 13  | No        | Show    | 13  | H      | 8  | 1  | 7  | 1.0928014 | 108.1724623 | -156.9199235 |  |

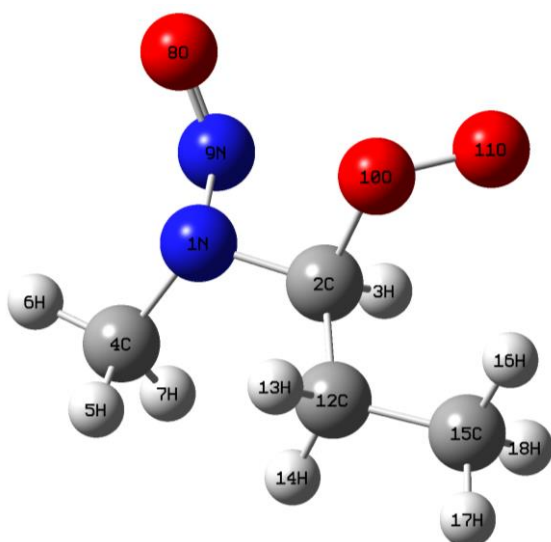
|     |      |    |      |    |   |    |    |   |           |             |             |
|-----|------|----|------|----|---|----|----|---|-----------|-------------|-------------|
| 502 | 14   | No | Show | 14 | O | 10 | 8  | 1 | 1.4529866 | 107.3743870 | 170.9059452 |
| 503 | 15   | No | Show | 15 | O | 14 | 10 | 8 | 1.3144352 | 112.3778313 | 133.6034651 |
| 504 | TS22 |    |      |    |   |    |    |   |           |             |             |



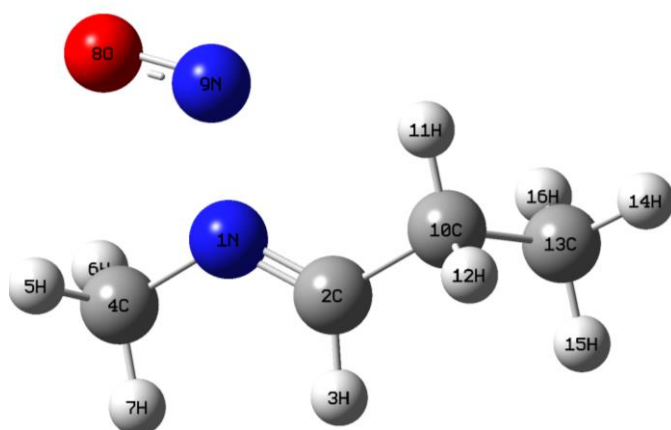
|     | Highlight |    |      |    |     |        | Display |           |             |             |              |          |  |  |  |
|-----|-----------|----|------|----|-----|--------|---------|-----------|-------------|-------------|--------------|----------|--|--|--|
|     | Row       |    |      |    | Tag | Symbol | NA      | NB        | NC          | Bond        | Angle        | Dihedral |  |  |  |
| 505 |           |    |      |    |     |        |         |           |             |             |              |          |  |  |  |
| 506 | 1         | No | Show | 1  | N   |        |         |           |             |             |              |          |  |  |  |
| 508 | 2         | No | Show | 2  | C   | 1      |         | 1.3335576 |             |             |              |          |  |  |  |
| 509 | 3         | No | Show | 3  | H   | 2      | 1       | 1.0787447 | 118.9218232 |             |              |          |  |  |  |
| 510 | 4         | No | Show | 4  | H   | 2      | 1       | 3         | 1.0803686   | 118.1273217 | 180.0000000  |          |  |  |  |
| 511 | 5         | No | Show | 5  | O   | 1      | 2       | 3         | 2.2234578   | 145.8482388 | 180.0000000  |          |  |  |  |
| 512 | 6         | No | Show | 6  | N   | 5      | 1       | 2         | 1.2484082   | 33.8175881  | 0.0000000    |          |  |  |  |
| 513 | 7         | No | Show | 7  | C   | 1      | 2       | 6         | 2.6220795   | 146.4092694 | 180.0000000  |          |  |  |  |
| 514 | 8         | No | Show | 8  | H   | 7      | 1       | 2         | 1.0897025   | 96.8966620  | 124.9248795  |          |  |  |  |
| 515 | 9         | No | Show | 9  | H   | 7      | 1       | 2         | 1.0897025   | 96.8966620  | -124.9248795 |          |  |  |  |
| 516 | 10        | No | Show | 10 | H   | 7      | 1       | 2         | 1.0961768   | 135.6895637 | 0.0000000    |          |  |  |  |
| 517 | 11        | No | Show | 11 | C   | 1      | 2       | 6         | 1.5059037   | 116.2221739 | 180.0000000  |          |  |  |  |
| 518 | 12        | No | Show | 12 | H   | 11     | 1       | 2         | 1.0924162   | 104.7086855 | 56.4345376   |          |  |  |  |
| 519 | 13        | No | Show | 13 | H   | 11     | 1       | 2         | 1.0924154   | 104.7086966 | -56.4345076  |          |  |  |  |
| 520 | TS23      |    |      |    |     |        |         |           |             |             |              |          |  |  |  |



|     |      |                   |      |    |   |     |        |           |             |             |              |       |          |
|-----|------|-------------------|------|----|---|-----|--------|-----------|-------------|-------------|--------------|-------|----------|
| 521 |      |                   |      |    |   |     |        |           |             |             |              |       |          |
| 522 | Row  | Highlight Display |      |    |   | Tag | Symbol | NA        | NB          | NC          | Bond         | Angle | Dihedral |
| 523 | 1    | No                | Show | 1  | N |     |        |           |             |             |              |       |          |
| 524 | 2    | No                | Show | 2  | C | 1   |        | 1.4509352 |             |             |              |       |          |
| 525 | 3    | No                | Show | 3  | H | 2   | 1      | 1.0941413 | 107.8921181 |             |              |       |          |
| 526 | 4    | No                | Show | 4  | H | 2   | 1      | 3         | 1.1403876   | 107.3624906 | -111.4931526 |       |          |
| 527 | 5    | No                | Show | 5  | C | 1   | 2      | 3         | 1.4574258   | 123.4802354 | -137.7828341 |       |          |
| 528 | 6    | No                | Show | 6  | H | 5   | 1      | 2         | 1.0914655   | 110.4563746 | 60.5080979   |       |          |
| 529 | 7    | No                | Show | 7  | H | 5   | 1      | 2         | 1.0894016   | 107.4361623 | -179.8486704 |       |          |
| 530 | 8    | No                | Show | 8  | H | 5   | 1      | 2         | 1.0929733   | 110.5247570 | -60.5316166  |       |          |
| 531 | 9    | No                | Show | 9  | O | 1   | 2      | 5         | 2.1612383   | 89.2385319  | -174.9954087 |       |          |
| 532 | 10   | No                | Show | 10 | N | 9   | 1      | 2         | 1.2435754   | 33.4008202  | 179.3909525  |       |          |
| 533 | 11   | No                | Show | 11 | C | 2   | 1      | 10        | 1.5206172   | 115.1898822 | 173.9219741  |       |          |
| 534 | 12   | No                | Show | 12 | H | 11  | 2      | 1         | 1.0945999   | 110.2545831 | 59.2164772   |       |          |
| 535 | 13   | No                | Show | 13 | H | 11  | 2      | 1         | 1.0968659   | 109.0170954 | -57.9908837  |       |          |
| 536 | 14   | No                | Show | 14 | C | 11  | 2      | 1         | 1.5294392   | 110.7479024 | -178.8480891 |       |          |
| 537 | 15   | No                | Show | 15 | H | 14  | 11     | 2         | 1.0951147   | 111.1712662 | 60.4290926   |       |          |
| 538 | 16   | No                | Show | 16 | H | 14  | 11     | 2         | 1.0936403   | 110.5850808 | -179.6845132 |       |          |
| 539 | 17   | No                | Show | 17 | H | 14  | 11     | 2         | 1.0952179   | 111.2541026 | -59.7341175  |       |          |
| 540 | 18   | No                | Show | 18 | O | 2   | 1      | 10        | 2.7013810   | 103.1199465 | -49.8972517  |       |          |
| 541 | 19   | No                | Show | 19 | H | 18  | 2      | 1         | 0.9770852   | 82.5940115  | 50.4462648   |       |          |
| 542 | TS24 |                   |      |    |   |     |        |           |             |             |              |       |          |

[illegible]





564

565

566

567

568

569

570

571

572

573

574

575

576

577

578

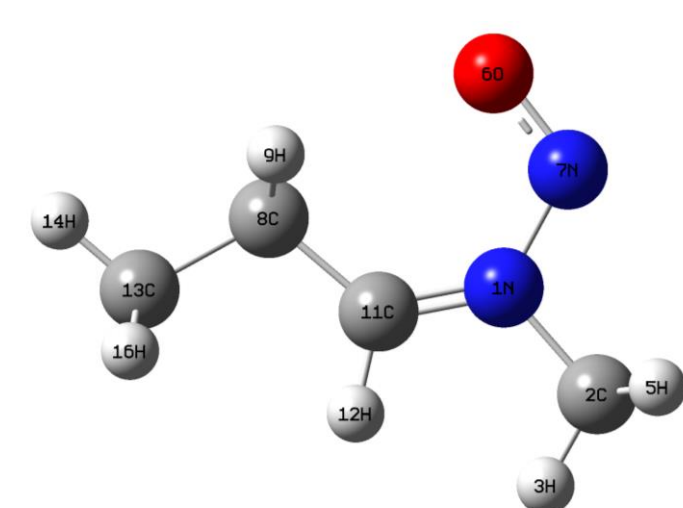
579

580

581

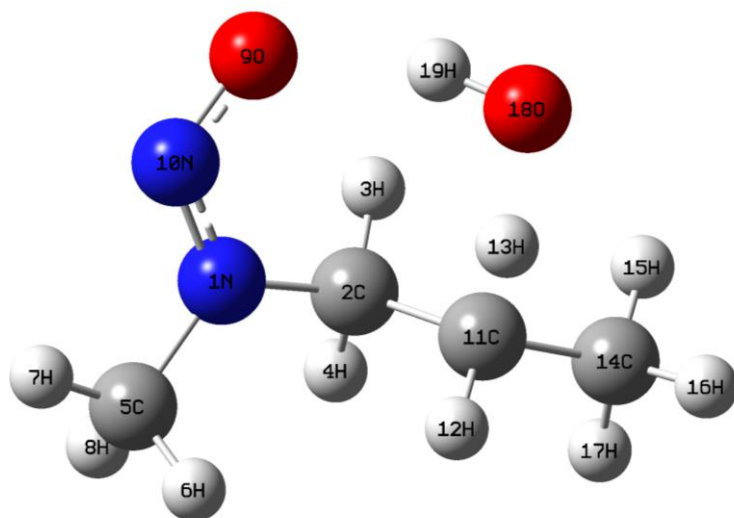
582

583



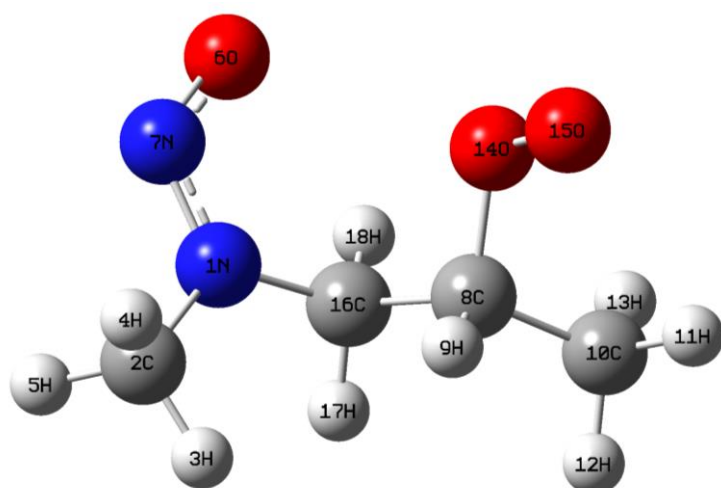
584

|     |      |           |         |     |        |    |    |    |           |             |              |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 585 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
| 586 | 1    | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 587 | 2    | No        | Show    | 2   | C      | 1  |    |    | 1.4700110 |             |              |
| 588 | 3    | No        | Show    | 3   | H      | 2  | 1  |    | 1.0874556 | 109.4595769 |              |
| 589 | 4    | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0907348 | 109.1250723 | 120.2866963  |
| 590 | 5    | No        | Show    | 5   | H      | 2  | 1  | 4  | 1.0907426 | 109.1346650 | 119.4151441  |
| 591 | 6    | No        | Show    | 6   | O      | 1  | 2  | 3  | 2.2251143 | 141.5430828 | -179.9948601 |
| 592 | 7    | No        | Show    | 7   | N      | 6  | 1  | 2  | 1.2614998 | 34.9869942  | 0.1325482    |
| 593 | 8    | No        | Show    | 8   | C      | 1  | 7  | 6  | 2.5414769 | 102.0578955 | 0.1007728    |
| 594 | 9    | No        | Show    | 9   | H      | 8  | 1  | 7  | 1.0952400 | 96.3824973  | -53.3673908  |
| 595 | 10   | No        | Show    | 10  | H      | 8  | 1  | 7  | 1.0950774 | 96.1842967  | 52.8709850   |
| 596 | 11   | No        | Show    | 11  | C      | 1  | 7  | 6  | 1.3229992 | 129.4044870 | 0.0746888    |
| 597 | 12   | No        | Show    | 12  | H      | 11 | 1  | 7  | 1.0844325 | 113.5524122 | -179.9593411 |
| 598 | 13   | No        | Show    | 13  | C      | 8  | 1  | 11 | 1.5317433 | 134.5861298 | -0.4146474   |
| 599 | 14   | No        | Show    | 14  | H      | 13 | 8  | 1  | 1.0933325 | 110.3592854 | -179.8222906 |
| 600 | 15   | No        | Show    | 15  | H      | 13 | 8  | 1  | 1.0949635 | 111.1442140 | -59.9679033  |
| 601 | 16   | No        | Show    | 16  | H      | 13 | 8  | 1  | 1.0949703 | 111.1524049 | 60.3243112   |
| 602 | TS27 |           |         |     |        |    |    |    |           |             |              |

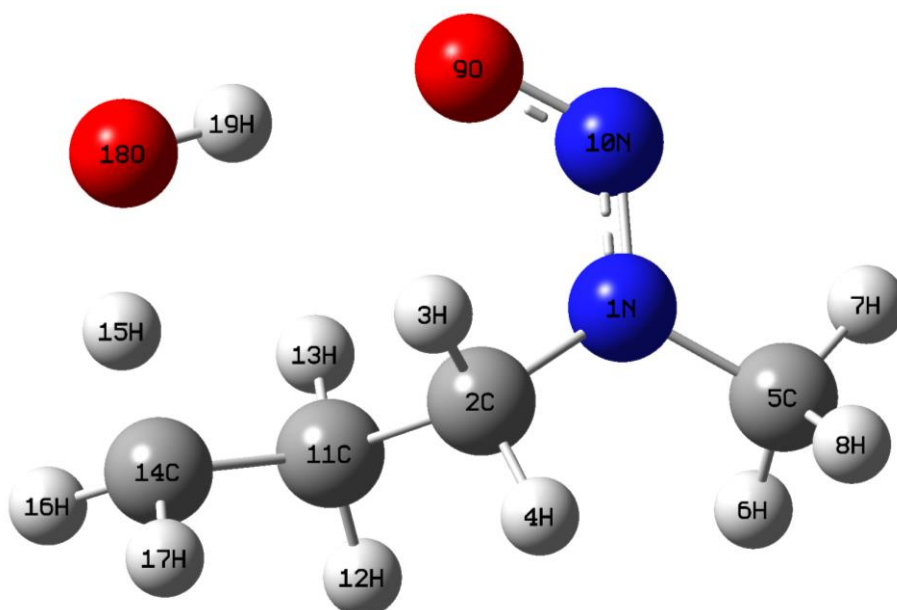


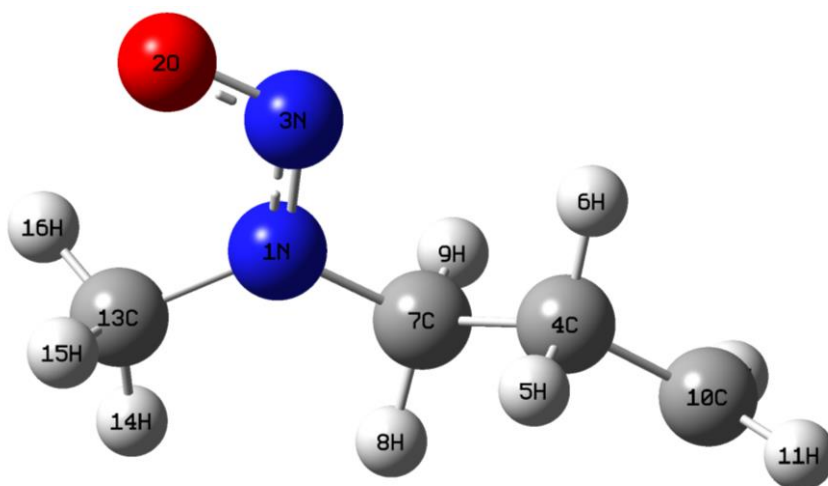
|     |     |           |         |     |        |    |    |    |           |             |              |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 603 |     |           |         |     |        |    |    |    |           |             |              |
| 604 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
| 605 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 606 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4661641 |             |              |
| 607 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0913764 | 107.4538649 |              |
| 608 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0946952 | 106.3777197 | -116.1646102 |
| 609 | 5   | No        | Show    | 5   | C      | 1  | 2  | 3  | 1.4557051 | 119.7724988 | 150.0077038  |
| 610 | 6   | No        | Show    | 6   | H      | 5  | 1  | 2  | 1.0932894 | 109.8401726 | 58.9229419   |
| 611 | 7   | No        | Show    | 7   | H      | 5  | 1  | 2  | 1.0895143 | 108.4238943 | 178.7701658  |
| 612 | 8   | No        | Show    | 8   | H      | 5  | 1  | 2  | 1.0934729 | 109.9301612 | -60.9277052  |
| 613 | 9   | No        | Show    | 9   | O      | 1  | 5  | 2  | 2.1681878 | 147.7531158 | -179.4426658 |





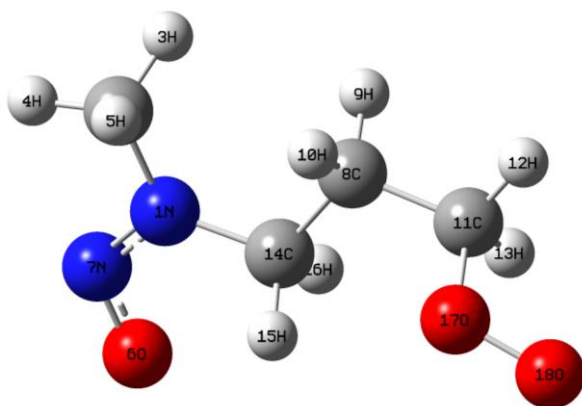
|     |      |    |                   |    |   |     |        |   |           |             |    |              |       |          |
|-----|------|----|-------------------|----|---|-----|--------|---|-----------|-------------|----|--------------|-------|----------|
| 644 |      |    |                   |    |   |     |        |   |           |             |    |              |       |          |
| 645 | Row  |    | Highlight Display |    |   | Tag | Symbol |   | NA        | NB          | NC | Bond         | Angle | Dihedral |
| 646 | 1    | No | Show              | 1  | N |     |        |   |           |             |    |              |       |          |
| 647 | 2    | No | Show              | 2  | C | 1   |        |   | 1.4637164 |             |    |              |       |          |
| 648 | 3    | No | Show              | 3  | H | 2   | 1      |   | 1.0891124 | 108.4828733 |    |              |       |          |
| 649 | 4    | No | Show              | 4  | H | 2   | 1      | 3 | 1.0917625 | 110.5244416 |    | 119.4089977  |       |          |
| 650 | 5    | No | Show              | 5  | H | 2   | 1      | 3 | 1.0925388 | 110.5344423 |    | -119.3225875 |       |          |
| 651 | 6    | No | Show              | 6  | O | 1   | 2      | 3 | 2.1698517 | 146.3259634 |    | -175.5419264 |       |          |
| 652 | 7    | No | Show              | 7  | N | 6   | 1      | 2 | 1.2384740 | 32.8005625  |    | -3.2705666   |       |          |
| 653 | 8    | No | Show              | 8  | C | 1   | 7      | 6 | 2.4997612 | 121.8164641 |    | 39.7564653   |       |          |
| 654 | 9    | No | Show              | 9  | H | 8   | 1      | 7 | 1.0921572 | 88.3309034  |    | 120.1540248  |       |          |
| 655 | 10   | No | Show              | 10 | C | 8   | 1      | 7 | 1.5177436 | 144.7992102 |    | -113.2124426 |       |          |
| 656 | 11   | No | Show              | 11 | H | 10  | 8      | 1 | 1.0924715 | 109.9511882 |    | -179.6435676 |       |          |
| 657 | 12   | No | Show              | 12 | H | 10  | 8      | 1 | 1.0933729 | 109.4327242 |    | -60.5418330  |       |          |
| 658 | 13   | No | Show              | 13 | H | 10  | 8      | 1 | 1.0939796 | 111.0313983 |    | 59.4450778   |       |          |
| 659 | 14   | No | Show              | 14 | O | 8   | 1      | 7 | 1.4784493 | 91.6342371  |    | 14.6399627   |       |          |
| 660 | 15   | No | Show              | 15 | O | 14  | 8      | 1 | 1.3102603 | 111.9432045 |    | 131.4824272  |       |          |
| 661 | 16   | No | Show              | 16 | C | 1   | 7      | 6 | 1.4624390 | 123.0167562 |    | -0.7126657   |       |          |
| 662 | 17   | No | Show              | 17 | H | 16  | 1      | 7 | 1.0916277 | 107.8177370 |    | -140.8570788 |       |          |
| 663 | 18   | No | Show              | 18 | H | 16  | 1      | 7 | 1.0903554 | 107.7692860 |    | -23.3413597  |       |          |
| 664 | TS31 |    |                   |    |   |     |        |   |           |             |    |              |       |          |

[illegible]



687

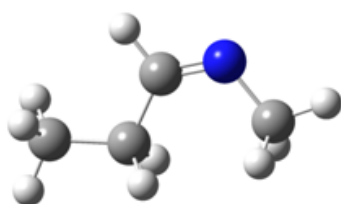
| 688 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond                  | Angle        | Dihedral |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------------------|--------------|----------|
| 689 | 1    | No        | Show    | 1   | N      |    |    |    |                       |              |          |
| 690 | 2    | No        | Show    | 2   | O      | 1  |    |    | 2.1526737             |              |          |
| 691 | 3    | No        | Show    | 3   | N      | 2  | 1  |    | 1.2451945 33.2925211  |              |          |
| 692 | 4    | No        | Show    | 4   | C      | 1  | 3  | 2  | 2.5165380 91.6622689  | -159.6102510 |          |
| 693 | 5    | No        | Show    | 5   | H      | 4  | 1  | 3  | 1.0964851 90.3446368  | 90.3812761   |          |
| 694 | 6    | No        | Show    | 6   | H      | 4  | 1  | 3  | 1.1012968 90.3474875  | -15.4400192  |          |
| 695 | 7    | No        | Show    | 7   | C      | 1  | 3  | 2  | 1.4716070 117.4387039 | 177.3775125  |          |
| 696 | 8    | No        | Show    | 8   | H      | 7  | 1  | 3  | 1.0902995 106.2943757 | 165.2885170  |          |
| 697 | 9    | No        | Show    | 9   | H      | 7  | 1  | 3  | 1.0959937 109.1868290 | -78.9974301  |          |
| 698 | 10   | No        | Show    | 10  | C      | 4  | 1  | 3  | 1.4877426 143.7503204 | -142.5283250 |          |
| 699 | 11   | No        | Show    | 11  | H      | 10 | 4  | 1  | 1.0837579 120.5164672 | -153.0416723 |          |
| 700 | 12   | No        | Show    | 12  | H      | 10 | 4  | 1  | 1.0853649 120.6739768 | 36.8804216   |          |
| 701 | 13   | No        | Show    | 13  | C      | 1  | 3  | 2  | 1.4601204 120.4367340 | 2.1339873    |          |
| 702 | 14   | No        | Show    | 14  | H      | 13 | 1  | 3  | 1.0876642 108.5118531 | 176.1905382  |          |
| 703 | 15   | No        | Show    | 15  | H      | 13 | 1  | 3  | 1.0937285 110.1531551 | -63.4019459  |          |
| 704 | 16   | No        | Show    | 16  | H      | 13 | 1  | 3  | 1.0935557 109.9657754 | 55.7940244   |          |
| 705 | TS33 |           |         |     |        |    |    |    |                       |              |          |



706

| 707 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral |
|-----|-----|-----------|---------|-----|--------|----|----|----|------|-------|----------|
| 708 | 1   | No        | Show    | 1   | N      |    |    |    |      |       |          |

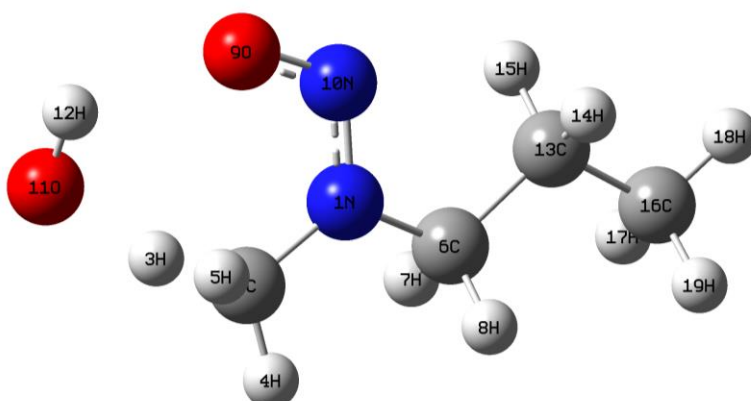
|     |           |    |      |    |   |    |    |           |             |             |
|-----|-----------|----|------|----|---|----|----|-----------|-------------|-------------|
| 709 | 2         | No | Show | 2  | C | 1  |    | 1.4561016 |             |             |
| 710 | 3         | No | Show | 3  | H | 2  | 1  | 1.0922147 | 110.8154809 |             |
| 711 | 4         | No | Show | 4  | H | 2  | 1  | 3         | 1.0896050   | 107.3500979 |
| 712 | 5         | No | Show | 5  | H | 2  | 1  | 4         | 1.0930188   | 110.7118426 |
| 713 | 6         | No | Show | 6  | O | 1  | 2  | 4         | 2.1558576   | 147.5786647 |
| 714 | 7         | No | Show | 7  | N | 6  | 1  | 2         | 1.2432460   | 33.3700593  |
| 715 | 8         | No | Show | 8  | C | 1  | 7  | 6         | 2.5066427   | 153.4650141 |
| 716 | 9         | No | Show | 9  | H | 8  | 1  | 7         | 1.0942404   | 93.7061345  |
| 717 | 10        | No | Show | 10 | H | 8  | 1  | 7         | 1.0940745   | 91.9998031  |
| 718 | 11        | No | Show | 11 | C | 8  | 1  | 7         | 1.5169171   | 143.8919264 |
| 719 | 12        | No | Show | 12 | H | 11 | 8  | 1         | 1.0920617   | 111.7457184 |
| 720 | 13        | No | Show | 13 | H | 11 | 8  | 1         | 1.0925208   | 113.2399474 |
| 721 | 14        | No | Show | 14 | C | 1  | 7  | 6         | 1.4691963   | 119.9112003 |
| 722 | 15        | No | Show | 15 | H | 14 | 1  | 7         | 1.0955613   | 107.9045322 |
| 723 | 16        | No | Show | 16 | H | 14 | 1  | 7         | 1.0948964   | 107.3716016 |
| 724 | 17        | No | Show | 17 | O | 11 | 8  | 1         | 1.4674058   | 107.7423747 |
| 725 | 18        | No | Show | 18 | O | 17 | 11 | 8         | 1.3101564   | 112.0202137 |
| 726 | TS34=TS28 |    |      |    |   |    |    |           |             |             |
| 727 | TS35      |    |      |    |   |    |    |           |             |             |



728

729

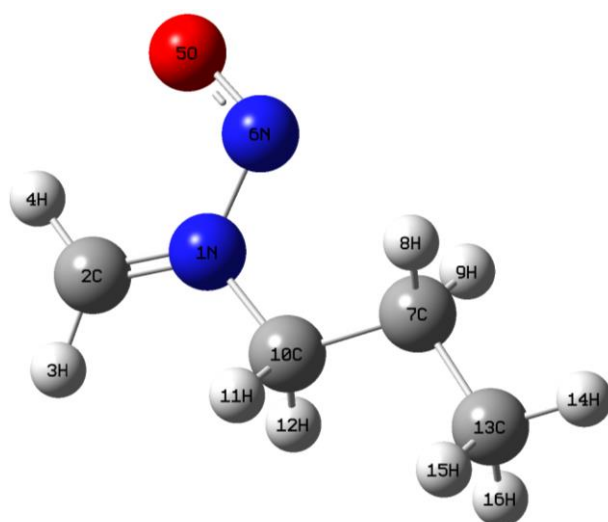
730 TS36



731

|     |     |           |         |     |        |    |    |    |           |             |             |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|-------------|
| 732 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral    |
| 733 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |             |
| 734 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4303963 |             |             |
| 735 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.1691815 | 109.4255091 |             |
| 736 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0882755 | 110.2618641 | 118.0764983 |

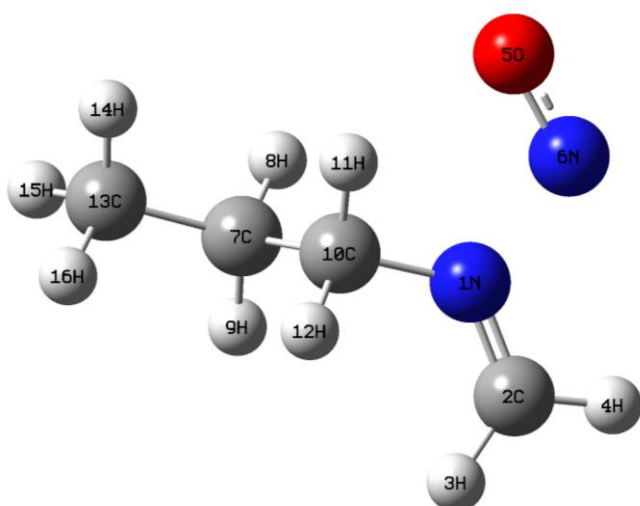
|     |      |    |      |    |   |    |    |    |           |             |              |
|-----|------|----|------|----|---|----|----|----|-----------|-------------|--------------|
| 737 | 5    | No | Show | 5  | H | 2  | 1  | 4  | 1.0908187 | 111.5701252 | 126.3301748  |
| 738 | 6    | No | Show | 6  | C | 1  | 2  | 4  | 1.4717076 | 120.1598414 | 8.7451413    |
| 739 | 7    | No | Show | 7  | H | 6  | 1  | 2  | 1.0962890 | 107.1390408 | 59.7087927   |
| 740 | 8    | No | Show | 8  | H | 6  | 1  | 2  | 1.0945403 | 106.7109809 | -54.8404867  |
| 741 | 9    | No | Show | 9  | O | 1  | 2  | 6  | 2.1545654 | 89.1363904  | 174.3937063  |
| 742 | 10   | No | Show | 10 | N | 9  | 1  | 2  | 1.2435462 | 33.6853335  | -179.7798586 |
| 743 | 11   | No | Show | 11 | O | 2  | 1  | 10 | 2.5993487 | 105.1548711 | 53.8999032   |
| 744 | 12   | No | Show | 12 | H | 11 | 2  | 1  | 0.9755007 | 85.2008735  | -53.9479400  |
| 745 | 13   | No | Show | 13 | C | 6  | 1  | 10 | 1.5237691 | 114.6515527 | 8.2765520    |
| 746 | 14   | No | Show | 14 | H | 13 | 6  | 1  | 1.0947542 | 109.7155511 | 57.6338222   |
| 747 | 15   | No | Show | 15 | H | 13 | 6  | 1  | 1.0938715 | 109.9577441 | -59.6645686  |
| 748 | 16   | No | Show | 16 | C | 13 | 6  | 1  | 1.5305744 | 110.2711610 | 178.9266653  |
| 749 | 17   | No | Show | 17 | H | 16 | 13 | 6  | 1.0953077 | 111.3005488 | 60.8518070   |
| 750 | 18   | No | Show | 18 | H | 16 | 13 | 6  | 1.0938048 | 110.4944155 | -179.3567397 |
| 751 | 19   | No | Show | 19 | H | 16 | 13 | 6  | 1.0954045 | 111.3845681 | -59.5279643  |
| 752 | TS37 |    |      |    |   |    |    |    |           |             |              |



|     |     |           |         |     |        |    |    |    |           |             |              |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 753 |     |           |         |     |        |    |    |    |           |             |              |
| 754 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
| 755 | 1   | No        | Show    | 1   | N      |    |    |    |           |             |              |
| 756 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.3198112 |             |              |
| 757 | 3   | No        | Show    | 3   | H      | 2  | 1  |    | 1.0798664 | 118.6665614 |              |
| 758 | 4   | No        | Show    | 4   | H      | 2  | 1  | 3  | 1.0789241 | 118.2734126 | 180.0000000  |
| 759 | 5   | No        | Show    | 5   | O      | 1  | 2  | 4  | 2.1976701 | 91.4856279  | 0.0000000    |
| 760 | 6   | No        | Show    | 6   | N      | 5  | 1  | 2  | 1.2518474 | 35.6769024  | -180.0000000 |
| 761 | 7   | No        | Show    | 7   | C      | 1  | 2  | 6  | 2.5360298 | 153.4919253 | -179.9991566 |
| 762 | 8   | No        | Show    | 8   | H      | 7  | 1  | 2  | 1.0935999 | 91.7867037  | -126.4632383 |
| 763 | 9   | No        | Show    | 9   | H      | 7  | 1  | 2  | 1.0936007 | 91.7864141  | 126.4616117  |
| 764 | 10  | No        | Show    | 10  | C      | 1  | 2  | 6  | 1.4827772 | 120.4856668 | -180.0000000 |
| 765 | 11  | No        | Show    | 11  | H      | 10 | 1  | 2  | 1.0934511 | 106.6983427 | -57.4107801  |





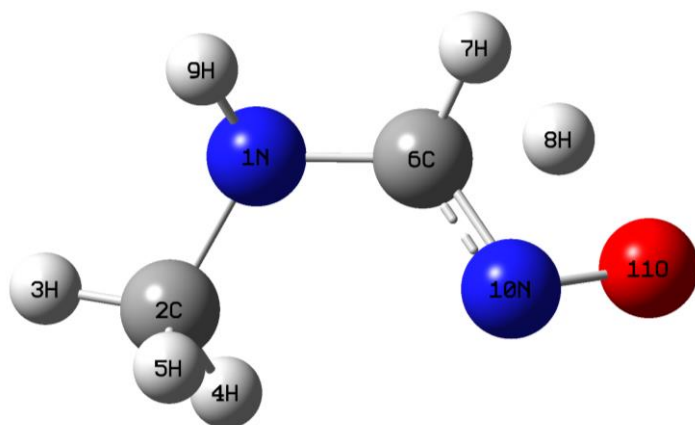


793

794 Row Highlight Display Tag Symbol NA NB NC Bond Angle Dihedral

|     |    |    |      |    |   |    |   |   |           |             |              |  |
|-----|----|----|------|----|---|----|---|---|-----------|-------------|--------------|--|
| 795 | 1  | No | Show | 1  | N |    |   |   |           |             |              |  |
| 796 | 2  | No | Show | 2  | C | 1  |   |   | 1.2725018 |             |              |  |
| 797 | 3  | No | Show | 3  | H | 2  | 1 |   | 1.0866470 | 121.5948551 |              |  |
| 798 | 4  | No | Show | 4  | H | 2  | 1 | 3 | 1.0876169 | 118.1789552 | -179.7733985 |  |
| 799 | 5  | No | Show | 5  | O | 1  | 2 | 3 | 2.3875984 | 146.2422880 | 179.5003000  |  |
| 800 | 6  | No | Show | 6  | N | 5  | 1 | 2 | 1.2274691 | 41.5661996  | 1.4934893    |  |
| 801 | 7  | No | Show | 7  | C | 1  | 2 | 6 | 2.4692123 | 117.6961869 | 137.4357158  |  |
| 802 | 8  | No | Show | 8  | H | 7  | 1 | 2 | 1.0951423 | 88.9623956  | -119.4032784 |  |
| 803 | 9  | No | Show | 9  | H | 7  | 1 | 2 | 1.0960589 | 90.6699810  | -12.2972426  |  |
| 804 | 10 | No | Show | 10 | C | 1  | 2 | 6 | 1.4529609 | 125.0388141 | 178.1186323  |  |
| 805 | 11 | No | Show | 11 | H | 10 | 1 | 2 | 1.0948155 | 106.2111942 | 150.6967086  |  |
| 806 | 12 | No | Show | 12 | H | 10 | 1 | 2 | 1.0934057 | 108.7609868 | 33.6470900   |  |
| 807 | 13 | No | Show | 13 | C | 7  | 1 | 2 | 1.5283500 | 144.6494318 | 115.7411966  |  |
| 808 | 14 | No | Show | 14 | H | 13 | 7 | 1 | 1.0953141 | 111.2891700 | 58.6060740   |  |
| 809 | 15 | No | Show | 15 | H | 13 | 7 | 1 | 1.0940796 | 110.6851876 | 178.5030168  |  |
| 810 | 16 | No | Show | 16 | H | 13 | 7 | 1 | 1.0955517 | 111.2859758 | -61.6352456  |  |

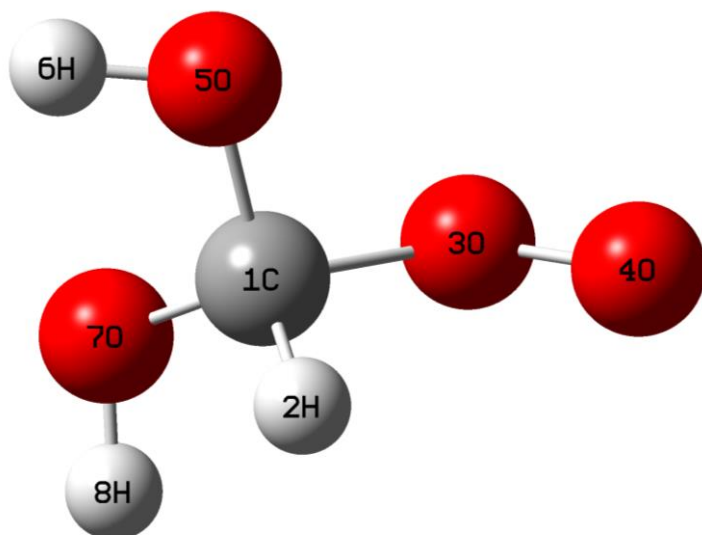
811 TS40



812

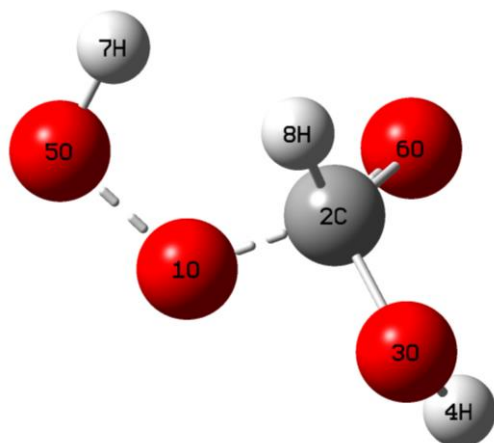
813 Row Highlight Display Tag Symbol NA NB NC Bond Angle Dihedral





838

| 839 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral     |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------|-------------|--------------|
| 840 | 1    | No        | Show    | 1   | C      |    |    |    |           |             |              |
| 841 | 2    | No        | Show    | 2   | H      | 1  |    |    | 1.0950145 |             |              |
| 842 | 3    | No        | Show    | 3   | O      | 1  | 2  |    | 1.4891424 | 104.9478713 |              |
| 843 | 4    | No        | Show    | 4   | O      | 3  | 1  | 2  | 1.3119434 | 111.0267162 | -33.6337657  |
| 844 | 5    | No        | Show    | 5   | O      | 1  | 3  | 4  | 1.3796067 | 104.8922413 | 86.8687018   |
| 845 | 6    | No        | Show    | 6   | H      | 5  | 1  | 3  | 0.9673515 | 107.7510176 | 148.5778547  |
| 846 | 7    | No        | Show    | 7   | O      | 1  | 5  | 3  | 1.3691767 | 110.4291964 | -115.1093192 |
| 847 | 8    | No        | Show    | 8   | H      | 7  | 1  | 5  | 0.9674666 | 108.9908847 | -160.7617545 |
| 848 | TS44 |           |         |     |        |    |    |    |           |             |              |



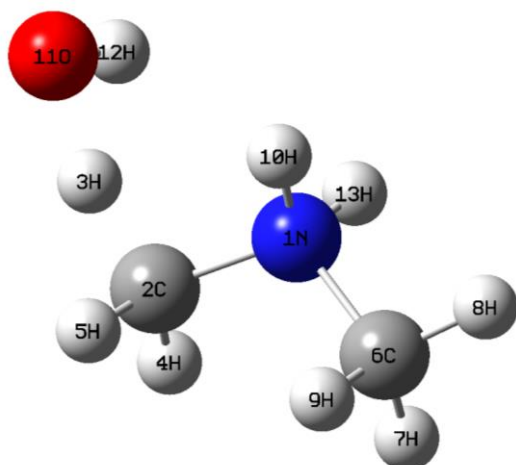
849

| 850 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond      | Angle       | Dihedral    |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------|-------------|-------------|
| 851 | 1   | No        | Show    | 1   | O      |    |    |    |           |             |             |
| 852 | 2   | No        | Show    | 2   | C      | 1  |    |    | 1.4778664 |             |             |
| 853 | 3   | No        | Show    | 3   | O      | 2  | 1  |    | 1.3733333 | 107.7530404 |             |
| 854 | 4   | No        | Show    | 4   | H      | 3  | 2  | 1  | 0.9703008 | 107.6711256 | 74.6589445  |
| 855 | 5   | No        | Show    | 5   | O      | 1  | 2  | 3  | 1.4192941 | 113.3318805 | 148.2526008 |
| 856 | 6   | No        | Show    | 6   | O      | 2  | 1  | 5  | 1.3440994 | 96.6870029  | -91.4846567 |

|     |   |    |      |   |   |   |   |   |           |             |            |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|
| 857 | 7 | No | Show | 7 | H | 5 | 1 | 2 | 0.9747164 | 105.1947390 | 20.6648108 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|

|     |   |    |      |   |   |   |   |   |           |             |            |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|
| 858 | 8 | No | Show | 8 | H | 2 | 1 | 5 | 1.0968676 | 108.8880392 | 30.5923668 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|

859 TS45



860

|     |     |                   |     |        |    |    |    |      |       |          |
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|
| 861 | Row | Highlight Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral |
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|

|     |   |    |      |   |   |
|-----|---|----|------|---|---|
| 862 | 1 | No | Show | 1 | N |
|-----|---|----|------|---|---|

|     |   |    |      |   |   |   |           |
|-----|---|----|------|---|---|---|-----------|
| 863 | 2 | No | Show | 2 | C | 1 | 1.4765832 |
|-----|---|----|------|---|---|---|-----------|

|     |   |    |      |   |   |   |   |           |             |
|-----|---|----|------|---|---|---|---|-----------|-------------|
| 864 | 3 | No | Show | 3 | H | 2 | 1 | 1.2310653 | 106.8814092 |
|-----|---|----|------|---|---|---|---|-----------|-------------|

|     |   |         |   |   |   |   |   |           |             |             |
|-----|---|---------|---|---|---|---|---|-----------|-------------|-------------|
| 865 | 4 | No Show | 4 | H | 2 | 1 | 3 | 1.0876667 | 111.0080794 | 117.3646271 |
|-----|---|---------|---|---|---|---|---|-----------|-------------|-------------|

|     |   |    |      |   |   |   |   |   |           |             |             |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|
| 866 | 5 | No | Show | 5 | H | 2 | 1 | 4 | 1.0890055 | 110.7158004 | 128.6950154 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|

|     |   |    |      |   |   |   |   |   |           |             |             |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|
| 867 | 6 | No | Show | 6 | C | 1 | 2 | 4 | 1.5003489 | 113.3113234 | -67.5202902 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|

|     |   |    |      |   |   |   |   |   |           |             |            |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|
| 868 | 7 | No | Show | 7 | H | 6 | 1 | 2 | 1.0891874 | 108.3365711 | 61.0319131 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|------------|

|     |   |    |      |   |   |   |   |   |           |             |              |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|
| 869 | 8 | No | Show | 8 | H | 6 | 1 | 2 | 1.0894204 | 108.0745001 | -179.0289128 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|

|     |   |    |      |   |   |   |   |   |           |             |             |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|
| 870 | 9 | No | Show | 9 | H | 6 | 1 | 2 | 1.0891052 | 108.1664610 | -59.1288467 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|

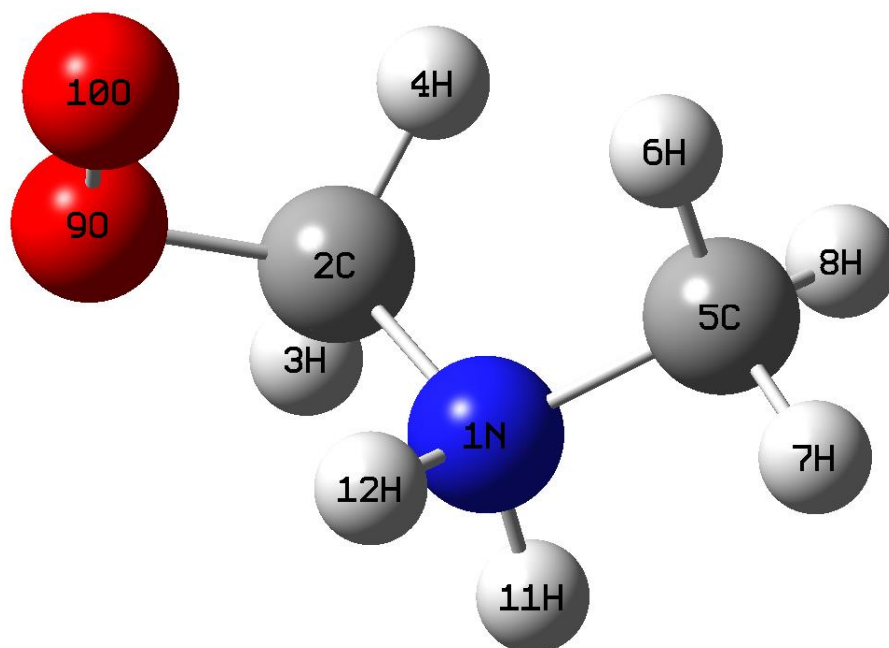
|     |    |    |      |    |   |   |   |   |           |             |              |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|--------------|
| 871 | 10 | No | Show | 10 | H | 1 | 2 | 6 | 1.0241826 | 108.9936541 | -121.7456967 |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|--------------|

|     |    |    |      |    |   |   |   |   |           |             |             |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|-------------|
| 872 | 11 | No | Show | 11 | O | 2 | 1 | 6 | 2.4913759 | 100.0533370 | 177.6741696 |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|-------------|

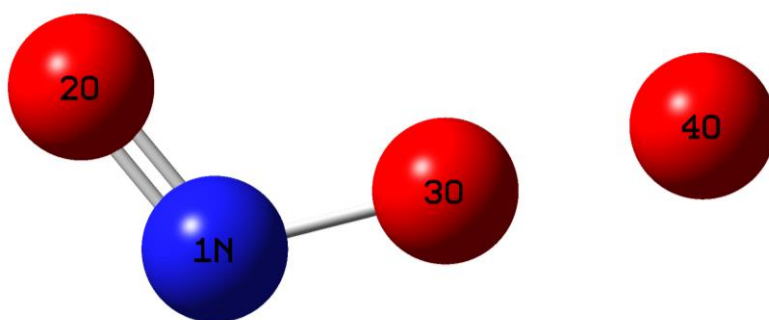
|     |    |    |      |    |   |    |   |   |           |            |            |
|-----|----|----|------|----|---|----|---|---|-----------|------------|------------|
| 873 | 12 | No | Show | 12 | H | 11 | 2 | 1 | 0.9736109 | 94.4453685 | 73.0574127 |
|-----|----|----|------|----|---|----|---|---|-----------|------------|------------|

|     |    |    |      |    |   |   |   |   |           |             |             |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|-------------|
| 874 | 13 | No | Show | 13 | H | 1 | 2 | 6 | 1.0241006 | 109.0557445 | 121.9436637 |
|-----|----|----|------|----|---|---|---|---|-----------|-------------|-------------|

875 TS46



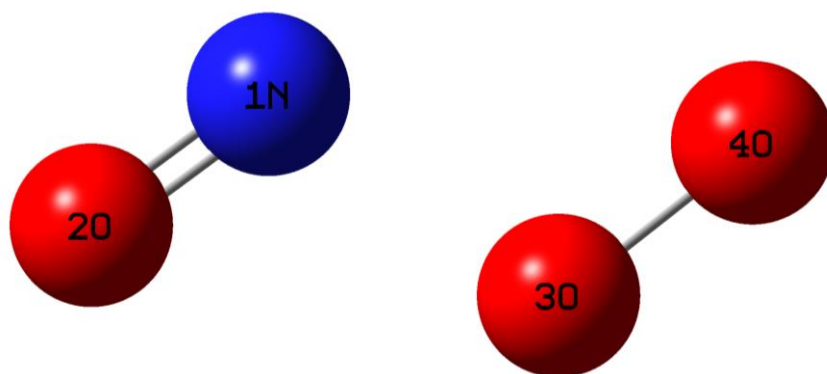
| 876 |      |                   |      |    |   |     |        |           |             |             |              |       |          |
|-----|------|-------------------|------|----|---|-----|--------|-----------|-------------|-------------|--------------|-------|----------|
| 877 | Row  | Highlight Display |      |    |   | Tag | Symbol | NA        | NB          | NC          | Bond         | Angle | Dihedral |
| 878 | 1    | No                | Show | 1  | N |     |        |           |             |             |              |       |          |
| 879 | 2    | No                | Show | 2  | C | 1   |        | 1.5016009 |             |             |              |       |          |
| 880 | 3    | No                | Show | 3  | H | 2   | 1      | 1.0875203 | 109.5701672 |             |              |       |          |
| 881 | 4    | No                | Show | 4  | H | 2   | 1      | 3         | 1.0879885   | 109.6774652 | -124.0622994 |       |          |
| 882 | 5    | No                | Show | 5  | C | 1   | 2      | 3         | 1.4999029   | 114.4170157 | 125.6096364  |       |          |
| 883 | 6    | No                | Show | 6  | H | 5   | 1      | 2         | 1.0886930   | 107.9789970 | 61.1720061   |       |          |
| 884 | 7    | No                | Show | 7  | H | 5   | 1      | 2         | 1.0888202   | 107.8464523 | -178.8636944 |       |          |
| 885 | 8    | No                | Show | 8  | H | 5   | 1      | 2         | 1.0891212   | 108.1595353 | -59.1377955  |       |          |
| 886 | 9    | No                | Show | 9  | O | 2   | 1      | 5         | 1.4315889   | 109.5771930 | -118.8517407 |       |          |
| 887 | 10   | No                | Show | 10 | O | 9   | 2      | 1         | 1.3181016   | 111.1902110 | 67.0223512   |       |          |
| 888 | 11   | No                | Show | 11 | H | 1   | 5      | 2         | 1.0239958   | 109.2463450 | 122.2394570  |       |          |
| 889 | 12   | No                | Show | 12 | H | 1   | 5      | 2         | 1.0258707   | 108.8909892 | -121.2371914 |       |          |
| 890 | TS47 |                   |      |    |   |     |        |           |             |             |              |       |          |



| Row | Highlight | Display | Tag | Symbol | NA | NB        | NC | Bond | Angle | Dihedral |
|-----|-----------|---------|-----|--------|----|-----------|----|------|-------|----------|
| 1   | No        | Show    | 1   | N      |    |           |    |      |       |          |
| 2   | No        | Show    | 2   | O      | 1  | 1.1888592 |    |      |       |          |

The diagram illustrates the decomposition of a 5N molecule into 5N, 4O, and 6O atoms, and the formation of 1O and 2H molecules from 1O and 2H atoms.

|     |      |                   |      |   |   |     |        |    |           |             |      |              |          |
|-----|------|-------------------|------|---|---|-----|--------|----|-----------|-------------|------|--------------|----------|
| 905 |      |                   |      |   |   |     |        |    |           |             |      |              |          |
| 906 | Row  | Highlight Display |      |   |   | Tag | Symbol | NA | NB        | NC          | Bond | Angle        | Dihedral |
| 907 | 1    | No                | Show | 1 | O |     |        |    |           |             |      |              |          |
| 908 | 2    | No                | Show | 2 | H | 1   |        |    | 0.9741814 |             |      |              |          |
| 909 | 3    | No                | Show | 3 | O | 1   | 2      |    | 1.4192722 | 100.8181308 |      |              |          |
| 910 | 4    | No                | Show | 4 | O | 3   | 1      | 2  | 2.1663143 | 92.9095041  |      | -179.9834816 |          |
| 911 | 5    | No                | Show | 5 | N | 4   | 3      | 1  | 1.2475313 | 108.7886270 |      | -179.5286391 |          |
| 912 | 6    | No                | Show | 6 | O | 5   | 4      | 3  | 1.2299882 | 117.5899412 |      | -0.1442372   |          |
| 913 | TS50 |                   |      |   |   |     |        |    |           |             |      |              |          |



914

| 915 | Row | Highlight Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral |
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|

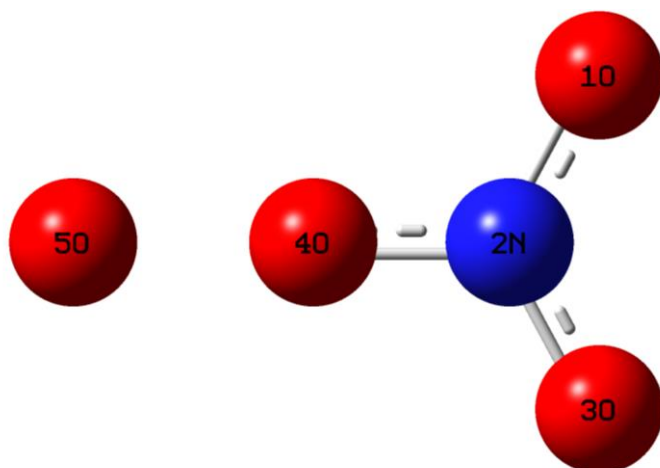
|     |   |    |      |   |   |
|-----|---|----|------|---|---|
| 916 | 1 | No | Show | 1 | N |
|-----|---|----|------|---|---|

|     |   |    |      |   |   |   |           |
|-----|---|----|------|---|---|---|-----------|
| 917 | 2 | No | Show | 2 | O | 1 | 1.1181846 |
|-----|---|----|------|---|---|---|-----------|

|     |   |         |   |   |   |   |           |             |
|-----|---|---------|---|---|---|---|-----------|-------------|
| 918 | 3 | No Show | 3 | O | 1 | 2 | 1.7925161 | 108.8293135 |
|-----|---|---------|---|---|---|---|-----------|-------------|

|     |   |    |      |   |   |   |   |   |           |             |              |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|
| 919 | 4 | No | Show | 4 | O | 3 | 1 | 2 | 1.2536053 | 107.1008677 | -179.9622208 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|

920 TS51



921

|     |     |                   |     |        |    |    |    |      |       |          |
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|
| 922 | Row | Highlight Display | Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral |
|-----|-----|-------------------|-----|--------|----|----|----|------|-------|----------|

923      1   No   Show   1   O

|     |   |    |      |   |   |   |           |
|-----|---|----|------|---|---|---|-----------|
| 924 | 2 | No | Show | 2 | N | 1 | 1.2256005 |
|-----|---|----|------|---|---|---|-----------|

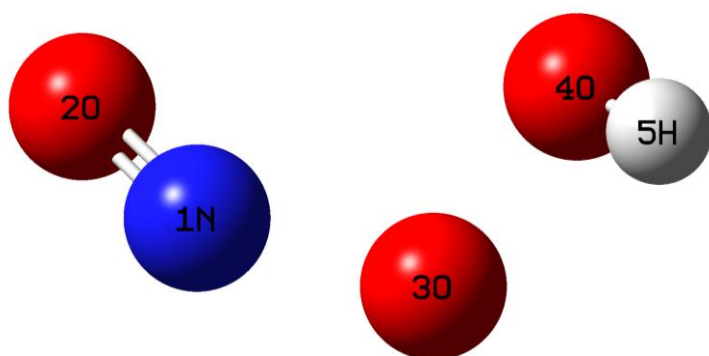
|     |   |    |      |   |   |   |   |           |             |
|-----|---|----|------|---|---|---|---|-----------|-------------|
| 925 | 3 | No | Show | 3 | O | 2 | 1 | 1.2256006 | 123.4897937 |
|-----|---|----|------|---|---|---|---|-----------|-------------|

|     |   |    |      |   |   |   |   |   |           |             |              |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|
| 926 | 4 | No | Show | 4 | O | 2 | 1 | 3 | 1.2710450 | 118.2542113 | -179.9967222 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|--------------|

|     |   |    |      |   |   |   |   |   |           |             |             |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|
| 927 | 5 | No | Show | 5 | O | 4 | 2 | 1 | 1.5530690 | 179.9977953 | -70.7925088 |
|-----|---|----|------|---|---|---|---|---|-----------|-------------|-------------|

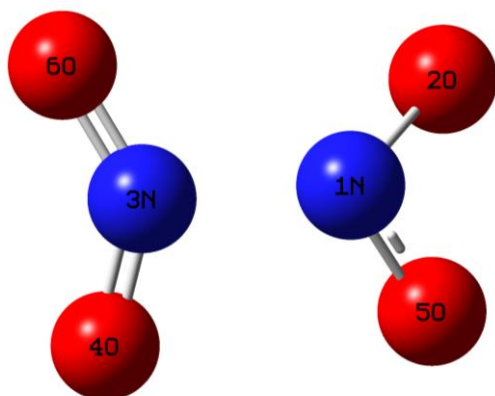
928 TS52





929

| 930 | Row  | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond                  | Angle      | Dihedral |
|-----|------|-----------|---------|-----|--------|----|----|----|-----------------------|------------|----------|
| 931 | 1    | No        | Show    | 1   | N      |    |    |    |                       |            |          |
| 932 | 2    | No        | Show    | 2   | O      | 1  |    |    | 1.1395924             |            |          |
| 933 | 3    | No        | Show    | 3   | O      | 1  | 2  |    | 1.5768614 109.1151508 |            |          |
| 934 | 4    | No        | Show    | 4   | O      | 3  | 1  | 2  | 1.4077887 101.9529810 | 85.6588239 |          |
| 935 | 5    | No        | Show    | 5   | H      | 4  | 3  | 1  | 0.9757984 102.6976776 | 91.3593034 |          |
| 936 | TS53 |           |         |     |        |    |    |    |                       |            |          |

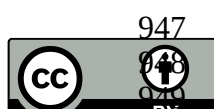


937

| 938 | Row | Highlight | Display | Tag | Symbol | NA | NB | NC | Bond                  | Angle        | Dihedral |
|-----|-----|-----------|---------|-----|--------|----|----|----|-----------------------|--------------|----------|
| 939 | 1   | No        | Show    | 1   | N      |    |    |    |                       |              |          |
| 940 | 2   | No        | Show    | 2   | O      | 1  |    |    | 1.3889452             |              |          |
| 941 | 3   | No        | Show    | 3   | N      | 1  | 2  |    | 1.6655300 109.1595436 |              |          |
| 942 | 4   | No        | Show    | 4   | O      | 3  | 1  | 2  | 1.1815411 110.2798928 | 118.4276055  |          |
| 943 | 5   | No        | Show    | 5   | O      | 1  | 2  | 3  | 1.2391592 87.0850850  | 108.2438695  |          |
| 944 | 6   | No        | Show    | 6   | O      | 3  | 1  | 5  | 1.1825345 115.2001144 | -158.4639506 |          |

945

946



947

© 2018 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).