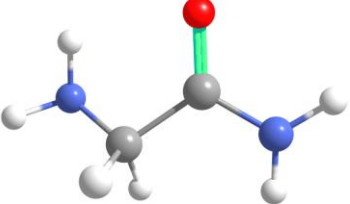
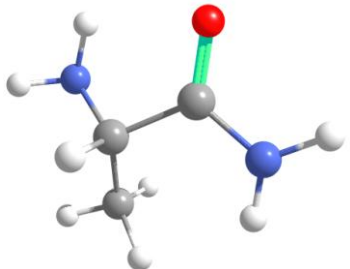
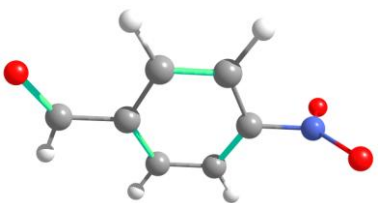
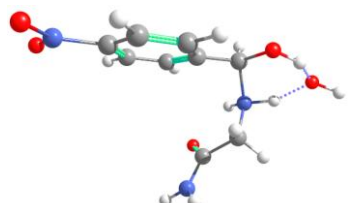
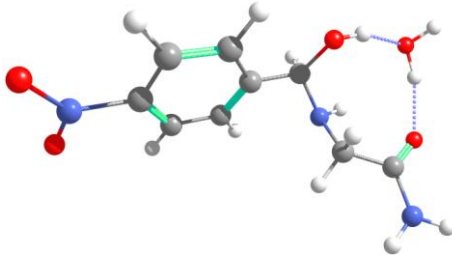
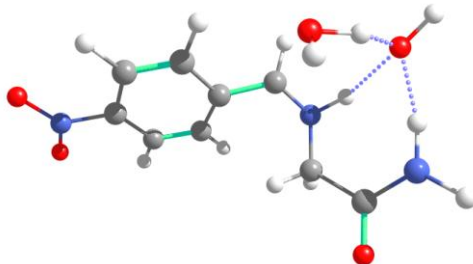
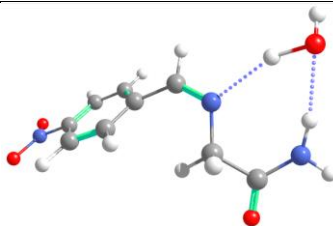
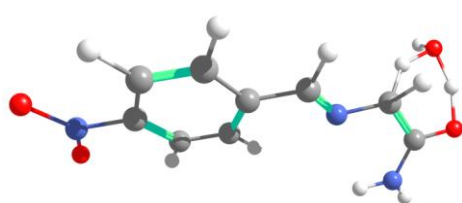


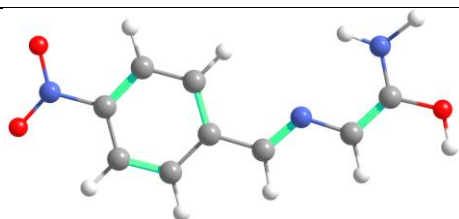
# **Additional Supplementary Information: Cartesian coordinates of the optimized structures**

**Supplementary Table 1.** Cartesian coordinates (Å) of the optimized structures of all intermediates and transition states at B3LYP/6-311++G(d,p) level of theory.  $E_e^S$  represents the absolute electronic energy in Hartree at M062X/6-311++G(d,p) level of theory in the solvent (water).

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |              |              |              |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|--------------|--------------|---|--------------|-------------|-------------|---|-------------|-------------|--------------|---|-------------|--------------|-------------|---|--------------|-------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|--------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|--------------|-------------|---|--------------|-------------|-------------|---|-------------|--------------|-------------|---|-------------|-------------|-------------|---|-------------|-------------|-------------|---|-------------|-------------|-------------|---|--------------|-------------|-------------|
|  <p><b>8a</b><br/><math>E_e^S = -264.549869</math></p> <table> <tr><td>N</td><td>0.089324000</td><td>0.834064000</td><td>0.861381000</td></tr> <tr><td>H</td><td>0.121903000</td><td>0.381564000</td><td>-0.048214000</td></tr> <tr><td>H</td><td>1.029925000</td><td>0.881351000</td><td>1.233363000</td></tr> <tr><td>C</td><td>-0.794681000</td><td>0.077094000</td><td>1.736008000</td></tr> <tr><td>C</td><td>-1.936694000</td><td>-0.525986000</td><td>0.919059000</td></tr> <tr><td>O</td><td>-1.797008000</td><td>-0.829475000</td><td>-0.252348000</td></tr> <tr><td>N</td><td>-3.091886000</td><td>-0.755414000</td><td>1.606862000</td></tr> <tr><td>H</td><td>-1.196683000</td><td>0.725115000</td><td>2.523115000</td></tr> <tr><td>H</td><td>-0.309651000</td><td>-0.775467000</td><td>2.240484000</td></tr> <tr><td>H</td><td>-3.242239000</td><td>-0.393448000</td><td>2.533481000</td></tr> <tr><td>H</td><td>-3.870466000</td><td>-1.163787000</td><td>1.113140000</td></tr> </table>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |              |              |              | N | 0.089324000  | 0.834064000 | 0.861381000 | H | 0.121903000 | 0.381564000 | -0.048214000 | H | 1.029925000 | 0.881351000  | 1.233363000 | C | -0.794681000 | 0.077094000 | 1.736008000 | C | -1.936694000 | -0.525986000 | 0.919059000 | O | -1.797008000 | -0.829475000 | -0.252348000 | N | -3.091886000 | -0.755414000 | 1.606862000 | H | -1.196683000 | 0.725115000  | 2.523115000 | H | -0.309651000 | -0.775467000 | 2.240484000 | H | -3.242239000 | -0.393448000 | 2.533481000 | H | -3.870466000 | -1.163787000 | 1.113140000 |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.089324000  | 0.834064000  | 0.861381000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.121903000  | 0.381564000  | -0.048214000 |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.029925000  | 0.881351000  | 1.233363000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.794681000 | 0.077094000  | 1.736008000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.936694000 | -0.525986000 | 0.919059000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.797008000 | -0.829475000 | -0.252348000 |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.091886000 | -0.755414000 | 1.606862000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.196683000 | 0.725115000  | 2.523115000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.309651000 | -0.775467000 | 2.240484000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.242239000 | -0.393448000 | 2.533481000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.870466000 | -1.163787000 | 1.113140000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
|  <p><b>8b</b><br/><math>E_e^S = -303.8561629</math></p> <table> <tr><td>N</td><td>-0.022422000</td><td>0.890479000</td><td>0.792664000</td></tr> <tr><td>H</td><td>0.008462000</td><td>0.394030000</td><td>-0.093246000</td></tr> <tr><td>H</td><td>0.924755000</td><td>1.012096000</td><td>1.131465000</td></tr> <tr><td>C</td><td>-0.830728000</td><td>0.133406000</td><td>1.745620000</td></tr> <tr><td>C</td><td>-1.940297000</td><td>-0.581554000</td><td>0.952495000</td></tr> <tr><td>O</td><td>-1.777307000</td><td>-0.900709000</td><td>-0.213339000</td></tr> <tr><td>N</td><td>-3.073943000</td><td>-0.905145000</td><td>1.637234000</td></tr> <tr><td>H</td><td>-0.267456000</td><td>-0.695255000</td><td>2.211280000</td></tr> <tr><td>H</td><td>-3.275384000</td><td>-0.540946000</td><td>2.552005000</td></tr> <tr><td>H</td><td>-3.809323000</td><td>-1.372968000</td><td>1.130301000</td></tr> <tr><td>C</td><td>-1.324361000</td><td>1.056899000</td><td>2.866175000</td></tr> <tr><td>H</td><td>-1.990812000</td><td>1.825889000</td><td>2.468976000</td></tr> <tr><td>H</td><td>-1.829909000</td><td>0.509093000</td><td>3.668027000</td></tr> <tr><td>H</td><td>-0.470130000</td><td>1.563751000</td><td>3.321472000</td></tr> </table>                                                                                                                                                                                                                                                                                                                                                                                                         |              |              |              | N | -0.022422000 | 0.890479000 | 0.792664000 | H | 0.008462000 | 0.394030000 | -0.093246000 | H | 0.924755000 | 1.012096000  | 1.131465000 | C | -0.830728000 | 0.133406000 | 1.745620000 | C | -1.940297000 | -0.581554000 | 0.952495000 | O | -1.777307000 | -0.900709000 | -0.213339000 | N | -3.073943000 | -0.905145000 | 1.637234000 | H | -0.267456000 | -0.695255000 | 2.211280000 | H | -3.275384000 | -0.540946000 | 2.552005000 | H | -3.809323000 | -1.372968000 | 1.130301000 | C | -1.324361000 | 1.056899000  | 2.866175000 | H | -1.990812000 | 1.825889000  | 2.468976000 | H | -1.829909000 | 0.509093000  | 3.668027000 | H | -0.470130000 | 1.563751000 | 3.321472000 |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.022422000 | 0.890479000  | 0.792664000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.008462000  | 0.394030000  | -0.093246000 |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.924755000  | 1.012096000  | 1.131465000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.830728000 | 0.133406000  | 1.745620000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.940297000 | -0.581554000 | 0.952495000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.777307000 | -0.900709000 | -0.213339000 |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.073943000 | -0.905145000 | 1.637234000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.267456000 | -0.695255000 | 2.211280000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.275384000 | -0.540946000 | 2.552005000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -3.809323000 | -1.372968000 | 1.130301000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.324361000 | 1.056899000  | 2.866175000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.990812000 | 1.825889000  | 2.468976000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -1.829909000 | 0.509093000  | 3.668027000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.470130000 | 1.563751000  | 3.321472000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
|  <p><b>2j</b><br/><math>E_e^S = -550.0103819</math></p> <table> <tr><td>C</td><td>1.803174000</td><td>0.639283000</td><td>2.673808000</td></tr> <tr><td>C</td><td>1.732218000</td><td>1.645644000</td><td>3.641718000</td></tr> <tr><td>C</td><td>2.221504000</td><td>-0.649345000</td><td>3.030635000</td></tr> <tr><td>C</td><td>2.074187000</td><td>1.378798000</td><td>4.963792000</td></tr> <tr><td>C</td><td>2.566801000</td><td>-0.932074000</td><td>4.344375000</td></tr> <tr><td>C</td><td>2.484361000</td><td>0.092375000</td><td>5.282096000</td></tr> <tr><td>H</td><td>1.407636000</td><td>2.642088000</td><td>3.360553000</td></tr> <tr><td>H</td><td>2.270076000</td><td>-1.415043000</td><td>2.265777000</td></tr> <tr><td>H</td><td>2.024724000</td><td>2.146369000</td><td>5.725842000</td></tr> <tr><td>H</td><td>2.892847000</td><td>-1.921514000</td><td>4.640258000</td></tr> <tr><td>N</td><td>2.853090000</td><td>-0.204333000</td><td>6.687039000</td></tr> <tr><td>O</td><td>1.959752000</td><td>-0.590848000</td><td>7.423901000</td></tr> <tr><td>O</td><td>4.021921000</td><td>-0.039411000</td><td>6.998685000</td></tr> <tr><td>C</td><td>1.433242000</td><td>0.947045000</td><td>1.269214000</td></tr> <tr><td>O</td><td>1.463040000</td><td>0.147888000</td><td>0.362553000</td></tr> <tr><td>H</td><td>1.114478000</td><td>1.995357000</td><td>1.092475000</td></tr> </table>                                                                                                                                                                                                                                                     |              |              |              | C | 1.803174000  | 0.639283000 | 2.673808000 | C | 1.732218000 | 1.645644000 | 3.641718000  | C | 2.221504000 | -0.649345000 | 3.030635000 | C | 2.074187000  | 1.378798000 | 4.963792000 | C | 2.566801000  | -0.932074000 | 4.344375000 | C | 2.484361000  | 0.092375000  | 5.282096000  | H | 1.407636000  | 2.642088000  | 3.360553000 | H | 2.270076000  | -1.415043000 | 2.265777000 | H | 2.024724000  | 2.146369000  | 5.725842000 | H | 2.892847000  | -1.921514000 | 4.640258000 | N | 2.853090000  | -0.204333000 | 6.687039000 | O | 1.959752000  | -0.590848000 | 7.423901000 | O | 4.021921000  | -0.039411000 | 6.998685000 | C | 1.433242000  | 0.947045000 | 1.269214000 | O | 1.463040000 | 0.147888000  | 0.362553000 | H | 1.114478000 | 1.995357000 | 1.092475000 |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.803174000  | 0.639283000  | 2.673808000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.732218000  | 1.645644000  | 3.641718000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.221504000  | -0.649345000 | 3.030635000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.074187000  | 1.378798000  | 4.963792000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.566801000  | -0.932074000 | 4.344375000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.484361000  | 0.092375000  | 5.282096000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.407636000  | 2.642088000  | 3.360553000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.270076000  | -1.415043000 | 2.265777000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.024724000  | 2.146369000  | 5.725842000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.892847000  | -1.921514000 | 4.640258000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.853090000  | -0.204333000 | 6.687039000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.959752000  | -0.590848000 | 7.423901000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 4.021921000  | -0.039411000 | 6.998685000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.433242000  | 0.947045000  | 1.269214000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.463040000  | 0.147888000  | 0.362553000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.114478000  | 1.995357000  | 1.092475000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
|  <p><b>8a-TS</b><br/><math>E_e^S = -891.0024184</math></p> <table> <tr><td>C</td><td>2.078859000</td><td>0.190598000</td><td>2.772074000</td></tr> <tr><td>C</td><td>2.255918000</td><td>1.396308000</td><td>3.460143000</td></tr> <tr><td>C</td><td>2.403134000</td><td>-1.014910000</td><td>3.399333000</td></tr> <tr><td>C</td><td>2.728812000</td><td>1.404143000</td><td>4.766329000</td></tr> <tr><td>C</td><td>2.877968000</td><td>-1.024915000</td><td>4.707152000</td></tr> <tr><td>C</td><td>3.027726000</td><td>0.187078000</td><td>5.372355000</td></tr> <tr><td>H</td><td>2.022717000</td><td>2.340522000</td><td>2.980117000</td></tr> <tr><td>H</td><td>2.294807000</td><td>-1.933034000</td><td>2.836308000</td></tr> <tr><td>H</td><td>2.868623000</td><td>2.325586000</td><td>5.314103000</td></tr> <tr><td>H</td><td>3.137178000</td><td>-1.946780000</td><td>5.209411000</td></tr> <tr><td>N</td><td>3.525938000</td><td>0.185031000</td><td>6.765559000</td></tr> <tr><td>O</td><td>3.665199000</td><td>1.267394000</td><td>7.321737000</td></tr> <tr><td>O</td><td>3.765215000</td><td>-0.899147000</td><td>7.282778000</td></tr> <tr><td>C</td><td>1.582722000</td><td>0.175510000</td><td>1.335141000</td></tr> <tr><td>O</td><td>1.602007000</td><td>-1.039882000</td><td>0.767472000</td></tr> <tr><td>H</td><td>2.109328000</td><td>0.954861000</td><td>0.757646000</td></tr> <tr><td>H</td><td>0.029686000</td><td>1.723982000</td><td>1.416934000</td></tr> <tr><td>N</td><td>0.085977000</td><td>0.713777000</td><td>1.252046000</td></tr> <tr><td>H</td><td>-0.132224000</td><td>0.436037000</td><td>0.193171000</td></tr> </table> |              |              |              | C | 2.078859000  | 0.190598000 | 2.772074000 | C | 2.255918000 | 1.396308000 | 3.460143000  | C | 2.403134000 | -1.014910000 | 3.399333000 | C | 2.728812000  | 1.404143000 | 4.766329000 | C | 2.877968000  | -1.024915000 | 4.707152000 | C | 3.027726000  | 0.187078000  | 5.372355000  | H | 2.022717000  | 2.340522000  | 2.980117000 | H | 2.294807000  | -1.933034000 | 2.836308000 | H | 2.868623000  | 2.325586000  | 5.314103000 | H | 3.137178000  | -1.946780000 | 5.209411000 | N | 3.525938000  | 0.185031000  | 6.765559000 | O | 3.665199000  | 1.267394000  | 7.321737000 | O | 3.765215000  | -0.899147000 | 7.282778000 | C | 1.582722000  | 0.175510000 | 1.335141000 | O | 1.602007000 | -1.039882000 | 0.767472000 | H | 2.109328000 | 0.954861000 | 0.757646000 | H | 0.029686000 | 1.723982000 | 1.416934000 | N | 0.085977000 | 0.713777000 | 1.252046000 | H | -0.132224000 | 0.436037000 | 0.193171000 |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.078859000  | 0.190598000  | 2.772074000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.255918000  | 1.396308000  | 3.460143000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.403134000  | -1.014910000 | 3.399333000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.728812000  | 1.404143000  | 4.766329000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.877968000  | -1.024915000 | 4.707152000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.027726000  | 0.187078000  | 5.372355000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.022717000  | 2.340522000  | 2.980117000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.294807000  | -1.933034000 | 2.836308000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.868623000  | 2.325586000  | 5.314103000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.137178000  | -1.946780000 | 5.209411000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.525938000  | 0.185031000  | 6.765559000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.665199000  | 1.267394000  | 7.321737000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 3.765215000  | -0.899147000 | 7.282778000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.582722000  | 0.175510000  | 1.335141000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1.602007000  | -1.039882000 | 0.767472000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2.109328000  | 0.954861000  | 0.757646000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.029686000  | 1.723982000  | 1.416934000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 0.085977000  | 0.713777000  | 1.252046000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |
| H                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -0.132224000 | 0.436037000  | 0.193171000  |   |              |             |             |   |             |             |              |   |             |              |             |   |              |             |             |   |              |              |             |   |              |              |              |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |              |             |   |              |             |             |   |             |              |             |   |             |             |             |   |             |             |             |   |             |             |             |   |              |             |             |

|                                                                                     |              |              |              |                                                                                      |              |              |              |
|-------------------------------------------------------------------------------------|--------------|--------------|--------------|--------------------------------------------------------------------------------------|--------------|--------------|--------------|
|                                                                                     |              |              |              | C                                                                                    | -0.879497000 | 0.056813000  | 2.150932000  |
|                                                                                     |              |              |              | C                                                                                    | -1.338802000 | 1.047978000  | 3.224101000  |
|                                                                                     |              |              |              | H                                                                                    | -0.425925000 | -0.836664000 | 2.583436000  |
|                                                                                     |              |              |              | H                                                                                    | -1.750221000 | -0.263813000 | 1.571667000  |
|                                                                                     |              |              |              | O                                                                                    | -1.094785000 | 2.239037000  | 3.121097000  |
|                                                                                     |              |              |              | N                                                                                    | -2.053103000 | 0.514210000  | 4.242707000  |
|                                                                                     |              |              |              | H                                                                                    | -2.184749000 | -0.478634000 | 4.346967000  |
|                                                                                     |              |              |              | H                                                                                    | -2.389836000 | 1.126442000  | 4.970425000  |
|                                                                                     |              |              |              | O                                                                                    | 0.187912000  | -0.322641000 | -1.011365000 |
|                                                                                     |              |              |              | H                                                                                    | 0.997084000  | -0.890886000 | -0.224289000 |
|                                                                                     |              |              |              | H                                                                                    | -0.376718000 | -0.884848000 | -1.546036000 |
|    |              |              |              |    |              |              |              |
| <b>8a-IN</b><br>$E_e^S = -900.5259926$                                              |              |              |              | <b>8a-TS'</b><br>$E_e^S = -900.5259926$                                              |              |              |              |
| C                                                                                   | 2.169721000  | 0.113636000  | 3.008229000  | C                                                                                    | 1.278365000  | -0.321384000 | 3.438340000  |
| C                                                                                   | 2.434773000  | 1.244373000  | 3.791191000  | C                                                                                    | 2.471398000  | 0.397281000  | 3.268797000  |
| C                                                                                   | 2.680675000  | -1.126151000 | 3.402383000  | C                                                                                    | 1.052464000  | -1.015313000 | 4.636532000  |
| C                                                                                   | 3.192908000  | 1.145394000  | 4.950218000  | C                                                                                    | 3.437644000  | 0.395562000  | 4.265299000  |
| C                                                                                   | 3.438185000  | -1.242645000 | 4.564224000  | C                                                                                    | 2.011176000  | -1.014518000 | 5.643332000  |
| C                                                                                   | 3.683667000  | -0.103581000 | 5.322339000  | C                                                                                    | 3.192255000  | -0.313822000 | 5.436640000  |
| H                                                                                   | 2.031299000  | 2.202427000  | 3.486997000  | H                                                                                    | 2.627968000  | 0.926658000  | 2.338166000  |
| H                                                                                   | 2.476862000  | -1.996125000 | 2.793606000  | H                                                                                    | 0.117226000  | -1.533895000 | 4.803456000  |
| H                                                                                   | 3.406179000  | 2.009200000  | 5.564551000  | H                                                                                    | 4.368688000  | 0.932694000  | 4.148682000  |
| H                                                                                   | 3.837334000  | -2.195054000 | 4.884881000  | H                                                                                    | 1.852915000  | -1.540080000 | 6.574710000  |
| N                                                                                   | 4.483281000  | -0.220110000 | 6.558561000  | N                                                                                    | 4.220716000  | -0.314622000 | 6.506217000  |
| O                                                                                   | 4.680764000  | 0.800185000  | 7.208986000  | O                                                                                    | 5.251110000  | 0.310248000  | 6.298222000  |
| O                                                                                   | 4.903648000  | -1.329649000 | 6.865269000  | O                                                                                    | 3.971853000  | -0.939479000 | 7.528075000  |
| C                                                                                   | 1.364815000  | 0.262920000  | 1.722538000  | C                                                                                    | 0.222739000  | -0.227063000 | 2.407059000  |
| O                                                                                   | 1.050151000  | -1.035007000 | 1.245247000  | O                                                                                    | 1.329147000  | 0.181518000  | 0.537987000  |
| H                                                                                   | 1.992951000  | 0.783353000  | 0.987191000  | H                                                                                    | -0.076192000 | 0.764251000  | 2.097647000  |
| H                                                                                   | -0.145053000 | 1.440867000  | 1.024764000  | H                                                                                    | -1.274973000 | -0.864366000 | 1.355539000  |
| N                                                                                   | 0.211918000  | 1.131804000  | 1.921453000  | N                                                                                    | -0.633075000 | -1.170520000 | 2.106939000  |
| H                                                                                   | -1.290166000 | 0.070949000  | -0.466442000 | H                                                                                    | 1.918015000  | -0.512007000 | 0.218654000  |
| C                                                                                   | -0.867024000 | 0.585791000  | 2.734804000  | C                                                                                    | -0.477188000 | -2.612364000 | 2.306596000  |
| C                                                                                   | -2.226974000 | 0.749655000  | 2.065094000  | C                                                                                    | -0.481084000 | -3.517127000 | 1.052374000  |
| H                                                                                   | -0.887919000 | 1.050670000  | 3.727395000  | H                                                                                    | -1.293579000 | -2.976854000 | 2.935228000  |
| H                                                                                   | -0.737149000 | -0.495226000 | 2.882519000  | H                                                                                    | 0.456410000  | -2.817142000 | 2.826202000  |
| O                                                                                   | -2.366977000 | 0.786556000  | 0.845040000  | O                                                                                    | -0.322569000 | -4.711244000 | 1.254360000  |
| N                                                                                   | -3.286866000 | 0.823178000  | 2.903885000  | N                                                                                    | -0.668775000 | -2.954716000 | -0.154913000 |
| H                                                                                   | -3.177183000 | 0.836273000  | 3.904313000  | H                                                                                    | -0.787595000 | -1.941131000 | -0.336553000 |
| H                                                                                   | -4.214920000 | 0.874729000  | 2.512435000  | H                                                                                    | -0.677608000 | -3.592891000 | -0.937573000 |
| O                                                                                   | -0.520652000 | -0.281160000 | -0.954660000 | O                                                                                    | -0.890025000 | -0.196719000 | -0.311665000 |
| H                                                                                   | 0.599219000  | -0.934478000 | 0.385944000  | H                                                                                    | -1.262250000 | 0.352290000  | -1.005559000 |
| H                                                                                   | -0.856126000 | -0.684714000 | -1.759871000 | H                                                                                    | 0.293926000  | 0.064237000  | -0.009070000 |
|  |              |              |              |  |              |              |              |
| <b>8a-IN1</b><br>$E_e^S = -814.5753457$                                             |              |              |              | <b>8a-TS1</b><br>$E_e^S = -814.527929$                                               |              |              |              |

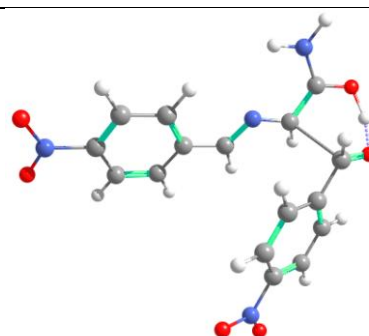
|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 1.155710000  | 0.964769000  | 3.267711000  | N | -1.577831000 | 0.804525000  | 0.075800000  |
| C | 1.325147000  | 2.169793000  | 3.966731000  | H | -3.662132000 | 0.300434000  | 1.398164000  |
| C | 1.438798000  | -0.244814000 | 3.919047000  | C | -2.961309000 | 0.622366000  | 0.165267000  |
| C | 1.723148000  | 2.174947000  | 5.296639000  | C | -3.494022000 | -0.525757000 | -0.553432000 |
| C | 1.855990000  | -0.254200000 | 5.244561000  | O | -4.692846000 | -0.923871000 | -0.327089000 |
| C | 1.981731000  | 0.956721000  | 5.915540000  | N | -2.723417000 | -1.226266000 | -1.391026000 |
| H | 1.132976000  | 3.111736000  | 3.465033000  | H | -3.591647000 | 1.513268000  | 0.048934000  |
| H | 1.361851000  | -1.183131000 | 3.386086000  | H | -1.765954000 | -0.935104000 | -1.519597000 |
| H | 1.841879000  | 3.095319000  | 5.851340000  | H | -3.044832000 | -2.113927000 | -1.744674000 |
| H | 2.085533000  | -1.177470000 | 5.758285000  | C | -1.046812000 | 1.943758000  | 0.321654000  |
| N | 2.420290000  | 0.950234000  | 7.331336000  | H | -1.661948000 | 2.818015000  | 0.573804000  |
| O | 2.532403000  | 2.031689000  | 7.892759000  | C | 0.400309000  | 2.167521000  | 0.291834000  |
| O | 2.643012000  | -0.135403000 | 7.849377000  | C | 1.312530000  | 1.117463000  | 0.079798000  |
| C | 0.749577000  | 1.046714000  | 1.840328000  | C | 0.898875000  | 3.466613000  | 0.484046000  |
| O | -0.383895000 | 0.555480000  | -1.650788000 | C | 2.675527000  | 1.357644000  | 0.051558000  |
| H | 1.213228000  | 1.876622000  | 1.299922000  | C | 2.263184000  | 3.722219000  | 0.457495000  |
| H | -0.393135000 | -1.705973000 | 1.418517000  | C | 3.136785000  | 2.661507000  | 0.239526000  |
| N | -0.053536000 | 0.327322000  | 1.160936000  | H | 0.930944000  | 0.113461000  | -0.053504000 |
| H | -0.170317000 | 1.389982000  | -2.077275000 | H | 0.206919000  | 4.284407000  | 0.653692000  |
| C | -0.827628000 | -0.753853000 | 1.748435000  | H | 3.388143000  | 0.560216000  | -0.108223000 |
| C | -2.309030000 | -0.799346000 | 1.320448000  | H | 2.657113000  | 4.718671000  | 0.601748000  |
| H | -0.058198000 | 0.610983000  | -0.728535000 | N | 4.586412000  | 2.920860000  | 0.209859000  |
| H | -0.843859000 | -0.751657000 | 2.839706000  | O | 4.964418000  | 4.075101000  | 0.379810000  |
| O | -3.114600000 | -1.297607000 | 2.090291000  | O | 5.333257000  | 1.967399000  | 0.016197000  |
| N | -2.633089000 | -0.316874000 | 0.100400000  | O | -4.722114000 | -0.028664000 | 1.885065000  |
| H | -1.957058000 | 0.020406000  | -0.577900000 | H | -4.931401000 | -0.540441000 | 0.796288000  |
| H | -3.594030000 | -0.424558000 | -0.187010000 | H | -4.615341000 | -0.684024000 | 2.584542000  |



**8a-IN2**

$$E_e^S = -738.1204458$$

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.506458000 | 0.517639000  | 0.670158000  |
| H | -3.048904000 | -1.550519000 | 2.574555000  |
| C | -1.462131000 | -0.090046000 | 1.430522000  |
| C | -1.972569000 | -1.294706000 | 1.021256000  |
| O | -2.884420000 | -1.994602000 | 1.734996000  |
| N | -1.663089000 | -1.900555000 | -0.152413000 |
| H | -1.837231000 | 0.366962000  | 2.348497000  |
| H | -0.887518000 | -1.497369000 | -0.656509000 |
| H | -1.799946000 | -2.897257000 | -0.215292000 |
| C | -0.014987000 | 1.662917000  | 1.001147000  |
| H | -0.359173000 | 2.185163000  | 1.902984000  |
| C | 1.013396000  | 2.338303000  | 0.220802000  |
| C | 1.547838000  | 1.782914000  | -0.958714000 |
| C | 1.495101000  | 3.588284000  | 0.651807000  |
| C | 2.523548000  | 2.448682000  | -1.678590000 |
| C | 2.472779000  | 4.266328000  | -0.060790000 |
| C | 2.978564000  | 3.687640000  | -1.221937000 |
| H | 1.182110000  | 0.821896000  | -1.295619000 |
| H | 1.094263000  | 4.030211000  | 1.557623000  |
| H | 2.940604000  | 2.031846000  | -2.585028000 |
| H | 2.847601000  | 5.227256000  | 0.263396000  |
| N | 4.014715000  | 4.397615000  | -1.984212000 |
| O | 4.392921000  | 5.486460000  | -1.561745000 |
| O | 4.445258000  | 3.862643000  | -3.001750000 |



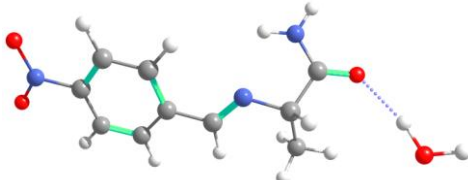
**8a-TS2**

$$E_e^S = -1288.136064$$

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|---|--------------|--------------|--------------|
| N | -0.535641000 | 0.680837000  | 0.245228000  |
| H | -2.557851000 | -2.000926000 | 1.922422000  |
| C | -1.404127000 | -0.020576000 | 1.047079000  |
| C | -2.417950000 | -0.800897000 | 0.384702000  |
| O | -3.193242000 | -1.582522000 | 1.050660000  |
| N | -2.518707000 | -0.779646000 | -0.950580000 |
| H | -1.664445000 | 0.350348000  | 2.036474000  |
| H | -1.908107000 | -0.171955000 | -1.475248000 |
| H | -3.151732000 | -1.412476000 | -1.413460000 |
| C | 0.171121000  | 1.642803000  | 0.733002000  |
| H | 0.057537000  | 1.954058000  | 1.778086000  |
| C | 1.139018000  | 2.395800000  | -0.060539000 |
| C | 1.417044000  | 2.073288000  | -1.402136000 |
| C | 1.815282000  | 3.477050000  | 0.529937000  |
| C | 2.334681000  | 2.809520000  | -2.131479000 |
| C | 2.737589000  | 4.223748000  | -0.190400000 |
| C | 2.984699000  | 3.879619000  | -1.515432000 |
| H | 0.903775000  | 1.236521000  | -1.857756000 |
| H | 1.613211000  | 3.734241000  | 1.563890000  |
| H | 2.559324000  | 2.574263000  | -3.162692000 |
| H | 3.262950000  | 5.058129000  | 0.253119000  |

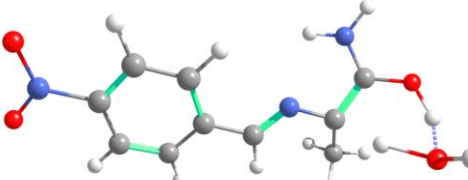
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|--|--|--|--|---|--------------|--------------|--------------|
|  |  |  |  | N | 3.961255000  | 4.667117000  | -2.291280000 |
|  |  |  |  | O | 4.507008000  | 5.610099000  | -1.730650000 |
|  |  |  |  | O | 4.168441000  | 4.331804000  | -3.452215000 |
|  |  |  |  | H | -0.263707000 | -2.266222000 | 1.094946000  |
|  |  |  |  | C | -0.543004000 | -1.807361000 | 2.051278000  |
|  |  |  |  | C | 0.563474000  | -1.172023000 | 2.787379000  |
|  |  |  |  | C | 0.420148000  | -0.858568000 | 4.148775000  |
|  |  |  |  | C | 1.771926000  | -0.887578000 | 2.134848000  |
|  |  |  |  | C | 1.463622000  | -0.269604000 | 4.845876000  |
|  |  |  |  | H | -0.511289000 | -1.099789000 | 4.645156000  |
|  |  |  |  | C | 2.825373000  | -0.298251000 | 2.823521000  |
|  |  |  |  | H | 1.889847000  | -1.135952000 | 1.086557000  |
|  |  |  |  | C | 2.652499000  | 0.004422000  | 4.169931000  |
|  |  |  |  | H | 1.379108000  | -0.026183000 | 5.896002000  |
|  |  |  |  | H | 3.766116000  | -0.074102000 | 2.340210000  |
|  |  |  |  | N | 3.768117000  | 0.633399000  | 4.909689000  |
|  |  |  |  | O | 3.590907000  | 0.888984000  | 6.094305000  |
|  |  |  |  | O | 4.800121000  | 0.865530000  | 4.292228000  |
|  |  |  |  | O | -1.578300000 | -2.236204000 | 2.674762000  |
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|   |              |              |             |  |  |  |
|---|--------------|--------------|-------------|--|--|--|
| C | 1.420074000  | -0.168324000 | 4.694866000 |  |  |  |
| H | -0.673001000 | -0.558959000 | 4.406950000 |  |  |  |
| C | 2.851922000  | -0.674381000 | 2.795325000 |  |  |  |
| H | 1.855137000  | -1.425326000 | 1.055613000 |  |  |  |
| C | 2.676188000  | -0.223830000 | 4.099509000 |  |  |  |
| H | 1.327229000  | 0.173307000  | 5.716600000 |  |  |  |
| H | 3.846172000  | -0.717470000 | 2.372647000 |  |  |  |
| N | 3.860222000  | 0.199088000  | 4.877589000 |  |  |  |
| O | 3.676752000  | 0.600297000  | 6.020228000 |  |  |  |
| O | 4.954782000  | 0.127821000  | 4.332049000 |  |  |  |
| O | -1.717140000 | -1.970786000 | 2.708537000 |  |  |  |



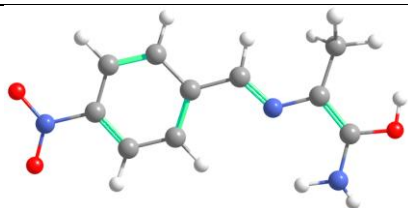
**8b-IN1**  
 $E_e^S = -853.8881817$

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| N | -1.257101000 | 0.273462000  | 0.831184000  | N | -1.631255000 | 0.908698000  | 0.041527000  |
| H | -2.447108000 | -0.761341000 | 2.148876000  | H | -3.620275000 | 0.290204000  | 1.342932000  |
| C | -2.588824000 | -0.189253000 | 1.221248000  | C | -3.019922000 | 0.724753000  | 0.088987000  |
| C | -3.091896000 | -1.249383000 | 0.216456000  | C | -3.443480000 | -0.506084000 | -0.582738000 |
| O | -4.192074000 | -1.775298000 | 0.348156000  | O | -4.593553000 | -1.019524000 | -0.324050000 |
| N | -2.250530000 | -1.557791000 | -0.791594000 | N | -2.619152000 | -1.160011000 | -1.405002000 |
| H | -1.327736000 | -1.150789000 | -0.805497000 | H | -1.688551000 | -0.791407000 | -1.534816000 |
| H | -2.511858000 | -2.286457000 | -1.437257000 | H | -2.845281000 | -2.098953000 | -1.696078000 |
| C | -0.895607000 | 1.476525000  | 1.018211000  | C | -1.075966000 | 2.048948000  | 0.237113000  |
| H | -1.555692000 | 2.232006000  | 1.456902000  | H | -1.654877000 | 2.959517000  | 0.420465000  |
| C | 0.451821000  | 1.960773000  | 0.658017000  | C | 0.380505000  | 2.216484000  | 0.244778000  |
| C | 1.455747000  | 1.088121000  | 0.210739000  | C | 1.259006000  | 1.122080000  | 0.142507000  |
| C | 0.734089000  | 3.328376000  | 0.772189000  | C | 0.923340000  | 3.507090000  | 0.361816000  |
| C | 2.710357000  | 1.571152000  | -0.126582000 | C | 2.630549000  | 1.309979000  | 0.146086000  |
| C | 1.986822000  | 3.828404000  | 0.435673000  | C | 2.296360000  | 3.710929000  | 0.365509000  |
| C | 2.956039000  | 2.938461000  | -0.010967000 | C | 3.135841000  | 2.606465000  | 0.255503000  |
| H | 1.239341000  | 0.029781000  | 0.143441000  | H | 0.843608000  | 0.125226000  | 0.070676000  |
| H | -0.034583000 | 4.007982000  | 1.123762000  | H | 0.258367000  | 4.359741000  | 0.447330000  |
| H | 3.498120000  | 0.915380000  | -0.470801000 | H | 3.316665000  | 0.477574000  | 0.070897000  |
| H | 2.219753000  | 4.881202000  | 0.513771000  | H | 2.723249000  | 4.700505000  | 0.451842000  |
| N | 4.294096000  | 3.459015000  | -0.371806000 | N | 4.593788000  | 2.810440000  | 0.259049000  |
| O | 4.486056000  | 4.662173000  | -0.251977000 | O | 5.010635000  | 3.959665000  | 0.359857000  |
| O | 5.126927000  | 2.654434000  | -0.769174000 | O | 5.309850000  | 1.819222000  | 0.160177000  |
| O | -5.591440000 | -1.673931000 | 2.796907000  | O | -4.602304000 | -0.155259000 | 1.900885000  |
| H | -5.206386000 | -1.816129000 | 1.913533000  | H | -4.817330000 | -0.679409000 | 0.801624000  |
| H | -6.322377000 | -2.293998000 | 2.864364000  | H | -4.361637000 | -0.800709000 | 2.575613000  |
| C | -3.665482000 | 0.873326000  | 1.472595000  | C | -3.944730000 | 1.933482000  | -0.112898000 |
| H | -3.823051000 | 1.492777000  | 0.584777000  | H | -3.661132000 | 2.490741000  | -1.014807000 |
| H | -4.604111000 | 0.387313000  | 1.733485000  | H | -4.981730000 | 1.615620000  | -0.219434000 |
| H | -3.393142000 | 1.519942000  | 2.309233000  | H | -3.903901000 | 2.620680000  | 0.735743000  |



**8b-TS1**  
 $E_e^S = -853.834017$

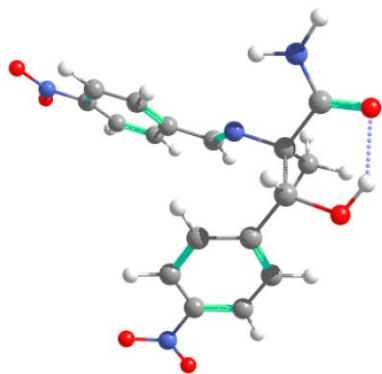
|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -1.631255000 | 0.908698000  | 0.041527000  |
| H | -3.620275000 | 0.290204000  | 1.342932000  |
| C | -3.019922000 | 0.724753000  | 0.088987000  |
| C | -3.443480000 | -0.506084000 | -0.582738000 |
| O | -4.593553000 | -1.019524000 | -0.324050000 |
| N | -2.619152000 | -1.160011000 | -1.405002000 |
| H | -1.688551000 | -0.791407000 | -1.534816000 |
| H | -2.845281000 | -2.098953000 | -1.696078000 |
| C | -1.075966000 | 2.048948000  | 0.237113000  |
| H | -1.654877000 | 2.959517000  | 0.420465000  |
| C | 0.380505000  | 2.216484000  | 0.244778000  |
| C | 1.259006000  | 1.122080000  | 0.142507000  |
| C | 0.923340000  | 3.507090000  | 0.361816000  |
| C | 2.630549000  | 1.309979000  | 0.146086000  |
| C | 2.296360000  | 3.710929000  | 0.365509000  |
| C | 3.135841000  | 2.606465000  | 0.255503000  |
| H | 0.843608000  | 0.125226000  | 0.070676000  |
| H | 0.258367000  | 4.359741000  | 0.447330000  |
| H | 3.316665000  | 0.477574000  | 0.070897000  |
| H | 2.723249000  | 4.700505000  | 0.451842000  |
| N | 4.593788000  | 2.810440000  | 0.259049000  |
| O | 5.010635000  | 3.959665000  | 0.359857000  |
| O | 5.309850000  | 1.819222000  | 0.160177000  |
| O | -4.602304000 | -0.155259000 | 1.900885000  |
| H | -4.817330000 | -0.679409000 | 0.801624000  |
| H | -4.361637000 | -0.800709000 | 2.575613000  |
| C | -3.944730000 | 1.933482000  | -0.112898000 |
| H | -3.661132000 | 2.490741000  | -1.014807000 |
| H | -4.981730000 | 1.615620000  | -0.219434000 |
| H | -3.903901000 | 2.620680000  | 0.735743000  |



**8b-IN2**

$$E_e^S = -777.4264296$$

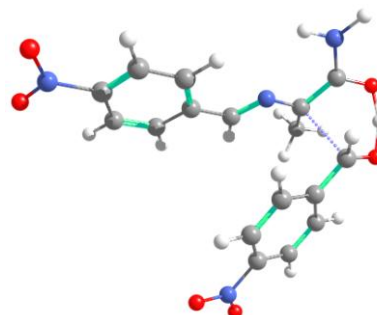
|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.662691000 | 0.838139000  | 0.362506000  |
| H | -3.281307000 | -1.438815000 | 1.935056000  |
| C | -1.639734000 | 0.208465000  | 1.089557000  |
| C | -2.248860000 | -0.848910000 | 0.443023000  |
| O | -3.180743000 | -1.654556000 | 1.002054000  |
| N | -2.016516000 | -1.179178000 | -0.853731000 |
| H | -1.234316000 | -0.703058000 | -1.278015000 |
| H | -2.195077000 | -2.133184000 | -1.126767000 |
| C | -0.003204000 | 1.856425000  | 0.806981000  |
| H | -0.191845000 | 2.286541000  | 1.794776000  |
| C | 1.044943000  | 2.507883000  | 0.029130000  |
| C | 1.410267000  | 2.071983000  | -1.259936000 |
| C | 1.722912000  | 3.612325000  | 0.578334000  |
| C | 2.410274000  | 2.711013000  | -1.970769000 |
| C | 2.727442000  | 4.262175000  | -0.122796000 |
| C | 3.062388000  | 3.803138000  | -1.394342000 |
| H | 0.894329000  | 1.223890000  | -1.690031000 |
| H | 1.454583000  | 3.962237000  | 1.569412000  |
| H | 2.697705000  | 2.384149000  | -2.960655000 |
| H | 3.252551000  | 5.110660000  | 0.293627000  |
| N | 4.125722000  | 4.482431000  | -2.145556000 |
| O | 4.683950000  | 5.437981000  | -1.613656000 |
| O | 4.398689000  | 4.057266000  | -3.264654000 |
| C | -2.021652000 | 0.655869000  | 2.477032000  |
| H | -2.320099000 | 1.710839000  | 2.481342000  |
| H | -2.866922000 | 0.103869000  | 2.897900000  |
| H | -1.188381000 | 0.551155000  | 3.181852000  |



**8b-IN3**

$$E_e^S = -1327.494915$$

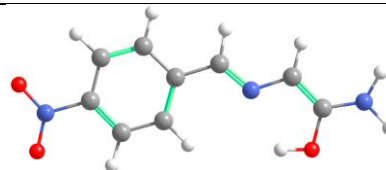
|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.476300000 | 0.625803000  | 0.321518000  |
| H | -2.431058000 | -2.180890000 | 2.079663000  |
| C | -1.445455000 | -0.078542000 | 1.152468000  |
| C | -2.532983000 | -0.686774000 | 0.220252000  |
| O | -3.409347000 | -1.413859000 | 0.680178000  |
| N | -2.455690000 | -0.371518000 | -1.087854000 |
| H | -1.652058000 | 0.132224000  | -1.430415000 |
| H | -3.115780000 | -0.791033000 | -1.724836000 |
| C | -0.030138000 | 1.773120000  | 0.642541000  |
| H | -0.352462000 | 2.303111000  | 1.543851000  |
| C | 0.967921000  | 2.487634000  | -0.174889000 |
| C | 1.534243000  | 1.912438000  | -1.323438000 |



**8b-TS2**

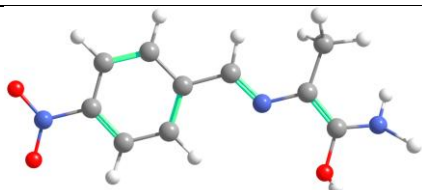
$$E_e^S = -1327.442875$$

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.527655000 | 0.813561000  | 0.444684000  |
| H | -2.427534000 | -2.083799000 | 1.910045000  |
| C | -1.462463000 | 0.161089000  | 1.212168000  |
| C | -2.330900000 | -0.725801000 | 0.462477000  |
| O | -3.097962000 | -1.573395000 | 1.049573000  |
| N | -2.295706000 | -0.717421000 | -0.879889000 |
| H | -1.677192000 | -0.071936000 | -1.346375000 |
| H | -2.800293000 | -1.423952000 | -1.391322000 |
| C | 0.153991000  | 1.819411000  | 0.887241000  |
| H | -0.007133000 | 2.235802000  | 1.884843000  |
| C | 1.171886000  | 2.486724000  | 0.079986000  |
| C | 1.523531000  | 2.037368000  | -1.207498000 |
| C | 1.824749000  | 3.618762000  | 0.599748000  |
| C | 2.486381000  | 2.697266000  | -1.951196000 |
| C | 2.791426000  | 4.290062000  | -0.135355000 |
| C | 3.110417000  | 3.820192000  | -1.405890000 |
| H | 1.030284000  | 1.162213000  | -1.610007000 |
| H | 1.567279000  | 3.975400000  | 1.591094000  |
| H | 2.765904000  | 2.363169000  | -2.940921000 |
| H | 3.297604000  | 5.161992000  | 0.255135000  |
| N | 4.134083000  | 4.525893000  | -2.196372000 |
| O | 4.656717000  | 5.516768000  | -1.698720000 |
| O | 4.403013000  | 4.080923000  | -3.307215000 |
| H | -0.223338000 | -2.107113000 | 1.024635000  |
| C | -0.463158000 | -1.826339000 | 2.054588000  |
| C | 0.629432000  | -1.258846000 | 2.838650000  |
| C | 0.523852000  | -1.151149000 | 4.237156000  |
| C | 1.800521000  | -0.821871000 | 2.196871000  |
| C | 1.567956000  | -0.622145000 | 4.979686000  |
| H | -0.376044000 | -1.505419000 | 4.723138000  |
| C | 2.851199000  | -0.289589000 | 2.931741000  |
| H | 1.887081000  | -0.905681000 | 1.120319000  |
| C | 2.717113000  | -0.197413000 | 4.314028000  |
| H | 1.513321000  | -0.537571000 | 6.056210000  |
| H | 3.761955000  | 0.049355000  | 2.458084000  |
| N | 3.832885000  | 0.367858000  | 5.103237000  |
| O | 3.689144000  | 0.440800000  | 6.317406000  |
| O | 4.831202000  | 0.732672000  | 4.494728000  |
| O | -1.490463000 | -2.340593000 | 2.625106000  |
| C | -1.964782000 | 0.713670000  | 2.523625000  |
| H | -2.445938000 | 1.686817000  | 2.363094000  |
| H | -2.701029000 | 0.049539000  | 2.972447000  |
| H | -1.158079000 | 0.862464000  | 3.246483000  |



**8a'-IN2**

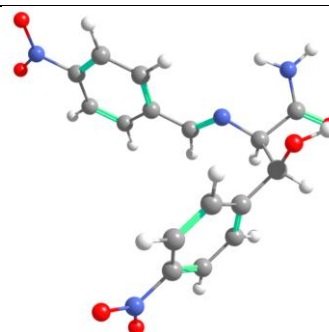
|   |              |              |              |                        |              |              |              |
|---|--------------|--------------|--------------|------------------------|--------------|--------------|--------------|
| C | 1.364209000  | 3.774326000  | 0.213521000  | $E_e^S = -738.1204907$ |              |              |              |
| C | 2.469702000  | 2.609187000  | -2.072101000 | N                      | -0.561056000 | 0.560465000  | 0.690707000  |
| C | 2.300132000  | 4.486118000  | -0.528086000 | H                      | -0.814172000 | -1.180632000 | -0.434238000 |
| C | 2.837037000  | 3.889809000  | -1.662258000 | C                      | -1.543317000 | -0.026817000 | 1.431984000  |
| H | 1.236280000  | 0.912972000  | -1.613472000 | C                      | -1.992275000 | -1.248937000 | 0.992882000  |
| H | 0.936527000  | 4.222873000  | 1.103474000  | O                      | -1.486455000 | -1.811576000 | -0.113362000 |
| H | 2.919531000  | 2.183862000  | -2.958627000 | N                      | -2.925064000 | -2.024669000 | 1.609890000  |
| H | 2.615654000  | 5.480302000  | -0.243772000 | H                      | -1.952394000 | 0.431098000  | 2.330585000  |
| N | 3.833916000  | 4.639351000  | -2.461912000 | H                      | -3.510053000 | -1.601907000 | 2.311794000  |
| O | 4.129225000  | 5.765935000  | -2.086587000 | H                      | -3.340536000 | -2.763022000 | 1.063285000  |
| O | 4.298628000  | 4.085211000  | -3.449357000 | C                      | -0.053569000 | 1.706415000  | 1.001065000  |
| H | -0.326753000 | -1.932627000 | 0.944392000  | H                      | -0.402509000 | 2.250019000  | 1.886765000  |
| C | -0.702637000 | -1.346236000 | 1.793922000  | C                      | 0.993518000  | 2.350734000  | 0.221897000  |
| C | 0.482002000  | -0.962839000 | 2.659830000  | C                      | 1.539528000  | 1.768624000  | -0.939737000 |
| C | 0.341165000  | -0.845815000 | 4.047429000  | C                      | 1.485067000  | 3.602754000  | 0.637643000  |
| C | 1.739154000  | -0.745266000 | 2.083717000  | C                      | 2.533808000  | 2.409911000  | -1.656434000 |
| C | 1.424592000  | -0.491718000 | 4.843856000  | C                      | 2.481402000  | 4.256006000  | -0.071640000 |
| H | -0.618226000 | -1.059098000 | 4.499159000  | C                      | 2.997216000  | 3.651166000  | -1.215095000 |
| C | 2.832635000  | -0.391313000 | 2.864702000  | H                      | 1.170345000  | 0.806273000  | -1.268788000 |
| H | 1.867114000  | -0.861546000 | 1.014161000  | H                      | 1.076602000  | 4.065269000  | 1.529651000  |
| C | 2.655175000  | -0.261547000 | 4.238293000  | H                      | 2.959175000  | 1.971786000  | -2.548843000 |
| H | 1.330902000  | -0.400258000 | 5.917240000  | H                      | 2.863283000  | 5.217653000  | 0.242015000  |
| H | 3.809383000  | -0.224557000 | 2.432113000  | N                      | 4.052808000  | 4.334770000  | -1.974120000 |
| N | 3.810924000  | 0.118901000  | 5.077844000  | O                      | 4.440859000  | 5.424572000  | -1.563023000 |
| O | 3.628872000  | 0.221266000  | 6.284719000  | O                      | 4.488685000  | 3.778505000  | -2.977920000 |
| O | 4.882385000  | 0.314184000  | 4.516556000  |                        |              |              |              |
| O | -1.594238000 | -2.107577000 | 2.573586000  |                        |              |              |              |
| C | -2.155387000 | 0.753171000  | 2.230756000  |                        |              |              |              |
| H | -2.656871000 | 1.615806000  | 1.783528000  |                        |              |              |              |
| H | -2.907717000 | 0.144223000  | 2.727941000  |                        |              |              |              |
| H | -1.455010000 | 1.108753000  | 2.988401000  |                        |              |              |              |



**8b'-IN2**

$$E_e^S = -777.4229146$$

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.694874000 | 0.880402000  | 0.322246000  |
| H | -2.148018000 | -2.000646000 | -1.064647000 |
| C | -1.702752000 | 0.253983000  | 1.022141000  |
| C | -2.317119000 | -0.792351000 | 0.389134000  |
| O | -2.078916000 | -1.048064000 | -0.920466000 |
| N | -3.188137000 | -1.700865000 | 0.974530000  |
| H | -3.357561000 | -1.585969000 | 1.961853000  |
| H | -4.038678000 | -1.880788000 | 0.453858000  |
| C | -0.038846000 | 1.879438000  | 0.795718000  |
| H | -0.231124000 | 2.308700000  | 1.785199000  |
| C | 1.031188000  | 2.519882000  | 0.029322000  |
| C | 1.378456000  | 2.079571000  | -1.261962000 |
| C | 1.733786000  | 3.601301000  | 0.587588000  |
| C | 2.393632000  | 2.698789000  | -1.970189000 |
| C | 2.753950000  | 4.230753000  | -0.111636000 |
| C | 3.072836000  | 3.770115000  | -1.386006000 |
| H | 0.832441000  | 1.247611000  | -1.687998000 |
| H | 1.475123000  | 3.950471000  | 1.581627000  |
| H | 2.671117000  | 2.372406000  | -2.963032000 |
| H | 3.301265000  | 5.063237000  | 0.308222000  |
| N | 4.152764000  | 4.430332000  | -2.135565000 |
| O | 4.731366000  | 5.370844000  | -1.599434000 |
| O | 4.416106000  | 4.004424000  | -3.255864000 |
| C | -2.097890000 | 0.701061000  | 2.408780000  |
| H | -2.294888000 | 1.778608000  | 2.423552000  |
| H | -3.007348000 | 0.216673000  | 2.766961000  |
| H | -1.306588000 | 0.508159000  | 3.142462000  |



**8a'-IN3**

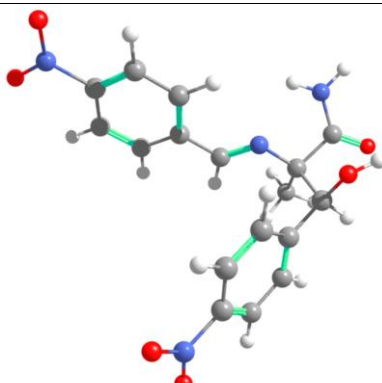
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|---|--------------|--------------|--------------|
| N | -0.489687000 | 0.666179000  | 0.273753000  |
| H | -1.358600000 | -2.731422000 | 0.356208000  |
| C | -1.286396000 | -0.077461000 | 1.223825000  |
| C | -2.692505000 | -0.401718000 | 0.677588000  |
| O | -3.487369000 | -1.022110000 | 1.366280000  |
| N | -2.951082000 | 0.036913000  | -0.574636000 |
| H | -1.448341000 | 0.479588000  | 2.158859000  |
| H | -2.208350000 | 0.443307000  | -1.123381000 |
| H | -3.841700000 | -0.181420000 | -0.994071000 |
| C | 0.120457000  | 1.707451000  | 0.675482000  |
| H | 0.038041000  | 2.059921000  | 1.713344000  |
| C | 0.973486000  | 2.522975000  | -0.205608000 |
| C | 1.247670000  | 2.133908000  | -1.526243000 |
| C | 1.524688000  | 3.711773000  | 0.290194000  |
| C | 2.046780000  | 2.922420000  | -2.338923000 |
| C | 2.327255000  | 4.512946000  | -0.513889000 |
| C | 2.572934000  | 4.103981000  | -1.818846000 |
| H | 0.832312000  | 1.205614000  | -1.897087000 |
| H | 1.322895000  | 4.013487000  | 1.312159000  |
| H | 2.272567000  | 2.641726000  | -3.358381000 |
| H | 2.759080000  | 5.434628000  | -0.149579000 |
| N | 3.424704000  | 4.951077000  | -2.685746000 |

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|  |  |  |  | O | 3.872349000  | 5.983693000  | -2.204988000 |
|  |  |  |  | O | 3.626399000  | 4.566499000  | -3.830143000 |
|  |  |  |  | H | -1.288593000 | -1.871305000 | 2.374125000  |
|  |  |  |  | C | -0.620026000 | -1.440743000 | 1.621571000  |
|  |  |  |  | C | 0.745723000  | -1.234383000 | 2.239263000  |
|  |  |  |  | C | 0.844616000  | -0.762824000 | 3.553954000  |
|  |  |  |  | C | 1.913635000  | -1.492258000 | 1.515983000  |
|  |  |  |  | C | 2.084093000  | -0.539100000 | 4.140285000  |
|  |  |  |  | H | -0.054264000 | -0.581411000 | 4.134011000  |
|  |  |  |  | C | 3.162269000  | -1.275820000 | 2.089298000  |
|  |  |  |  | H | 1.837317000  | -1.875264000 | 0.507443000  |
|  |  |  |  | C | 3.229205000  | -0.796864000 | 3.393004000  |
|  |  |  |  | H | 2.175811000  | -0.182515000 | 5.156856000  |
|  |  |  |  | H | 4.075599000  | -1.472688000 | 1.544896000  |
|  |  |  |  | N | 4.553122000  | -0.560524000 | 4.006719000  |
|  |  |  |  | O | 4.579402000  | -0.121550000 | 5.150406000  |
|  |  |  |  | O | 5.545336000  | -0.814031000 | 3.335365000  |
|  |  |  |  | O | -0.504245000 | -2.315048000 | 0.509876000  |
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|---|--------------|--------------|-------------|
| O | -0.348883000 | -2.291951000 | 0.840853000 |
| C | -2.224883000 | 0.740500000  | 2.178507000 |
| H | -2.711105000 | 1.601265000  | 1.712104000 |
| H | -2.998059000 | 0.124805000  | 2.638844000 |
| H | -1.560925000 | 1.104602000  | 2.964147000 |

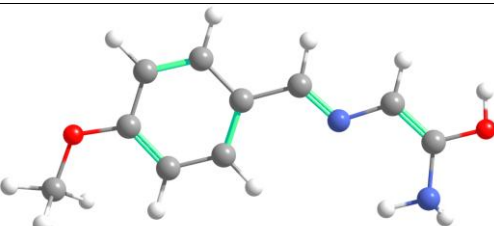
  



**10-TS1**  
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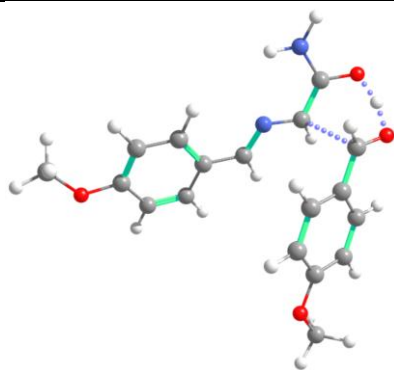
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|---|--------------|--------------|--------------|
| N | -0.192066000 | 1.910915000  | -0.346604000 |
| H | 1.715851000  | 3.304567000  | 1.649913000  |
| C | 1.045148000  | 2.543949000  | -0.786997000 |
| C | 0.925974000  | 4.084324000  | -0.563923000 |
| O | 1.759642000  | 4.847154000  | -1.020210000 |
| N | -0.105929000 | 4.482385000  | 0.222678000  |
| H | -0.802500000 | 3.804028000  | 0.494347000  |
| H | -0.265648000 | 5.470997000  | 0.343895000  |
| C | -0.718671000 | 0.953047000  | -0.995479000 |
| H | -0.294507000 | 0.560153000  | -1.925020000 |
| C | -1.958506000 | 0.288813000  | -0.549722000 |
| C | -2.550826000 | 0.584085000  | 0.687962000  |
| C | -2.554496000 | -0.665351000 | -1.384908000 |
| C | -3.719973000 | -0.049928000 | 1.078098000  |
| C | -3.728487000 | -1.307749000 | -1.008512000 |
| C | -4.293822000 | -0.985998000 | 0.219259000  |
| H | -2.076072000 | 1.307114000  | 1.338677000  |
| H | -2.097697000 | -0.905275000 | -2.338874000 |
| H | -4.191251000 | 0.160961000  | 2.028122000  |
| H | -4.203761000 | -2.043416000 | -1.642284000 |
| N | -5.545361000 | -1.662781000 | 0.630701000  |
| O | -6.028378000 | -2.479530000 | -0.142291000 |
| O | -6.020270000 | -1.361829000 | 1.718045000  |
| H | 3.092962000  | 2.684581000  | -0.145022000 |
| C | 2.227664000  | 2.098737000  | 0.185481000  |
| C | 2.565635000  | 0.627499000  | 0.085964000  |
| C | 3.568094000  | 0.192205000  | -0.788477000 |
| C | 1.895660000  | -0.314583000 | 0.876072000  |
| C | 3.885858000  | -1.156858000 | -0.897799000 |
| H | 4.118181000  | 0.914127000  | -1.381321000 |
| C | 2.203215000  | -1.666699000 | 0.781750000  |
| H | 1.147979000  | 0.022403000  | 1.580989000  |
| C | 3.190654000  | -2.069012000 | -0.111855000 |
| H | 4.661146000  | -1.505106000 | -1.566056000 |
| H | 1.697385000  | -2.405656000 | 1.387815000  |
| N | 3.519393000  | -3.506851000 | -0.221404000 |
| O | 4.398164000  | -3.830678000 | -1.010934000 |
| O | 2.890788000  | -4.288981000 | 0.480650000  |
| O | 1.936002000  | 2.371916000  | 1.546587000  |
| C | 1.440684000  | 2.320540000  | -2.253971000 |
| H | 2.316083000  | 2.924605000  | -2.489174000 |
| H | 1.670174000  | 1.275479000  | -2.463181000 |
| H | 0.632362000  | 2.639777000  | -2.916963000 |



**10-IN2**  
 $E_e^S = -648.1430488$

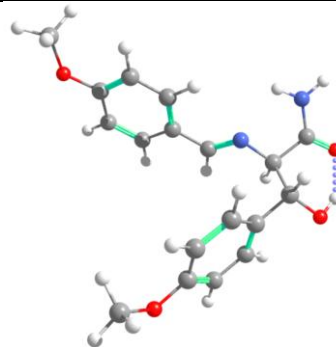
|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.516994000 | 0.485625000  | 0.650287000  |
| H | -3.058273000 | -1.521220000 | 2.642001000  |
| C | -1.487928000 | -0.095372000 | 1.432421000  |
| C | -2.023671000 | -1.289459000 | 1.056479000  |
| O | -2.943250000 | -1.966725000 | 1.795463000  |
| N | -1.750430000 | -1.926473000 | -0.123168000 |
| H | -1.848319000 | 0.394755000  | 2.339727000  |
| H | -0.962484000 | -1.533928000 | -0.619525000 |
| H | -1.802413000 | -2.934590000 | -0.103296000 |
| C | -0.017449000 | 1.628449000  | 0.960838000  |
| H | -0.363836000 | 2.167798000  | 1.854179000  |
| C | 1.023187000  | 2.297492000  | 0.184156000  |
| C | 1.569311000  | 1.743926000  | -0.981922000 |
| C | 1.509500000  | 3.548518000  | 0.604437000  |
| C | 2.557923000  | 2.403329000  | -1.704132000 |
| C | 2.494260000  | 4.217050000  | -0.104640000 |
| C | 3.027447000  | 3.648743000  | -1.267158000 |
| H | 1.206706000  | 0.781320000  | -1.320947000 |
| H | 1.104322000  | 4.001522000  | 1.503955000  |
| H | 2.953928000  | 1.943376000  | -2.599816000 |
| H | 2.866970000  | 5.180742000  | 0.220990000  |
| O | 3.991930000  | 4.377581000  | -1.900102000 |
| C | 4.570940000  | 3.856513000  | -3.088584000 |
| H | 5.078867000  | 2.903997000  | -2.902226000 |
| H | 3.819432000  | 3.721484000  | -3.874050000 |
| H | 5.301191000  | 4.596324000  | -3.412502000 |



**10-TS2**

$E_e^S = -1108.183688$

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.624092000 | 0.698116000  | 0.211212000  |
| H | -2.552285000 | -2.019123000 | 1.974139000  |
| C | -1.488224000 | 0.004148000  | 1.028868000  |
| C | -2.475533000 | -0.817518000 | 0.406752000  |
| O | -3.240296000 | -1.591784000 | 1.098312000  |
| N | -2.566010000 | -0.860652000 | -0.938365000 |
| H | -1.713431000 | 0.362332000  | 2.030779000  |
| H | -1.935016000 | -0.290305000 | -1.479973000 |
| H | -3.137880000 | -1.566619000 | -1.372072000 |
| C | 0.097942000  | 1.652371000  | 0.690443000  |
| H | 0.000382000  | 1.954274000  | 1.741222000  |
| C | 1.067315000  | 2.406570000  | -0.098243000 |
| C | 1.331647000  | 2.122196000  | -1.445266000 |
| C | 1.776553000  | 3.464297000  | 0.499669000  |
| C | 2.259013000  | 2.858732000  | -2.173809000 |
| C | 2.703091000  | 4.206643000  | -0.213373000 |
| C | 2.952151000  | 3.909701000  | -1.558669000 |
| H | 0.798936000  | 1.307669000  | -1.920741000 |
| H | 1.593669000  | 3.703733000  | 1.542341000  |
| H | 2.435844000  | 2.608881000  | -3.211529000 |
| H | 3.247886000  | 5.021307000  | 0.248225000  |
| H | -0.300620000 | -2.241669000 | 1.100089000  |
| C | -0.557990000 | -1.808382000 | 2.072950000  |
| C | 0.543993000  | -1.182973000 | 2.799948000  |
| C | 0.428929000  | -0.884537000 | 4.164026000  |
| C | 1.751651000  | -0.879768000 | 2.145721000  |
| C | 1.482241000  | -0.307266000 | 4.863198000  |
| H | -0.495996000 | -1.126997000 | 4.673163000  |
| C | 2.807635000  | -0.304862000 | 2.831700000  |
| H | 1.858743000  | -1.101870000 | 1.089835000  |
| C | 2.680447000  | -0.013905000 | 4.196474000  |
| H | 1.367070000  | -0.097780000 | 5.918170000  |
| H | 3.740673000  | -0.068832000 | 2.335004000  |
| O | -1.598698000 | -2.243657000 | 2.694741000  |
| O | 3.879915000  | 4.691937000  | -2.180026000 |
| C | 4.177312000  | 4.444422000  | -3.547991000 |
| H | 4.583493000  | 3.437589000  | -3.693064000 |
| H | 3.292205000  | 4.575928000  | -4.179626000 |
| H | 4.930443000  | 5.179907000  | -3.825721000 |
| O | 3.770634000  | 0.547291000  | 4.786408000  |
| C | 3.717701000  | 0.858873000  | 6.173910000  |
| H | 2.932509000  | 1.591253000  | 6.388851000  |
| H | 3.556164000  | -0.039686000 | 6.778392000  |
| H | 4.687853000  | 1.288229000  | 6.417603000  |



**10-IN3**

$E_e^S = -1108.233658$

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.453990000 | 0.475001000  | 0.200732000  |
| H | -2.560420000 | -2.009593000 | 2.242218000  |
| C | -1.406221000 | -0.202467000 | 1.054366000  |
| C | -2.596607000 | -0.728395000 | 0.234231000  |
| O | -3.523921000 | -1.324356000 | 0.778272000  |
| N | -2.543512000 | -0.504834000 | -1.095332000 |
| H | -1.823723000 | 0.454678000  | 1.831369000  |
| H | -1.720056000 | -0.071680000 | -1.486761000 |
| H | -3.277580000 | -0.868870000 | -1.682373000 |
| C | 0.021440000  | 1.591740000  | 0.592072000  |
| H | -0.295384000 | 2.038967000  | 1.544676000  |
| C | 1.006312000  | 2.368556000  | -0.164498000 |
| C | 1.563451000  | 1.906166000  | -1.362804000 |
| C | 1.416890000  | 3.621434000  | 0.320020000  |
| C | 2.492564000  | 2.664031000  | -2.064980000 |
| C | 2.341101000  | 4.388909000  | -0.368384000 |
| C | 2.885944000  | 3.915336000  | -1.568800000 |
| H | 1.264037000  | 0.935027000  | -1.738071000 |
| H | 1.002659000  | 3.995119000  | 1.250918000  |
| H | 2.905735000  | 2.277115000  | -2.986713000 |
| H | 2.659387000  | 5.356043000  | 0.000854000  |
| H | -0.440111000 | -2.149823000 | 1.053736000  |
| C | -0.753489000 | -1.422771000 | 1.816500000  |
| C | 0.462037000  | -1.004166000 | 2.614049000  |
| C | 0.322460000  | -0.458464000 | 3.897413000  |
| C | 1.744813000  | -1.133724000 | 2.090095000  |
| C | 1.430357000  | -0.045595000 | 4.621833000  |
| H | -0.665950000 | -0.384651000 | 4.334523000  |
| C | 2.872521000  | -0.723215000 | 2.805508000  |
| H | 1.879732000  | -1.562876000 | 1.102686000  |
| C | 2.715039000  | -0.171783000 | 4.078304000  |
| H | 1.327394000  | 0.368307000  | 5.618001000  |
| H | 3.852813000  | -0.844240000 | 2.364551000  |
| O | -1.699981000 | -1.996463000 | 2.698442000  |
| O | 3.785574000  | 4.734180000  | -2.175026000 |
| C | 4.379871000  | 4.318478000  | -3.400071000 |
| H | 4.954632000  | 3.395590000  | -3.270876000 |
| H | 3.625255000  | 4.175576000  | -4.180358000 |
| H | 5.051443000  | 5.124190000  | -3.690674000 |
| O | 3.742043000  | 0.262386000  | 4.868522000  |
| C | 5.069957000  | 0.146913000  | 4.378366000  |
| H | 5.337595000  | -0.898557000 | 4.189309000  |
| H | 5.211052000  | 0.730069000  | 3.461511000  |
| H | 5.712553000  | 0.546496000  | 5.161437000  |

