Supporting Information for

DFT insight into axial ligand effects on electronic structure and mechanistic reactivity of oxoiron(IV) porphyrin

Zhifeng Ma\textsuperscript{a}, Naoki Nakatani\textsuperscript{a}, Hiroshi Fujii\textsuperscript{b}, and Masahiko Hada\textsuperscript{*a},

a) Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University,
1-1 Minami-Osawa, Hachioji, Tokyo, 192-0397, Japan

b) Department of Chemistry, Graduate School of Humanities and Science, Nara Women’s University, Kitauoyanishi, Nara, 630-8506, Japan

E-mail addresses:
ma-zhifeng@ed.tmu.ac.jp; naokin@tmu.ac.jp; fujii@cc.nara-wu.ac.jp; hada@tmu.ac.jp

*Corresponding Author:
E-mail: hada@tmu.ac.jp, Tel: +81-48-858-9113.
Figure S1. Geometry scans for the generation of radical complexes from reactants and epoxide formation scans starting from radical intermediates. Each point is a full geometry optimization.
Figure S2. Change in spin population along ethylene oxidation by Fe(IV)OL-porphyrin complexes in the quartet ground spin state.
Figure S3. Change in Mulliken charge during ethylene oxidation by Fe(IV)OL-porphyrin complexes.
Figure S4. 2D potential energy surfaces of the quartet (blue) and sextet (red) spin states of the ring-closing reactions (from Imt to P through TS2) by the Fe(IV)OL-porphyrin complexes with Ac, Cl, and NO$_3$ as the axial ligands.
### Table S1. Activation energies (kcal/mol) for optimized Comp-Ac, Comp-Cl, Comp-F and Comp-NO₃ using various basis sets for other atoms, cc-pVTZ for iron atom in combination with PBE0 functional.

<table>
<thead>
<tr>
<th></th>
<th>Comp-Ac</th>
<th>Comp-Cl</th>
<th>Comp-F</th>
<th>Comp-NO₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-31G</td>
<td>9.5</td>
<td>13.7</td>
<td>6.6</td>
<td>12.3</td>
</tr>
<tr>
<td>6-31G(d)</td>
<td>12.1</td>
<td>14.1</td>
<td>9.2</td>
<td>14.2</td>
</tr>
<tr>
<td>6-31+G(d)</td>
<td>13.2</td>
<td>14.6</td>
<td>11.0</td>
<td>15.5</td>
</tr>
<tr>
<td>6-31++G(d,p)</td>
<td>13.2</td>
<td>14.6</td>
<td>10.9</td>
<td>15.4</td>
</tr>
</tbody>
</table>

### Table S2. Bond lengths (Å) for optimized Comp-Ac, Comp-Cl, Comp-F and Comp-NO₃ using various basis sets for other atoms, cc-pVTZ for iron atom in combination with PBE0 functional.

<table>
<thead>
<tr>
<th></th>
<th>Fe–O</th>
<th>Fe–L (L=Ligand)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Comp-Ac</td>
<td>Comp-Cl</td>
</tr>
<tr>
<td>6-31G</td>
<td>1.637</td>
<td>1.630</td>
</tr>
<tr>
<td>6-31G(d)</td>
<td>1.627</td>
<td>1.623</td>
</tr>
<tr>
<td>6-31+G(d)</td>
<td>1.626</td>
<td>1.623</td>
</tr>
<tr>
<td>6-31++G(d,p)</td>
<td>1.626</td>
<td>1.623</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Transition states (TS1)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fe–O</td>
</tr>
<tr>
<td>6-31G</td>
<td>1.759</td>
</tr>
<tr>
<td>6-31G(d)</td>
<td>1.716</td>
</tr>
<tr>
<td>6-31+G(d)</td>
<td>1.706</td>
</tr>
<tr>
<td>6-31++G(d,p)</td>
<td>1.707</td>
</tr>
</tbody>
</table>

### Table S3. Mulliken spin population ($P$) of key atoms based on optimized structures during the epoxidation of ethylene in the quartet state.

<table>
<thead>
<tr>
<th></th>
<th>$P_{Fe}$</th>
<th>$P_{Por}$</th>
<th>$P_{N×4}$</th>
<th>$P_{O}$</th>
<th>$P_{L}$</th>
<th>$P_{CH2}$</th>
<th>$P_{CH2}^{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{4}$Ac+C_{2}H_{4}</td>
<td>1.17</td>
<td>0.89</td>
<td>0.76</td>
<td>0.87</td>
<td>0.03</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$Cl+C_{2}H_{4}</td>
<td>1.16</td>
<td>0.88</td>
<td>0.76</td>
<td>0.87</td>
<td>0.09</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$F+C_{2}H_{4}</td>
<td>1.19</td>
<td>0.91</td>
<td>0.75</td>
<td>0.84</td>
<td>0.06</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$NO₃+C_{2}H_{4}</td>
<td>1.16</td>
<td>0.93</td>
<td>0.73</td>
<td>0.89</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$Ac-TS1</td>
<td>1.68</td>
<td>0.04</td>
<td>-0.01</td>
<td>0.95</td>
<td>0.05</td>
<td>-0.11</td>
<td>0.38</td>
</tr>
<tr>
<td>$^{4}$Cl-TS1</td>
<td>1.47</td>
<td>0.28</td>
<td>0.25</td>
<td>0.81</td>
<td>0.11</td>
<td>-0.13</td>
<td>0.45</td>
</tr>
<tr>
<td>$^{4}$F-TS1</td>
<td>1.75</td>
<td>-0.03</td>
<td>-0.08</td>
<td>0.94</td>
<td>0.09</td>
<td>-0.11</td>
<td>0.36</td>
</tr>
<tr>
<td>$^{4}$NO₃-TS1</td>
<td>1.54</td>
<td>0.22</td>
<td>0.17</td>
<td>0.88</td>
<td>0.03</td>
<td>-0.10</td>
<td>0.42</td>
</tr>
<tr>
<td>$^{4}$Ac-Imt1</td>
<td>1.95</td>
<td>-0.15</td>
<td>-0.19</td>
<td>0.20</td>
<td>0.05</td>
<td>-0.04</td>
<td>0.97</td>
</tr>
<tr>
<td>$^{4}$Cl-Imt1</td>
<td>2.06</td>
<td>-0.15</td>
<td>-0.20</td>
<td>0.15</td>
<td>0.05</td>
<td>-0.04</td>
<td>0.94</td>
</tr>
<tr>
<td>$^{4}$F-Imt1</td>
<td>1.96</td>
<td>-0.17</td>
<td>-0.20</td>
<td>0.18</td>
<td>0.10</td>
<td>-0.04</td>
<td>0.97</td>
</tr>
<tr>
<td>$^{4}$NO₃-Imt1</td>
<td>2.04</td>
<td>-0.14</td>
<td>-0.20</td>
<td>0.16</td>
<td>0.02</td>
<td>-0.04</td>
<td>0.94</td>
</tr>
<tr>
<td>$^{4}$Ac-TS2</td>
<td>2.46</td>
<td>-0.16</td>
<td>-0.24</td>
<td>-0.16</td>
<td>0.10</td>
<td>-0.04</td>
<td>0.77</td>
</tr>
<tr>
<td>$^{4}$Cl-TS2</td>
<td>2.37</td>
<td>-0.16</td>
<td>-0.23</td>
<td>-0.09</td>
<td>0.10</td>
<td>-0.04</td>
<td>0.83</td>
</tr>
<tr>
<td>$^{4}$F-TS2</td>
<td>2.46</td>
<td>-0.18</td>
<td>-0.24</td>
<td>-0.18</td>
<td>0.16</td>
<td>-0.04</td>
<td>0.77</td>
</tr>
<tr>
<td>$^{4}$NO₃-TS2</td>
<td>2.34</td>
<td>-0.17</td>
<td>-0.24</td>
<td>-0.06</td>
<td>0.06</td>
<td>-0.03</td>
<td>0.84</td>
</tr>
<tr>
<td>$^{4}$Ac-P</td>
<td>2.87</td>
<td>-0.08</td>
<td>-0.18</td>
<td>0.02</td>
<td>0.15</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$Cl-P</td>
<td>2.82</td>
<td>-0.07</td>
<td>-0.18</td>
<td>0.02</td>
<td>0.22</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{4}$F-P</td>
<td>2.84</td>
<td>-0.08</td>
<td>-0.17</td>
<td>0.02</td>
<td>0.22</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table S4. Mulliken spin population ($P$) of key atoms based on optimized structures during the epoxidation of ethylene in the sextet state.

<table>
<thead>
<tr>
<th></th>
<th>$P_{Fe}$</th>
<th>$P_{Por}$</th>
<th>$P_{CH2}$</th>
<th>$P_{O}$</th>
<th>$P_{L}$</th>
<th>$P_{CH2}$</th>
<th>$P_{CH2}$*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{6}$Ac+${C_2}H_4$</td>
<td>3.21</td>
<td>1.18</td>
<td>1.02</td>
<td>0.59</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$Cl+${C_2}H_4$</td>
<td>3.22</td>
<td>1.17</td>
<td>1.02</td>
<td>0.56</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$F+${C_2}H_4$</td>
<td>3.22</td>
<td>1.18</td>
<td>1.00</td>
<td>0.55</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$NO$_3$+${C_2}H_4$</td>
<td>3.22</td>
<td>1.21</td>
<td>1.00</td>
<td>0.56</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$Ac-TS1</td>
<td>3.98</td>
<td>1.20</td>
<td>1.02</td>
<td>0.01</td>
<td>0.09</td>
<td>0.17</td>
<td>-0.46</td>
</tr>
<tr>
<td>$^{6}$Cl-TS1</td>
<td>3.94</td>
<td>1.16</td>
<td>1.01</td>
<td>0.03</td>
<td>0.17</td>
<td>0.16</td>
<td>-0.48</td>
</tr>
<tr>
<td>$^{6}$F-TS1</td>
<td>3.98</td>
<td>1.18</td>
<td>1.01</td>
<td>-0.04</td>
<td>0.14</td>
<td>0.17</td>
<td>-0.44</td>
</tr>
<tr>
<td>$^{6}$NO$_3$-TS1</td>
<td>3.83</td>
<td>1.22</td>
<td>0.99</td>
<td>0.09</td>
<td>0.05</td>
<td>0.15</td>
<td>-0.34</td>
</tr>
<tr>
<td>$^{6}$Ac-Imt1</td>
<td>4.30</td>
<td>-0.42</td>
<td>-0.32</td>
<td>0.15</td>
<td>0.11</td>
<td>-0.05</td>
<td>0.89</td>
</tr>
<tr>
<td>$^{6}$Cl-Imt1</td>
<td>2.61</td>
<td>0.82</td>
<td>0.63</td>
<td>0.42</td>
<td>0.20</td>
<td>-0.06</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{6}$F-Imt1</td>
<td>3.75</td>
<td>0.30</td>
<td>0.23</td>
<td>-0.03</td>
<td>0.11</td>
<td>-0.03</td>
<td>0.90</td>
</tr>
<tr>
<td>$^{6}$NO$_3$-Imt1</td>
<td>2.64</td>
<td>0.90</td>
<td>0.62</td>
<td>0.42</td>
<td>0.06</td>
<td>-0.06</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{6}$Ac-TS2</td>
<td>4.31</td>
<td>-0.34</td>
<td>-0.26</td>
<td>0.04</td>
<td>0.12</td>
<td>-0.03</td>
<td>0.88</td>
</tr>
<tr>
<td>$^{6}$Cl-TS2</td>
<td>4.26</td>
<td>-0.64</td>
<td>-0.48</td>
<td>0.31</td>
<td>0.07</td>
<td>0.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{6}$F-TS2</td>
<td>4.36</td>
<td>0.23</td>
<td>0.17</td>
<td>-0.62</td>
<td>0.23</td>
<td>-0.09</td>
<td>0.88</td>
</tr>
<tr>
<td>$^{6}$NO$_3$-TS2</td>
<td>4.29</td>
<td>-0.59</td>
<td>-0.42</td>
<td>0.27</td>
<td>0.05</td>
<td>-0.01</td>
<td>0.97</td>
</tr>
<tr>
<td>$^{6}$Ac-P</td>
<td>4.34</td>
<td>0.41</td>
<td>0.32</td>
<td>0.02</td>
<td>0.18</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$Cl-P</td>
<td>4.28</td>
<td>0.43</td>
<td>0.33</td>
<td>0.03</td>
<td>0.25</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$F-P</td>
<td>4.34</td>
<td>0.40</td>
<td>0.31</td>
<td>0.02</td>
<td>0.23</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$^{6}$NO$_3$-P</td>
<td>4.36</td>
<td>0.43</td>
<td>0.32</td>
<td>0.03</td>
<td>0.13</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

* Terminal CH$_2$ group in ethylene

Table S5. Absolute energies (Hartree) in the 1-hexene solvent and the group Mulliken charges ($Q$) of optimized structures in the epoxidation in the quartet state.

<table>
<thead>
<tr>
<th></th>
<th>Energy</th>
<th>$Q_{Fe}$</th>
<th>$Q_{Por}$</th>
<th>$Q_{CH2}$</th>
<th>$Q_{O}$</th>
<th>$Q_{L}$</th>
<th>$Q_{CH2}$</th>
<th>$Q_{CH2}$*</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{4}$Ac+${C_2}H_4$</td>
<td>-2632.28493</td>
<td>1.06</td>
<td>-0.24</td>
<td>-2.76</td>
<td>-0.27</td>
<td>-0.58</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$^{4}$Cl+${C_2}H_4$</td>
<td>-2864.17171</td>
<td>0.78</td>
<td>-0.12</td>
<td>-2.69</td>
<td>-0.26</td>
<td>-0.40</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$^{4}$F+${C_2}H_4$</td>
<td>-2503.87022</td>
<td>0.86</td>
<td>-0.19</td>
<td>-2.68</td>
<td>-0.29</td>
<td>-0.38</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$^{4}$NO$_3$+${C_2}H_4$</td>
<td>-2684.02848</td>
<td>1.11</td>
<td>-0.16</td>
<td>-2.79</td>
<td>-0.24</td>
<td>-0.42</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$^{4}$Ac-TS1</td>
<td>-2632.26976</td>
<td>1.24</td>
<td>-0.68</td>
<td>-2.95</td>
<td>-0.29</td>
<td>-0.56</td>
<td>0.12</td>
<td>0.07</td>
</tr>
<tr>
<td>$^{4}$Cl-TS1</td>
<td>-2864.14995</td>
<td>0.87</td>
<td>-0.48</td>
<td>-2.83</td>
<td>-0.30</td>
<td>-0.30</td>
<td>0.15</td>
<td>0.07</td>
</tr>
<tr>
<td>$^{4}$F-TS1</td>
<td>-2503.85971</td>
<td>1.07</td>
<td>-0.66</td>
<td>-2.91</td>
<td>-0.28</td>
<td>-0.31</td>
<td>0.11</td>
<td>0.07</td>
</tr>
<tr>
<td>$^{4}$NO$_3$-TS1</td>
<td>-2684.00879</td>
<td>1.28</td>
<td>-0.56</td>
<td>-2.93</td>
<td>-0.28</td>
<td>-0.41</td>
<td>0.14</td>
<td>0.08</td>
</tr>
<tr>
<td>$^{4}$Ac-Imt1</td>
<td>-2632.30281</td>
<td>1.39</td>
<td>-0.78</td>
<td>-3.03</td>
<td>-0.48</td>
<td>-0.56</td>
<td>0.25</td>
<td>0.08</td>
</tr>
<tr>
<td>$^{4}$Cl-Imt1</td>
<td>-2864.18366</td>
<td>1.04</td>
<td>-0.63</td>
<td>-2.96</td>
<td>-0.49</td>
<td>-0.25</td>
<td>0.25</td>
<td>0.10</td>
</tr>
<tr>
<td>$^{4}$F-Imt1</td>
<td>-2503.89290</td>
<td>1.21</td>
<td>-0.75</td>
<td>-2.98</td>
<td>-0.48</td>
<td>-0.30</td>
<td>0.25</td>
<td>0.08</td>
</tr>
<tr>
<td>$^{4}$NO$_3$-Imt1</td>
<td>-2684.04028</td>
<td>1.15</td>
<td>-0.71</td>
<td>-3.06</td>
<td>-0.47</td>
<td>-0.41</td>
<td>0.26</td>
<td>0.10</td>
</tr>
<tr>
<td>$^{4}$Ac-TS2</td>
<td>-2632.30035</td>
<td>1.43</td>
<td>-0.82</td>
<td>-3.06</td>
<td>-0.51</td>
<td>-0.58</td>
<td>0.26</td>
<td>0.16</td>
</tr>
<tr>
<td>$^{4}$Cl-TS2</td>
<td>-2864.18352</td>
<td>1.08</td>
<td>-0.67</td>
<td>-2.98</td>
<td>-0.51</td>
<td>-0.30</td>
<td>0.25</td>
<td>0.17</td>
</tr>
<tr>
<td>$^{4}$F-TS2</td>
<td>-2503.89035</td>
<td>1.24</td>
<td>-0.81</td>
<td>-3.00</td>
<td>-0.51</td>
<td>-0.34</td>
<td>0.26</td>
<td>0.15</td>
</tr>
<tr>
<td>$^{4}$NO$_3$-TS2</td>
<td>-2684.03990</td>
<td>1.44</td>
<td>-0.72</td>
<td>-3.08</td>
<td>-0.49</td>
<td>-0.41</td>
<td>0.26</td>
<td>0.15</td>
</tr>
<tr>
<td>$^{4}$Ac-P</td>
<td>-2632.35050</td>
<td>1.43</td>
<td>-0.91</td>
<td>-3.11</td>
<td>-0.50</td>
<td>-0.62</td>
<td>0.29</td>
<td>0.29</td>
</tr>
<tr>
<td>$^{4}$Cl-P</td>
<td>-2864.23693</td>
<td>1.15</td>
<td>-0.81</td>
<td>-3.07</td>
<td>-0.51</td>
<td>-0.41</td>
<td>0.29</td>
<td>0.29</td>
</tr>
</tbody>
</table>

* Terminal CH$_2$ group in ethylene
Table S6. Absolute energies (Hartree) in the 1-hexene solvent and group Mulliken charges ($Q$) of optimized structures in the epoxidation in the sextet state.

<table>
<thead>
<tr>
<th>Energy</th>
<th>$Q_{Fe}$</th>
<th>$Q_{Por}$</th>
<th>$Q_{N} \times 4$</th>
<th>$Q_{O}$</th>
<th>$Q_{X}$</th>
<th>$Q_{CH2}$</th>
<th>$Q_{CH2}^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^6$Ac+$C_2H_4$</td>
<td>-2632.27542</td>
<td>1.22</td>
<td>-0.39</td>
<td>-2.89</td>
<td>-0.29</td>
<td>-0.58</td>
<td>0.0</td>
</tr>
<tr>
<td>$^6$Cl+$C_2H_4$</td>
<td>-2864.16140</td>
<td>0.94</td>
<td>-0.28</td>
<td>-2.82</td>
<td>-0.28</td>
<td>-0.38</td>
<td>0.00</td>
</tr>
<tr>
<td>$^6$F+$C_2H_4$</td>
<td>-2503.86280</td>
<td>1.03</td>
<td>-0.36</td>
<td>-2.83</td>
<td>-0.30</td>
<td>-0.37</td>
<td>0.00</td>
</tr>
<tr>
<td>$^6$NO$_3$+$C_2H_4$</td>
<td>-2684.01733</td>
<td>1.27</td>
<td>-0.31</td>
<td>-2.92</td>
<td>-0.26</td>
<td>-0.43</td>
<td>0.00</td>
</tr>
<tr>
<td>$^6$Ac-TS1</td>
<td>-2632.25771</td>
<td>1.36</td>
<td>-0.49</td>
<td>-2.93</td>
<td>-0.43</td>
<td>-0.60</td>
<td>0.12</td>
</tr>
<tr>
<td>$^6$Cl-TS1</td>
<td>-2864.14727</td>
<td>1.14</td>
<td>-0.42</td>
<td>-2.88</td>
<td>-0.44</td>
<td>-0.47</td>
<td>0.13</td>
</tr>
<tr>
<td>$^6$F-TS1</td>
<td>-2503.84426</td>
<td>1.16</td>
<td>-0.47</td>
<td>-2.87</td>
<td>-0.42</td>
<td>-0.40</td>
<td>0.11</td>
</tr>
<tr>
<td>$^6$NO$_3$-TS1</td>
<td>-2684.00395</td>
<td>1.36</td>
<td>-0.40</td>
<td>-2.95</td>
<td>-0.36</td>
<td>-0.43</td>
<td>0.10</td>
</tr>
<tr>
<td>$^6$Ac-Imt1</td>
<td>-2632.28790</td>
<td>1.54</td>
<td>-0.68</td>
<td>-3.06</td>
<td>-0.58</td>
<td>-0.61</td>
<td>0.23</td>
</tr>
<tr>
<td>$^6$Cl-Imt1</td>
<td>-2864.17683</td>
<td>1.12</td>
<td>-0.27</td>
<td>-2.79</td>
<td>-0.60</td>
<td>-0.48</td>
<td>0.20</td>
</tr>
<tr>
<td>$^6$F-Imt1</td>
<td>-2503.84743</td>
<td>1.39</td>
<td>-1.01</td>
<td>-3.17</td>
<td>-0.47</td>
<td>-0.30</td>
<td>0.27</td>
</tr>
<tr>
<td>$^6$NO$_3$-Imt1</td>
<td>-2684.03394</td>
<td>1.34</td>
<td>-0.25</td>
<td>-2.87</td>
<td>-0.60</td>
<td>-0.41</td>
<td>0.21</td>
</tr>
<tr>
<td>$^6$Ac-TS2</td>
<td>-2632.28711</td>
<td>1.54</td>
<td>-0.72</td>
<td>-3.08</td>
<td>-0.58</td>
<td>-0.61</td>
<td>0.25</td>
</tr>
<tr>
<td>$^6$Cl-TS2</td>
<td>-2864.15196</td>
<td>1.29</td>
<td>-0.45</td>
<td>-2.94</td>
<td>-0.63</td>
<td>-0.48</td>
<td>0.25</td>
</tr>
<tr>
<td>$^6$F-TS2</td>
<td>-2503.87837</td>
<td>1.41</td>
<td>-1.04</td>
<td>-3.17</td>
<td>-0.41</td>
<td>-0.38</td>
<td>0.30</td>
</tr>
<tr>
<td>$^6$NO$_3$-TS2</td>
<td>-2684.00792</td>
<td>1.54</td>
<td>-0.50</td>
<td>-3.05</td>
<td>-0.61</td>
<td>-0.42</td>
<td>0.26</td>
</tr>
<tr>
<td>$^6$Ac-P</td>
<td>-2632.35829</td>
<td>1.61</td>
<td>-1.14</td>
<td>-3.24</td>
<td>-0.51</td>
<td>-0.63</td>
<td>0.29</td>
</tr>
<tr>
<td>$^6$Cl-P</td>
<td>-2864.24198</td>
<td>1.30</td>
<td>-1.04</td>
<td>-3.21</td>
<td>-0.51</td>
<td>-0.34</td>
<td>0.29</td>
</tr>
<tr>
<td>$^6$F-P</td>
<td>-2503.94950</td>
<td>1.46</td>
<td>-1.15</td>
<td>-3.21</td>
<td>-0.51</td>
<td>-0.38</td>
<td>0.29</td>
</tr>
<tr>
<td>$^6$NO$_3$-P</td>
<td>-2684.09614</td>
<td>1.67</td>
<td>-1.07</td>
<td>-3.28</td>
<td>-0.52</td>
<td>-0.45</td>
<td>0.30</td>
</tr>
</tbody>
</table>

*a Terminal CH$_2$ group in ethylene

Figure S5. Cartesian coordinates of representative stationary structures and an estimated structure of the minimum energy point as follows.

Reactant (4R) for Comp-F

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.00000000</td>
<td>0.00000000</td>
<td>0.08294900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>0.00000000</td>
<td>0.00000000</td>
<td>1.72517300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1.42315900</td>
<td>-1.42318600</td>
<td>0.01366900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-1.42318600</td>
<td>-1.42315900</td>
<td>0.01366900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-1.42315900</td>
<td>1.42318600</td>
<td>0.01366900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1.42318600</td>
<td>1.42315900</td>
<td>0.01366900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.23531100</td>
<td>-2.78456500</td>
<td>0.00455700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.00000000</td>
<td>-3.41677100</td>
<td>0.00205500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.23531400</td>
<td>-2.78456800</td>
<td>0.00468600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.50578900</td>
<td>-3.46949300</td>
<td>-0.00800000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.46951900</td>
<td>-2.50580800</td>
<td>-0.00787000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.78456600</td>
<td>-1.23531100</td>
<td>0.00455700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.41677100</td>
<td>0.00000000</td>
<td>0.00205500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.78456800</td>
<td>1.23531400</td>
<td>0.00468600</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Element</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.469493</td>
<td>2.505789</td>
<td>-0.008000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.505808</td>
<td>3.469519</td>
<td>-0.007800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.235311</td>
<td>2.784656</td>
<td>0.004557</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.000000</td>
<td>3.416771</td>
<td>0.002055</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.235314</td>
<td>2.784568</td>
<td>-0.008000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.505789</td>
<td>3.469493</td>
<td>-0.007870</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.469519</td>
<td>2.505808</td>
<td>-0.007870</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.784656</td>
<td>1.235311</td>
<td>0.004557</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.416771</td>
<td>0.000000</td>
<td>0.002055</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.784568</td>
<td>-1.235314</td>
<td>0.004686</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.469493</td>
<td>-2.505789</td>
<td>-0.008000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.628465</td>
<td>-4.542232</td>
<td>-0.018729</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.542232</td>
<td>-2.628465</td>
<td>-0.018729</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.542252</td>
<td>2.628538</td>
<td>0.000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.628538</td>
<td>4.542252</td>
<td>0.000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.628465</td>
<td>-4.542232</td>
<td>0.000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.542232</td>
<td>-2.628465</td>
<td>0.000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>0.000000</td>
<td>0.000000</td>
<td>-1.784139</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.501750</td>
<td>0.000000</td>
<td>-0.006165</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.000060</td>
<td>-4.501750</td>
<td>-0.006165</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.501750</td>
<td>0.000000</td>
<td>-0.006165</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Reactant (4R) for Comp-Ac**

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>-0.117187</td>
<td>0.000047</td>
<td>-0.406984</td>
</tr>
<tr>
<td>O</td>
<td>-0.218849</td>
<td>0.000355</td>
<td>-2.040596</td>
</tr>
<tr>
<td>N</td>
<td>1.300847</td>
<td>1.413958</td>
<td>-0.427506</td>
</tr>
<tr>
<td>N</td>
<td>-1.535362</td>
<td>1.419062</td>
<td>-0.248439</td>
</tr>
<tr>
<td>N</td>
<td>-1.533953</td>
<td>-1.420352</td>
<td>-0.248748</td>
</tr>
<tr>
<td>N</td>
<td>1.302182</td>
<td>-1.412481</td>
<td>-0.428320</td>
</tr>
<tr>
<td>C</td>
<td>1.121762</td>
<td>2.773733</td>
<td>-0.301917</td>
</tr>
<tr>
<td>C</td>
<td>-0.103422</td>
<td>3.403668</td>
<td>-0.150707</td>
</tr>
<tr>
<td>C</td>
<td>-1.342741</td>
<td>2.775237</td>
<td>-0.148218</td>
</tr>
<tr>
<td>C</td>
<td>-2.610515</td>
<td>3.460578</td>
<td>-0.086650</td>
</tr>
<tr>
<td>C</td>
<td>-3.577804</td>
<td>2.502105</td>
<td>-0.163173</td>
</tr>
<tr>
<td>C</td>
<td>-2.897955</td>
<td>1.233076</td>
<td>-0.253610</td>
</tr>
<tr>
<td>C</td>
<td>-3.530834</td>
<td>-0.001635</td>
<td>-0.280086</td>
</tr>
<tr>
<td>C</td>
<td>-2.896704</td>
<td>-1.235712</td>
<td>-0.252786</td>
</tr>
<tr>
<td>C</td>
<td>-3.575261</td>
<td>-2.505365</td>
<td>-0.161536</td>
</tr>
<tr>
<td>C</td>
<td>-2.606994</td>
<td>-3.462875</td>
<td>-0.085406</td>
</tr>
<tr>
<td>C</td>
<td>-1.339930</td>
<td>-2.776320</td>
<td>-0.148041</td>
</tr>
<tr>
<td>C</td>
<td>-0.100038</td>
<td>-3.403562</td>
<td>-0.151392</td>
</tr>
<tr>
<td>C</td>
<td>1.124467</td>
<td>-2.772416</td>
<td>-0.303348</td>
</tr>
<tr>
<td>C</td>
<td>2.389591</td>
<td>-3.456453</td>
<td>-0.425768</td>
</tr>
<tr>
<td>C</td>
<td>3.332190</td>
<td>-2.499129</td>
<td>-0.651264</td>
</tr>
<tr>
<td>C</td>
<td>2.647108</td>
<td>-1.229374</td>
<td>-0.642100</td>
</tr>
<tr>
<td>C</td>
<td>3.269223</td>
<td>0.001777</td>
<td>-0.776223</td>
</tr>
</tbody>
</table>
C                  2.64597200    1.23228800   -0.64094400
C                  3.32987900    2.50266600   -0.64906500
C                  2.38627100    3.45900400   -0.42353800
H                 -2.73038900    4.53044200   -0.00302200
H                 -4.64748400   -2.63218100   -0.14681300
H                 -2.72569600   -4.53284200   -0.00139000
H                  4.39491900   -2.62365800   -0.79511600
H                  2.51643400    4.52855600   -0.35325300
H                  2.52078500   -4.52591800   -0.35607300
H                  4.39254800    2.62830500   -0.79237600
H                 -4.65016400    2.62786200   -0.14923700
O                 -0.13000400   -0.00069400    1.55857500
O                  2.07211700    0.00038000    2.17968800
C                  0.35956700   -0.00100700    3.87740000
H                 -0.26300300   -0.88311300    4.05748500
H                 -0.26475100    0.87977000    4.05785400
H                  1.20660300   -0.00035500    4.56451400
C                  0.84951300   -0.00028400    2.44369900
H                  4.34002100    0.00232300   -0.95018200
H                 -0.09234900   -4.48527000   -0.06621200
H                 -4.61598700   -0.00216900   -0.28231400
H                 -0.09680600    4.48539000   -0.06556700

Reactant (dR) for Comp-Cl

Fe     0.00000000    0.00000000    0.21114500
O      0.00000000    0.00000000    1.84088800
N      0.72283200   -1.87196800    0.12359800
N     -1.87196800   -0.72283200    0.12359800
N     -0.72283200    1.87196800    0.12359800
N      1.87196800    0.72283200    0.12359800
C     -0.00000000   -3.04320200    0.11303500
C     -1.38358700   -3.12375200    0.11000100
C     -2.25381300   -2.04520400    0.11210800
C     -3.69148900   -2.15538900    0.09395200
C     -4.18214700   -0.88431800    0.09468000
C     -3.04320200    0.00000000    0.11303500
C     -3.12375200    1.38358700    0.11000100
C     -2.04520400   -2.25381300    0.11210800
C     -2.15538900    3.69148900    0.09395200
C     -0.88431800   -4.18214700    0.09468000
C     -0.00000000    3.04320200    0.11303500
C      1.38358700    3.12375200    0.11000100
C      2.25381300    2.04520400    0.11210800
C      3.69148900    2.15538900    0.09395200
C      4.18214700    0.88431800    0.09468000
C      3.04320200    0.00000000    0.11303500
C      3.12375200   -1.38358700    0.11000100
C      2.04520400   -2.25381300    0.11210800
C      2.15538900   -3.69148900    0.09395200
C      0.88431800   -4.18214700    0.09468000
H  -4.23677300  -3.08705900  0.07887300
H  -3.08705900  4.23677300  0.07887300
H  -0.56066600  5.21207000  0.08015800
H   5.21207000  -0.56066600  0.08015800
H   4.23677300  3.08705900  0.07887300
H   3.08705900 -4.23677300  0.07887300
H  -5.21207000  -0.56066600  0.08015800
H   4.11568500 -1.82289600  0.09940300
H   1.82289600  4.11568500  0.09940300
H  -1.82289600 -4.11568500  0.09940300
H  -4.11568500  1.82289600  0.09940300
Cl  0.00000000  0.00000000 -2.19305700

Reactant (4R) for Comp-NO₃

Fe  -0.11588800  0.00382400 -0.40244600
O  -0.21486100  0.00950100 -2.02586800
N   1.29139200  1.42756800 -0.40614100
N  -1.54052800  1.41077000 -0.22759500
N  -1.52525800 -1.42352500 -0.23954600
N   1.30702500 -1.40406400 -0.23954600
C   1.10600100  2.78615100 -0.28635300
C  -0.12314300  3.41046400 -0.13509200
C  -1.35660200  2.77299400 -0.12789000
C  -2.62730100  3.44974900 -0.05715000
C  -3.58895700  2.48533100 -0.12691700
C  -2.90215100  1.22158000 -0.22317400
C  -3.53016700 -0.01555100 -0.25028200
C  -2.88892500 -1.24595100 -0.23374800
C  -3.56183900 -2.51789300 -0.14684400
C  -2.58964700 -3.47210200 -0.08354500
C  -1.32645300 -2.78080300 -0.14884600
C  -0.08588100 -3.40443900 -0.15774800
C   1.13646900 -2.76560100 -0.30272000
C   2.40448500 -3.44171600 -0.42024400
C   3.34508500 -2.47690200 -0.62686000
C   2.65319400 -1.21255500 -0.61338500
C   3.27102300  0.02364400 -0.73176600
C   2.63958200  1.25206400 -0.60764800
C   3.31736600  2.52422700 -0.61431700
C   2.36633200  3.47717100 -0.40114900
H  -2.75288500  4.51842900  0.03083100
H  -4.63329800  2.64832500 -0.12341000
H  -2.70339000 -4.54269600 -0.00294700
H   4.40979300 -2.59476700 -0.76071300
H   2.49064000  4.54737600 -0.33247200
H   2.54072000 -4.51085500 -0.35777100
H   4.38055900  2.65475400 -0.74841100
H  -4.66179800  2.60372500 -0.10267600
O  -0.20365400 -0.00872700  1.61463300
Transition state (\(^4\)TS1) for Comp-F

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.14970100</td>
<td>0.00088500</td>
<td>-0.21691700</td>
</tr>
<tr>
<td>O</td>
<td>0.15277900</td>
<td>-0.03282400</td>
<td>1.55310500</td>
</tr>
<tr>
<td>N</td>
<td>-0.44106300</td>
<td>-1.91615200</td>
<td>-0.30316300</td>
</tr>
<tr>
<td>N</td>
<td>-1.75961900</td>
<td>0.58195100</td>
<td>-0.33022900</td>
</tr>
<tr>
<td>N</td>
<td>0.73276300</td>
<td>1.91703200</td>
<td>-0.20859900</td>
</tr>
<tr>
<td>N</td>
<td>2.02343500</td>
<td>-0.57056300</td>
<td>-0.01644700</td>
</tr>
<tr>
<td>C</td>
<td>-1.72408100</td>
<td>-2.38601400</td>
<td>-0.50700100</td>
</tr>
<tr>
<td>C</td>
<td>-2.85731800</td>
<td>-1.60529400</td>
<td>-0.61097400</td>
</tr>
<tr>
<td>C</td>
<td>-2.86603900</td>
<td>-0.22555100</td>
<td>-0.51173400</td>
</tr>
<tr>
<td>C</td>
<td>-4.05558000</td>
<td>0.58066900</td>
<td>-0.58553600</td>
</tr>
<tr>
<td>C</td>
<td>-3.66399500</td>
<td>1.88240100</td>
<td>-0.45961000</td>
</tr>
<tr>
<td>C</td>
<td>-2.23204800</td>
<td>1.87884800</td>
<td>-0.31980900</td>
</tr>
<tr>
<td>C</td>
<td>-1.45949900</td>
<td>3.03338400</td>
<td>-0.21699600</td>
</tr>
<tr>
<td>C</td>
<td>0.72230100</td>
<td>4.23068100</td>
<td>-0.19619500</td>
</tr>
<tr>
<td>C</td>
<td>2.02447600</td>
<td>3.83452300</td>
<td>-0.17228200</td>
</tr>
<tr>
<td>C</td>
<td>2.02516400</td>
<td>2.39180800</td>
<td>-0.16565200</td>
</tr>
<tr>
<td>C</td>
<td>3.16134900</td>
<td>1.61366100</td>
<td>-0.06296300</td>
</tr>
<tr>
<td>C</td>
<td>3.14885100</td>
<td>0.23806200</td>
<td>0.03386100</td>
</tr>
<tr>
<td>C</td>
<td>4.32468700</td>
<td>-0.57079600</td>
<td>0.20701100</td>
</tr>
<tr>
<td>C</td>
<td>3.91617300</td>
<td>-1.87064600</td>
<td>0.26483300</td>
</tr>
<tr>
<td>C</td>
<td>2.48691200</td>
<td>-1.87451300</td>
<td>0.11419300</td>
</tr>
<tr>
<td>C</td>
<td>1.72132000</td>
<td>-3.01858200</td>
<td>0.04632500</td>
</tr>
<tr>
<td>C</td>
<td>0.35676100</td>
<td>-3.03101800</td>
<td>-0.17474700</td>
</tr>
<tr>
<td>C</td>
<td>-0.43675600</td>
<td>-4.22697700</td>
<td>-0.31254500</td>
</tr>
<tr>
<td>C</td>
<td>-1.72197900</td>
<td>-3.82835200</td>
<td>-0.52575200</td>
</tr>
<tr>
<td>H</td>
<td>-5.05205300</td>
<td>0.18931700</td>
<td>-0.72793100</td>
</tr>
<tr>
<td>H</td>
<td>0.32394400</td>
<td>5.23443400</td>
<td>-0.20195100</td>
</tr>
<tr>
<td>H</td>
<td>2.91430800</td>
<td>4.44595400</td>
<td>-0.14995500</td>
</tr>
<tr>
<td>H</td>
<td>4.51883900</td>
<td>-2.75889900</td>
<td>0.38289700</td>
</tr>
<tr>
<td>H</td>
<td>-2.59985800</td>
<td>-4.43927800</td>
<td>-0.67552900</td>
</tr>
<tr>
<td>H</td>
<td>5.32905700</td>
<td>-0.17939300</td>
<td>0.27146600</td>
</tr>
<tr>
<td>H</td>
<td>-0.04442600</td>
<td>-5.23145500</td>
<td>-0.25530200</td>
</tr>
<tr>
<td>H</td>
<td>-4.27437300</td>
<td>2.77309100</td>
<td>-0.48129500</td>
</tr>
<tr>
<td>F</td>
<td>0.21556400</td>
<td>0.00853300</td>
<td>-2.00835800</td>
</tr>
<tr>
<td>H</td>
<td>2.22826700</td>
<td>-3.97148900</td>
<td>0.14418100</td>
</tr>
<tr>
<td>H</td>
<td>4.12106600</td>
<td>2.11552400</td>
<td>-0.02465400</td>
</tr>
<tr>
<td>H</td>
<td>-3.80652400</td>
<td>-2.10634100</td>
<td>-0.76225900</td>
</tr>
<tr>
<td>H</td>
<td>-1.97329800</td>
<td>3.97861700</td>
<td>-0.25160700</td>
</tr>
<tr>
<td>C</td>
<td>-1.52430800</td>
<td>-0.62179200</td>
<td>2.81291000</td>
</tr>
<tr>
<td>H</td>
<td>-0.78201300</td>
<td>-0.98146400</td>
<td>3.51578300</td>
</tr>
</tbody>
</table>
Transition state ("TS1") for Comp-Ac

Fe  -0.02526400  0.11839700  -0.11955400
O   0.19358400  0.14313300  -1.86491100
N  -0.31452200 -1.85841100  -0.12755000
N   1.93239000 -0.18608400  0.22512900
N   0.27839200  2.09401400  -0.03510200
N  -1.90759900  0.42201100  -0.51580000
C   0.59661000 -2.83927400   0.22048800
C   1.92225200 -2.62625700   0.54093000
C   2.54482300 -1.38890700   0.51061400
C   3.95109600 -1.18241200   0.73706000
C   4.18603000  0.15498000   0.58596200
C   2.91794600  0.77219300   0.29031500
C   2.72793000  2.13929300   0.17949000
C   1.49507100  2.74558100   0.06011900
C   1.28686900  4.17312200   0.07299100
C  -0.05703800  4.38106800  -0.00039200
C  -0.67878700  3.08204800  -0.08531300
C  -2.03108200  2.86990300  -0.27844300
C  -2.58690500  1.63102700  -0.52067400
C  -3.96348100  1.41601000  -0.87772400
C  -4.11810700  0.08154700  -1.10910000
C  -2.84829500  0.54428400  -0.86484500
C  -2.64115800 -1.90390800  -0.88914600
C  -1.46362000 -2.51554400  -0.49615600
C  -1.28111700 -3.93969400  -0.37220900
C  -0.01354300 -4.13959700   0.08751500
H   4.65442000 -1.96497900   0.98114200
H   2.07820500  4.90516800   0.13941300
H  -0.59356600  5.31816700  -0.01441300
H  -5.01331800 -0.44963300  -1.39597300
H   0.48295300 -5.07350200   0.30621800
H  -4.70416700  2.19895800  -0.94541100
H  -2.03817100 -4.67581800  -0.59800400
H   5.11940100  0.68862400   0.68846800
O  -0.22442300  0.12965200   1.74322000
O  -2.21166700  0.93021100   2.16800300
C  -0.83720900 -0.17960300   4.00657300
H  -0.70094300  0.88437900   4.22162500
H   0.10531700 -0.68306200   4.24303100
H  -1.63803100 -0.58383300   4.62629900
C  -1.16776700 -0.37218600   2.54712000
H  -3.47503800 -2.53782700  -1.16714200
H  -2.68519600  3.73353400  -0.30475800
H   3.60022100  2.77838800   0.24980200
Transition state (\textsuperscript{4}TS1) for Comp-Cl
Transition state (TS1) for Comp-NO₃
Intermediate (\textsuperscript{4}Imt) for Comp-F

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.06624300</td>
<td>0.00008700</td>
<td>-0.21170700</td>
</tr>
<tr>
<td>O</td>
<td>0.02595700</td>
<td>0.00121100</td>
<td>1.55509800</td>
</tr>
<tr>
<td>N</td>
<td>-1.34374900</td>
<td>-1.40932500</td>
<td>-0.28822200</td>
</tr>
<tr>
<td>N</td>
<td>-1.34131800</td>
<td>1.41214200</td>
<td>-0.28820000</td>
</tr>
<tr>
<td>N</td>
<td>1.48568500</td>
<td>1.41182100</td>
<td>-0.18139400</td>
</tr>
<tr>
<td>N</td>
<td>1.48310000</td>
<td>-1.41436800</td>
<td>-0.18159500</td>
</tr>
<tr>
<td>C</td>
<td>-2.70357800</td>
<td>-1.21878500</td>
<td>-0.54401300</td>
</tr>
<tr>
<td>C</td>
<td>-3.34156300</td>
<td>0.00323000</td>
<td>0.00010200</td>
</tr>
<tr>
<td>C</td>
<td>-2.70146500</td>
<td>3.45216700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-3.37145700</td>
<td>2.49835500</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-2.41469200</td>
<td>3.45694000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-1.14877300</td>
<td>2.77855000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>0.07015800</td>
<td>3.41953000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>1.29210700</td>
<td>2.77643200</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>2.56524100</td>
<td>3.45216700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>3.52799800</td>
<td>2.49061000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>2.85136300</td>
<td>1.21856700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>3.49464600</td>
<td>0.00312700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>2.84913000</td>
<td>-1.22363400</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>3.52342500</td>
<td>-2.49696000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>2.55901600</td>
<td>-3.45673500</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>1.28713900</td>
<td>-2.77863700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>0.06400800</td>
<td>-3.41944200</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-1.15372700</td>
<td>-2.77645500</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-2.42088000</td>
<td>-3.45214400</td>
<td>0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>-3.37590500</td>
<td>-2.49172700</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>-4.43713200</td>
<td>2.62598000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>2.68738500</td>
<td>4.52371600</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>4.60104300</td>
<td>2.61231500</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>2.67922100</td>
<td>-4.52854100</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>-4.44182700</td>
<td>-2.61733600</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>4.39623100</td>
<td>-2.62067500</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>2.54532200</td>
<td>-4.52447300</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>2.53713500</td>
<td>4.52949000</td>
<td>0.00134200</td>
</tr>
<tr>
<td>F</td>
<td>0.12831200</td>
<td>0.00010200</td>
<td>0.00134200</td>
</tr>
<tr>
<td>H</td>
<td>0.06021600</td>
<td>-4.50197100</td>
<td>-0.04977700</td>
</tr>
<tr>
<td>H</td>
<td>4.57835000</td>
<td>-0.04122000</td>
<td>-0.24617400</td>
</tr>
<tr>
<td>H</td>
<td>-4.41754600</td>
<td>0.00414900</td>
<td>-0.67401000</td>
</tr>
<tr>
<td>H</td>
<td>0.06834900</td>
<td>4.50208600</td>
<td>-0.04920300</td>
</tr>
<tr>
<td>C</td>
<td>-1.14200700</td>
<td>-0.00375400</td>
<td>2.43725200</td>
</tr>
<tr>
<td>H</td>
<td>-1.73794000</td>
<td>-0.89845900</td>
<td>2.22539200</td>
</tr>
<tr>
<td>H</td>
<td>-1.74724500</td>
<td>0.88412800</td>
<td>2.22244500</td>
</tr>
<tr>
<td>C</td>
<td>-0.61652300</td>
<td>0.00134200</td>
<td>3.82126000</td>
</tr>
<tr>
<td>H</td>
<td>-0.31891700</td>
<td>0.93366700</td>
<td>4.28916000</td>
</tr>
</tbody>
</table>
### Intermediate (I)nt for Comp-Ac

<table>
<thead>
<tr>
<th>Atom</th>
<th>x-Coord</th>
<th>y-Coord</th>
<th>z-Coord</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.08832500</td>
<td>0.05931700</td>
<td>-0.10737600</td>
</tr>
<tr>
<td>O</td>
<td>0.28864200</td>
<td>-0.00960700</td>
<td>-1.86429700</td>
</tr>
<tr>
<td>N</td>
<td>-1.10904100</td>
<td>-1.51841900</td>
<td>-0.13896600</td>
</tr>
<tr>
<td>N</td>
<td>1.66282000</td>
<td>-1.14312900</td>
<td>0.15236000</td>
</tr>
<tr>
<td>N</td>
<td>1.30172600</td>
<td>1.65460700</td>
<td>-0.04284900</td>
</tr>
<tr>
<td>N</td>
<td>-1.47435700</td>
<td>1.26676800</td>
<td>-0.32816700</td>
</tr>
<tr>
<td>C</td>
<td>0.08832500</td>
<td>0.05931700</td>
<td>-0.10737600</td>
</tr>
<tr>
<td>C</td>
<td>0.50252100</td>
<td>-3.29325700</td>
<td>0.41783400</td>
</tr>
<tr>
<td>C</td>
<td>1.63726100</td>
<td>-2.50393700</td>
<td>0.39431500</td>
</tr>
<tr>
<td>C</td>
<td>2.98055900</td>
<td>-2.99649000</td>
<td>0.55373900</td>
</tr>
<tr>
<td>C</td>
<td>3.81870300</td>
<td>-1.93179500</td>
<td>0.39449200</td>
</tr>
<tr>
<td>C</td>
<td>2.99442200</td>
<td>-0.77425700</td>
<td>0.16139100</td>
</tr>
<tr>
<td>C</td>
<td>3.47754100</td>
<td>0.51545300</td>
<td>0.04233100</td>
</tr>
<tr>
<td>C</td>
<td>2.68140100</td>
<td>1.64265400</td>
<td>-0.02185100</td>
</tr>
<tr>
<td>C</td>
<td>3.18256900</td>
<td>2.99455500</td>
<td>-0.00134200</td>
</tr>
<tr>
<td>C</td>
<td>2.09913300</td>
<td>3.82129000</td>
<td>0.01178100</td>
</tr>
<tr>
<td>C</td>
<td>0.92755500</td>
<td>2.98157600</td>
<td>-0.02657000</td>
</tr>
<tr>
<td>C</td>
<td>-0.36969200</td>
<td>3.45219900</td>
<td>-0.10002200</td>
</tr>
<tr>
<td>C</td>
<td>-1.47787000</td>
<td>2.64597400</td>
<td>-0.27482800</td>
</tr>
<tr>
<td>C</td>
<td>-2.81071600</td>
<td>3.14035700</td>
<td>-0.51431800</td>
</tr>
<tr>
<td>C</td>
<td>-3.60440200</td>
<td>2.05618400</td>
<td>-0.74033600</td>
</tr>
<tr>
<td>C</td>
<td>-2.77103500</td>
<td>0.88824000</td>
<td>-0.61076400</td>
</tr>
<tr>
<td>C</td>
<td>-3.23053700</td>
<td>-0.40974100</td>
<td>-0.70102900</td>
</tr>
<tr>
<td>C</td>
<td>-2.45863000</td>
<td>-1.52309100</td>
<td>-0.43520600</td>
</tr>
<tr>
<td>C</td>
<td>-2.96985700</td>
<td>-2.86560300</td>
<td>-0.35459200</td>
</tr>
<tr>
<td>C</td>
<td>-1.93315600</td>
<td>-3.66927800</td>
<td>0.01865300</td>
</tr>
<tr>
<td>H</td>
<td>3.23442000</td>
<td>-4.02724000</td>
<td>0.75272500</td>
</tr>
<tr>
<td>H</td>
<td>4.22978600</td>
<td>3.25823900</td>
<td>0.01527500</td>
</tr>
<tr>
<td>H</td>
<td>2.07728700</td>
<td>4.90087400</td>
<td>0.03289400</td>
</tr>
<tr>
<td>H</td>
<td>-4.66163200</td>
<td>2.03072000</td>
<td>-0.95869100</td>
</tr>
<tr>
<td>H</td>
<td>-1.93764000</td>
<td>-4.73551800</td>
<td>0.19035800</td>
</tr>
<tr>
<td>H</td>
<td>-3.08214700</td>
<td>4.18562300</td>
<td>-0.51956800</td>
</tr>
<tr>
<td>H</td>
<td>-3.99780900</td>
<td>-3.13912400</td>
<td>-0.54055000</td>
</tr>
<tr>
<td>H</td>
<td>4.89742500</td>
<td>-1.91334200</td>
<td>0.44484500</td>
</tr>
<tr>
<td>O</td>
<td>-0.02095000</td>
<td>0.16789200</td>
<td>1.74901400</td>
</tr>
<tr>
<td>O</td>
<td>-2.22306700</td>
<td>-0.11041100</td>
<td>2.33107800</td>
</tr>
<tr>
<td>C</td>
<td>-0.56529300</td>
<td>0.27825300</td>
<td>4.04460400</td>
</tr>
<tr>
<td>H</td>
<td>-0.09866700</td>
<td>1.26195900</td>
<td>4.15467900</td>
</tr>
<tr>
<td>H</td>
<td>0.19251400</td>
<td>-0.47135700</td>
<td>4.29136700</td>
</tr>
<tr>
<td>H</td>
<td>-1.41042100</td>
<td>0.19139500</td>
<td>4.72819100</td>
</tr>
<tr>
<td>C</td>
<td>-1.03381600</td>
<td>0.08964500</td>
<td>2.62276500</td>
</tr>
<tr>
<td>H</td>
<td>-4.27980900</td>
<td>-0.56236200</td>
<td>-0.92502700</td>
</tr>
<tr>
<td>H</td>
<td>-0.52269500</td>
<td>4.52492900</td>
<td>-0.07689400</td>
</tr>
<tr>
<td>H</td>
<td>4.55227700</td>
<td>0.65538200</td>
<td>0.06106900</td>
</tr>
<tr>
<td>H</td>
<td>0.62377700</td>
<td>-4.35117300</td>
<td>0.61982200</td>
</tr>
<tr>
<td>C</td>
<td>0.59445700</td>
<td>-0.70731400</td>
<td>-4.09488600</td>
</tr>
<tr>
<td>H</td>
<td>-0.31308200</td>
<td>-0.53042600</td>
<td>-4.66219200</td>
</tr>
</tbody>
</table>
Intermediate (4Imt) for Comp-Cl

Fe  -0.06125400  0.00001300  -0.10086100
O   -0.01270000  0.00072600   1.67645500
N   -1.47862800  1.40941200   -0.06480500
N    1.34567400  1.40957600   -0.18319100
N    1.34771100 -1.40737000   -0.18305600
N   -1.47648400 -1.41159300   -0.06480500
C    1.53824000  2.77756600   -0.11231000
C    2.41832500  3.45509500   -0.22510400
C    3.37484600  2.49623800   -0.38401700
C    2.70614800  1.22256300   -0.35453800
C    3.34624300  0.00260100   -0.44943500
C    2.70795500 -1.21827400   -0.35427400
C    3.37860200 -2.49090100   -0.38351700
C    2.42354900 -3.45123800   -0.22462000
C    1.15798800 -2.77569000   -0.11211600
C   -0.05889800 -3.41906200   -0.00115300
C   -1.28090700 -2.77718600   0.00339400
C   -2.55187800 -3.45484900   0.03822000
C   -3.51681300 -2.49494200   -0.02126300
C   -2.84358900 -1.22209500   -0.07754300
C   -3.48987500 -0.00260500   -0.10445800
C   -2.84543400  1.21786800   -0.07715200
C   -3.52055700  2.48967800   -0.02045200
C   -2.55704100  3.45101500   0.03915300
H    2.54029100  4.52776200   -0.19815100
H    4.44390600 -2.61664100   -0.50824900
H    2.54718300 -4.52371200   -0.19757900
H   -4.58962000 -2.61847700   -0.02168200
H   -2.67814300  4.52274300   0.09314500
H   -2.67137000  4.52677600   0.09187600
H   -4.59354900  2.61160800   -0.02064600
H    4.43994000  2.62361500   -0.50886800
Cl  -0.14888800  0.00005900  -0.23948240
C    1.17024600 -0.02618000  2.54222400
H    1.77045500  0.88716300  2.32484100
H    1.76329300 -0.89785700  2.32773100
C    0.62754200  0.00181400  3.91788700
H    0.32046100 -0.92687300  4.38659800
H    0.32760300  0.93443500  4.38339900
H   -0.06230200  4.50175300  0.04645400
H   -4.57351000 -0.00342000 -0.11618100
H   -0.05549800 -4.50177700  0.04629000
Intermediate (4\textsuperscript{1}int) for Comp-NO$_3$

<table>
<thead>
<tr>
<th>Element</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>-0.08666400</td>
<td>0.05638500</td>
<td>0.11003000</td>
</tr>
<tr>
<td>O</td>
<td>-0.29881800</td>
<td>-0.02276100</td>
<td>1.85526200</td>
</tr>
<tr>
<td>N</td>
<td>0.93316700</td>
<td>-1.63587700</td>
<td>0.09775800</td>
</tr>
<tr>
<td>N</td>
<td>-1.77257900</td>
<td>-0.95867700</td>
<td>-0.19530200</td>
</tr>
<tr>
<td>N</td>
<td>-1.11648600</td>
<td>1.77013800</td>
<td>0.04731000</td>
</tr>
<tr>
<td>N</td>
<td>1.59465300</td>
<td>1.08458400</td>
<td>0.32349500</td>
</tr>
<tr>
<td>C</td>
<td>0.45872300</td>
<td>-2.90053700</td>
<td>-0.21008000</td>
</tr>
<tr>
<td>C</td>
<td>-0.85213900</td>
<td>-3.21746600</td>
<td>-0.50868400</td>
</tr>
<tr>
<td>C</td>
<td>-1.89342900</td>
<td>-2.31029800</td>
<td>-0.46953800</td>
</tr>
<tr>
<td>C</td>
<td>-3.28048500</td>
<td>-2.65219000</td>
<td>-0.63518900</td>
</tr>
<tr>
<td>C</td>
<td>-4.00130000</td>
<td>-1.50965600</td>
<td>-0.44341200</td>
</tr>
<tr>
<td>C</td>
<td>-3.06004100</td>
<td>-0.45215900</td>
<td>-0.18748000</td>
</tr>
<tr>
<td>C</td>
<td>-3.40409400</td>
<td>0.87751000</td>
<td>-0.03873600</td>
</tr>
<tr>
<td>C</td>
<td>-2.49025000</td>
<td>1.90973900</td>
<td>0.03549400</td>
</tr>
<tr>
<td>C</td>
<td>-2.84122000</td>
<td>3.30713700</td>
<td>0.02665500</td>
</tr>
<tr>
<td>C</td>
<td>-1.67472300</td>
<td>4.01134000</td>
<td>0.00787600</td>
</tr>
<tr>
<td>C</td>
<td>-0.60134300</td>
<td>3.05056800</td>
<td>0.03482900</td>
</tr>
<tr>
<td>C</td>
<td>0.73807700</td>
<td>3.37959900</td>
<td>0.10475300</td>
</tr>
<tr>
<td>C</td>
<td>1.75068700</td>
<td>2.45696300</td>
<td>0.27884700</td>
</tr>
<tr>
<td>C</td>
<td>3.12612500</td>
<td>2.80050100</td>
<td>0.53136500</td>
</tr>
<tr>
<td>C</td>
<td>3.79404000</td>
<td>1.63514700</td>
<td>0.76307600</td>
</tr>
<tr>
<td>C</td>
<td>2.84095700</td>
<td>0.56619500</td>
<td>0.62121900</td>
</tr>
<tr>
<td>C</td>
<td>3.15611700</td>
<td>-0.77449500</td>
<td>0.70377700</td>
</tr>
<tr>
<td>C</td>
<td>2.27109400</td>
<td>-1.79359200</td>
<td>0.41430500</td>
</tr>
<tr>
<td>C</td>
<td>2.63393000</td>
<td>-3.18106200</td>
<td>0.31575400</td>
</tr>
<tr>
<td>C</td>
<td>1.52233200</td>
<td>-3.86072700</td>
<td>-0.08921200</td>
</tr>
<tr>
<td>H</td>
<td>-3.64242200</td>
<td>-3.64407900</td>
<td>-0.86156700</td>
</tr>
<tr>
<td>H</td>
<td>-3.85354100</td>
<td>3.68287900</td>
<td>0.01601200</td>
</tr>
<tr>
<td>H</td>
<td>-1.53578100</td>
<td>5.08196900</td>
<td>-0.01286300</td>
</tr>
<tr>
<td>H</td>
<td>4.83929200</td>
<td>1.49450000</td>
<td>0.99156100</td>
</tr>
<tr>
<td>H</td>
<td>1.41555100</td>
<td>-4.91765700</td>
<td>-0.28314500</td>
</tr>
<tr>
<td>H</td>
<td>3.51135300</td>
<td>3.80921700</td>
<td>0.54018300</td>
</tr>
<tr>
<td>H</td>
<td>3.62255600</td>
<td>-3.56862200</td>
<td>0.51185100</td>
</tr>
<tr>
<td>H</td>
<td>-5.07179500</td>
<td>-1.37639400</td>
<td>-0.48879100</td>
</tr>
<tr>
<td>O</td>
<td>-0.03362400</td>
<td>0.21016100</td>
<td>-1.82141000</td>
</tr>
<tr>
<td>N</td>
<td>1.02201200</td>
<td>0.11446600</td>
<td>-2.66626100</td>
</tr>
<tr>
<td>O</td>
<td>2.13459300</td>
<td>-2.63993000</td>
<td>-2.23919600</td>
</tr>
<tr>
<td>O</td>
<td>0.78233000</td>
<td>0.41726300</td>
<td>-3.85476700</td>
</tr>
<tr>
<td>H</td>
<td>-1.08591100</td>
<td>-4.25062300</td>
<td>-0.73683400</td>
</tr>
<tr>
<td>H</td>
<td>4.17918700</td>
<td>-1.04276300</td>
<td>0.93953600</td>
</tr>
<tr>
<td>H</td>
<td>1.00579400</td>
<td>4.42934600</td>
<td>0.08306900</td>
</tr>
<tr>
<td>H</td>
<td>-4.45738900</td>
<td>1.13222900</td>
<td>-0.05068700</td>
</tr>
<tr>
<td>C</td>
<td>-0.70964400</td>
<td>-0.69364300</td>
<td>4.05211000</td>
</tr>
<tr>
<td>H</td>
<td>0.19858200</td>
<td>-0.61877000</td>
<td>4.64002800</td>
</tr>
<tr>
<td>H</td>
<td>-1.60358500</td>
<td>-0.20491500</td>
<td>4.42389500</td>
</tr>
<tr>
<td>C</td>
<td>-0.65880200</td>
<td>-1.19533200</td>
<td>2.66295800</td>
</tr>
<tr>
<td>H</td>
<td>-1.62476100</td>
<td>-1.57556600</td>
<td>2.31521300</td>
</tr>
</tbody>
</table>
Transition state (\textsuperscript{4}TS2) for Comp-F

<table>
<thead>
<tr>
<th>Element</th>
<th>X (Å)</th>
<th>Y (Å)</th>
<th>Z (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>-0.05855400</td>
<td>0.00000300</td>
<td>-0.25473000</td>
</tr>
<tr>
<td>O</td>
<td>-0.03147900</td>
<td>0.00000500</td>
<td>1.63313200</td>
</tr>
<tr>
<td>N</td>
<td>1.35828700</td>
<td>1.41332500</td>
<td>-0.26988600</td>
</tr>
<tr>
<td>N</td>
<td>1.35888000</td>
<td>-1.41272500</td>
<td>-0.26983600</td>
</tr>
<tr>
<td>N</td>
<td>-1.47790400</td>
<td>-1.41550600</td>
<td>-0.18636800</td>
</tr>
<tr>
<td>N</td>
<td>-1.47849000</td>
<td>1.41492200</td>
<td>-0.18632600</td>
</tr>
<tr>
<td>C</td>
<td>2.72265900</td>
<td>1.22381000</td>
<td>-0.39255500</td>
</tr>
<tr>
<td>C</td>
<td>3.36373200</td>
<td>0.00071700</td>
<td>-0.45821300</td>
</tr>
<tr>
<td>C</td>
<td>2.72317700</td>
<td>-1.22264400</td>
<td>-0.39247900</td>
</tr>
<tr>
<td>C</td>
<td>3.39430000</td>
<td>-2.49680400</td>
<td>-0.41241300</td>
</tr>
<tr>
<td>C</td>
<td>2.43277000</td>
<td>-3.45759600</td>
<td>-0.30019000</td>
</tr>
<tr>
<td>C</td>
<td>1.16410800</td>
<td>-2.78026100</td>
<td>-0.22026100</td>
</tr>
<tr>
<td>C</td>
<td>-0.05766500</td>
<td>-3.42147800</td>
<td>-0.13924800</td>
</tr>
<tr>
<td>C</td>
<td>-1.28192500</td>
<td>2.78046500</td>
<td>-0.13591000</td>
</tr>
<tr>
<td>C</td>
<td>-2.55423900</td>
<td>3.45859400</td>
<td>-0.10524000</td>
</tr>
<tr>
<td>C</td>
<td>-3.51896900</td>
<td>2.49700000</td>
<td>-0.14641200</td>
</tr>
<tr>
<td>C</td>
<td>-2.84390400</td>
<td>-1.22340500</td>
<td>-0.19161700</td>
</tr>
<tr>
<td>C</td>
<td>-3.48761700</td>
<td>0.00070700</td>
<td>-0.20817100</td>
</tr>
<tr>
<td>C</td>
<td>-2.84412000</td>
<td>1.22225600</td>
<td>-0.19151200</td>
</tr>
<tr>
<td>C</td>
<td>-3.52000100</td>
<td>2.49556900</td>
<td>-0.14617400</td>
</tr>
<tr>
<td>C</td>
<td>-2.55566800</td>
<td>3.45756100</td>
<td>-0.10500000</td>
</tr>
<tr>
<td>C</td>
<td>-1.28307800</td>
<td>2.77995900</td>
<td>-0.13547500</td>
</tr>
<tr>
<td>C</td>
<td>-0.05908500</td>
<td>3.42148500</td>
<td>-0.13920200</td>
</tr>
<tr>
<td>C</td>
<td>1.16294900</td>
<td>2.78078100</td>
<td>-0.22032300</td>
</tr>
<tr>
<td>C</td>
<td>2.43132700</td>
<td>3.45864300</td>
<td>-0.30031800</td>
</tr>
<tr>
<td>C</td>
<td>3.39325300</td>
<td>2.49824900</td>
<td>-0.41255700</td>
</tr>
<tr>
<td>H</td>
<td>4.46303000</td>
<td>-2.62391700</td>
<td>-0.50281600</td>
</tr>
<tr>
<td>H</td>
<td>-2.67549800</td>
<td>-4.53106700</td>
<td>-0.06537000</td>
</tr>
<tr>
<td>H</td>
<td>-4.59185800</td>
<td>2.62088900</td>
<td>-0.14396900</td>
</tr>
<tr>
<td>H</td>
<td>-2.67736200</td>
<td>4.52998500</td>
<td>-0.06542400</td>
</tr>
<tr>
<td>H</td>
<td>4.46193000</td>
<td>2.62579900</td>
<td>-0.50300400</td>
</tr>
<tr>
<td>H</td>
<td>-4.59293900</td>
<td>2.61901800</td>
<td>-0.14365300</td>
</tr>
<tr>
<td>H</td>
<td>2.55313800</td>
<td>4.53166300</td>
<td>-0.28341400</td>
</tr>
<tr>
<td>H</td>
<td>2.55502500</td>
<td>-4.53056600</td>
<td>-0.28326300</td>
</tr>
<tr>
<td>F</td>
<td>-0.11450400</td>
<td>0.00000500</td>
<td>-2.07454100</td>
</tr>
<tr>
<td>H</td>
<td>-0.05768100</td>
<td>4.50501000</td>
<td>-0.10510100</td>
</tr>
<tr>
<td>H</td>
<td>-4.57158800</td>
<td>0.00003500</td>
<td>-0.21327300</td>
</tr>
<tr>
<td>H</td>
<td>4.44328100</td>
<td>0.00004400</td>
<td>-0.55613900</td>
</tr>
<tr>
<td>H</td>
<td>-0.05501000</td>
<td>4.50500600</td>
<td>-0.10519500</td>
</tr>
<tr>
<td>C</td>
<td>1.15448300</td>
<td>-0.00003500</td>
<td>2.48283500</td>
</tr>
<tr>
<td>H</td>
<td>1.75749900</td>
<td>0.89767600</td>
<td>2.32669000</td>
</tr>
<tr>
<td>H</td>
<td>1.75741700</td>
<td>-0.89780500</td>
<td>2.32663400</td>
</tr>
<tr>
<td>C</td>
<td>0.36003200</td>
<td>0.00001100</td>
<td>3.72150500</td>
</tr>
<tr>
<td>H</td>
<td>-0.03334900</td>
<td>-0.93137000</td>
<td>4.11254600</td>
</tr>
<tr>
<td>H</td>
<td>-0.03324900</td>
<td>0.93143100</td>
<td>4.11255600</td>
</tr>
</tbody>
</table>

Transition state (\textsuperscript{4}TS2) for Comp-Ac
<table>
<thead>
<tr>
<th>Element</th>
<th>X-coordinates</th>
<th>Y-coordinates</th>
<th>Z-coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.08848000</td>
<td>0.05374800</td>
<td>-0.07872700</td>
</tr>
<tr>
<td>O</td>
<td>0.30426300</td>
<td>-0.00569200</td>
<td>-1.94785500</td>
</tr>
<tr>
<td>N</td>
<td>-1.12249100</td>
<td>-1.52318600</td>
<td>-0.17452800</td>
</tr>
<tr>
<td>N</td>
<td>1.65676700</td>
<td>-1.17351500</td>
<td>0.13317000</td>
</tr>
<tr>
<td>N</td>
<td>1.32145800</td>
<td>1.63765900</td>
<td>-0.03560200</td>
</tr>
<tr>
<td>N</td>
<td>-1.46191000</td>
<td>1.27971200</td>
<td>-0.33755600</td>
</tr>
<tr>
<td>C</td>
<td>-0.79009600</td>
<td>-2.84680700</td>
<td>0.05370200</td>
</tr>
<tr>
<td>C</td>
<td>0.48150400</td>
<td>-3.32654800</td>
<td>0.30685500</td>
</tr>
<tr>
<td>C</td>
<td>1.62095500</td>
<td>-2.54324300</td>
<td>0.32223200</td>
</tr>
<tr>
<td>C</td>
<td>2.95860700</td>
<td>-3.04865600</td>
<td>0.48814400</td>
</tr>
<tr>
<td>C</td>
<td>3.80442000</td>
<td>-1.98227700</td>
<td>0.39059800</td>
</tr>
<tr>
<td>C</td>
<td>2.99036700</td>
<td>-0.81281400</td>
<td>0.18299700</td>
</tr>
<tr>
<td>C</td>
<td>3.48380400</td>
<td>0.47626800</td>
<td>0.10353100</td>
</tr>
<tr>
<td>C</td>
<td>2.70017000</td>
<td>1.61186800</td>
<td>0.02319900</td>
</tr>
<tr>
<td>C</td>
<td>3.21550800</td>
<td>2.95826900</td>
<td>0.04209900</td>
</tr>
<tr>
<td>C</td>
<td>2.14124500</td>
<td>3.79694600</td>
<td>0.01001100</td>
</tr>
<tr>
<td>C</td>
<td>0.96205200</td>
<td>2.96958400</td>
<td>-0.04762800</td>
</tr>
<tr>
<td>C</td>
<td>-0.32875300</td>
<td>3.45400900</td>
<td>-0.14714000</td>
</tr>
<tr>
<td>C</td>
<td>-1.44828800</td>
<td>2.65981600</td>
<td>-0.30763700</td>
</tr>
<tr>
<td>C</td>
<td>-2.77831900</td>
<td>3.16754600</td>
<td>-0.53413300</td>
</tr>
<tr>
<td>C</td>
<td>-3.59035300</td>
<td>2.08930700</td>
<td>-0.72170800</td>
</tr>
<tr>
<td>C</td>
<td>-2.76833100</td>
<td>0.91340200</td>
<td>-0.58899000</td>
</tr>
<tr>
<td>C</td>
<td>-3.24381500</td>
<td>-0.38030000</td>
<td>-0.66770200</td>
</tr>
<tr>
<td>C</td>
<td>-2.47845800</td>
<td>-1.50698400</td>
<td>-0.44030200</td>
</tr>
<tr>
<td>C</td>
<td>-3.00979000</td>
<td>-2.84714200</td>
<td>-0.39198100</td>
</tr>
<tr>
<td>C</td>
<td>-1.96273400</td>
<td>-3.67241000</td>
<td>-0.07350800</td>
</tr>
<tr>
<td>H</td>
<td>3.20423700</td>
<td>-0.08744400</td>
<td>0.65312200</td>
</tr>
<tr>
<td>H</td>
<td>4.26461200</td>
<td>3.21141900</td>
<td>0.08578000</td>
</tr>
<tr>
<td>H</td>
<td>2.13139000</td>
<td>4.87693800</td>
<td>0.01575900</td>
</tr>
<tr>
<td>H</td>
<td>-4.65216300</td>
<td>2.07368400</td>
<td>-0.91793500</td>
</tr>
<tr>
<td>H</td>
<td>-1.97355600</td>
<td>-4.74384400</td>
<td>0.06214400</td>
</tr>
<tr>
<td>H</td>
<td>-3.03729100</td>
<td>4.21585900</td>
<td>-0.55341700</td>
</tr>
<tr>
<td>H</td>
<td>-4.03559000</td>
<td>-3.10578200</td>
<td>-0.56215400</td>
</tr>
<tr>
<td>H</td>
<td>4.88187200</td>
<td>-1.97165200</td>
<td>0.46541900</td>
</tr>
<tr>
<td>O</td>
<td>-0.04046800</td>
<td>0.15596600</td>
<td>1.82174800</td>
</tr>
<tr>
<td>O</td>
<td>-2.23672100</td>
<td>-0.11048200</td>
<td>2.41139800</td>
</tr>
<tr>
<td>C</td>
<td>-0.57951400</td>
<td>0.26675500</td>
<td>4.12580800</td>
</tr>
<tr>
<td>H</td>
<td>-0.11503500</td>
<td>1.25113100</td>
<td>4.24135300</td>
</tr>
<tr>
<td>H</td>
<td>0.17953800</td>
<td>-0.48190500</td>
<td>4.37236900</td>
</tr>
<tr>
<td>H</td>
<td>-1.42590400</td>
<td>0.17601600</td>
<td>4.80769900</td>
</tr>
<tr>
<td>C</td>
<td>-1.04148600</td>
<td>0.08318200</td>
<td>2.69910500</td>
</tr>
<tr>
<td>H</td>
<td>-4.30028400</td>
<td>-0.51933200</td>
<td>-0.86588400</td>
</tr>
<tr>
<td>H</td>
<td>-0.46817800</td>
<td>4.52896000</td>
<td>-0.14184200</td>
</tr>
<tr>
<td>H</td>
<td>4.55880200</td>
<td>0.60756000</td>
<td>0.15296900</td>
</tr>
<tr>
<td>H</td>
<td>0.59677200</td>
<td>-4.39180100</td>
<td>0.47071200</td>
</tr>
<tr>
<td>C</td>
<td>0.54933600</td>
<td>-0.46433500</td>
<td>-0.4019723000</td>
</tr>
<tr>
<td>H</td>
<td>-0.38700600</td>
<td>-0.21807300</td>
<td>-4.50750400</td>
</tr>
<tr>
<td>H</td>
<td>1.45128800</td>
<td>0.03860100</td>
<td>-4.34968200</td>
</tr>
<tr>
<td>C</td>
<td>0.54225400</td>
<td>-1.20370300</td>
<td>-2.74706800</td>
</tr>
<tr>
<td>H</td>
<td>1.49460800</td>
<td>-1.67155000</td>
<td>-2.48577200</td>
</tr>
</tbody>
</table>
Transition state ($^4$TS2) for Comp-C1

Fe  -0.05727700  0.00000000  -0.12039600
O   -0.01583800  -0.00000800  1.72491200
N   -1.47363300  1.41137500  -0.06593000
N    1.35519500  1.40921600  -0.17021000
N    1.35506000  -1.40935900  -0.17021500
N   -1.47377400  -1.41123600  -0.06592400
C   -1.27887000  2.77756200  -0.01010000
C    0.05668000  3.42008800  -0.01908600
C    1.16248300  2.77787000  -0.11369600
C    2.42866200  3.45465000  -0.21243400
C    3.38795900  2.49435300  -0.34553700
C    2.71843500  1.22098300  -0.31740500
C    3.35899700  -0.00017100  -0.39820400
C    2.71831300  -1.22126300  -0.31741500
C    3.38771000  -2.49469900  -0.34554000
C    2.42831800  -3.45490100  -0.21244900
C    1.16220700  -2.77799400  -0.11370200
C    -0.05702000  -3.42008800  -0.01907900
C    -1.27914600  -2.77744200  -0.01907900
C    -2.55051700  -3.45449500  0.02413900
C    -3.51515000  -2.49313600  -0.02145100
C    -2.84097600  -1.22060700  -0.07128000
C    -3.48581000  0.00016900  -0.09212100
C    -2.84085500  1.22088200  -0.07129700
C    -3.51490200  2.49347900  -0.02149200
C    -2.55017500  3.45474200  0.02409600
H    2.55052900  4.52754300  -0.19378100
H    4.45466600  -2.62160000  -0.45427000
H    2.55007800  -4.52780600  -0.19379800
H    -4.58802800  -2.61628200  -0.01816600
H    -2.67064000  4.52702300  0.06843200
H    -2.67108800  -4.52676300  0.06849000
H    -4.58776800  2.61673100  -0.01821900
H    4.45492800  2.62114600  -0.45424800
Cl   -0.13973000  0.00000800  -2.44623500
C    1.17664100  0.00003300  2.57034100
H    1.77609900  0.89621500  2.38885800
H    1.77618000  -0.89609000  2.38883000
C    0.47743900  -0.00002400  3.86818800
H    0.11377700  -0.93111100  4.28848200
H    0.11366600  0.93101000  4.28850000
H   -0.05474500  4.50332900  0.01733600
H   -4.56956200  0.00002300  -0.09937300
H   -0.05519300  -4.50333000  0.01734700
H    4.43615400  -0.00022400  -0.51777600

Transition state ($^4$TS2) for Comp-NO$_3$
<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>-0.09937300</td>
<td>0.06394800</td>
<td>0.07117600</td>
</tr>
<tr>
<td>O</td>
<td>-0.39590400</td>
<td>0.07188000</td>
<td>1.86119300</td>
</tr>
<tr>
<td>N</td>
<td>-0.01604300</td>
<td>-1.92159400</td>
<td>0.05845900</td>
</tr>
<tr>
<td>N</td>
<td>-2.05043300</td>
<td>-0.01057700</td>
<td>-0.30584300</td>
</tr>
<tr>
<td>N</td>
<td>-0.17776000</td>
<td>2.06459100</td>
<td>0.07231900</td>
</tr>
<tr>
<td>N</td>
<td>1.87079500</td>
<td>0.14436700</td>
<td>0.34954900</td>
</tr>
<tr>
<td>C</td>
<td>-1.03719900</td>
<td>-2.79604000</td>
<td>-0.27357600</td>
</tr>
<tr>
<td>C</td>
<td>-2.33144200</td>
<td>-2.43815500</td>
<td>-0.59589400</td>
</tr>
<tr>
<td>C</td>
<td>-2.80281200</td>
<td>-1.13950100</td>
<td>-0.58591500</td>
</tr>
<tr>
<td>C</td>
<td>-4.17473300</td>
<td>-0.76950400</td>
<td>-0.80480300</td>
</tr>
<tr>
<td>C</td>
<td>-2.93295800</td>
<td>1.05663000</td>
<td>-0.34069400</td>
</tr>
<tr>
<td>C</td>
<td>-2.60134600</td>
<td>2.38577000</td>
<td>-0.16975700</td>
</tr>
<tr>
<td>C</td>
<td>-1.31163100</td>
<td>2.84924100</td>
<td>-0.00228000</td>
</tr>
<tr>
<td>C</td>
<td>-0.94955700</td>
<td>4.24288100</td>
<td>0.05284500</td>
</tr>
<tr>
<td>C</td>
<td>0.40908400</td>
<td>4.29823300</td>
<td>0.14043800</td>
</tr>
<tr>
<td>C</td>
<td>0.88624000</td>
<td>2.93875900</td>
<td>0.16066700</td>
</tr>
<tr>
<td>C</td>
<td>2.21354300</td>
<td>2.58148400</td>
<td>0.29185000</td>
</tr>
<tr>
<td>C</td>
<td>2.65958000</td>
<td>1.28055800</td>
<td>0.41029000</td>
</tr>
<tr>
<td>C</td>
<td>4.02191800</td>
<td>0.91597000</td>
<td>0.69282800</td>
</tr>
<tr>
<td>C</td>
<td>4.05366700</td>
<td>-0.43953500</td>
<td>0.83744400</td>
</tr>
<tr>
<td>C</td>
<td>2.71529400</td>
<td>-0.91935900</td>
<td>0.62233300</td>
</tr>
<tr>
<td>C</td>
<td>2.35011600</td>
<td>-2.25003300</td>
<td>0.64657900</td>
</tr>
<tr>
<td>C</td>
<td>1.08338800</td>
<td>-2.71040500</td>
<td>0.34685300</td>
</tr>
<tr>
<td>C</td>
<td>0.73584800</td>
<td>-4.09986500</td>
<td>0.21698900</td>
</tr>
<tr>
<td>C</td>
<td>-0.56785200</td>
<td>-4.15247000</td>
<td>-0.17985900</td>
</tr>
<tr>
<td>H</td>
<td>-4.96404200</td>
<td>-1.46573800</td>
<td>-1.04650400</td>
</tr>
<tr>
<td>H</td>
<td>-1.65445100</td>
<td>5.05988000</td>
<td>0.01083700</td>
</tr>
<tr>
<td>H</td>
<td>1.04490800</td>
<td>5.16955600</td>
<td>0.19029300</td>
</tr>
<tr>
<td>H</td>
<td>4.90105800</td>
<td>-1.07175200</td>
<td>1.05680800</td>
</tr>
<tr>
<td>H</td>
<td>-1.17004000</td>
<td>-5.02300000</td>
<td>-0.39332500</td>
</tr>
<tr>
<td>H</td>
<td>4.83689100</td>
<td>1.61948800</td>
<td>0.77559900</td>
</tr>
<tr>
<td>H</td>
<td>1.41939700</td>
<td>-4.91828200</td>
<td>0.38710700</td>
</tr>
<tr>
<td>H</td>
<td>-5.12706700</td>
<td>1.21703000</td>
<td>-0.72620300</td>
</tr>
<tr>
<td>O</td>
<td>0.13096100</td>
<td>0.12622000</td>
<td>-1.87577700</td>
</tr>
<tr>
<td>N</td>
<td>1.32079400</td>
<td>-0.14733700</td>
<td>-2.47292500</td>
</tr>
<tr>
<td>O</td>
<td>1.66457300</td>
<td>-1.34421100</td>
<td>-2.58300700</td>
</tr>
<tr>
<td>O</td>
<td>1.97813300</td>
<td>0.82186700</td>
<td>-2.90686300</td>
</tr>
<tr>
<td>H</td>
<td>-3.03110200</td>
<td>-3.22956000</td>
<td>-0.83804600</td>
</tr>
<tr>
<td>H</td>
<td>3.11907900</td>
<td>-2.98360300</td>
<td>0.85806000</td>
</tr>
<tr>
<td>H</td>
<td>2.94936300</td>
<td>3.37489700</td>
<td>0.34724700</td>
</tr>
<tr>
<td>H</td>
<td>-3.40013700</td>
<td>3.11642200</td>
<td>-0.22207600</td>
</tr>
<tr>
<td>C</td>
<td>-1.05896800</td>
<td>-0.27790900</td>
<td>3.95317800</td>
</tr>
<tr>
<td>H</td>
<td>-0.19051200</td>
<td>-0.56458700</td>
<td>4.53569200</td>
</tr>
<tr>
<td>H</td>
<td>-1.63304700</td>
<td>0.58385200</td>
<td>4.27506300</td>
</tr>
<tr>
<td>C</td>
<td>-1.26409800</td>
<td>-0.84284900</td>
<td>2.60705900</td>
</tr>
<tr>
<td>H</td>
<td>-2.29292400</td>
<td>-0.76175600</td>
<td>2.24538200</td>
</tr>
<tr>
<td>H</td>
<td>-0.90935400</td>
<td>-1.87118800</td>
<td>2.50019400</td>
</tr>
</tbody>
</table>

**Product (4P) for Comp-F**
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.08139200</td>
<td>-0.00223000</td>
<td>-0.36943800</td>
</tr>
<tr>
<td>O</td>
<td>0.07977300</td>
<td>-0.01175300</td>
<td>2.03676800</td>
</tr>
<tr>
<td>N</td>
<td>-0.00656800</td>
<td>-2.00309500</td>
<td>-0.19801300</td>
</tr>
<tr>
<td>N</td>
<td>-1.93078000</td>
<td>0.07452600</td>
<td>-0.27960600</td>
</tr>
<tr>
<td>C</td>
<td>-2.44214100</td>
<td>-2.33265800</td>
<td>-0.32368600</td>
</tr>
<tr>
<td>C</td>
<td>-2.80463000</td>
<td>-0.99736500</td>
<td>-0.34022000</td>
</tr>
<tr>
<td>C</td>
<td>-1.13950400</td>
<td>-2.79389100</td>
<td>-0.25363100</td>
</tr>
<tr>
<td>C</td>
<td>-2.41099200</td>
<td>0.84039900</td>
<td>-0.42511700</td>
</tr>
<tr>
<td>C</td>
<td>-2.72059600</td>
<td>1.20997600</td>
<td>-0.34023500</td>
</tr>
<tr>
<td>C</td>
<td>-2.25788300</td>
<td>2.51385700</td>
<td>-0.31782800</td>
</tr>
<tr>
<td>C</td>
<td>-0.92384000</td>
<td>2.87460700</td>
<td>-0.24861700</td>
</tr>
<tr>
<td>C</td>
<td>-0.45016900</td>
<td>4.23534200</td>
<td>-0.21915500</td>
</tr>
<tr>
<td>C</td>
<td>0.91103200</td>
<td>4.18242900</td>
<td>-0.15444800</td>
</tr>
<tr>
<td>C</td>
<td>2.58141000</td>
<td>2.32693200</td>
<td>-0.09489700</td>
</tr>
<tr>
<td>C</td>
<td>2.94268900</td>
<td>0.99211800</td>
<td>-0.08783700</td>
</tr>
<tr>
<td>C</td>
<td>4.30301000</td>
<td>0.51898600</td>
<td>-0.01943200</td>
</tr>
<tr>
<td>C</td>
<td>4.25113500</td>
<td>-0.84309400</td>
<td>-0.01945200</td>
</tr>
<tr>
<td>C</td>
<td>2.39700300</td>
<td>-2.51463700</td>
<td>-0.09576800</td>
</tr>
<tr>
<td>C</td>
<td>1.06324800</td>
<td>-2.87649500</td>
<td>-0.14669000</td>
</tr>
<tr>
<td>C</td>
<td>0.59030500</td>
<td>-2.37616000</td>
<td>-0.15868900</td>
</tr>
<tr>
<td>C</td>
<td>-0.77085000</td>
<td>-4.18673400</td>
<td>-0.22532800</td>
</tr>
<tr>
<td>H</td>
<td>-5.03161500</td>
<td>-1.16058500</td>
<td>-0.48697800</td>
</tr>
<tr>
<td>H</td>
<td>-1.08706800</td>
<td>5.10714900</td>
<td>-0.25019000</td>
</tr>
<tr>
<td>H</td>
<td>1.61347600</td>
<td>5.00224600</td>
<td>-0.12154400</td>
</tr>
<tr>
<td>H</td>
<td>5.06986700</td>
<td>-1.54625800</td>
<td>0.02257500</td>
</tr>
<tr>
<td>H</td>
<td>-1.47225000</td>
<td>-5.00748900</td>
<td>-0.25828300</td>
</tr>
<tr>
<td>H</td>
<td>5.17286900</td>
<td>1.15779200</td>
<td>0.02258300</td>
</tr>
<tr>
<td>H</td>
<td>1.22822900</td>
<td>-5.10856600</td>
<td>-0.12591100</td>
</tr>
<tr>
<td>H</td>
<td>-4.92872000</td>
<td>1.54249800</td>
<td>-0.48307300</td>
</tr>
<tr>
<td>F</td>
<td>0.14499200</td>
<td>-0.00283600</td>
<td>-2.22559200</td>
</tr>
<tr>
<td>H</td>
<td>3.13331200</td>
<td>-3.30974700</td>
<td>-0.06113300</td>
</tr>
<tr>
<td>H</td>
<td>3.37596900</td>
<td>3.06383100</td>
<td>-0.06027200</td>
</tr>
<tr>
<td>H</td>
<td>-3.23514900</td>
<td>3.07033500</td>
<td>-0.37510000</td>
</tr>
<tr>
<td>H</td>
<td>-2.99281100</td>
<td>3.30956600</td>
<td>-0.36690000</td>
</tr>
<tr>
<td>C</td>
<td>-0.94208500</td>
<td>-0.70954100</td>
<td>2.86345800</td>
</tr>
<tr>
<td>H</td>
<td>-0.52395000</td>
<td>1.26715600</td>
<td>3.69362400</td>
</tr>
<tr>
<td>H</td>
<td>-1.70797100</td>
<td>-1.21320700</td>
<td>2.28515400</td>
</tr>
<tr>
<td>C</td>
<td>-0.88635700</td>
<td>0.76269300</td>
<td>2.86248000</td>
</tr>
<tr>
<td>H</td>
<td>-1.61323600</td>
<td>1.31865700</td>
<td>2.28211000</td>
</tr>
<tr>
<td>H</td>
<td>-0.42622500</td>
<td>1.28478100</td>
<td>3.69318200</td>
</tr>
</tbody>
</table>

**Product (4P) for Comp-Ac**

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>0.12729100</td>
<td>0.05085100</td>
<td>0.01784200</td>
</tr>
<tr>
<td>O</td>
<td>0.38003900</td>
<td>-0.00797000</td>
<td>-2.35635000</td>
</tr>
</tbody>
</table>
Product (1P) for Comp-Cl
Product (4P) for Comp-NO₃

Fe     0.12220900  0.04852400  -0.00320200
O      0.42415600  -0.06842300  -2.28677300
N  -0.50868000  -1.85175600  -0.03667300
N   2.00967000  -0.59162900   0.15698500
N   0.78260500   1.92827400  -0.20441500
N  -1.73766100   0.66655700  -0.37124300
C   0.24925100  -2.98495400   0.21875000
C   1.61826800  -3.00999400   0.40771000
C   2.43357600  -1.89390800   0.36708000
C   3.86317900  -1.92829000   0.51959100
C   4.30926300  -0.64419500   0.40124200
C   3.15519700   0.18585300   0.18324100
C   3.20126100   1.55959300   0.04076000
C   2.09208300   2.36509000  -0.12948900
C   2.14096400   3.80036200  -0.23642000
C   0.85544200   4.23501700  -0.36559000
C   0.01259600   3.06768600  -0.34684400
C  -1.36310600   3.09852000  -0.47186500
C  -2.17082000   1.97777900  -0.49391700
C  -3.59676500   2.01038700  -0.67526800
C  -4.03121900   0.71715300  -0.67069600
C  -2.87644500  -0.11653900  -0.47539500
C  -2.91773500  -1.49492300  -0.39252000
C  -1.81517800  -2.29557400  -0.16437900
C  -1.86850700  -3.72399300  -0.00808000
C  -0.59504100  -4.14909000   0.23503800
H   4.43870900  -2.82481000   0.69649500
H   3.04794700   4.38563100  -0.20554500
H   0.49549100   5.24840900  -0.46329500
H  -5.04078400   0.34851400  -0.77544500
H  -0.24678300  -5.15525000   0.41593800
H  -4.17846800   2.91319500  -0.78775500
H  -2.77271600  -4.31187700  -0.06311000
H   5.32328500  -0.27788800   0.46305300
O   0.04382000   0.28846800   2.01427300
N  -1.05006900   0.32571600   2.78317300
O  -1.99557600  -0.46759300   2.53547400
O  -1.06315100  1.14815300   3.72961400
H   2.08514700  -3.97007700   0.59540100
H  -3.88452000  -1.97754800  -0.47691200
H  -1.84048900   4.06647700  -0.57103200
H   4.17213300   2.03938100   0.86686600
C  -0.46860600  -0.77280900  -3.25140000
H  -1.30365900  -1.28191200  -2.78463700
H  -0.69218700  -0.18665600  -4.13475700
C   0.89724100   1.27357300  -3.02609100
H   1.67947800  -1.05648200  -3.74356100
H   1.04553200  -2.14329500  -2.39674800

a point for Comp-F

Fe  -0.27767700   0.00903400  -0.30122800
O   0.08860100  -0.00471100   1.43052600
N   0.70945300  1.74345000  -0.53228700  
N   1.41157800  -0.98212600  -0.50862700  
N  -1.27804400  -1.72670700  -0.13731300  
N  -1.90178900   0.99781700   0.20670600  
C   2.05127200   1.90647000  -0.80571800  
C   2.97874900   0.88977600  -0.88788800  
C   2.67508400  -0.44777000  -0.73624700  
C   3.63349100  -1.50480400  -0.86898500  
C   2.95441000  -2.68469500  -0.74688400  
C   1.57483600  -2.36285700  -0.53703700  
C   0.57101100  -3.30476200  -0.44443600  
C  -0.76212800  -2.99887500  -0.26931400  
C  -1.81047000  -3.97233000  -0.11272900  
C  -2.95715500  -3.29127400   0.14836700  
C  -2.61690400  -1.88961200   0.15109800  
C  -3.49431000  -0.87356200   0.46590500  
C  -3.15052000   0.46264000   0.50221400  
C  -4.07932300   1.51825800   0.77816900  
C  -3.40845000   2.69003000   0.62766000  
C  -2.06114700   2.37847500   0.25943300  
C  -1.10297000   3.32152000  -0.05286700  
C   0.18760700   3.01611100  -0.43110300  
C   1.21270200   3.99490700  -0.69949100  
C   1.05503700   5.06306300  -0.69216600  
H   4.68638800  -1.35383300  -1.05486500  
H  -1.66523800  -5.04509000  -0.18069500  
H  -3.94614400  -3.68073000   0.33875000  
H  -3.78869200   3.70399300   0.73437200  
H   3.34850000   3.69768900  -1.14890600  
H  -5.11739200   1.36493400  -1.03047000  
H  -1.05503700   5.06306300  -0.69216600  
H   3.34189900  -3.69033000  -0.81253000  
F  -0.65023000   0.02647300  -0.36150300  
H  -1.38332200   4.36618400   0.01677000  
H  -4.51930700  -1.13724200   0.69819300  
H   4.01073400   1.15507100  -1.08394700  
H   0.85123500  -4.34963200  -0.50650300  
C   2.84654600   0.24781200   3.36814600  
H   1.95421600   0.18106300   2.75173700  
H   2.80615300   0.93426600   4.21069100  
C   3.94398200  -0.46342900   3.10098800  
H   4.84212000  -0.39183700   3.70951600  
H   3.98747300  -1.14866300   2.25833600  

*a point for Comp-Ac*

Fe  -0.05349600   0.12294200  -0.13495300  
O   0.13800100   0.17278600  -1.76553600  
N  -0.11975900  -1.88339400  -0.09620700  
N   1.93099700   0.03612000   0.27751600  
N   0.03675600   2.12542400  -0.03473000
<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>-1.97283800</td>
<td>0.20084600</td>
<td>-0.50742100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.88543100</td>
<td>-2.75412000</td>
<td>0.27999800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.17262700</td>
<td>-2.37945100</td>
<td>0.61691700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.66701600</td>
<td>-1.07925400</td>
<td>0.58561000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.04180900</td>
<td>-0.72539800</td>
<td>0.83762900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.13355900</td>
<td>0.62594700</td>
<td>0.66983300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.80940400</td>
<td>1.09048100</td>
<td>0.33912900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.45807600</td>
<td>2.42614100</td>
<td>0.20639200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.16646100</td>
<td>2.90651700</td>
<td>0.06208700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.81196400</td>
<td>4.30442400</td>
<td>0.04054600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.54646800</td>
<td>4.36416000</td>
<td>-0.06065800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.01606900</td>
<td>3.00156300</td>
<td>-0.12389200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.33253900</td>
<td>2.62180200</td>
<td>-0.34918100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.76300800</td>
<td>1.32394700</td>
<td>-0.57633800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.09716100</td>
<td>0.96651900</td>
<td>-0.99774900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.09614500</td>
<td>-0.37545300</td>
<td>-1.21740300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.77209500</td>
<td>-0.85405400</td>
<td>-0.90187800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.39841500</td>
<td>-2.18192900</td>
<td>-0.91221200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.16842600</td>
<td>-2.67026200</td>
<td>-0.48308800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.83482500</td>
<td>-4.06653700</td>
<td>-0.34396100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.43563700</td>
<td>-4.11848700</td>
<td>0.14865100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.82062400</td>
<td>-1.42446800</td>
<td>1.10400300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.51713000</td>
<td>5.11945400</td>
<td>0.10206800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.17932300</td>
<td>5.23781700</td>
<td>-0.10606800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.91216900</td>
<td>-1.00231400</td>
<td>-1.54365700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.02929300</td>
<td>-4.98864500</td>
<td>0.38647800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.91078200</td>
<td>1.66609200</td>
<td>-1.11639300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.49723900</td>
<td>-4.88555600</td>
<td>-0.58076100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.00113400</td>
<td>1.25957400</td>
<td>0.77884400</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-0.25867600</td>
<td>0.12264800</td>
<td>1.79659000</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>-2.15435800</td>
<td>-1.11133600</td>
<td>2.13729700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.93111800</td>
<td>-0.24323100</td>
<td>4.02973300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.91042100</td>
<td>0.82804100</td>
<td>4.25210600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.04656900</td>
<td>-0.65118500</td>
<td>4.30436700</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.71191200</td>
<td>-0.72794300</td>
<td>4.61664900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.17387500</td>
<td>-0.45360300</td>
<td>2.55154400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.14219400</td>
<td>-2.90650700</td>
<td>-1.22633900</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.07477900</td>
<td>3.41003100</td>
<td>-0.41973800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.25549900</td>
<td>3.15909000</td>
<td>0.27291300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.86879400</td>
<td>-3.16876500</td>
<td>0.88109000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.89803500</td>
<td>-0.25598400</td>
<td>-3.04735500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.95763900</td>
<td>0.58543400</td>
<td>-3.73253600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.65820900</td>
<td>-0.29915200</td>
<td>-2.27276500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.92555500</td>
<td>-1.16336400</td>
<td>-3.13486500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.84564800</td>
<td>-1.98982800</td>
<td>-2.43675500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.15018600</td>
<td>-1.10589700</td>
<td>-3.89255400</td>
<td></td>
</tr>
</tbody>
</table>

*a point for Comp-Cl*

<p>| Fe | 0.15907600 | 0.02170100 | -0.03244100 |
| O | 0.06226300 | 0.05156800 | 1.60735500 |</p>
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>2.01056100</td>
<td>-0.65937300</td>
<td>0.09308800</td>
</tr>
<tr>
<td>N</td>
<td>-0.53664900</td>
<td>-1.87266500</td>
<td>-0.15431700</td>
</tr>
<tr>
<td>N</td>
<td>-1.73202400</td>
<td>0.69551900</td>
<td>-0.27165700</td>
</tr>
<tr>
<td>C</td>
<td>2.40470100</td>
<td>-1.97743900</td>
<td>0.23601000</td>
</tr>
<tr>
<td>C</td>
<td>1.56344300</td>
<td>-3.07249500</td>
<td>0.21398100</td>
</tr>
<tr>
<td>C</td>
<td>0.19073000</td>
<td>-3.02482500</td>
<td>0.00137000</td>
</tr>
<tr>
<td>C</td>
<td>-0.65299600</td>
<td>-4.18196700</td>
<td>-0.15573700</td>
</tr>
<tr>
<td>C</td>
<td>-1.90611800</td>
<td>-3.71761000</td>
<td>-0.42851100</td>
</tr>
<tr>
<td>C</td>
<td>-1.82675300</td>
<td>-2.27913800</td>
<td>-0.41982500</td>
</tr>
<tr>
<td>C</td>
<td>-2.90743400</td>
<td>-1.43183500</td>
<td>-0.60618600</td>
</tr>
<tr>
<td>C</td>
<td>-2.86467000</td>
<td>-0.04924600</td>
<td>-0.52171300</td>
</tr>
<tr>
<td>C</td>
<td>-4.01426700</td>
<td>0.81159700</td>
<td>-0.63550200</td>
</tr>
<tr>
<td>C</td>
<td>-3.57087900</td>
<td>2.08690400</td>
<td>-0.44217200</td>
</tr>
<tr>
<td>C</td>
<td>-2.14874400</td>
<td>2.00137200</td>
<td>-0.22828100</td>
</tr>
<tr>
<td>C</td>
<td>-1.07899000</td>
<td>3.09639300</td>
<td>-0.06788500</td>
</tr>
<tr>
<td>C</td>
<td>0.06993700</td>
<td>3.03864500</td>
<td>0.00682200</td>
</tr>
<tr>
<td>C</td>
<td>0.92872500</td>
<td>4.19546700</td>
<td>0.06039000</td>
</tr>
<tr>
<td>C</td>
<td>2.21010700</td>
<td>3.73851100</td>
<td>0.04500500</td>
</tr>
<tr>
<td>C</td>
<td>2.13935600</td>
<td>2.29933400</td>
<td>-0.00277700</td>
</tr>
<tr>
<td>C</td>
<td>3.23837000</td>
<td>1.45797500</td>
<td>0.03532700</td>
</tr>
<tr>
<td>C</td>
<td>3.17380700</td>
<td>0.07688000</td>
<td>0.10432500</td>
</tr>
<tr>
<td>C</td>
<td>4.31722300</td>
<td>-0.78848600</td>
<td>0.25184400</td>
</tr>
<tr>
<td>C</td>
<td>3.84005000</td>
<td>-2.05913800</td>
<td>0.34617700</td>
</tr>
<tr>
<td>H</td>
<td>-0.31728200</td>
<td>-5.20537000</td>
<td>-0.08054300</td>
</tr>
<tr>
<td>H</td>
<td>-5.02048200</td>
<td>0.47320800</td>
<td>-0.83255600</td>
</tr>
<tr>
<td>H</td>
<td>-4.13886000</td>
<td>3.00501400</td>
<td>-0.45569800</td>
</tr>
<tr>
<td>H</td>
<td>3.12713000</td>
<td>4.30774300</td>
<td>0.06772200</td>
</tr>
<tr>
<td>H</td>
<td>4.39451400</td>
<td>-2.97770100</td>
<td>0.46665700</td>
</tr>
<tr>
<td>H</td>
<td>0.58021800</td>
<td>5.21703700</td>
<td>0.09221900</td>
</tr>
<tr>
<td>H</td>
<td>5.34222100</td>
<td>-0.45122400</td>
<td>0.28515600</td>
</tr>
<tr>
<td>H</td>
<td>-2.80617900</td>
<td>-4.28405600</td>
<td>-0.61516800</td>
</tr>
<tr>
<td>Cl</td>
<td>0.28161400</td>
<td>-0.02823900</td>
<td>-2.37330000</td>
</tr>
<tr>
<td>C</td>
<td>-1.64517900</td>
<td>-0.68870400</td>
<td>2.79979300</td>
</tr>
<tr>
<td>H</td>
<td>-0.90871800</td>
<td>-0.94395900</td>
<td>3.55494200</td>
</tr>
<tr>
<td>H</td>
<td>-1.78707300</td>
<td>-1.41425600</td>
<td>2.00529700</td>
</tr>
<tr>
<td>C</td>
<td>-2.40585400</td>
<td>0.40583000</td>
<td>2.89877800</td>
</tr>
<tr>
<td>H</td>
<td>-3.15472200</td>
<td>0.65202800</td>
<td>2.15120700</td>
</tr>
<tr>
<td>H</td>
<td>-2.27460000</td>
<td>1.12326400</td>
<td>3.70397200</td>
</tr>
<tr>
<td>H</td>
<td>2.01727000</td>
<td>-4.05154600</td>
<td>0.32607200</td>
</tr>
<tr>
<td>H</td>
<td>4.22141600</td>
<td>1.91609300</td>
<td>0.04545700</td>
</tr>
<tr>
<td>H</td>
<td>-1.76715200</td>
<td>4.07906500</td>
<td>-0.04541400</td>
</tr>
<tr>
<td>H</td>
<td>-3.87005400</td>
<td>-1.88917700</td>
<td>-0.80958200</td>
</tr>
</tbody>
</table>

*a point for Comp-NO*

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>-0.03856500</td>
<td>0.14213300</td>
<td>-0.15565000</td>
</tr>
<tr>
<td>O</td>
<td>0.13993100</td>
<td>0.22400300</td>
<td>-1.78375500</td>
</tr>
<tr>
<td>N</td>
<td>-0.19233300</td>
<td>-1.85286300</td>
<td>-0.13137400</td>
</tr>
<tr>
<td>N</td>
<td>1.93808100</td>
<td>-0.03103300</td>
<td>0.21957900</td>
</tr>
<tr>
<td>N</td>
<td>0.12303100</td>
<td>2.12330800</td>
<td>-0.01692200</td>
</tr>
</tbody>
</table>
Estimated minimum energy point for Comp-F

Fe  0.08119700  0.03535400  -0.37726500
O  0.19165700  0.01059600   1.78775000
N  0.63483100  0.37987300  -3.65183400
H  3.44283200  -0.63788800  -2.20210700
C   1.53808400  -1.09441900  -3.02662700
N  -1.91136100  -0.54355500  -0.23919400
N  -0.50558500  2.00925500  -0.18849400

N  -1.97145100  0.30654600  -0.45125700
C   0.77381500  -2.76925900   0.23553300
C   2.08008000  -2.45255700   0.56730000
C   2.63059800  -1.17630500   0.52355700
C   4.02580700  -0.88126500   0.73353000
C   4.17431700   0.46177800   0.54295100
C   2.86421800   0.98344600   0.24553000
C   2.56300800   2.33169600   0.12362800
C   1.28350100   2.85766000   0.07879700
C   0.98119900   4.26832700   0.07879700
C  -0.37737900   4.37986500   0.07004000
C  -0.90148000   3.04040800  -0.00775400
C  -2.24249400   2.72210300  -0.15531000
C  -2.30547000   1.44876300  -0.41275300
C  -4.08159000  1.15290100  -0.76228300
C  -4.15302100  -0.17705200  -1.04424000
C  -2.82861900  -0.70567700  -0.83123600
C  -2.50647200  -2.04716800  -0.88757400
C  -1.28216800  -2.59018200  -0.50747900
C  -1.00992000  -3.99796800  -0.37941400
C   0.26228800  -4.10908500   0.10242200
H   4.78056200  -1.61048100   0.98802200
H   1.71887700   5.05591000   0.12432400
H  -0.97765400   5.27681100   0.09767700
H  -5.00791100  -0.76245400  -1.34785800
H   0.81533200  -5.00716200   0.33389000
H  -4.89599900   1.87961800  -0.79690100
H  -1.70987900  -4.78686300  -0.61043000
H   5.07384500   1.05430500   0.61866300
O  -0.13412600   0.13861800   1.82188200
N  -0.99635900  -0.51463400   2.60154000
O  -2.00422600  -1.07721900   2.09619000
O  -0.74024400  -0.51812200   3.82891000
H   2.74089400  -3.27148700   0.83039800
H  -3.28946700  -2.73631300  -1.18502600
H  -2.95749200   3.53724900  -0.13792400
H   3.38855500   3.03403400   0.16552200
C   2.69438000  -0.42535500  -2.96011200
H   2.92736000   0.37987300  -3.65183400
H   3.44283200  -0.63788800  -2.20210700
C   1.53808400  -1.09441900  -3.02662700
H   1.30166100  -1.90507800  -2.34880200
H   0.80715000  -0.88927500  -3.80054800
<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>2.04801300</td>
<td>0.59772300</td>
<td>-0.11965500</td>
</tr>
<tr>
<td>C</td>
<td>-0.20531200</td>
<td>-3.04577400</td>
<td>-0.23562800</td>
</tr>
<tr>
<td>C</td>
<td>-1.59699700</td>
<td>-2.98837200</td>
<td>-0.29906700</td>
</tr>
<tr>
<td>C</td>
<td>-2.38552700</td>
<td>-1.83752600</td>
<td>-0.31326900</td>
</tr>
<tr>
<td>C</td>
<td>-3.82762900</td>
<td>-1.80638300</td>
<td>-0.41168800</td>
</tr>
<tr>
<td>C</td>
<td>-4.20643700</td>
<td>-0.49201700</td>
<td>-0.40982000</td>
</tr>
<tr>
<td>C</td>
<td>-3.00175900</td>
<td>1.69533200</td>
<td>-0.28834300</td>
</tr>
<tr>
<td>C</td>
<td>-2.94570900</td>
<td>0.30173000</td>
<td>-0.31067900</td>
</tr>
<tr>
<td>C</td>
<td>-1.79755000</td>
<td>2.48437900</td>
<td>-0.22643100</td>
</tr>
<tr>
<td>C</td>
<td>-1.69026000</td>
<td>3.93124300</td>
<td>-0.18949000</td>
</tr>
<tr>
<td>C</td>
<td>-0.45639500</td>
<td>4.30756100</td>
<td>-0.12977600</td>
</tr>
<tr>
<td>C</td>
<td>0.33678700</td>
<td>3.09665600</td>
<td>-0.13059000</td>
</tr>
<tr>
<td>C</td>
<td>1.72890000</td>
<td>3.03874300</td>
<td>-0.07594100</td>
</tr>
<tr>
<td>C</td>
<td>4.34265300</td>
<td>0.54890300</td>
<td>0.01295200</td>
</tr>
<tr>
<td>C</td>
<td>0.13500500</td>
<td>-0.24535300</td>
<td>-0.06851600</td>
</tr>
<tr>
<td>C</td>
<td>3.07723700</td>
<td>-1.63784000</td>
<td>-0.08216600</td>
</tr>
<tr>
<td>C</td>
<td>1.92919200</td>
<td>-2.42641800</td>
<td>-0.13386400</td>
</tr>
<tr>
<td>C</td>
<td>1.90238200</td>
<td>-3.87301300</td>
<td>-0.15859400</td>
</tr>
<tr>
<td>C</td>
<td>0.59107600</td>
<td>-4.25377100</td>
<td>-0.22231800</td>
</tr>
<tr>
<td>H</td>
<td>-4.46107500</td>
<td>-2.67875000</td>
<td>-0.48364000</td>
</tr>
<tr>
<td>H</td>
<td>-2.64177900</td>
<td>4.56785300</td>
<td>-0.21093800</td>
</tr>
<tr>
<td>H</td>
<td>-0.05444000</td>
<td>5.30975500</td>
<td>-0.09316800</td>
</tr>
<tr>
<td>H</td>
<td>5.34439700</td>
<td>0.14722800</td>
<td>0.06153500</td>
</tr>
<tr>
<td>H</td>
<td>0.19277700</td>
<td>-5.25732800</td>
<td>-0.26203300</td>
</tr>
<tr>
<td>H</td>
<td>4.59729000</td>
<td>2.73541000</td>
<td>0.06594700</td>
</tr>
<tr>
<td>H</td>
<td>2.77684900</td>
<td>-4.50722600</td>
<td>-0.13757600</td>
</tr>
<tr>
<td>H</td>
<td>-5.20707400</td>
<td>-0.09044900</td>
<td>-0.48040900</td>
</tr>
<tr>
<td>F</td>
<td>0.11486100</td>
<td>0.03108200</td>
<td>-2.21642100</td>
</tr>
<tr>
<td>H</td>
<td>4.02607900</td>
<td>-2.16383700</td>
<td>-0.04869200</td>
</tr>
<tr>
<td>H</td>
<td>2.25263700</td>
<td>3.98852000</td>
<td>-0.03377000</td>
</tr>
<tr>
<td>H</td>
<td>-2.12100800</td>
<td>-3.93716100</td>
<td>-0.35657600</td>
</tr>
<tr>
<td>H</td>
<td>-3.89461400</td>
<td>2.22024800</td>
<td>-0.33717300</td>
</tr>
<tr>
<td>C</td>
<td>-0.48717000</td>
<td>-0.88105700</td>
<td>2.65284900</td>
</tr>
<tr>
<td>H</td>
<td>0.14300600</td>
<td>-1.22251400</td>
<td>3.47658200</td>
</tr>
<tr>
<td>H</td>
<td>-0.92460700</td>
<td>-1.73704300</td>
<td>2.13639300</td>
</tr>
<tr>
<td>C</td>
<td>-1.38113500</td>
<td>0.20359100</td>
<td>2.94180700</td>
</tr>
<tr>
<td>H</td>
<td>-2.22824600</td>
<td>0.39499500</td>
<td>2.29223000</td>
</tr>
<tr>
<td>H</td>
<td>-1.12817600</td>
<td>0.93828300</td>
<td>3.69810300</td>
</tr>
</tbody>
</table>