

**Supporting Information for**

**The potential of d<sup>6</sup> non-noble metal NHC catalysts for Carbon  
Dioxide Hydrogenation: group and row effects**

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All calculations were performed with Gaussian 16 program.<sup>1</sup> The solvation effect of DMSO simulated by the SMD continuum solvent model.<sup>2</sup> Vibration frequency calculations based on the optimized structures were performed at the same level of theory to verify the stationary point as minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations<sup>3</sup> were performed for all transition states to confirm whether they connect two correct minima or not. Natural bond orbital (NBO) analyses were performed using the NBO 3.1 package<sup>4</sup> in order to simulate the alkaline experimental conditions, our DFT calculations at pH 9, which based on the equation  $\Delta G = RT \ln(Q/K_{eq})$ .<sup>5,6</sup>

To test the reliability of our calculations, M06 functional which was the most suitable and B3LYP functional which overestimated slightly the barrier in the study of yang et al.<sup>7</sup> are used to recalculate the rate-determining transition state for all complexes. As shown in Table S1, the conclusions using M06, B3LYP and M06-L functionals are identical, suggesting that M06-L functional is applicable for our system.

**Table S1.** Relative free energies of the rate-determining transition states for all catalytic reactions obtained using different density functionals. Free energies are in kcal/mol

| functional | Cr-TS1 | Mn-TS1 | Fe-TS1 | Co-TS1 | Mo-TS1 | W-TS1 |
|------------|--------|--------|--------|--------|--------|-------|
| M06L       | 28.0   | 26.9   | 31.4   | 33.2   | 24.3   | 25.7  |
| M06        | 26.7   | 26.9   | 32.6   | 32.2   | 28.4   | 27.2  |
| B3LYP      | 27.5   | 27.1   | 30.0   | 29.0   | 24.7   | 25.0  |

The relative free energies of key structures of oxidation addition and inner-sphere mechanisms of all reaction systems were calculated systematically (see Figs. S1-S6), For Cr<sup>0</sup>/Mo<sup>0</sup>/W<sup>0</sup>/Mn<sup>I</sup>/<sup>I</sup> complexes, reactions proceeded along the outer sphere mechanism. For Co<sup>III</sup> complex, the innner sphere and the outer sphere mechanisms are competitive. Therefore, after the revision, all the discussion and analysis of the metal center effects are on the basis of their most preferred outer-sphere mechanism.

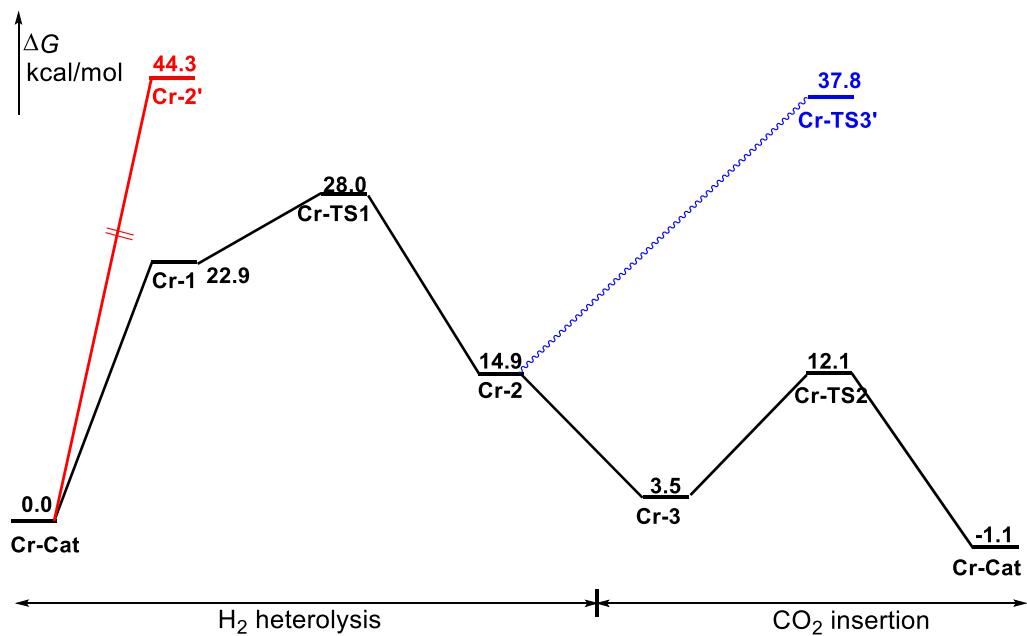


Fig. S1 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid Catalysed by  $\text{Cr}^0$ -NHC Complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies are shown in kcal/mol.

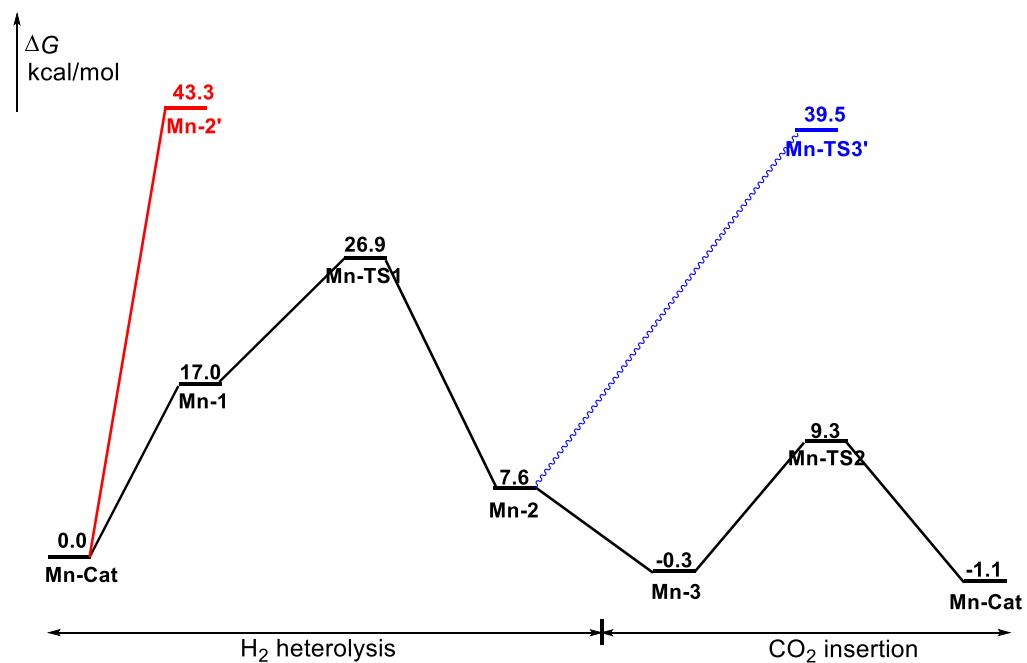


Fig. S2 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid Catalysed by  $\text{Mn}^1$ -NHC Complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies are shown in kcal/mol.

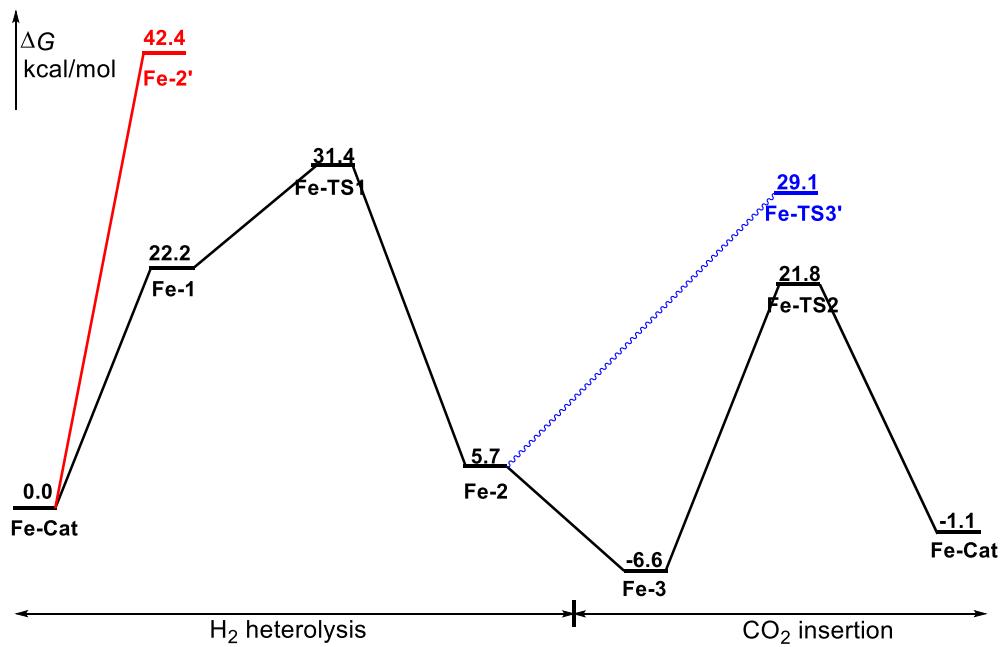


Fig. S3 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid Catalysed by  $\text{Fe}^{\text{II}}$ -NHC Complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies are shown in kcal/mol.

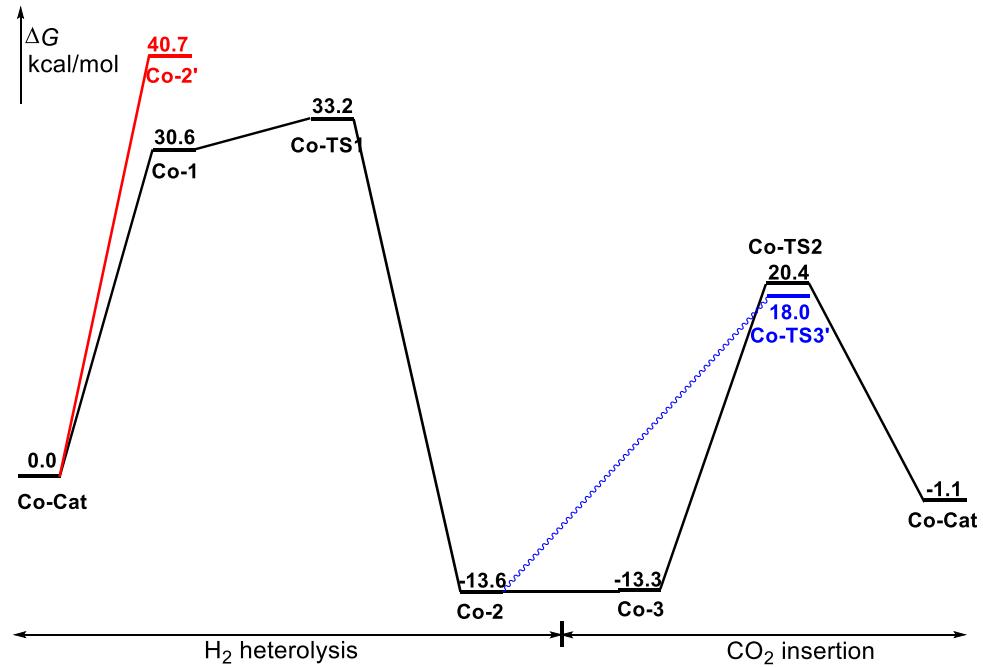


Fig. S4 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid Catalysed by  $\text{Co}^{\text{III}}$ -NHC Complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies are shown in kcal/mol.

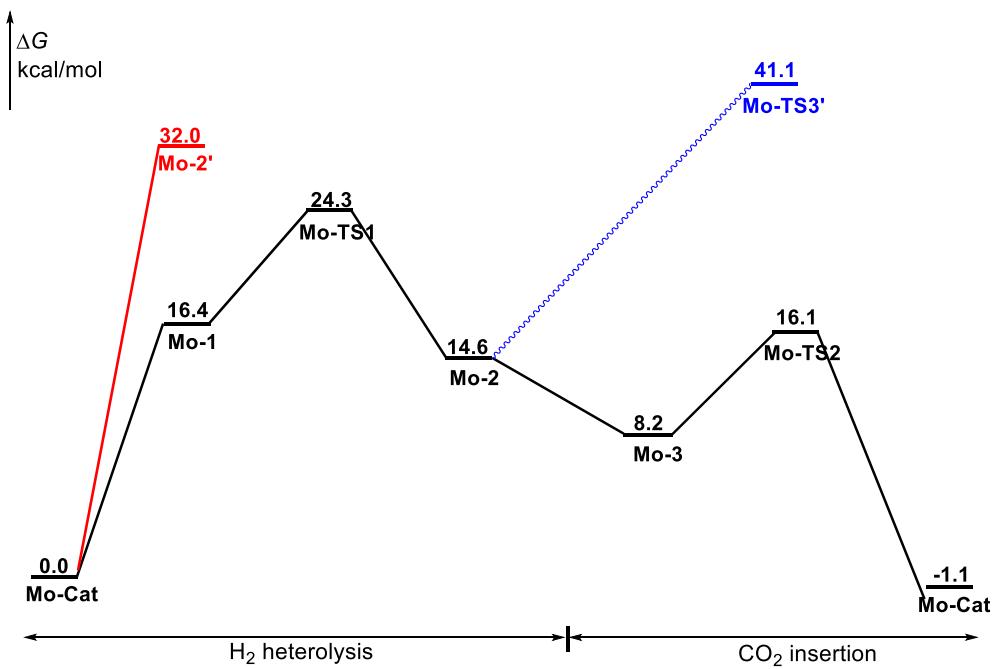


Fig. S5 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid catalysed by  $\text{Mo}^0\text{-NHC}$  complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies are shown in kcal/mol.

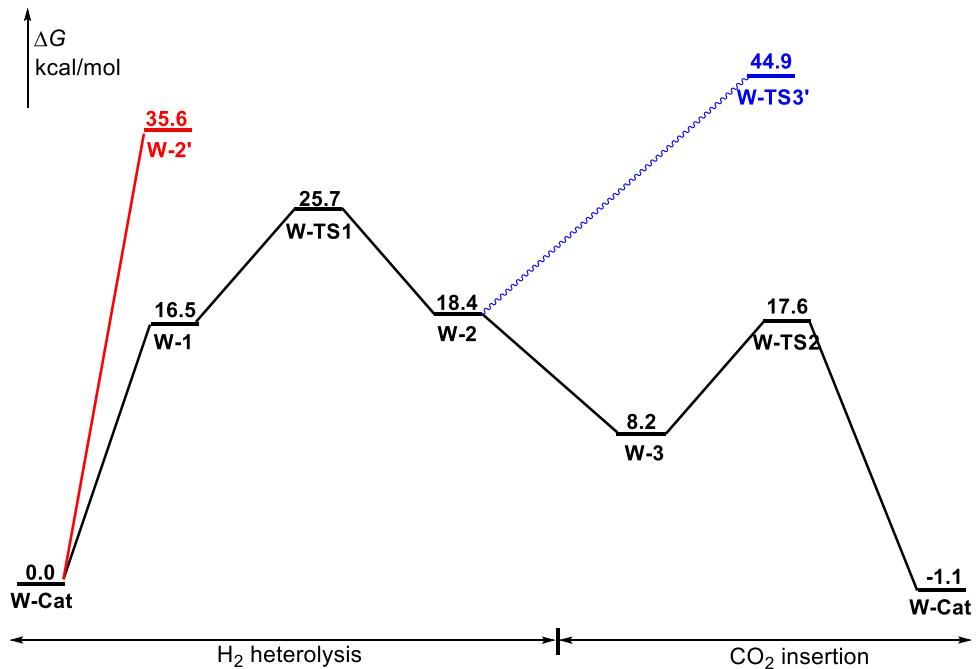


Fig. S6 PES for the Hydrogenation of  $\text{CO}_2$  to formic acid Catalysed by  $\text{W}^0\text{-NHC}$  Complexes along outer sphere (black), oxidative addition (red), and inner sphere (blue) mechanisms. Free energies

are shown in kcal/mol.

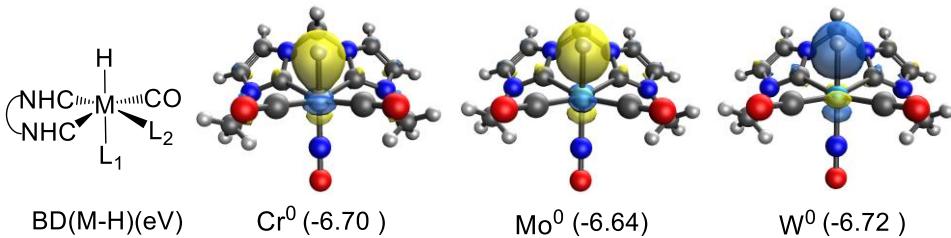


Fig. S7 M-H bond orbitals of Cr<sup>0</sup>, Mo<sup>0</sup>, and W<sup>0</sup> monohydride complexes.

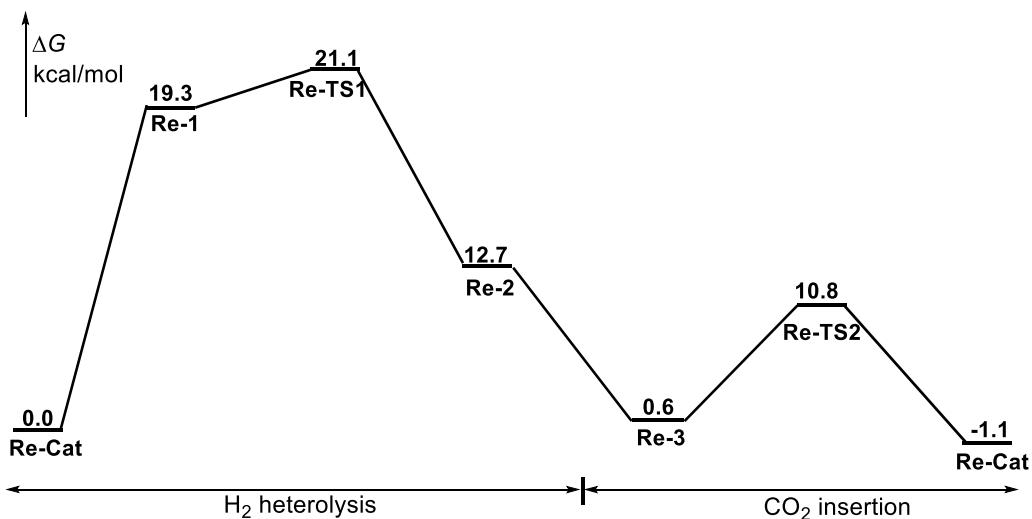


Fig. S8 PES for the Hydrogenation of CO<sub>2</sub> to formic acid Catalysed by Re<sup>I</sup>-NHC Complexes along outer-sphere mechanism. Free energies are shown in kcal/mol.

## References

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### **Cartesian coordinates of optimized reactants, intermediates and transition states**

#### **Mn-cat**

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.17609500  | 1.94374900  | 0.12107100  |
| N | 2.78202300  | 0.66227600  | -0.46024300 |
| C | -0.12046800 | 2.42691500  | 0.54519600  |
| C | 2.27340700  | 2.76351100  | -0.06893700 |
| C | 3.29148700  | 1.94800000  | -0.43351900 |
| C | 1.46992300  | 0.63422200  | -0.10567300 |
| C | -1.24101000 | 0.49139100  | -0.54363100 |
| C | -2.25561100 | 2.51925200  | -0.74542000 |
| C | -3.02140800 | 1.61125900  | -1.39683000 |
| N | -2.38378000 | 0.39037500  | -1.27226600 |
| N | -1.17718200 | 1.81777000  | -0.23753000 |
| H | -0.26780600 | 2.20369900  | 1.60411100  |
| H | -0.15405100 | 3.50400300  | 0.38593800  |
| C | -2.92982100 | -0.84345500 | -1.80345300 |
| H | -3.56260000 | -0.61127400 | -2.65998100 |
| H | -2.12398200 | -1.50073800 | -2.12935500 |
| H | -3.53043300 | -1.35535300 | -1.04716800 |
| H | 4.31850700  | 2.15920000  | -0.68639700 |
| H | 2.22109800  | 3.83243600  | 0.06519900  |
| H | -2.36673200 | 3.58262500  | -0.60294600 |
| H | -3.94580500 | 1.71837100  | -1.94247300 |
| C | -1.37435200 | 0.09361100  | 2.47134300  |
| O | -0.19014500 | -0.07184400 | 1.99880900  |
| C | -1.12096600 | -2.16820600 | 0.37042700  |
| O | -1.86553200 | -3.04667300 | 0.55767100  |
| C | 1.35538100  | -1.97837200 | 0.82897000  |
| O | 2.11742100  | -2.70464600 | 1.32862200  |
| C | 3.59763000  | -0.49301400 | -0.78421400 |
| H | 4.10167200  | -0.87111300 | 0.10862400  |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | 2.97778900  | -1.28247100 | -1.20681400 |
| H            | 4.34907500  | -0.20239200 | -1.51883200 |
| C            | 0.43407900  | -1.47261600 | -1.54208300 |
| O            | 0.63404900  | -1.84771500 | -2.63320100 |
| Mn           | 0.12196100  | -0.90084500 | 0.09286900  |
| O            | -1.67160200 | 0.78334900  | 3.44563800  |
| H            | -2.18900500 | -0.44981200 | 1.91778900  |
| <b>Mn-1</b>  |             |             |             |
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| N            | -2.59611000 | 0.60036500  | 0.48276400  |
| C            | -0.00129200 | 2.31238900  | -1.20098300 |
| C            | -2.25392500 | 2.67873700  | -0.15520500 |
| C            | -3.14700200 | 1.86942700  | 0.46341300  |
| C            | -1.38076400 | 0.58096900  | -0.11910400 |
| C            | 1.37916400  | 0.58277800  | -0.11683500 |
| C            | 2.25291900  | 2.67955900  | -0.15888300 |
| C            | 3.14761400  | 1.87065100  | 0.45794500  |
| N            | 2.59645700  | 0.60181700  | 0.48086400  |
| N            | 1.18317300  | 1.87347900  | -0.49653800 |
| H            | -0.00156100 | 1.89562300  | -2.21227100 |
| H            | -0.00146800 | 3.39885200  | -1.25721800 |
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| H            | 3.95335100  | -0.20252500 | 1.83408500  |
| H            | 2.58650700  | -1.25885900 | 1.44875600  |
| H            | 3.89800300  | -1.03439400 | 0.26637300  |
| H            | -4.11203200 | 2.07387300  | 0.89932300  |
| H            | -2.26975700 | 3.73380600  | -0.37723500 |
| H            | 2.26849000  | 3.73428800  | -0.38243100 |
| H            | 4.11396900  | 2.07526400  | 0.89080000  |
| C            | 1.27096400  | -2.14117100 | -0.75999200 |
| O            | 2.04821900  | -2.97168500 | -0.99330200 |
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| H            | -2.58331400 | -1.26159500 | 1.44800500  |
| H            | -3.94762700 | -0.20510800 | 1.84088900  |
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| O            | 0.00039300  | -1.41199500 | 2.47600200  |
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| H            | 0.40985300  | -0.37034700 | -2.03384300 |
| <b>Mn-2'</b> |             |             |             |
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|    |             |             |             |
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| C  | -3.08626200 | 1.55207700  | 0.00930500  |
| C  | -3.67090200 | 0.38788100  | 0.38893800  |
| C  | -1.56944000 | -0.11211300 | -0.27722700 |
| C  | 1.05183300  | 0.71545800  | -0.09139200 |
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| C  | 2.32357800  | 2.37510900  | 0.79202200  |
| N  | 2.20374300  | 1.01430100  | 0.56954400  |
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| H  | 3.83500400  | 0.51711400  | 1.74705700  |
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| H  | 3.85656300  | -0.20830200 | 0.12748600  |
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| H  | 3.17917100  | 2.79206700  | 1.29943100  |
| C  | 1.78468900  | -1.77461000 | -1.04982500 |
| O  | 2.77050400  | -2.35616500 | -1.28832800 |
| C  | -2.95080400 | -2.00401400 | 0.54876200  |
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| H  | -2.12115900 | -2.59702400 | 0.16279000  |
| H  | -3.01244200 | -2.12722000 | 1.63255000  |
| C  | 0.28527900  | -1.61017300 | 0.96464800  |
| O  | 0.32433500  | -2.02222200 | 2.05840600  |
| Mn | 0.23352900  | -0.96730100 | -0.67023500 |
| H  | 0.48240900  | -0.54234800 | -2.38371400 |
| H  | -0.24469800 | -0.23296300 | -2.23448600 |

### Mn-TS1

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| N | 2.92083100  | 0.84455800 | -0.17867900 |
| C | -0.20523400 | 2.34766800 | 0.53138100  |
| C | 2.21182200  | 2.89906300 | 0.15881400  |
| C | 3.32066600  | 2.16629000 | -0.10986100 |
| C | 1.58862200  | 0.71536400 | 0.05060300  |
| C | -1.04222400 | 0.37682400 | -0.69104600 |
| C | -2.13662500 | 2.33186000 | -1.06075100 |
| C | -2.76185700 | 1.36731200 | -1.78101900 |
| N | -2.07671900 | 0.18942200 | -1.55154200 |
| N | -1.08627700 | 1.70877200 | -0.42213500 |
| H | -0.49856900 | 2.02717400 | 1.53728200  |

|             |             |             |             |
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| H           | -1.65191000 | -1.74214600 | -2.23748500 |
| H           | -3.22883300 | -1.55933300 | -1.42708100 |
| H           | 4.34653400  | 2.45902900  | -0.26936400 |
| H           | 2.06429700  | 3.95969100  | 0.28809500  |
| H           | -2.33272900 | 3.38670200  | -0.95008300 |
| H           | -3.61503100 | 1.40877200  | -2.43955300 |
| C           | -2.65443600 | 0.26396000  | 1.93287800  |
| O           | -1.98886600 | -0.70693500 | 2.38769300  |
| C           | -0.92381100 | -2.19895000 | 0.35755300  |
| O           | -1.63783300 | -3.11176200 | 0.42608300  |
| C           | 1.53772000  | -1.89835700 | 1.02365800  |
| O           | 2.29213800  | -2.58417200 | 1.58487900  |
| C           | 3.85291500  | -0.24520200 | -0.40259400 |
| H           | 4.26861200  | -0.59547400 | 0.54517300  |
| H           | 3.35160300  | -1.07148600 | -0.90446700 |
| H           | 4.66581700  | 0.10829100  | -1.03710400 |
| C           | 0.81487000  | -1.53919900 | -1.38797300 |
| O           | 1.13985800  | -1.94789500 | -2.43492900 |
| Mn          | 0.32562800  | -0.89302200 | 0.14609500  |
| O           | -2.61160600 | 1.46878300  | 2.25014500  |
| H           | -3.40941600 | -0.01406800 | 1.12522300  |
| H           | -0.08317500 | 0.07556900  | 2.64504000  |
| H           | 0.65837500  | 0.23090400  | 2.55596000  |
| <b>Mn-2</b> |             |             |             |
| N           | -1.03403000 | 2.06881200  | -0.13547200 |
| N           | -2.90558100 | 1.06601700  | 0.08847300  |
| C           | 0.37364400  | 2.28351400  | -0.36722200 |
| C           | -1.98297500 | 3.06254000  | 0.02351700  |
| C           | -3.16976600 | 2.42397900  | 0.16057700  |
| C           | -1.58044400 | 0.82113500  | -0.10308000 |
| C           | 0.94698000  | 0.15795900  | 0.73125000  |
| C           | 2.24116400  | 1.95403400  | 1.27925700  |
| C           | 2.72844800  | 0.87836700  | 1.94418300  |
| N           | 1.92304500  | -0.19739000 | 1.61078900  |
| N           | 1.15935600  | 1.49292200  | 0.55291000  |
| H           | 0.63150300  | 1.98278400  | -1.38765500 |
| H           | 0.60695500  | 3.33746600  | -0.22211800 |
| C           | 2.16035100  | -1.54353300 | 2.08926500  |
| H           | 2.64237100  | -1.49664900 | 3.06624600  |
| H           | 1.21325500  | -2.07496000 | 2.18385100  |
| H           | 2.80859800  | -2.09059000 | 1.39912600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.16919700 | 2.80238700  | 0.30796000  |
| H  | -1.72468100 | 4.10961500  | 0.02470100  |
| H  | 2.55220500  | 2.98645300  | 1.25397000  |
| H  | 3.55295100  | 0.78014900  | 2.63293500  |
| C  | 3.45130200  | 0.63101400  | -1.83965100 |
| O  | 2.84562900  | -0.51537500 | -1.55060100 |
| C  | 0.56567600  | -2.32190500 | -0.50844800 |
| O  | 1.19579700  | -3.28629200 | -0.71331500 |
| C  | -1.69154000 | -1.58626100 | -1.37781900 |
| O  | -2.45382100 | -2.02575700 | -2.14836000 |
| C  | -3.94934400 | 0.06388300  | 0.17801400  |
| H  | -4.48227100 | -0.02334500 | -0.77251000 |
| H  | -3.51140700 | -0.90087600 | 0.42816400  |
| H  | -4.65865700 | 0.34767800  | 0.95696400  |
| C  | -1.19206200 | -1.58331200 | 1.23987000  |
| O  | -1.64767300 | -2.04862400 | 2.21419900  |
| Mn | -0.49043600 | -0.90653700 | -0.25042900 |
| O  | 2.91169200  | 1.69051700  | -2.07711900 |
| H  | 4.54407500  | 0.48248300  | -1.84347300 |
| H  | 1.86344400  | -0.37445100 | -1.51394900 |
| H  | 0.17061000  | -0.18148400 | -1.56709600 |

### Mn-3

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|---|-------------|-------------|-------------|
| N | -1.51383300 | 1.67809500  | -0.84811600 |
| N | -3.07058500 | 0.38272400  | -0.17240700 |
| C | -0.19547700 | 2.15254000  | -1.19246700 |
| C | -2.69606600 | 2.36928100  | -1.04190600 |
| C | -3.68265400 | 1.54353000  | -0.61780500 |
| C | -1.71723300 | 0.44029800  | -0.31265300 |
| C | 0.83159700  | 0.82017900  | 0.59277100  |
| C | 1.54171500  | 2.98303900  | 0.42272400  |
| C | 2.23981300  | 2.39914000  | 1.42667900  |
| N | 1.78857000  | 1.09294800  | 1.52126100  |
| N | 0.69357300  | 2.00633800  | -0.06577200 |
| H | 0.19225500  | 1.55123300  | -2.02360100 |
| H | -0.25186300 | 3.20207200  | -1.47724200 |
| C | 2.33879200  | 0.13506000  | 2.45695900  |
| H | 2.62213400  | 0.64953900  | 3.37623600  |
| H | 1.59052000  | -0.62290900 | 2.68546200  |
| H | 3.22312800  | -0.35278000 | 2.03663700  |
| H | -4.75288200 | 1.67345900  | -0.57979800 |
| H | -2.71958900 | 3.36747200  | -1.45028200 |
| H | 1.55818400  | 3.98481500  | 0.02287600  |
| H | 2.99555000  | 2.78941800  | 2.09021900  |
| C | 1.26943200  | -1.84657500 | 0.22007500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | 2.23959100  | -2.50380000 | 0.24119000  |
| C  | -1.10718100 | -2.20948000 | -0.63235800 |
| O  | -1.66085400 | -3.09850500 | -1.15653400 |
| C  | -3.81319600 | -0.74700000 | 0.34744100  |
| H  | -4.23466300 | -1.34215500 | -0.46711000 |
| H  | -3.14866200 | -1.37382500 | 0.94004500  |
| H  | -4.62648400 | -0.38840200 | 0.98047000  |
| C  | -0.75461500 | -1.22329600 | 1.77962300  |
| O  | -1.09996700 | -1.51150200 | 2.86419200  |
| Mn | -0.21263100 | -0.86885400 | 0.11991200  |
| H  | 0.27490700  | -0.48825300 | -1.37658800 |
| C  | 2.98147000  | -0.50516900 | -2.13086800 |
| O  | 2.72011900  | -1.31165400 | -2.93598400 |
| O  | 3.28746000  | 0.31066600  | -1.35151200 |

### Mn-TS2

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.09340400  | 1.89930000  | 0.29921400  |
| N | 2.34060100  | 0.93206200  | -1.13834300 |
| C | 0.02973400  | 2.13227800  | 1.24815300  |
| C | 2.13660800  | 2.77068000  | 0.05125500  |
| C | 2.92807800  | 2.15396400  | -0.85937900 |
| C | 1.20195700  | 0.74557000  | -0.41732100 |
| C | -1.49903500 | 0.63778400  | 0.03207400  |
| C | -2.36419100 | 2.64234900  | 0.69070000  |
| C | -3.35186700 | 1.95144400  | 0.07184000  |
| N | -2.80712500 | 0.74198400  | -0.32638200 |
| N | -1.25016900 | 1.82421900  | 0.65465500  |
| H | 0.18737700  | 1.49592900  | 2.12397100  |
| H | 0.04241300  | 3.17888200  | 1.54732400  |
| C | -3.58131900 | -0.28832700 | -0.99060100 |
| H | -4.35358800 | 0.18222100  | -1.59972400 |
| H | -2.93427000 | -0.88375600 | -1.63344900 |
| H | -4.05801500 | -0.94511900 | -0.25824300 |
| H | 3.83865300  | 2.47072500  | -1.34358900 |
| H | 2.20987600  | 3.73314300  | 0.53259700  |
| H | -2.34480600 | 3.62165400  | 1.14253900  |
| H | -4.38002900 | 2.20611300  | -0.13172600 |
| C | -1.24552600 | -2.10185300 | 0.20945600  |
| O | -1.96247900 | -2.96228400 | 0.54041400  |
| C | 1.25791700  | -1.97847200 | -0.23065100 |
| O | 2.12867700  | -2.75425100 | -0.15978300 |
| C | 2.91769000  | -0.02178000 | -2.06556900 |
| H | 3.68131700  | -0.62863100 | -1.57231000 |
| H | 2.13834700  | -0.67636100 | -2.45409100 |
| H | 3.37705000  | 0.51666700  | -2.89544700 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | -0.40191200 | -0.96605000 | -1.99536700 |
| O            | -0.60071200 | -1.08566100 | -3.14390300 |
| Mn           | -0.09636600 | -0.81662400 | -0.25488300 |
| H            | 0.18113000  | -0.59164100 | 1.39035200  |
| C            | 1.00103800  | -0.98199900 | 2.66835600  |
| O            | 0.36120900  | -1.85137800 | 3.18481300  |
| O            | 1.94976800  | -0.24901500 | 2.65623200  |
| <b>Mn-4'</b> |             |             |             |
| N            | -1.78647500 | 1.23261400  | -0.41156600 |
| N            | -2.75967700 | -0.56813100 | 0.19641200  |
| C            | -0.76019700 | 2.09734100  | -0.94874000 |
| C            | -3.06479800 | 1.59969700  | -0.03077600 |
| C            | -3.68286000 | 0.45378500  | 0.34958100  |
| C            | -1.57341900 | -0.10678900 | -0.28049900 |
| C            | 1.05233900  | 0.67341100  | -0.05814400 |
| C            | 1.25321200  | 2.92595400  | 0.30565200  |
| C            | 2.34216100  | 2.32566000  | 0.83991800  |
| N            | 2.20385800  | 0.96413600  | 0.62116300  |
| N            | 0.47956500  | 1.91014100  | -0.23353600 |
| H            | -0.60582600 | 1.83819700  | -2.00313800 |
| H            | -1.07479700 | 3.13592000  | -0.85752700 |
| C            | 3.18868800  | -0.00717400 | 1.04694600  |
| H            | 3.68165800  | 0.35631300  | 1.94970600  |
| H            | 2.69980900  | -0.95703100 | 1.26163400  |
| H            | 3.94352800  | -0.16788100 | 0.27224200  |
| H            | -4.68262100 | 0.27256500  | 0.71287800  |
| H            | -3.40883400 | 2.62140700  | -0.07054700 |
| H            | 0.95404800  | 3.96118500  | 0.25720700  |
| H            | 3.19508500  | 2.73281200  | 1.36038100  |
| C            | 1.75673500  | -1.66469000 | -1.19773000 |
| O            | 2.77183300  | -2.12676500 | -1.57798900 |
| C            | -3.01768500 | -1.95186700 | 0.53954800  |
| H            | -2.15906200 | -2.55274300 | 0.23793000  |
| H            | -3.16978400 | -2.05808000 | 1.61695900  |
| H            | -3.90789400 | -2.31118000 | 0.01877700  |
| C            | 0.31087600  | -1.71254600 | 0.94574200  |
| O            | 0.37183200  | -2.22193600 | 2.00883700  |
| Mn           | 0.22323000  | -0.97030700 | -0.65091400 |
| H            | 0.01341100  | -0.39222800 | -2.20674900 |
| <b>Mn-5'</b> |             |             |             |
| N            | -1.36388800 | 1.74535600  | -0.64233700 |
| N            | -2.83557500 | 0.45157900  | 0.22368500  |
| C            | -0.12400500 | 2.20474700  | -1.21763700 |
| C            | -2.52281200 | 2.49614300  | -0.53344100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.45145700 | 1.67451100  | 0.00970300  |
| C  | -1.53051600 | 0.46162500  | -0.18428500 |
| C  | 1.18278300  | 0.67749500  | 0.17701600  |
| C  | 1.92922300  | 2.83386800  | 0.10490600  |
| C  | 2.78090300  | 2.13226900  | 0.89309900  |
| N  | 2.30762800  | 0.83071800  | 0.93256700  |
| N  | 0.97497100  | 1.93001200  | -0.32069100 |
| H  | 0.05400000  | 1.66665200  | -2.15615400 |
| H  | -0.18456600 | 3.27681400  | -1.39885000 |
| C  | 2.95473200  | -0.22829300 | 1.68119900  |
| H  | 3.17385200  | 0.11200700  | 2.69503600  |
| H  | 2.28786200  | -1.08907600 | 1.72739000  |
| H  | 3.89155200  | -0.52420700 | 1.19957300  |
| H  | -4.48450800 | 1.84324200  | 0.27127700  |
| H  | -2.56918000 | 3.52758800  | -0.84548300 |
| H  | 1.91317000  | 3.87213200  | -0.18706500 |
| H  | 3.66521900  | 2.43445600  | 1.43222800  |
| C  | -1.17764400 | -2.17585900 | -0.69036600 |
| O  | -1.86454600 | -3.07085900 | -1.02810300 |
| C  | -3.52483900 | -0.70144100 | 0.76273700  |
| H  | -3.87724900 | -1.35549900 | -0.03924600 |
| H  | -2.85427700 | -1.26866000 | 1.40866100  |
| H  | -4.38212000 | -0.36321900 | 1.34574500  |
| C  | -0.29428400 | -1.26514000 | 1.52855500  |
| O  | -0.43035000 | -1.56041300 | 2.66314600  |
| Mn | -0.11091900 | -0.86227700 | -0.17897800 |
| H  | 0.16345900  | -0.52088400 | -1.79194600 |
| C  | 2.40282900  | -1.62741500 | -1.31741500 |
| O  | 1.80470500  | -2.23940900 | -0.50862200 |
| O  | 3.07073200  | -1.08596100 | -2.10438600 |

#### Mn-TS3'

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -0.96575000 | 1.93867500 | -0.76264700 |
| N | -2.53539500 | 1.01473500 | 0.36090900  |
| C | 0.27648000  | 2.12196500 | -1.47168300 |
| C | -1.96356000 | 2.89074000 | -0.63966500 |
| C | -2.95661000 | 2.30144600 | 0.06644700  |
| C | -1.29482400 | 0.75836200 | -0.14937800 |
| C | 1.41280800  | 0.56874900 | 0.03120300  |
| C | 2.52560300  | 2.51336600 | -0.39416100 |
| C | 3.30194100  | 1.76656900 | 0.42924300  |
| N | 2.60592200  | 0.59537500 | 0.68325700  |
| N | 1.38635800  | 1.76359100 | -0.62027800 |
| H | 0.28292800  | 1.46706200 | -2.35078800 |

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | 0.36982300   | 3.16395000  | -1.77390100 |
| C  | 3.10424300   | -0.45178500 | 1.55216600  |
| H  | 3.46006200   | -0.01643200 | 2.48807200  |
| H  | 2.29641800   | -1.15094300 | 1.76062600  |
| H  | 3.92660600   | -0.99080700 | 1.07564900  |
| H  | -3.91479000  | 2.67293600  | 0.39416100  |
| H  | -1.866691000 | 3.87916700  | -1.06011200 |
| H  | 2.67180400   | 3.48844900  | -0.83137500 |
| H  | 4.27093800   | 1.95963500  | 0.86270900  |
| C  | -1.42974000  | -1.94637500 | -0.28409100 |
| O  | -2.30333800  | -2.72338800 | -0.41598900 |
| C  | -3.35048900  | 0.06457300  | 1.08958100  |
| H  | -3.82208700  | -0.64790300 | 0.40886800  |
| H  | -2.73874800  | -0.48424600 | 1.80643200  |
| H  | -4.12737200  | 0.60712300  | 1.62825500  |
| C  | -0.23396000  | -0.97467000 | 1.70042500  |
| O  | -0.34070900  | -1.12043300 | 2.86319100  |
| Mn | -0.10003200  | -0.79683200 | -0.05660600 |
| H  | 0.13237500   | -0.59412700 | -1.67992700 |
| C  | 0.92065400   | -2.48384200 | -1.37444300 |
| O  | 1.53759100   | -2.27610600 | -0.36201000 |
| O  | 0.63727000   | -3.05435800 | -2.36970000 |

#### Mn-6'

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.04371100 | 1.83888200  | -0.73585900 |
| N | -2.66140800 | 0.82504300  | 0.23037200  |
| C | 0.25769000  | 2.10373800  | -1.30698400 |
| C | -2.09081500 | 2.74259100  | -0.68847200 |
| C | -3.11366400 | 2.09652000  | -0.07893400 |
| C | -1.37319800 | 0.63165800  | -0.17432300 |
| C | 1.32397900  | 0.53702900  | 0.23109000  |
| C | 2.37539300  | 2.54374000  | 0.01111300  |
| C | 3.10975300  | 1.78142300  | 0.86086100  |
| N | 2.45388700  | 0.56735800  | 0.97799400  |
| N | 1.29415600  | 1.76352200  | -0.35528600 |
| H | 0.39267500  | 1.49555700  | -2.20780100 |
| H | 0.33126800  | 3.15916600  | -1.56412700 |
| C | 2.90030400  | -0.52369000 | 1.82228400  |
| H | 2.68237700  | -0.31274100 | 2.87258400  |
| H | 2.38240300  | -1.43108300 | 1.51271900  |
| H | 3.97645600  | -0.66210400 | 1.70519900  |
| H | -4.11224000 | 2.41976900  | 0.17036100  |
| H | -2.00585900 | 3.74107400  | -1.08740000 |
| H | 2.52218300  | 3.54318400  | -0.36740400 |
| H | 4.02750500  | 1.98908700  | 1.38887200  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| C             | -1.35187800 | -2.12752300 | -0.34591900 |
| O             | -2.16089500 | -2.96706500 | -0.48975400 |
| C             | -3.48519100 | -0.17462700 | 0.87908400  |
| H             | -3.89585200 | -0.87631200 | 0.14911100  |
| H             | -2.89590500 | -0.72847700 | 1.61037400  |
| H             | -4.30716300 | 0.32432400  | 1.39236400  |
| C             | -0.32083500 | -1.11106400 | 1.65521700  |
| O             | -0.44740400 | -1.27477900 | 2.81528200  |
| Mn            | -0.11575000 | -0.88586500 | -0.05068900 |
| H             | 0.41483400  | -0.87146500 | -1.84884000 |
| C             | 1.30598300  | -1.65425600 | -1.80138300 |
| O             | 1.48762200  | -2.14402400 | -0.65180400 |
| O             | 1.85261100  | -1.82416300 | -2.88136600 |
| <b>Cr-cat</b> |             |             |             |
| N             | 1.15959100  | 1.99151400  | 0.14877200  |
| N             | 2.77845700  | 0.75755200  | -0.49211000 |
| C             | -0.14467800 | 2.43341800  | 0.59752600  |
| C             | 2.23365300  | 2.83959400  | -0.05264200 |
| C             | 3.26102400  | 2.05321900  | -0.45680500 |
| C             | 1.47745400  | 0.69341200  | -0.10781100 |
| C             | -1.24741700 | 0.52186600  | -0.55240600 |
| C             | -2.27564600 | 2.54685600  | -0.70523200 |
| C             | -3.02874500 | 1.65154700  | -1.38981600 |
| N             | -2.38213100 | 0.43319600  | -1.29282600 |
| N             | -1.19608700 | 1.83947400  | -0.20737200 |
| H             | -0.28436100 | 2.16241500  | 1.64721300  |
| H             | -0.19911100 | 3.51555500  | 0.48472700  |
| C             | -2.91069800 | -0.79874500 | -1.84639900 |
| H             | -3.52435600 | -0.56538300 | -2.71657900 |
| H             | -2.09178400 | -1.44902200 | -2.15318500 |
| H             | -3.52628800 | -1.31754800 | -1.10633100 |
| H             | 4.27659400  | 2.29255300  | -0.73056300 |
| H             | 2.16165500  | 3.90495200  | 0.10057100  |
| H             | -2.39674900 | 3.60520500  | -0.53524800 |
| H             | -3.94791800 | 1.76849800  | -1.94249900 |
| C             | -1.39118600 | 0.08061000  | 2.43690500  |
| O             | -0.20455900 | -0.13645000 | 1.98832300  |
| C             | -1.16427100 | -2.22989000 | 0.41976300  |
| O             | -1.91242500 | -3.09852200 | 0.62223000  |
| C             | 1.42878300  | -2.01271300 | 0.90375600  |
| O             | 2.19400200  | -2.71481700 | 1.42661400  |
| C             | 3.59870000  | -0.38572200 | -0.84518900 |
| H             | 4.08502900  | -0.79933200 | 0.04198000  |
| H             | 2.98252900  | -1.15450200 | -1.30988300 |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | 4.36477800  | -0.06953800 | -1.55362500 |
| O             | 0.63453500  | -2.08962700 | -2.51273900 |
| O             | -1.68560000 | 0.84582400  | 3.35303800  |
| H             | -2.20955300 | -0.48976900 | 1.91904000  |
| Cr            | 0.14377800  | -0.92856700 | 0.06222000  |
| N             | 0.44437100  | -1.58322900 | -1.45196600 |
| <b>Cr-1</b>   |             |             |             |
| N             | -1.20432400 | 1.90387700  | -0.50121700 |
| N             | -2.60192000 | 0.65278900  | 0.52112800  |
| C             | -0.02217100 | 2.33778800  | -1.21466200 |
| C             | -2.26867500 | 2.71671400  | -0.16264300 |
| C             | -3.15391700 | 1.92033300  | 0.48476000  |
| C             | -1.39279600 | 0.61974600  | -0.09225800 |
| C             | 1.38025300  | 0.64561600  | -0.09262800 |
| C             | 2.22070900  | 2.75587000  | -0.16856300 |
| C             | 3.12275000  | 1.97390600  | 0.47393600  |
| N             | 2.59203700  | 0.69800400  | 0.51366300  |
| N             | 1.16787300  | 1.92597500  | -0.50050000 |
| H             | -0.01777200 | 1.89821600  | -2.21590100 |
| H             | -0.03169300 | 3.42273700  | -1.29485900 |
| C             | 3.29106000  | -0.43523100 | 1.09295300  |
| H             | 3.99385400  | -0.07145600 | 1.84203700  |
| H             | 2.58218900  | -1.10799600 | 1.57411100  |
| H             | 3.84502400  | -0.97767400 | 0.32315700  |
| H             | -4.11191700 | 2.13556100  | 0.93139900  |
| H             | -2.28870800 | 3.76713900  | -0.40575500 |
| H             | 2.22288600  | 3.80630400  | -0.41219500 |
| H             | 4.07948200  | 2.20501900  | 0.91532300  |
| C             | 1.35152000  | -2.16331900 | -0.83553000 |
| O             | 2.13400300  | -2.97330900 | -1.11222400 |
| C             | -1.31781600 | -2.16317600 | -0.85867800 |
| O             | -2.10684400 | -2.95847900 | -1.15834300 |
| C             | -3.28404800 | -0.48309000 | 1.11446100  |
| H             | -4.01377100 | -0.89798000 | 0.41496600  |
| H             | -2.56153900 | -1.25271200 | 1.37974600  |
| H             | -3.80150500 | -0.15992600 | 2.01802900  |
| O             | 0.02143500  | -1.82783300 | 2.34959600  |
| Cr            | 0.01208500  | -0.92940600 | -0.35765500 |
| N             | 0.01395000  | -1.44597100 | 1.23352500  |
| H             | -0.33970800 | -0.48577200 | -2.23714400 |
| H             | 0.42986100  | -0.39241900 | -2.19451400 |
| <b>Cr-TS1</b> |             |             |             |
| N             | -1.08678700 | 2.06696500  | -0.25181900 |
| N             | -2.90129900 | 1.02342100  | 0.18222800  |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| C           | 0.31118200  | 2.34527700  | -0.51896900 |
| C           | -2.07665400 | 3.02757000  | -0.18306400 |
| C           | -3.22689700 | 2.36276400  | 0.09089800  |
| C           | -1.57852900 | 0.81501300  | -0.03699300 |
| C           | 1.03176100  | 0.33927200  | 0.72329100  |
| C           | 2.21210100  | 2.23924300  | 1.10896800  |
| C           | 2.77057000  | 1.24989500  | 1.85094200  |
| N           | 2.03415700  | 0.10591500  | 1.60773600  |
| N           | 1.14830700  | 1.66465700  | 0.44674200  |
| H           | 0.60202500  | 2.01203800  | -1.52053000 |
| H           | 0.47670400  | 3.41835500  | -0.43345200 |
| C           | 2.37004100  | -1.18925600 | 2.16574300  |
| H           | 2.81169800  | -1.05120800 | 3.15290800  |
| H           | 1.47124800  | -1.79709400 | 2.26331400  |
| H           | 3.08893400  | -1.70545400 | 1.52309000  |
| H           | -4.23517600 | 2.71631600  | 0.23935800  |
| H           | -1.86975200 | 4.07621600  | -0.32849600 |
| H           | 2.46413300  | 3.28216700  | 0.99785700  |
| H           | 3.60690400  | 1.25579600  | 2.53233500  |
| C           | 2.86461000  | 0.33521500  | -1.83151400 |
| O           | 2.28621600  | -0.70067600 | -2.25599400 |
| C           | 0.88154400  | -2.28317700 | -0.44744700 |
| O           | 1.56181000  | -3.21535800 | -0.54751900 |
| C           | -1.67302800 | -1.84547500 | -1.17718900 |
| O           | -2.43821500 | -2.46608400 | -1.79302600 |
| C           | -3.88170800 | -0.02221200 | 0.40981900  |
| H           | -4.27039700 | -0.39598800 | -0.54062300 |
| H           | -3.42700700 | -0.84303300 | 0.96334600  |
| H           | -4.70718100 | 0.38520300  | 0.99352700  |
| O           | -1.32382900 | -2.17296000 | 2.25277600  |
| O           | 2.72377900  | 1.52387800  | -2.18415300 |
| H           | 3.64044800  | 0.14775800  | -1.01590400 |
| H           | 0.34400500  | -0.01996000 | -2.52420400 |
| H           | -0.40732600 | 0.12214000  | -2.58281900 |
| Cr          | -0.41112700 | -0.91822900 | -0.12932900 |
| N           | -0.94155800 | -1.65537800 | 1.25519900  |
| <b>Cr-2</b> |             |             |             |
| N           | -0.95120700 | 2.13247500  | -0.10226900 |
| N           | -2.86816000 | 1.22849000  | 0.14797800  |
| C           | 0.46324600  | 2.27796300  | -0.35231900 |
| C           | -1.84625400 | 3.17439700  | 0.06062600  |
| C           | -3.06296000 | 2.59784700  | 0.21683700  |
| C           | -1.56088000 | 0.91534400  | -0.05634900 |
| C           | 0.95896300  | 0.13898400  | 0.76955900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.34618500  | 1.87968600  | 1.26119400  |
| C  | 2.79213600  | 0.79387800  | 1.94003300  |
| N  | 1.93183300  | -0.24665100 | 1.63741900  |
| N  | 1.22912200  | 1.45932900  | 0.56327300  |
| H  | 0.69343200  | 1.96302000  | -1.37495700 |
| H  | 0.74630000  | 3.32104300  | -0.21803100 |
| C  | 2.10893700  | -1.59955900 | 2.12372300  |
| H  | 2.55193500  | -1.57104700 | 3.11986600  |
| H  | 1.14024600  | -2.09701200 | 2.17519700  |
| H  | 2.76665500  | -2.16462800 | 1.45694300  |
| H  | -4.03950600 | 3.02742800  | 0.37691200  |
| H  | -1.53614800 | 4.20735000  | 0.05361800  |
| H  | 2.70573200  | 2.89563900  | 1.21242200  |
| H  | 3.62127400  | 0.67033300  | 2.61927200  |
| C  | 3.47699100  | 0.62116700  | -1.80826200 |
| O  | 2.84421700  | -0.51278400 | -1.52780900 |
| C  | 0.55450700  | -2.36605300 | -0.57587900 |
| O  | 1.19307800  | -3.30717800 | -0.83916000 |
| C  | -1.77186200 | -1.50357800 | -1.47838000 |
| O  | -2.50537400 | -1.86672900 | -2.31021400 |
| C  | -3.95091100 | 0.26862200  | 0.23701100  |
| H  | -4.44840700 | 0.15946700  | -0.73045400 |
| H  | -3.55580900 | -0.69818700 | 0.54624000  |
| H  | -4.67995600 | 0.61104800  | 0.97264000  |
| O  | -1.80065400 | -2.37924600 | 1.97146200  |
| O  | 2.96229500  | 1.68447900  | -2.08113600 |
| H  | 4.56669800  | 0.45663600  | -1.76906200 |
| H  | 1.86389300  | -0.35778700 | -1.53078200 |
| H  | 0.16139100  | -0.25648200 | -1.59827100 |
| Cr | -0.56335500 | -0.92814500 | -0.19126900 |
| N  | -1.28934300 | -1.72105400 | 1.11745600  |

### Cr-3

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.51095400 | 1.71849900 | -0.83083300 |
| N | -3.09594900 | 0.45398600 | -0.16216200 |
| C | -0.17929400 | 2.17288600 | -1.15938900 |
| C | -2.67874000 | 2.43438300 | -1.02445900 |
| C | -3.68348000 | 1.62866000 | -0.60218300 |
| C | -1.74285100 | 0.48482100 | -0.29866800 |
| C | 0.81579600  | 0.83311100 | 0.64085800  |
| C | 1.52906800  | 2.99518800 | 0.49459300  |
| C | 2.19887500  | 2.40909300 | 1.51764400  |
| N | 1.74726900  | 1.10245000 | 1.59377600  |
| N | 0.69535400  | 2.01918000 | -0.02032300 |
| H | 0.21085000  | 1.56624300 | -1.98539300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.21794800 | 3.22203900  | -1.44804200 |
| C  | 2.26622200  | 0.12843400  | 2.53185600  |
| H  | 2.52236000  | 0.62578600  | 3.46840100  |
| H  | 1.50738500  | -0.63083400 | 2.72086600  |
| H  | 3.16190400  | -0.35536100 | 2.13043500  |
| H  | -4.75080900 | 1.78167700  | -0.56406500 |
| H  | -2.68204100 | 3.43316200  | -1.43226700 |
| H  | 1.55827800  | 3.99767500  | 0.09712100  |
| H  | 2.93500800  | 2.79956500  | 2.20272600  |
| C  | 1.33366400  | -1.87140000 | 0.13890200  |
| O  | 2.32704400  | -2.48717300 | 0.09648900  |
| C  | -1.14298500 | -2.19992800 | -0.81307800 |
| O  | -1.68784100 | -3.00504800 | -1.46097500 |
| C  | -3.85386500 | -0.66837900 | 0.35271600  |
| H  | -4.37500300 | -1.18417300 | -0.45841500 |
| H  | -3.17140000 | -1.36443100 | 0.83889600  |
| H  | -4.58889000 | -0.31642000 | 1.07877900  |
| O  | -1.06497900 | -1.94233800 | 2.73509300  |
| H  | 0.28191500  | -0.57209400 | -1.40504800 |
| C  | 3.08419200  | -0.40665000 | -2.12153600 |
| O  | 2.81684100  | -1.20467000 | -2.93257300 |
| O  | 3.38962900  | 0.39969800  | -1.33203700 |
| Cr | -0.24755300 | -0.90572000 | 0.16694200  |
| N  | -0.74650700 | -1.43563000 | 1.69923900  |

### Cr-TS2

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.10641400  | 1.92415200  | 0.35993600  |
| N | 2.36282500  | 1.03133700  | -1.11677500 |
| C | 0.03353900  | 2.10491700  | 1.31271400  |
| C | 2.12907000  | 2.82589200  | 0.13209600  |
| C | 2.92601600  | 2.25616100  | -0.80496100 |
| C | 1.23290800  | 0.79881900  | -0.39757300 |
| C | -1.49228700 | 0.69355700  | -0.00541100 |
| C | -2.34733200 | 2.67139900  | 0.73902900  |
| C | -3.32617100 | 2.03212600  | 0.05257200  |
| N | -2.78645000 | 0.83846200  | -0.39488900 |
| N | -1.24395300 | 1.83900000  | 0.68907600  |
| H | 0.18079000  | 1.41464600  | 2.14836100  |
| H | 0.04701200  | 3.13168000  | 1.67431300  |
| C | -3.54559000 | -0.14336500 | -1.14403600 |
| H | -4.20231500 | 0.36607900  | -1.85043600 |
| H | -2.86117900 | -0.78813300 | -1.69342500 |
| H | -4.15396600 | -0.75449400 | -0.47181200 |
| H | 3.82616300  | 2.60854200  | -1.28420200 |
| H | 2.18735300  | 3.77284000  | 0.64549600  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | -2.32866800 | 3.62287600  | 1.24692600  |
| H             | -4.34385200 | 2.31466100  | -0.16711200 |
| C             | -1.28584400 | -2.12402100 | 0.22543100  |
| O             | -2.01170800 | -2.95501900 | 0.59963800  |
| C             | 1.33390200  | -2.01368600 | -0.18823100 |
| O             | 2.20061900  | -2.78167600 | -0.05112600 |
| C             | 2.95213200  | 0.10862500  | -2.06743200 |
| H             | 3.77960600  | -0.43917900 | -1.60879900 |
| H             | 2.19545900  | -0.59981000 | -2.40211300 |
| H             | 3.32897700  | 0.66340400  | -2.92795900 |
| O             | -0.49657300 | -1.37181500 | -3.14682400 |
| H             | 0.16704700  | -0.70996500 | 1.38633100  |
| C             | 0.87410500  | -1.09123900 | 2.75161900  |
| O             | 0.18972000  | -1.96179900 | 3.20209800  |
| O             | 1.81705100  | -0.35525400 | 2.81554500  |
| Cr            | -0.08637600 | -0.82173100 | -0.35193600 |
| N             | -0.33154700 | -1.08898100 | -2.00001500 |
| <b>Fe-cat</b> |             |             |             |
| N             | 1.19100800  | 1.90514200  | 0.22146500  |
| N             | 2.78376800  | 0.61844800  | -0.39831900 |
| C             | -0.10462500 | 2.39394400  | 0.64051400  |
| C             | 2.30892300  | 2.70777100  | 0.09934600  |
| C             | 3.31600100  | 1.89066500  | -0.29009500 |
| C             | 1.46849500  | 0.60749000  | -0.06929200 |
| C             | -1.22224900 | 0.52084700  | -0.54955000 |
| C             | -2.24279000 | 2.54445800  | -0.64404000 |
| C             | -3.01247800 | 1.66314000  | -1.32665800 |
| N             | -2.36889800 | 0.44032700  | -1.26823900 |
| N             | -1.15406000 | 1.82783000  | -0.18285100 |
| H             | -0.27377900 | 2.13404600  | 1.68757100  |
| H             | -0.11967600 | 3.47616500  | 0.52098600  |
| C             | -2.92314700 | -0.77356300 | -1.83685700 |
| H             | -3.56324400 | -0.51017000 | -2.67833400 |
| H             | -2.12505600 | -1.42132700 | -2.19885000 |
| H             | -3.51967100 | -1.30718400 | -1.09219200 |
| H             | 4.35230400  | 2.09141900  | -0.51072500 |
| H             | 2.27662200  | 3.76751400  | 0.29674300  |
| H             | -2.35605200 | 3.59952500  | -0.45128200 |
| H             | -3.94349700 | 1.79018900  | -1.85617100 |
| C             | -1.44338700 | -0.06658700 | 2.39761200  |
| O             | -0.24197400 | -0.18860600 | 1.93758100  |
| C             | -1.07944400 | -2.17556200 | 0.28454700  |
| O             | -1.75522600 | -3.09100600 | 0.48945900  |
| C             | 1.42024400  | -2.02335000 | 0.81780700  |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| C           | 3.59446900  | -0.52171100 | -0.78943600 |
| H           | 4.11340300  | -0.93547300 | 0.07746800  |
| H           | 2.97130800  | -1.29931400 | -1.22416300 |
| H           | 4.32511600  | -0.19245200 | -1.52880100 |
| C           | 0.46435100  | -1.32311000 | -1.59878800 |
| O           | -1.73968200 | 0.44498600  | 3.47209500  |
| H           | -2.25311800 | -0.46627700 | 1.73016000  |
| O           | 0.70872800  | -1.62300900 | -2.69338000 |
| N           | 2.20133200  | -2.73270300 | 1.33947700  |
| Fe          | 0.09624400  | -0.85174900 | 0.03039100  |
| <b>Fe-1</b> |             |             |             |
| N           | -1.18144300 | 1.84722000  | -0.52171500 |
| N           | -2.55030500 | 0.57032900  | 0.51733400  |
| C           | -0.00127900 | 2.29208600  | -1.23038500 |
| C           | -2.24098200 | 2.64827900  | -0.14591300 |
| C           | -3.10733500 | 1.83649900  | 0.50665900  |
| C           | -1.35957800 | 0.56255600  | -0.12383400 |
| C           | 1.35808900  | 0.56521000  | -0.12342400 |
| C           | 2.22811300  | 2.65616600  | -0.12623300 |
| C           | 3.09337400  | 1.84559700  | 0.52927100  |
| N           | 2.54339000  | 0.57626800  | 0.52801900  |
| N           | 1.17651400  | 1.85099200  | -0.51582600 |
| H           | 0.00339600  | 1.87543300  | -2.24128700 |
| H           | -0.00313000 | 3.37817600  | -1.28521200 |
| C           | 3.21845300  | -0.56576800 | 1.12238800  |
| H           | 3.84692500  | -0.21012500 | 1.93848300  |
| H           | 2.48730400  | -1.26424600 | 1.52738000  |
| H           | 3.85087100  | -1.06207400 | 0.38306100  |
| H           | -4.05868000 | 2.03623800  | 0.97347100  |
| H           | -2.26852000 | 3.70204200  | -0.37213400 |
| H           | 2.25195100  | 3.71129800  | -0.34650800 |
| H           | 4.03964800  | 2.04813700  | 1.00518800  |
| C           | 1.28726600  | -2.09573600 | -0.76652000 |
| O           | 2.07746300  | -2.90684300 | -0.97545000 |
| C           | -1.27322200 | -2.11490700 | -0.74180200 |
| O           | -2.05156200 | -2.94466000 | -0.92021800 |
| C           | -3.22239600 | -0.57185100 | 1.11463300  |
| H           | -3.84380400 | -1.07921800 | 0.37350100  |
| H           | -2.48945200 | -1.26067200 | 1.53299000  |
| H           | -3.86186800 | -0.21394100 | 1.92110500  |
| C           | 0.00372000  | -1.23136300 | 1.37638500  |
| N           | 0.00297100  | -1.44267100 | 2.53335000  |
| Fe          | 0.00087700  | -0.87541600 | -0.47123600 |
| H           | -0.41610900 | -0.37104600 | -2.04044000 |

|               |             |              |             |
|---------------|-------------|--------------|-------------|
| H             | 0.38822700  | -0.49273800  | -2.08759000 |
| <b>Fe-TS1</b> |             |              |             |
| N             | -1.19868600 | 1.97474600   | -0.17364900 |
| N             | -2.92593400 | 0.75263300   | 0.15022300  |
| C             | 0.17298400  | 2.36763100   | -0.40846700 |
| C             | -2.26123100 | 2.84272800   | -0.02936200 |
| C             | -3.35449100 | 2.06576600   | 0.17285600  |
| C             | -1.59053700 | 0.67950900   | -0.07564200 |
| C             | 0.98972900  | 0.33381600   | 0.73039600  |
| C             | 2.11177200  | 2.24861000   | 1.17227100  |
| C             | 2.72600100  | 1.24360000   | 1.84569600  |
| N             | 2.01847200  | 0.08813000   | 1.57700100  |
| N             | 1.04404900  | 1.67253000   | 0.51753700  |
| H             | 0.50116200  | 2.10648300   | -1.42340700 |
| H             | 0.26585100  | 3.43982600   | -0.24277200 |
| C             | 2.41978700  | -1.21375900  | 2.07512600  |
| H             | 2.93533100  | -1.08309000  | 3.02657400  |
| H             | 1.54017300  | -1.83752500  | 2.23587000  |
| H             | 3.09730700  | -1.69639300  | 1.36647700  |
| H             | -4.38860500 | 2.32138200   | 0.34176900  |
| H             | -2.13760500 | 3.91280500   | -0.07916300 |
| H             | 2.32044100  | 3.30495700   | 1.11109300  |
| H             | 3.58084000  | 1.24466000   | 2.50320100  |
| C             | 2.84875300  | 0.52200100   | -2.13688500 |
| O             | 2.44877200  | -0.58993700  | -1.70205300 |
| C             | 0.91371200  | -2.173333500 | -0.37555500 |
| O             | 1.58429800  | -3.10583800  | -0.47874500 |
| C             | -1.49070600 | -1.84673700  | -1.11384200 |
| O             | -2.21845800 | -2.52467200  | -1.70236200 |
| C             | -3.83104000 | -0.37256200  | 0.30610700  |
| H             | -4.21485300 | -0.69321100  | -0.66518200 |
| H             | -3.31638500 | -1.19754100  | 0.79809900  |
| H             | -4.66981200 | -0.06442800  | 0.93000700  |
| C             | -0.88333300 | -1.53393300  | 1.41459000  |
| O             | 2.22587200  | 1.57290200   | -2.39032500 |
| H             | 3.96332500  | 0.55395700   | -2.33939500 |
| H             | 0.18903500  | 0.22134500   | -2.55816300 |
| H             | -0.54304900 | 0.10469100   | -2.70240600 |
| Fe            | -0.30547800 | -0.85461600  | -0.20331600 |
| N             | -1.24261800 | -1.94768700  | 2.45856700  |
| <b>Fe-2</b>   |             |              |             |
| N             | -1.04071700 | 2.03076000   | -0.16804200 |
| N             | -2.89454300 | 0.99555400   | 0.08195300  |
| C             | 0.36688300  | 2.25754000   | -0.39400500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.00198400 | 3.00745500  | 0.01419500  |
| C  | -3.17643400 | 2.34893900  | 0.16595000  |
| C  | -1.57195800 | 0.78145000  | -0.12951200 |
| C  | 0.92080100  | 0.13465200  | 0.71341500  |
| C  | 2.19432200  | 1.92241700  | 1.30391500  |
| C  | 2.64785000  | 0.84610200  | 1.99183600  |
| N  | 1.85384800  | -0.22847000 | 1.62884500  |
| N  | 1.14458500  | 1.46365200  | 0.53157500  |
| H  | 0.63120800  | 1.96386900  | -1.41413100 |
| H  | 0.59422300  | 3.31145100  | -0.24244000 |
| C  | 2.05972800  | -1.57334200 | 2.13054200  |
| H  | 2.48564900  | -1.51623600 | 3.13245300  |
| H  | 1.10365000  | -2.09549400 | 2.18015800  |
| H  | 2.74907400  | -2.12338200 | 1.48423600  |
| H  | -4.17941000 | 2.70973300  | 0.33115400  |
| H  | -1.75841400 | 4.05783800  | 0.02024700  |
| H  | 2.50911800  | 2.95365500  | 1.28857800  |
| H  | 3.44251700  | 0.74455600  | 2.71395200  |
| C  | 3.50855000  | 0.64048500  | -1.78019500 |
| O  | 2.89305000  | -0.51217900 | -1.52058900 |
| C  | 0.55455900  | -2.30156200 | -0.49533400 |
| O  | 1.18261400  | -3.26040900 | -0.68426200 |
| C  | -1.67453800 | -1.55453000 | -1.38474300 |
| O  | -2.42642700 | -1.96490500 | -2.16976800 |
| C  | -3.92014400 | -0.02713700 | 0.17760300  |
| H  | -4.41540800 | -0.16363100 | -0.78690300 |
| H  | -3.47072800 | -0.96602200 | 0.49832300  |
| H  | -4.66167200 | 0.28143700  | 0.91534800  |
| O  | 2.96866500  | 1.69713400  | -2.02338800 |
| H  | 4.59982100  | 0.49242100  | -1.75071200 |
| H  | 1.91798900  | -0.36170200 | -1.52155100 |
| H  | 0.14368100  | -0.20872600 | -1.54794200 |
| C  | -1.22885000 | -1.52415100 | 1.36985000  |
| N  | -1.68345200 | -1.89117600 | 2.39444000  |
| Fe | -0.47558600 | -0.88842500 | -0.28843100 |

### Fe-3

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.44740300 | 1.63614600 | -0.89658900 |
| N | -3.01753800 | 0.39091700 | -0.15227400 |
| C | -0.11924200 | 2.08009700 | -1.24919900 |
| C | -2.61898600 | 2.34415800 | -1.08800800 |
| C | -3.61310900 | 1.55023500 | -0.62219400 |
| C | -1.67152800 | 0.42533700 | -0.32025900 |
| C | 0.85895600  | 0.76249800 | 0.57202700  |
| C | 1.60862800  | 2.90132800 | 0.38803400  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| C             | 2.26764200  | 2.31917600  | 1.41939300  |
| N             | 1.79263000  | 1.02200900  | 1.52068900  |
| N             | 0.75874500  | 1.93321600  | -0.11239300 |
| H             | 0.25939800  | 1.46327400  | -2.07237900 |
| H             | -0.15506100 | 3.12590100  | -1.54860700 |
| C             | 2.30699700  | 0.06347800  | 2.47911700  |
| H             | 2.56596300  | 0.58460900  | 3.40157800  |
| H             | 1.54169100  | -0.68277500 | 2.69234200  |
| H             | 3.20227800  | -0.42732500 | 2.08698500  |
| H             | -4.67987400 | 1.70085300  | -0.56989100 |
| H             | -2.62963400 | 3.33096600  | -1.52322500 |
| H             | 1.65283700  | 3.89680000  | -0.02468500 |
| H             | 3.01285200  | 2.70457000  | 2.09711700  |
| C             | 1.21816000  | -1.87282200 | 0.26098800  |
| O             | 2.16613000  | -2.54838200 | 0.27944800  |
| C             | -1.16116600 | -2.17678300 | -0.55062800 |
| O             | -1.75829500 | -3.04056000 | -1.05086600 |
| C             | -3.77229300 | -0.71296400 | 0.41019300  |
| H             | -4.13618200 | -1.37362500 | -0.38076600 |
| H             | -3.13794500 | -1.27440800 | 1.09547300  |
| H             | -4.62678600 | -0.31579500 | 0.95910500  |
| H             | 0.26013700  | -0.55931200 | -1.32123700 |
| C             | 2.88467900  | -0.53641000 | -2.14991100 |
| O             | 2.50751100  | -1.24082200 | -3.00301500 |
| O             | 3.29165500  | 0.17337300  | -1.31470800 |
| Fe            | -0.20681000 | -0.86499900 | 0.11304700  |
| C             | -0.81234000 | -1.03918300 | 1.94255100  |
| N             | -1.18172300 | -1.13678700 | 3.05906600  |
| <b>Fe-TS2</b> |             |             |             |
| N             | 1.37047600  | 1.76932600  | 0.36635200  |
| N             | 2.69863700  | 0.48372700  | -0.70966500 |
| C             | 0.19781800  | 2.24541000  | 1.07066900  |
| C             | 2.52841300  | 2.49475900  | 0.16845400  |
| C             | 3.36958500  | 1.67624600  | -0.51024900 |
| C             | 1.45934800  | 0.52118500  | -0.16386500 |
| C             | -1.24967100 | 0.76646300  | -0.27932600 |
| C             | -1.96894400 | 2.90051100  | -0.00704900 |
| C             | -2.87527200 | 2.25306400  | -0.78067200 |
| N             | -2.41741800 | 0.95963800  | -0.94111300 |
| N             | -0.98623900 | 1.97664600  | 0.28101600  |
| H             | 0.11787500  | 1.74641900  | 2.04119800  |
| H             | 0.28564900  | 3.31999200  | 1.21808900  |
| C             | -3.14562100 | -0.04252700 | -1.69983800 |
| H             | -3.69394100 | 0.45413200  | -2.49983600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.44547100 | -0.75034100 | -2.14239000 |
| H  | -3.85583800 | -0.56624600 | -1.05619900 |
| H  | 4.37155400  | 1.83045700  | -0.87821400 |
| H  | 2.63674000  | 3.50791600  | 0.52182700  |
| H  | -1.92618200 | 3.91527500  | 0.35546300  |
| H  | -3.79204800 | 2.59073300  | -1.23765000 |
| C  | -1.43382500 | -1.96448800 | -0.00524900 |
| O  | -2.28729100 | -2.74102200 | -0.00630400 |
| C  | 1.08465400  | -2.17231200 | 0.22227800  |
| O  | 1.76492500  | -3.06997500 | 0.48185700  |
| C  | 3.30532500  | -0.65866100 | -1.37031800 |
| H  | 3.82491300  | -1.28723900 | -0.64319200 |
| H  | 2.53970100  | -1.23756500 | -1.88603500 |
| H  | 4.02662200  | -0.29780000 | -2.10349500 |
| H  | 0.67417900  | -0.43308400 | 2.02892700  |
| C  | -0.20157700 | -0.63692500 | 2.74891600  |
| O  | -0.96015100 | -1.58061000 | 2.39949000  |
| O  | -0.23919100 | 0.09275100  | 3.74642100  |
| Fe | -0.03945800 | -0.82054000 | -0.09899200 |
| N  | 0.09492600  | -1.09783200 | -3.11543500 |
| C  | 0.04862300  | -1.00077400 | -1.94116800 |

#### Co-cat

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.37047600  | 1.76932600  | 0.36635200  |
| N | 2.69863700  | 0.48372700  | -0.70966500 |
| C | 0.19781800  | 2.24541000  | 1.07066900  |
| C | 2.52841300  | 2.49475900  | 0.16845400  |
| C | 3.36958500  | 1.67624600  | -0.51024900 |
| C | 1.45934800  | 0.52118500  | -0.16386500 |
| C | -1.24967100 | 0.76646300  | -0.27932600 |
| C | -1.96894400 | 2.90051100  | -0.00704900 |
| C | -2.87527200 | 2.25306400  | -0.78067200 |
| N | -2.41741800 | 0.95963800  | -0.94111300 |
| N | -0.98623900 | 1.97664600  | 0.28101600  |
| H | 0.11787500  | 1.74641900  | 2.04119800  |
| H | 0.28564900  | 3.31999200  | 1.21808900  |
| C | -3.14562100 | -0.04252700 | -1.69983800 |
| H | -3.69394100 | 0.45413200  | -2.49983600 |
| H | -2.44547100 | -0.75034100 | -2.14239000 |
| H | -3.85583800 | -0.56624600 | -1.05619900 |
| H | 4.37155400  | 1.83045700  | -0.87821400 |
| H | 2.63674000  | 3.50791600  | 0.52182700  |
| H | -1.92618200 | 3.91527500  | 0.35546300  |
| H | -3.79204800 | 2.59073300  | -1.23765000 |
| C | -1.43382500 | -1.96448800 | -0.00524900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -2.28729100 | -2.74102200 | -0.00630400 |
| C  | 1.08465400  | -2.17231200 | 0.22227800  |
| O  | 1.76492500  | -3.06997500 | 0.48185700  |
| C  | 3.30532500  | -0.65866100 | -1.37031800 |
| H  | 3.82491300  | -1.28723900 | -0.64319200 |
| H  | 2.53970100  | -1.23756500 | -1.88603500 |
| H  | 4.02662200  | -0.29780000 | -2.10349500 |
| H  | 0.67417900  | -0.43308400 | 2.02892700  |
| C  | -0.20157700 | -0.63692500 | 2.74891600  |
| O  | -0.96015100 | -1.58061000 | 2.39949000  |
| O  | -0.23919100 | 0.09275100  | 3.74642100  |
| Fe | -0.03945800 | -0.82054000 | -0.09899200 |
| N  | 0.09492600  | -1.09783200 | -3.11543500 |
| C  | 0.04862300  | -1.00077400 | -1.94116800 |

### Co-1

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.14270300 | 1.85101300  | -0.49819400 |
| N | -2.53698000 | 0.56819600  | 0.51911200  |
| C | 0.04070200  | 2.29925400  | -1.20367500 |
| C | -2.21858500 | 2.64405100  | -0.15881500 |
| C | -3.09549900 | 1.83188800  | 0.48058600  |
| C | -1.33749000 | 0.57222100  | -0.09700900 |
| C | 1.38751100  | 0.54891900  | -0.12293400 |
| C | 2.29938100  | 2.61039000  | -0.13266700 |
| C | 3.16206500  | 1.77265700  | 0.49471800  |
| N | 2.58310600  | 0.51721200  | 0.49881500  |
| N | 1.21740900  | 1.83679200  | -0.49899500 |
| H | 0.03805600  | 1.89105800  | -2.21789800 |
| H | 0.04526400  | 3.38597900  | -1.23996300 |
| C | 3.23553300  | -0.65485500 | 1.06003900  |
| H | 3.93703700  | -0.32711700 | 1.82590100  |
| H | 2.49724800  | -1.30862100 | 1.52444100  |
| H | 3.78676500  | -1.18916200 | 0.28330200  |
| H | -4.05926700 | 2.02967300  | 0.92182000  |
| H | -2.24928700 | 3.69439200  | -0.39955000 |
| H | 2.34473500  | 3.66593800  | -0.34745800 |
| H | 4.12544800  | 1.94780500  | 0.94610700  |
| C | 1.19142300  | -2.20792400 | -0.74004000 |
| O | 1.85126700  | -3.11993900 | -0.92847300 |
| C | -1.39176800 | -2.11131300 | -0.75736900 |
| C | -3.22345100 | -0.56140400 | 1.13088900  |
| H | -3.81411300 | -1.09172500 | 0.38264600  |
| H | -2.50259100 | -1.24233200 | 1.57851500  |
| H | -3.88161300 | -0.17445300 | 1.90814500  |
| C | -0.03006700 | -1.15384700 | 1.36143100  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| Co            | -0.00570700 | -0.82391000 | -0.44802900 |
| N             | -2.21438100 | -2.91445700 | -0.98988400 |
| N             | -0.03250300 | -1.37011400 | 2.51514100  |
| H             | -0.47059400 | -0.56547400 | -2.14150000 |
| H             | 0.31071200  | -0.47157900 | -2.21283000 |
| <b>Co-TS1</b> |             |             |             |
| N             | -1.50949000 | 1.79206400  | -0.56589500 |
| N             | -3.02667700 | 0.41154600  | 0.05687200  |
| C             | -0.21660800 | 2.32963500  | -0.93179500 |
| C             | -2.69612200 | 2.49760000  | -0.57203200 |
| C             | -3.65340500 | 1.62116000  | -0.17915800 |
| C             | -1.70278200 | 0.50095600  | -0.19146300 |
| C             | 0.89051200  | 0.71431600  | 0.57143600  |
| C             | 1.68425100  | 2.82957600  | 0.63271500  |
| C             | 2.39655900  | 2.09058400  | 1.51948400  |
| N             | 1.88955400  | 0.80634000  | 1.47787200  |
| N             | 0.76350600  | 1.96850300  | 0.07220500  |
| H             | 0.09364700  | 1.93193500  | -1.90216700 |
| H             | -0.28453300 | 3.41388800  | -0.98850200 |
| C             | 2.45115100  | -0.28724600 | 2.25207100  |
| H             | 2.82315500  | 0.10716900  | 3.19712400  |
| H             | 1.68229000  | -1.03024100 | 2.45822500  |
| H             | 3.28109900  | -0.74727900 | 1.70796100  |
| H             | -4.71509000 | 1.74370700  | -0.03457800 |
| H             | -2.74049000 | 3.53906900  | -0.84765700 |
| H             | 1.73373800  | 3.87108100  | 0.35802900  |
| H             | 3.20446700  | 2.35807800  | 2.18181900  |
| C             | 2.82640300  | -0.23731700 | -1.61537800 |
| O             | 1.91258600  | -1.13451200 | -1.83413200 |
| C             | 1.27302900  | -1.95215700 | -0.14331400 |
| O             | 1.92948200  | -2.85538100 | 0.16655200  |
| C             | -1.25474500 | -2.20655200 | -0.80225500 |
| C             | -3.75185000 | -0.77886800 | 0.47090100  |
| H             | -4.18318800 | -1.27717400 | -0.39982100 |
| H             | -3.07691200 | -1.46191900 | 0.98194600  |
| H             | -4.55013600 | -0.48217400 | 1.15158400  |
| O             | 3.20180400  | 0.60557000  | -2.42143300 |
| H             | 3.30014100  | -0.29081100 | -0.60260900 |
| H             | 0.12325600  | -0.30352000 | -2.40738400 |
| H             | -0.62080300 | -0.18573100 | -2.31657600 |
| C             | -0.63370200 | -1.27854400 | 1.58702100  |
| N             | -0.92666200 | -1.60683100 | 2.67799100  |
| Co            | -0.19399600 | -0.78204000 | -0.10092900 |
| N             | -1.88449700 | -3.09380300 | -1.24613200 |

**Co-2**

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -0.95035000 | 2.06218800  | -0.13653600 |
| N  | -2.85106900 | 1.10462000  | 0.10981500  |
| C  | 0.46543000  | 2.23043600  | -0.36266700 |
| C  | -1.86929900 | 3.07813200  | 0.04341100  |
| C  | -3.07023600 | 2.46950800  | 0.19396500  |
| C  | -1.54189200 | 0.84164800  | -0.10241800 |
| C  | 0.90885000  | 0.05989400  | 0.69448300  |
| C  | 2.30498300  | 1.73853200  | 1.29368100  |
| C  | 2.70543900  | 0.61377000  | 1.93665600  |
| N  | 1.83432900  | -0.39684800 | 1.56734300  |
| N  | 1.20601300  | 1.37340800  | 0.53934300  |
| H  | 0.71036700  | 1.95378700  | -1.39305300 |
| H  | 0.74242900  | 3.26779100  | -0.18403800 |
| C  | 1.98415600  | -1.77363500 | 1.99912700  |
| H  | 2.40240900  | -1.78629900 | 3.00539900  |
| H  | 1.00948300  | -2.26164100 | 2.01682700  |
| H  | 2.66033900  | -2.30966300 | 1.32772300  |
| H  | -4.05709000 | 2.87135500  | 0.36025800  |
| H  | -1.58101500 | 4.11686700  | 0.04902100  |
| H  | 2.68247400  | 2.74872500  | 1.30303100  |
| H  | 3.51049900  | 0.43998100  | 2.63286800  |
| C  | 3.59454100  | 0.65726300  | -1.49029700 |
| O  | 2.93860600  | -0.50902700 | -1.46869200 |
| C  | 0.41917400  | -2.27949600 | -0.67130900 |
| O  | 0.98624400  | -3.23254100 | -0.97980500 |
| C  | -1.89662000 | -1.49838200 | -1.43711900 |
| C  | -3.92785300 | 0.13533400  | 0.22077900  |
| H  | -4.40949300 | -0.00811700 | -0.74876900 |
| H  | -3.53151200 | -0.81574000 | 0.57051200  |
| H  | -4.65906700 | 0.50992200  | 0.93773200  |
| O  | 3.15752100  | 1.69942200  | -1.92148500 |
| H  | 4.60130200  | 0.52146800  | -1.06572400 |
| H  | 2.03596900  | -0.35249600 | -1.81491800 |
| H  | 0.04664300  | -0.18058900 | -1.51883400 |
| C  | -1.31996200 | -1.56468300 | 1.31664000  |
| N  | -1.79571100 | -2.00698100 | 2.29777300  |
| Co | -0.53475000 | -0.82353400 | -0.28754400 |
| N  | -2.71817300 | -1.90677400 | -2.17260500 |

**Co-3**

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.39753800 | 1.67781800 | -0.86480500 |
| N | -2.98498500 | 0.41779600 | -0.17108800 |
| C | -0.06264100 | 2.12765200 | -1.18464000 |
| C | -2.56349700 | 2.39324100 | -1.05560700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.56578300 | 1.59156100  | -0.62221300 |
| C  | -1.64173200 | 0.45774000  | -0.32301400 |
| C  | 0.86408100  | 0.74453400  | 0.61127000  |
| C  | 1.67502600  | 2.85468500  | 0.49629700  |
| C  | 2.31121700  | 2.21861400  | 1.51081700  |
| N  | 1.79881600  | 0.93386000  | 1.56926700  |
| N  | 0.79800300  | 1.93130500  | -0.03926400 |
| H  | 0.32478700  | 1.54286000  | -2.02646900 |
| H  | -0.08841800 | 3.18342900  | -1.44603700 |
| C  | 2.28523900  | -0.07675500 | 2.49052800  |
| H  | 2.58265000  | 0.40587500  | 3.42153700  |
| H  | 1.49248000  | -0.79537600 | 2.69992800  |
| H  | 3.15187500  | -0.59136200 | 2.06616800  |
| H  | -4.63257200 | 1.74391700  | -0.57976800 |
| H  | -2.56391800 | 3.38927900  | -1.46874300 |
| H  | 1.75122600  | 3.86091600  | 0.11623000  |
| H  | 3.06412600  | 2.55944200  | 2.20352600  |
| C  | 1.16752500  | -1.91448200 | 0.18457600  |
| O  | 2.05540500  | -2.64867300 | 0.15149400  |
| C  | -1.25555300 | -2.22787800 | -0.62249500 |
| C  | -3.76567100 | -0.68412100 | 0.36351300  |
| H  | -4.10416100 | -1.33680700 | -0.44384400 |
| H  | -3.16001500 | -1.25772800 | 1.06245500  |
| H  | -4.63132100 | -0.27460800 | 0.88488600  |
| H  | 0.23239000  | -0.53173200 | -1.29886200 |
| C  | 2.84113400  | -0.51159400 | -2.20520600 |
| O  | 2.43199100  | -1.18258500 | -3.06997200 |
| O  | 3.26989300  | 0.15644200  | -1.34644400 |
| C  | -0.85292500 | -1.09948300 | 1.90804400  |
| N  | -1.23799500 | -1.27491100 | 3.00617900  |
| Co | -0.21418700 | -0.80693700 | 0.10232100  |
| N  | -1.87814400 | -3.10794800 | -1.09250700 |

### Co-TS2

|   |             |            |             |
|---|-------------|------------|-------------|
| N | 1.41085900  | 1.73770300 | 0.41002100  |
| N | 2.77189800  | 0.38342700 | -0.54465000 |
| C | 0.20426100  | 2.27516400 | 1.00130200  |
| C | 2.60226500  | 2.42039000 | 0.28078700  |
| C | 3.46052000  | 1.56064100 | -0.32180100 |
| C | 1.50559400  | 0.47608800 | -0.08213800 |
| C | -1.17911500 | 0.77973400 | -0.39896300 |
| C | -1.90861800 | 2.90803500 | -0.19539300 |
| C | -2.79202600 | 2.23682100 | -0.97598300 |
| N | -2.32531200 | 0.94175400 | -1.09480000 |
| N | -0.92728900 | 1.99856500 | 0.13909500  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| H             | 0.04019800  | 1.82384900  | 1.98436500  |
| H             | 0.31123200  | 3.35210600  | 1.11110700  |
| C             | -3.04187700 | -0.09729600 | -1.81488400 |
| H             | -3.62410400 | 0.36736600  | -2.60963700 |
| H             | -2.33635800 | -0.79703900 | -2.26236900 |
| H             | -3.72014100 | -0.62320100 | -1.13922700 |
| H             | 4.48988800  | 1.67584000  | -0.62205100 |
| H             | 2.71929900  | 3.43607600  | 0.62371000  |
| H             | -1.88113000 | 3.93072500  | 0.14509700  |
| H             | -3.69822000 | 2.55765300  | -1.46486900 |
| C             | -1.39436900 | -1.99915000 | 0.03173200  |
| O             | -2.14907900 | -2.86373800 | -0.01877900 |
| C             | 1.14502200  | -2.22021400 | 0.37279800  |
| C             | 3.39441000  | -0.77008500 | -1.17551100 |
| H             | 3.88334300  | -1.39353500 | -0.42495300 |
| H             | 2.64484200  | -1.35512600 | -1.70394200 |
| H             | 4.13613300  | -0.41049400 | -1.88874600 |
| H             | 0.41158100  | -0.49497600 | 2.10920800  |
| C             | -0.57111000 | -0.54983800 | 2.68906000  |
| O             | -1.52138300 | -1.16911100 | 2.11080800  |
| O             | -0.58169100 | -0.01582300 | 3.79651400  |
| N             | 0.29941300  | -1.19585700 | -3.03526300 |
| C             | 0.18425000  | -1.03124800 | -1.87662700 |
| Co            | -0.01811900 | -0.77265300 | -0.07743800 |
| N             | 1.83823600  | -3.11594900 | 0.68538200  |
| <b>Mo-cat</b> |             |             |             |
| N             | 0.99608400  | 2.21452200  | 0.21862100  |
| N             | 2.74247900  | 1.18605200  | -0.45343400 |
| C             | -0.34689700 | 2.49099800  | 0.69236500  |
| C             | 1.95810100  | 3.18520000  | 0.00731300  |
| C             | 3.06669800  | 2.52924500  | -0.41695200 |
| C             | 1.46553800  | 0.96364600  | -0.05191000 |
| C             | -1.35202600 | 0.58443600  | -0.56124400 |
| C             | -2.44010100 | 2.57974900  | -0.67219300 |
| C             | -3.14871500 | 1.68385500  | -1.40336800 |
| N             | -2.46619100 | 0.48460800  | -1.32912100 |
| N             | -1.34989900 | 1.89235500  | -0.17257700 |
| H             | -0.46408700 | 2.10336300  | 1.70782300  |
| H             | -0.49752900 | 3.56948000  | 0.68647300  |
| C             | -2.93495700 | -0.74640900 | -1.93673600 |
| H             | -3.46492900 | -0.51375000 | -2.86090200 |
| H             | -2.08237800 | -1.38736900 | -2.16341500 |
| H             | -3.61441700 | -1.27169200 | -1.25983200 |
| H             | 4.04171000  | 2.89040000  | -0.70463300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.76260500  | 4.23331400  | 0.17148600  |
| H  | -2.60118200 | 3.62702700  | -0.46936800 |
| H  | -4.05868200 | 1.79019400  | -1.97305200 |
| C  | -1.51657100 | -0.00889600 | 2.47178900  |
| O  | -0.29458300 | -0.13440700 | 2.07760800  |
| C  | -1.11688100 | -2.44349600 | 0.35205400  |
| O  | -1.85693700 | -3.33474800 | 0.46599700  |
| C  | 1.70779800  | -2.03650100 | 0.91859500  |
| O  | 2.56015200  | -2.68547600 | 1.37286500  |
| C  | 3.67487100  | 0.14404300  | -0.84116200 |
| H  | 4.20830300  | -0.23972800 | 0.03238000  |
| H  | 3.13183200  | -0.67188400 | -1.31884000 |
| H  | 4.39766200  | 0.55456800  | -1.54640500 |
| O  | 0.84126900  | -2.00114700 | -2.66622800 |
| O  | -1.93962300 | 0.84377400  | 3.24744000  |
| H  | -2.22989900 | -0.76428100 | 2.04363200  |
| N  | 0.61775600  | -1.55455300 | -1.58238300 |
| Mo | 0.21681000  | -0.91761200 | 0.08462200  |

### Mo-1

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.33207200 | 1.97642200  | -0.52376100 |
| N | -2.70935200 | 0.75182700  | 0.55614800  |
| C | -0.16411000 | 2.38886200  | -1.28119700 |
| C | -2.40170700 | 2.79093000  | -0.20759200 |
| C | -3.27578000 | 2.01023800  | 0.47638400  |
| C | -1.50606900 | 0.70508900  | -0.06447300 |
| C | 1.40053300  | 0.88261100  | -0.11274500 |
| C | 1.98235200  | 3.08037900  | -0.16792000 |
| C | 2.94475000  | 2.41382100  | 0.51862700  |
| N | 2.56804000  | 1.08427400  | 0.54535500  |
| N | 1.05468300  | 2.12775700  | -0.54176600 |
| H | -0.13582400 | 1.83967800  | -2.22488300 |
| H | -0.23261100 | 3.45539900  | -1.48498800 |
| C | 3.35541400  | 0.03993700  | 1.17515300  |
| H | 3.90261000  | 0.46369800  | 2.01712400  |
| H | 2.69681500  | -0.74790800 | 1.54024200  |
| H | 4.06699100  | -0.38598100 | 0.46339600  |
| H | -4.23471500 | 2.23330700  | 0.91733100  |
| H | -2.43684900 | 3.83087500  | -0.49128300 |
| H | 1.87361300  | 4.12307400  | -0.42235200 |
| H | 3.84925100  | 2.75995900  | 0.99404800  |
| C | 1.62499900  | -2.18527800 | -0.77393000 |
| O | 2.51123600  | -2.91543400 | -0.94605100 |
| C | -1.30799700 | -2.41345600 | -0.71020700 |
| O | -2.07646300 | -3.27214000 | -0.85339700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.36123600 | -0.38621700 | 1.17926200  |
| H  | -3.97400700 | -0.92204000 | 0.44967100  |
| H  | -2.60851100 | -1.06187500 | 1.58579000  |
| H  | -4.00065300 | -0.03410700 | 1.98893000  |
| O  | 0.17981600  | -1.72355000 | 2.51478700  |
| N  | 0.13338300  | -1.41218800 | 1.36794400  |
| H  | -0.35331900 | -0.70951300 | -2.97078200 |
| H  | 0.31989200  | -0.37323300 | -2.92247700 |
| Mo | 0.06192700  | -0.92477400 | -0.36138400 |

### Mo-TS1

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.26031900 | 2.16314000  | -0.44785000 |
| N | -3.00695900 | 1.05353200  | 0.07983000  |
| C | 0.10738100  | 2.47471000  | -0.80729200 |
| C | -2.27187600 | 3.09178200  | -0.29259000 |
| C | -3.38004400 | 2.38496700  | 0.04212900  |
| C | -1.69293000 | 0.89153200  | -0.21855500 |
| C | 1.07159100  | 0.69768000  | 0.61598700  |
| C | 2.04473100  | 2.74661600  | 0.76333000  |
| C | 2.73408300  | 1.90118900  | 1.57251600  |
| N | 2.11873600  | 0.66945700  | 1.47520700  |
| N | 1.03361000  | 1.99334900  | 0.20042800  |
| H | 0.36617100  | 2.00274400  | -1.75918800 |
| H | 0.21237700  | 3.55499000  | -0.89173100 |
| C | 2.61980500  | -0.53740800 | 2.10215200  |
| H | 3.20622600  | -0.26989900 | 2.98141100  |
| H | 1.78199700  | -1.16639000 | 2.40770900  |
| H | 3.24554200  | -1.08084100 | 1.38938600  |
| H | -4.38967700 | 2.70087200  | 0.25324900  |
| H | -2.11200400 | 4.14776700  | -0.44437000 |
| H | 2.16903800  | 3.79663900  | 0.54942400  |
| H | 3.58496200  | 2.06659600  | 2.21503100  |
| C | 3.11855800  | 0.39671100  | -1.80232000 |
| O | 3.31356100  | -0.65023800 | -1.16998800 |
| C | 1.11038000  | -2.40592800 | -0.05164300 |
| O | 1.84492300  | -3.29759600 | 0.04861200  |
| C | -1.56763400 | -2.16655400 | -1.16255500 |
| O | -2.26253400 | -2.87605000 | -1.77117900 |
| C | -3.90705700 | -0.01487400 | 0.46856300  |
| H | -4.89141400 | 0.16170400  | 0.03311700  |
| H | -3.51608800 | -0.96433500 | 0.10263600  |
| H | -4.00000800 | -0.06123300 | 1.55633900  |
| O | -1.49540800 | -1.89319400 | 2.46373900  |
| O | 2.11751100  | 0.73459300  | -2.51703200 |
| H | 3.92660500  | 1.18455900  | -1.77477800 |

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| H           | 0.91017200  | -0.20194000 | -2.18206500 |
| H           | 0.18791600  | -0.65072700 | -2.13958600 |
| N           | -1.01152600 | -1.48328100 | 1.45601800  |
| Mo          | -0.33007100 | -0.92610800 | -0.12984700 |
| <b>Mo-2</b> |             |             |             |
| N           | -0.76696600 | 2.33988000  | -0.21876400 |
| N           | -2.75262800 | 1.64333000  | 0.14292400  |
| C           | 0.64816300  | 2.33489300  | -0.51837300 |
| C           | -1.54250800 | 3.47037400  | -0.03555800 |
| C           | -2.80381600 | 3.02456900  | 0.19030700  |
| C           | -1.49780000 | 1.19456800  | -0.11486700 |
| C           | 1.10938900  | 0.26917900  | 0.76412200  |
| C           | 2.53361100  | 2.01241200  | 1.10535400  |
| C           | 2.97396600  | 0.96828700  | 1.85162000  |
| N           | 2.09037700  | -0.07349000 | 1.63792200  |
| N           | 1.39673100  | 1.56690900  | 0.45847100  |
| H           | 0.81323600  | 1.88911500  | -1.50376200 |
| H           | 1.01568900  | 3.35966200  | -0.51493800 |
| C           | 2.25675100  | -1.39722500 | 2.20451500  |
| H           | 2.68142700  | -1.31372700 | 3.20559800  |
| H           | 1.28581700  | -1.89058300 | 2.26505000  |
| H           | 2.92613300  | -1.99731100 | 1.58098000  |
| H           | -3.72169400 | 3.55679200  | 0.38575700  |
| H           | -1.13066600 | 4.46634600  | -0.08207400 |
| H           | 2.91322900  | 3.01419200  | 0.97779800  |
| H           | 3.81464500  | 0.87724000  | 2.52174900  |
| C           | 3.57805400  | 0.39753400  | -1.78187400 |
| O           | 2.91905400  | -0.71730700 | -1.48734500 |
| C           | 0.51591100  | -2.57456800 | -0.40960700 |
| O           | 1.13036600  | -3.55374300 | -0.55787200 |
| C           | -2.02585800 | -1.60125900 | -1.42627500 |
| O           | -2.84264300 | -1.99676000 | -2.15831400 |
| C           | -3.90838000 | 0.78305200  | 0.30917100  |
| H           | -4.34150800 | 0.52679900  | -0.66149000 |
| H           | -3.60859400 | -0.13301400 | 0.81965400  |
| H           | -4.65919400 | 1.30020100  | 0.90686700  |
| O           | -1.93051200 | -2.17069700 | 2.22795800  |
| O           | 3.09920800  | 1.42627600  | -2.21007200 |
| H           | 4.65478200  | 0.25360600  | -1.58827800 |
| H           | 1.94202900  | -0.56776600 | -1.61076700 |
| H           | 0.29878600  | -0.43526800 | -1.79562600 |
| N           | -1.41652500 | -1.58654500 | 1.32310800  |
| Mo          | -0.58975500 | -0.88880800 | -0.18233800 |

**Mo-3**

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -1.59266100 | 1.84635200  | -0.87246600 |
| N  | -3.18921000 | 0.56563500  | -0.26212500 |
| C  | -0.25923400 | 2.31106000  | -1.19077000 |
| C  | -2.75594400 | 2.57279900  | -1.04837400 |
| C  | -3.76845000 | 1.75632600  | -0.66389500 |
| C  | -1.83769900 | 0.59484700  | -0.38908800 |
| C  | 0.82492400  | 1.04731500  | 0.62820300  |
| C  | 1.38437400  | 3.25005800  | 0.46160200  |
| C  | 2.09613600  | 2.72065200  | 1.48773300  |
| N  | 1.73710000  | 1.38741300  | 1.57480000  |
| N  | 0.61770100  | 2.21615400  | -0.04271800 |
| H  | 0.14795100  | 1.68640000  | -1.99294500 |
| H  | -0.31272500 | 3.34932600  | -1.51337700 |
| C  | 2.31600500  | 0.45943300  | 2.52562300  |
| H  | 2.42133500  | 0.94547400  | 3.49673900  |
| H  | 1.65942300  | -0.40595200 | 2.62218700  |
| H  | 3.30142600  | 0.12672700  | 2.18611100  |
| H  | -4.83526900 | 1.91344000  | -0.63124100 |
| H  | -2.75214900 | 3.58559600  | -1.41974900 |
| H  | 1.34516900  | 4.24838600  | 0.05470300  |
| H  | 2.80732000  | 3.16634900  | 2.16535800  |
| C  | 1.53092100  | -1.91472300 | 0.18783000  |
| O  | 2.55703700  | -2.47140400 | 0.20784900  |
| C  | -1.18775800 | -2.41817000 | -0.80679400 |
| O  | -1.74328600 | -3.28404400 | -1.35711400 |
| C  | -3.94294100 | -0.58924700 | 0.18567900  |
| H  | -4.27235900 | -1.18771600 | -0.66807100 |
| H  | -3.30966700 | -1.20131700 | 0.82919000  |
| H  | -4.81779800 | -0.25857700 | 0.74666400  |
| O  | -1.07486800 | -1.95153900 | 2.83269800  |
| H  | 0.33351800  | -0.58048100 | -1.64966400 |
| C  | 3.40983900  | -0.31498900 | -2.07588900 |
| O  | 3.28299600  | -1.14310300 | -2.89110200 |
| O  | 3.55883500  | 0.51877400  | -1.26978700 |
| N  | -0.75293200 | -1.44850400 | 1.79820400  |
| Mo | -0.21340300 | -0.89425400 | 0.10506500  |

### Mo-TS2

|   |             |            |             |
|---|-------------|------------|-------------|
| N | 0.43098400  | 2.31379000 | 0.31437600  |
| N | 1.69382100  | 1.91366800 | -1.36025400 |
| C | -0.49367800 | 2.10421600 | 1.41341800  |
| C | 1.05037100  | 3.50955000 | 0.00835200  |
| C | 1.85288600  | 3.25390300 | -1.05575200 |
| C | 0.82194700  | 1.30639700 | -0.51723000 |
| C | -1.76839600 | 0.32579300 | 0.29843700  |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | -2.98592400 | 2.10710000  | 1.02503500  |
| C            | -3.84078200 | 1.23769200  | 0.42966700  |
| N            | -3.08120900 | 0.16403400  | -0.00173800 |
| N            | -1.73297600 | 1.52873000  | 0.93699200  |
| H            | -0.02906900 | 1.41617200  | 2.12470600  |
| H            | -0.70095400 | 3.06069600  | 1.89003100  |
| C            | -3.60895300 | -0.95632400 | -0.75540000 |
| H            | -4.62803600 | -1.16693700 | -0.42945400 |
| H            | -3.61467900 | -0.73185700 | -1.82543600 |
| H            | -2.98138400 | -1.83144600 | -0.57880700 |
| H            | 2.50567300  | 3.89650700  | -1.62555900 |
| H            | 0.85927500  | 4.41539500  | 0.56243900  |
| H            | -3.14998000 | 3.05699600  | 1.50915200  |
| H            | -4.90801100 | 1.28041900  | 0.27791500  |
| C            | -0.53104800 | -2.56927900 | 0.59743400  |
| O            | -0.85206700 | -3.54788000 | 1.14266100  |
| C            | 1.95386800  | -1.60393000 | -0.54013300 |
| O            | 3.01881400  | -2.04074900 | -0.71907500 |
| C            | 2.40532200  | 1.24079800  | -2.42942100 |
| H            | 3.43646400  | 1.03142700  | -2.13269500 |
| H            | 1.89742500  | 0.30235000  | -2.65614200 |
| H            | 2.41284400  | 1.87100800  | -3.31996600 |
| O            | -0.79652700 | -1.75098200 | -2.99756400 |
| H            | 0.59460700  | -0.64949500 | 1.60809700  |
| C            | 1.94462800  | -0.64349700 | 2.55132300  |
| O            | 2.10833100  | -1.79546200 | 2.81609600  |
| O            | 2.23416200  | 0.51392300  | 2.63523000  |
| N            | -0.44941800 | -1.31412200 | -1.94298000 |
| Mo           | 0.08986400  | -0.83569600 | -0.24291000 |
| <b>W-cat</b> |             |             |             |
| N            | 0.84632500  | 2.38159100  | 0.20358900  |
| N            | 2.62842800  | 1.42377000  | -0.48418000 |
| C            | -0.50398300 | 2.61005900  | 0.68381900  |
| C            | 1.77072200  | 3.38778000  | -0.00445000 |
| C            | 2.90113000  | 2.77685700  | -0.43855400 |
| C            | 1.36194700  | 1.15065500  | -0.07811500 |
| C            | -1.41919000 | 0.64192900  | -0.53989000 |
| C            | -2.60134500 | 2.58067100  | -0.67941500 |
| C            | -3.25837700 | 1.64427800  | -1.40846300 |
| N            | -2.52084400 | 0.48055900  | -1.31657300 |
| N            | -1.48457100 | 1.95150600  | -0.16259900 |
| H            | -0.59928200 | 2.24041300  | 1.70806900  |
| H            | -0.69855200 | 3.68110200  | 0.65583500  |
| C            | -2.91431700 | -0.77673600 | -1.92567400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.55757800 | -0.57201800 | -2.78122200 |
| H | -2.02785600 | -1.31541400 | -2.26271400 |
| H | -3.45986900 | -1.39431200 | -1.20725200 |
| H | 3.85990100  | 3.17687900  | -0.72914900 |
| H | 1.53739400  | 4.42663000  | 0.16838000  |
| H | -2.81517700 | 3.62016500  | -0.48675700 |
| H | -4.16674000 | 1.70012300  | -1.98739700 |
| C | -1.43938300 | -0.00044000 | 2.56579000  |
| O | -0.26003200 | 0.00311100  | 2.03352400  |
| C | -1.03569900 | -2.34481500 | 0.33884400  |
| O | -1.73736700 | -3.27362500 | 0.43554200  |
| C | 1.75022900  | -1.83811800 | 0.85598400  |
| O | 2.63468300  | -2.47094600 | 1.27950400  |
| C | 3.59813100  | 0.42150800  | -0.88546800 |
| H | 4.15034200  | 0.05185500  | -0.01763500 |
| H | 3.08450600  | -0.41077800 | -1.36723000 |
| H | 4.30079500  | 0.86644800  | -1.59005800 |
| O | 0.83705700  | -1.79682200 | -2.70818500 |
| O | -1.87165700 | 0.84078800  | 3.34502600  |
| H | -2.08664800 | -0.86569400 | 2.26480800  |
| N | 0.60888300  | -1.38017400 | -1.60680700 |
| W | 0.21419700  | -0.77227000 | 0.07038600  |

### W -1

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.33450200 | 2.10088300  | -0.51781400 |
| N | -2.69273600 | 0.88436800  | 0.59659700  |
| C | -0.16925300 | 2.50807500  | -1.28043700 |
| C | -2.40370300 | 2.91361000  | -0.20079100 |
| C | -3.26487700 | 2.13818300  | 0.50535900  |
| C | -1.49502100 | 0.83455700  | -0.03733700 |
| C | 1.37376000  | 1.01802100  | -0.06799000 |
| C | 1.98283100  | 3.20569300  | -0.17648400 |
| C | 2.93264100  | 2.54487000  | 0.53301300  |
| N | 2.54204700  | 1.22127900  | 0.58997900  |
| N | 1.04604800  | 2.25641000  | -0.53190700 |
| H | -0.13769600 | 1.94512100  | -2.21613000 |
| H | -0.23982500 | 3.57156800  | -1.49851200 |
| C | 3.31721100  | 0.18248300  | 1.24489500  |
| H | 3.87411300  | 0.62211500  | 2.07211300  |
| H | 2.64946300  | -0.58565800 | 1.63428400  |
| H | 4.01961700  | -0.27157800 | 0.54163600  |
| H | -4.21886300 | 2.36282700  | 0.95608400  |
| H | -2.44714800 | 3.94929100  | -0.49802900 |
| H | 1.88819500  | 4.24307700  | -0.45637100 |
| H | 3.83786800  | 2.89217100  | 1.00602000  |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | 1.60404300  | -2.04333500 | -0.68345900 |
| O            | 2.48947300  | -2.78190000 | -0.84678400 |
| C            | -1.30861900 | -2.26065400 | -0.63150000 |
| O            | -2.08160400 | -3.12038900 | -0.77205900 |
| C            | -3.33411500 | -0.24486900 | 1.24628000  |
| H            | -3.94867500 | -0.79773300 | 0.53116700  |
| H            | -2.57571600 | -0.90791300 | 1.66243000  |
| H            | -3.97018800 | 0.12136400  | 2.05224200  |
| O            | 0.15135000  | -1.55015400 | 2.59988400  |
| N            | 0.11071900  | -1.25505800 | 1.44172700  |
| H            | -0.36443200 | -0.65243100 | -2.94041100 |
| H            | 0.30177900  | -0.30256700 | -2.90655300 |
| W            | 0.05064000  | -0.78115000 | -0.29118500 |
| <b>W-TS1</b> |             |             |             |
| N            | -1.20352600 | 2.31026500  | -0.38484700 |
| N            | -2.96438400 | 1.19897900  | 0.09524600  |
| C            | 0.16484500  | 2.62251900  | -0.74353100 |
| C            | -2.22516700 | 3.23463400  | -0.28747900 |
| C            | -3.34212400 | 2.52636800  | 0.01384100  |
| C            | -1.63977800 | 1.03903200  | -0.15411900 |
| C            | 1.13228000  | 0.81131500  | 0.63542100  |
| C            | 2.14394800  | 2.84213700  | 0.77277400  |
| C            | 2.84778100  | 1.97485800  | 1.54542500  |
| N            | 2.21111500  | 0.75430000  | 1.45465900  |
| N            | 1.09951000  | 2.11486700  | 0.24073600  |
| H            | 0.40820000  | 2.17233500  | -1.70982500 |
| H            | 0.27495800  | 3.70360500  | -0.80708300 |
| C            | 2.70575000  | -0.46386600 | 2.06619900  |
| H            | 3.33793400  | -0.20581700 | 2.91591200  |
| H            | 1.86556900  | -1.06662000 | 2.41447100  |
| H            | 3.28403500  | -1.02991400 | 1.33155100  |
| H            | -4.35997600 | 2.84075400  | 0.18349400  |
| H            | -2.06244400 | 4.29007600  | -0.43939100 |
| H            | 2.27984400  | 3.89197900  | 0.56544200  |
| H            | 3.72310500  | 2.11869600  | 2.15956100  |
| C            | 3.25050400  | 0.34151400  | -1.83592900 |
| O            | 3.34811500  | -0.76085400 | -1.28410100 |
| C            | 1.08031900  | -2.28142200 | -0.03311000 |
| O            | 1.77345700  | -3.20822800 | 0.08703400  |
| C            | -1.57992000 | -1.97738300 | -1.08276200 |
| O            | -2.32843700 | -2.68065000 | -1.63854600 |
| C            | -3.90083300 | 0.11465800  | 0.32966500  |
| H            | -4.73438600 | 0.48633900  | 0.92572300  |
| H            | -4.28525800 | -0.26814000 | -0.61952100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.40593400 | -0.69209300 | 0.86924400  |
| O | -1.42486100 | -1.71965500 | 2.52137800  |
| O | 2.24691300  | 0.86201400  | -2.43320400 |
| H | 4.15733400  | 1.01053100  | -1.84679900 |
| H | 1.00476100  | 0.09155300  | -2.14246100 |
| H | 0.20218400  | -0.24586500 | -2.09662500 |
| N | -0.95302500 | -1.33647300 | 1.48993400  |
| W | -0.29412000 | -0.77078600 | -0.09936000 |

### **W-2**

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.50757500 | 2.49461800  | -0.19792000 |
| N | -2.53778800 | 1.92344800  | 0.14272700  |
| C | 0.90662300  | 2.40275200  | -0.48768200 |
| C | -1.21273100 | 3.67032400  | -0.02456900 |
| C | -2.50178500 | 3.30475200  | 0.18763700  |
| C | -1.31010000 | 1.39644800  | -0.10107600 |
| C | 1.19226900  | 0.30185000  | 0.78318100  |
| C | 2.75577200  | 1.91679000  | 1.14256100  |
| C | 3.09716000  | 0.83754500  | 1.89138200  |
| N | 2.12988000  | -0.12384500 | 1.66858700  |
| N | 1.59105000  | 1.57151800  | 0.48422300  |
| H | 1.05134900  | 1.96185900  | -1.47836700 |
| H | 1.34066900  | 3.40120000  | -0.46546900 |
| C | 2.16701100  | -1.45490100 | 2.24174300  |
| H | 2.70106500  | -1.42275900 | 3.19162100  |
| H | 1.14939900  | -1.80913600 | 2.41171600  |
| H | 2.68018800  | -2.14642100 | 1.56761900  |
| H | -3.38656500 | 3.89290800  | 0.37462000  |
| H | -0.73837400 | 4.63809300  | -0.06819100 |
| H | 3.22022700  | 2.88254000  | 1.02019200  |
| H | 3.91994900  | 0.67351400  | 2.56952500  |
| C | 3.70089600  | 0.30091100  | -1.79649600 |
| O | 2.98579800  | -0.77464400 | -1.48501200 |
| C | 0.42348800  | -2.47780500 | -0.38667000 |
| O | 0.97419800  | -3.49835700 | -0.53107700 |
| C | -2.05914700 | -1.37301300 | -1.35240200 |
| O | -2.92448400 | -1.74971800 | -2.04187200 |
| C | -3.74994200 | 1.14129000  | 0.29161900  |
| H | -4.18801600 | 0.92227100  | -0.68583000 |
| H | -3.51893300 | 0.20432600  | 0.79966200  |
| H | -4.46945700 | 1.70535700  | 0.88535500  |
| O | -1.93903400 | -1.83565100 | 2.30875600  |
| O | 3.26886800  | 1.35828100  | -2.20384100 |
| H | 4.77258300  | 0.09310300  | -1.63801000 |
| H | 2.01942800  | -0.56521100 | -1.58977700 |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| H            | 0.38547800  | -0.30898500 | -1.74917000 |
| N            | -1.40758400 | -1.33608900 | 1.35764200  |
| W            | -0.55668600 | -0.72474500 | -0.16274800 |
| <b>W-3</b>   |             |             |             |
| N            | -1.55413100 | 1.98783500  | -0.86514900 |
| N            | -3.14300600 | 0.71796500  | -0.20836600 |
| C            | -0.22451400 | 2.44604500  | -1.20849700 |
| C            | -2.71478600 | 2.72678700  | -0.99415700 |
| C            | -3.72164900 | 1.91738300  | -0.58084500 |
| C            | -1.79564100 | 0.73483300  | -0.38135000 |
| C            | 0.86658700  | 1.13900100  | 0.57249900  |
| C            | 1.45748300  | 3.33453500  | 0.43586300  |
| C            | 2.16685600  | 2.77798700  | 1.44965200  |
| N            | 1.78878700  | 1.44992800  | 1.51966000  |
| N            | 0.67321300  | 2.32073600  | -0.08014100 |
| H            | 0.15836100  | 1.83158600  | -2.03014400 |
| H            | -0.27532400 | 3.49058000  | -1.51035400 |
| C            | 2.35907200  | 0.49701800  | 2.45088200  |
| H            | 2.58245300  | 0.99940900  | 3.39291600  |
| H            | 1.64178000  | -0.30485200 | 2.62907200  |
| H            | 3.28173600  | 0.06951700  | 2.04767700  |
| H            | -4.78501000 | 2.08466300  | -0.51006100 |
| H            | -2.71347200 | 3.74204500  | -1.35836100 |
| H            | 1.43072100  | 4.33932800  | 0.04445400  |
| H            | 2.88879100  | 3.20212800  | 2.12956500  |
| C            | 1.51881300  | -1.82601500 | 0.12988200  |
| O            | 2.52464600  | -2.42381800 | 0.16549100  |
| C            | -1.20165000 | -2.26675100 | -0.84477600 |
| O            | -1.78177000 | -3.12783000 | -1.38272400 |
| C            | -3.89331500 | -0.43063400 | 0.26163700  |
| H            | -4.18769700 | -1.06695600 | -0.57731600 |
| H            | -3.27566800 | -1.00902900 | 0.94960100  |
| H            | -4.78957100 | -0.08795300 | 0.77950100  |
| O            | -1.03239300 | -1.75272100 | 2.80604900  |
| H            | 0.32480400  | -0.41445800 | -1.70968400 |
| C            | 3.44353600  | -0.20292400 | -1.95200600 |
| O            | 3.33259200  | -1.00105200 | -2.79861000 |
| O            | 3.57532900  | 0.60224200  | -1.11431700 |
| N            | -0.71101000 | -1.29861700 | 1.74300500  |
| W            | -0.19149800 | -0.76458300 | 0.04757100  |
| <b>W-TS2</b> |             |             |             |
| N            | 0.46336100  | 2.43201300  | 0.35791300  |
| N            | 1.84849700  | 1.95672100  | -1.19842900 |
| C            | -0.55736100 | 2.27554300  | 1.37538800  |

|              |             |             |             |
|--------------|-------------|-------------|-------------|
| C            | 1.10167500  | 3.61420100  | 0.03880200  |
| C            | 1.98264100  | 3.30937500  | -0.94732500 |
| C            | 0.91526300  | 1.38706400  | -0.39382600 |
| C            | -1.74628700 | 0.49775800  | 0.15607100  |
| C            | -3.02693200 | 2.23553500  | 0.87626000  |
| C            | -3.84267500 | 1.35599500  | 0.24193400  |
| N            | -3.04537400 | 0.31303700  | -0.19239900 |
| N            | -1.75832400 | 1.69255600  | 0.81127800  |
| H            | -0.17071900 | 1.61450900  | 2.15613900  |
| H            | -0.79632600 | 3.25224900  | 1.79195200  |
| C            | -3.54890400 | -0.85905600 | -0.88419200 |
| H            | -2.79687300 | -1.22223600 | -1.58513400 |
| H            | -3.78588300 | -1.65397100 | -0.17185200 |
| H            | -4.45219000 | -0.59239000 | -1.43336900 |
| H            | 2.67774500  | 3.92572900  | -1.49563200 |
| H            | 0.87141100  | 4.54458200  | 0.53402300  |
| H            | -3.22576000 | 3.17916700  | 1.35940700  |
| H            | -4.90450300 | 1.37816400  | 0.05296900  |
| C            | -0.69854300 | -2.43281000 | 0.42413800  |
| O            | -1.14735600 | -3.42781100 | 0.83856400  |
| C            | 1.95606700  | -1.53593200 | -0.26139200 |
| O            | 3.01800400  | -2.02059500 | -0.29019200 |
| C            | 2.64029100  | 1.23289600  | -2.17469500 |
| H            | 3.57674000  | 0.88691100  | -1.72902600 |
| H            | 2.07211400  | 0.37273000  | -2.53018300 |
| H            | 2.86658500  | 1.88964800  | -3.01510700 |
| O            | -0.36595200 | -1.41222300 | -3.12547100 |
| H            | 0.32193100  | -0.51835500 | 1.69609600  |
| C            | 1.43983500  | -0.63354200 | 2.82608300  |
| O            | 1.51577800  | -1.80253700 | 3.06588100  |
| O            | 1.77029400  | 0.49949200  | 3.03807300  |
| N            | -0.17150800 | -1.08233800 | -1.98938800 |
| W            | 0.11314300  | -0.69747900 | -0.21664100 |
| <b>Cr-2'</b> |             |             |             |
| N            | -1.88074500 | 1.15474500  | -0.43119400 |
| N            | -2.73588700 | -0.69146700 | 0.21811900  |
| C            | -0.91739600 | 2.09075600  | -0.97121700 |
| C            | -3.16680700 | 1.45257100  | -0.02389300 |
| C            | -3.70811100 | 0.27737700  | 0.38710500  |
| C            | -1.59620400 | -0.16685100 | -0.28958000 |
| C            | 1.00554000  | 0.79468500  | -0.07030100 |
| C            | 1.03117900  | 3.04702900  | 0.27476100  |
| C            | 2.14673200  | 2.52897100  | 0.84246100  |
| N            | 2.11150600  | 1.16337200  | 0.62687100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 0.34501400  | 1.97664900  | -0.27036300 |
| H  | -0.76996600 | 1.89075100  | -2.03737700 |
| H  | -1.29641000 | 3.10410500  | -0.85134200 |
| C  | 3.16934200  | 0.26211800  | 1.04397000  |
| H  | 3.75832700  | 0.75015800  | 1.81974000  |
| H  | 2.74602600  | -0.65775600 | 1.44648700  |
| H  | 3.82024000  | 0.01999900  | 0.20079400  |
| H  | -4.68483400 | 0.04465500  | 0.78187300  |
| H  | -3.57002200 | 2.45181900  | -0.07295600 |
| H  | 0.66108900  | 4.05778000  | 0.20656500  |
| H  | 2.95536900  | 2.99895300  | 1.37938200  |
| C  | 1.93762800  | -1.69686400 | -1.13883500 |
| O  | 2.96578600  | -2.18490900 | -1.40739600 |
| C  | -2.90097900 | -2.08399800 | 0.59270000  |
| H  | -3.86453300 | -2.45046000 | 0.23615600  |
| H  | -2.10273700 | -2.67005800 | 0.13712900  |
| H  | -2.85624900 | -2.19438000 | 1.67897800  |
| O  | 0.54259800  | -2.18719400 | 1.94519200  |
| H  | 0.49435600  | -0.48055200 | -2.51882300 |
| H  | -0.17833800 | -0.13492900 | -2.35967500 |
| N  | 0.43169600  | -1.69342200 | 0.86865400  |
| Cr | 0.28808300  | -1.00654800 | -0.63820500 |

#### Cr-TS3'

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.07722900 | 1.866698900 | -0.68229200 |
| N | -2.68677000 | 0.84988300  | 0.29899300  |
| C | 0.23313700  | 2.12572100  | -1.23171800 |
| C | -2.08029400 | 2.80740300  | -0.50810700 |
| C | -3.09603200 | 2.16070600  | 0.11310500  |
| C | -1.42885300 | 0.64021100  | -0.18146900 |
| C | 1.25783200  | 0.51376400  | 0.30177400  |
| C | 2.32492900  | 2.51933200  | 0.13757300  |
| C | 3.03096900  | 1.74638200  | 1.00154300  |
| N | 2.36491500  | 0.53573600  | 1.08874800  |
| N | 1.25454300  | 1.74842000  | -0.27423200 |
| H | 0.37086700  | 1.52791300  | -2.13935000 |
| H | 0.32678600  | 3.18587100  | -1.46240000 |
| C | 2.80364200  | -0.57603600 | 1.90909000  |
| H | 2.97209500  | -0.24188300 | 2.93473200  |
| H | 2.02799300  | -1.34192300 | 1.89978300  |
| H | 3.73137400  | -0.99973700 | 1.51594300  |
| H | -4.06749700 | 2.50420700  | 0.43282300  |
| H | -1.98035800 | 3.82433300  | -0.85385600 |
| H | 2.47935200  | 3.52810600  | -0.21262600 |
| H | 3.92909300  | 1.94855500  | 1.56429000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.37656700 | -2.06929600 | -0.95227900 |
| O  | -2.13475400 | -2.78249500 | -1.49737400 |
| C  | -3.46647500 | -0.14726000 | 1.00132700  |
| H  | -3.28921800 | -1.12787500 | 0.55759900  |
| H  | -3.18900800 | -0.18581700 | 2.05807100  |
| H  | -4.52497700 | 0.10223300  | 0.92011900  |
| O  | -0.84892700 | -1.98877400 | 2.47468900  |
| H  | 0.24581600  | -0.65619700 | -1.78794500 |
| C  | 1.90563400  | -1.46345800 | -1.51398000 |
| O  | 1.63552400  | -2.23433400 | -0.63357900 |
| O  | 2.58630300  | -0.95603200 | -2.33415900 |
| N  | -0.57465800 | -1.48705600 | 1.41873800  |
| Cr | -0.18960900 | -0.93822100 | -0.12144300 |

### Fe-2'

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.78022300 | 1.22746700  | -0.38341000 |
| N | -2.68387600 | -0.61445100 | 0.22536900  |
| C | -0.79235700 | 2.13793000  | -0.92314500 |
| C | -3.06434700 | 1.54494100  | 0.01202000  |
| C | -3.63593200 | 0.37463500  | 0.39379100  |
| C | -1.53425500 | -0.09959100 | -0.25887200 |
| C | 1.04673300  | 0.70022100  | -0.09636000 |
| C | 1.25685800  | 2.92333100  | 0.29492100  |
| C | 2.33975300  | 2.30443000  | 0.82133500  |
| N | 2.19153500  | 0.94907300  | 0.58524100  |
| N | 0.47556300  | 1.92585600  | -0.25857200 |
| H | -0.67983900 | 1.96154600  | -1.99744400 |
| H | -1.11510100 | 3.16325900  | -0.75592300 |
| C | 3.16491200  | -0.03456100 | 1.02623000  |
| H | 3.74118600  | 0.39700700  | 1.84363200  |
| H | 2.65558800  | -0.92726700 | 1.39033100  |
| H | 3.84698600  | -0.29351500 | 0.21363200  |
| H | -4.62327100 | 0.15438200  | 0.76821600  |
| H | -3.44256100 | 2.55420900  | -0.02304900 |
| H | 0.96530000  | 3.96061300  | 0.25838600  |
| H | 3.19711000  | 2.69198000  | 1.34834700  |
| C | 1.77171400  | -1.74987500 | -1.04594300 |
| O | 2.73026400  | -2.34335400 | -1.30247700 |
| C | -2.89839300 | -2.01076400 | 0.56286500  |
| H | -3.86868400 | -2.33036800 | 0.18069300  |
| H | -2.11417500 | -2.61312000 | 0.10633400  |
| H | -2.87412200 | -2.14583300 | 1.64640800  |
| H | 0.46036700  | -0.43174200 | -2.30979800 |
| H | -0.32072400 | -0.27776400 | -2.16913100 |
| C | 0.24949600  | -1.60867100 | 1.07127600  |

|                |             |             |             |
|----------------|-------------|-------------|-------------|
| N              | 0.24510300  | -2.04897900 | 2.16447100  |
| Fe             | 0.22184700  | -0.92621000 | -0.67543200 |
| <b>Fe-TS3'</b> |             |             |             |
| N              | -1.13532700 | 1.81906800  | -0.63069600 |
| N              | -2.67959800 | 0.66522900  | 0.30642600  |
| C              | 0.13525300  | 2.16173100  | -1.22312100 |
| C              | -2.21309300 | 2.67240300  | -0.47556700 |
| C              | -3.18909000 | 1.93884500  | 0.11002800  |
| C              | -1.40344900 | 0.56936000  | -0.15304500 |
| C              | 1.26539800  | 0.53528000  | 0.20590600  |
| C              | 2.28853600  | 2.55848600  | 0.04024600  |
| C              | 3.05907100  | 1.76764000  | 0.82859200  |
| N              | 2.41691000  | 0.54417000  | 0.92200600  |
| N              | 1.20627100  | 1.78289800  | -0.32783100 |
| H              | 0.25299200  | 1.61609500  | -2.16595900 |
| H              | 0.17267200  | 3.23432100  | -1.40509900 |
| C              | 2.95248300  | -0.58389500 | 1.66074500  |
| H              | 3.35038800  | -0.23523500 | 2.61487200  |
| H              | 2.15394200  | -1.30162400 | 1.84149600  |
| H              | 3.75444300  | -1.06409100 | 1.09408600  |
| H              | -4.19145500 | 2.19882700  | 0.41178700  |
| H              | -2.17817600 | 3.70287500  | -0.79126600 |
| H              | 2.40111100  | 3.58134400  | -0.28313200 |
| H              | 3.99064500  | 1.96130800  | 1.33710600  |
| C              | -1.32968000 | -2.04524600 | -0.62893600 |
| O              | -2.09477500 | -2.84203300 | -0.99688200 |
| C              | -3.45218800 | -0.41184000 | 0.89548800  |
| H              | -4.00128600 | -0.96002000 | 0.12566100  |
| H              | -2.78561700 | -1.09125900 | 1.42619100  |
| H              | -4.16527600 | 0.01136900  | 1.60325400  |
| H              | 0.09159500  | -0.59886500 | -1.68569900 |
| C              | 1.61738400  | -1.58956100 | -1.48315500 |
| O              | 1.45871200  | -2.26906700 | -0.49184300 |
| O              | 2.22755500  | -1.26871000 | -2.44645100 |
| C              | -0.33768200 | -1.17850300 | 1.73561100  |
| N              | -0.45308500 | -1.39093200 | 2.89162500  |
| Fe             | -0.13160700 | -0.85876100 | -0.14805200 |
| <b>Co-2'</b>   |             |             |             |
| N              | -1.76213500 | 1.24604600  | -0.36397500 |
| N              | -2.67427500 | -0.60288000 | 0.22440400  |
| C              | -0.76617500 | 2.15416300  | -0.88899300 |
| C              | -3.05239600 | 1.55879500  | 0.01236700  |
| C              | -3.62753900 | 0.38569600  | 0.38236700  |
| C              | -1.52711200 | -0.07901400 | -0.24406300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.04625800  | 0.66825300  | -0.06288500 |
| C  | 1.34007500  | 2.87068100  | 0.27414300  |
| C  | 2.41189100  | 2.21905600  | 0.78624500  |
| N  | 2.21120900  | 0.86599000  | 0.58652900  |
| N  | 0.50234700  | 1.89866500  | -0.23339600 |
| H  | -0.65868300 | 2.00335300  | -1.96709400 |
| H  | -1.06613100 | 3.18035900  | -0.69046800 |
| C  | 3.17389000  | -0.13327700 | 1.02878000  |
| H  | 3.71999700  | 0.28208300  | 1.87470900  |
| H  | 2.65722200  | -1.03780700 | 1.34407900  |
| H  | 3.87043400  | -0.36693900 | 0.22261200  |
| H  | -4.61996500 | 0.16267400  | 0.74104500  |
| H  | -3.43147900 | 2.56740300  | -0.02801400 |
| H  | 1.08932300  | 3.91787400  | 0.21985700  |
| H  | 3.29753200  | 2.58270500  | 1.28245100  |
| C  | 1.82308700  | -1.78738900 | -1.11988800 |
| C  | -2.88460000 | -2.00142800 | 0.56075000  |
| H  | -3.85328400 | -2.32129000 | 0.17612000  |
| H  | -2.09840000 | -2.60134600 | 0.10413200  |
| H  | -2.86194900 | -2.13317800 | 1.64437600  |
| H  | 0.46864800  | -0.42621200 | -2.33332200 |
| H  | -0.30011400 | -0.27720400 | -2.23058000 |
| C  | 0.27046800  | -1.55635900 | 1.06723600  |
| N  | 0.28198500  | -2.00144500 | 2.15498000  |
| N  | 2.77277600  | -2.39017800 | -1.45804200 |
| Co | 0.19320100  | -0.90522000 | -0.64851000 |

#### Co-TS3'

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.07438600 | 1.79384500  | -0.74628300 |
| N | -2.61700400 | 0.72988400  | 0.30560500  |
| C | 0.19926800  | 2.08158200  | -1.36742200 |
| C | -2.15214800 | 2.65460400  | -0.67037700 |
| C | -3.12407700 | 1.97937100  | -0.01115000 |
| C | -1.35162800 | 0.60403200  | -0.15329100 |
| C | 1.30318700  | 0.55294900  | 0.18385700  |
| C | 2.36777800  | 2.52448700  | -0.14192800 |
| C | 3.12012900  | 1.77847800  | 0.70548700  |
| N | 2.45011000  | 0.58158200  | 0.89672100  |
| N | 1.26443200  | 1.75185000  | -0.44601200 |
| H | 0.30492100  | 1.47404900  | -2.27171200 |
| H | 0.24593000  | 3.13868100  | -1.62006800 |
| C | 2.95483000  | -0.49431600 | 1.73054200  |
| H | 3.26571100  | -0.09072400 | 2.69531800  |
| H | 2.16627500  | -1.22840800 | 1.88371800  |
| H | 3.81062100  | -0.97324400 | 1.24964200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.12484400 | 2.26486700  | 0.27144900  |
| H  | -2.11796500 | 3.64932300  | -1.08495000 |
| H  | 2.50808200  | 3.51259600  | -0.55009000 |
| H  | 4.05869100  | 1.98655500  | 1.19476500  |
| C  | -1.41496400 | -2.12179100 | -0.42424900 |
| C  | -3.39788900 | -0.27332000 | 1.00984800  |
| H  | -3.93728500 | -0.90265600 | 0.29972800  |
| H  | -2.74137500 | -0.89269300 | 1.61813900  |
| H  | -4.11158200 | 0.24003700  | 1.65407900  |
| H  | 0.14628500  | -0.67540700 | -1.57259200 |
| C  | 1.31503900  | -1.88672200 | -1.60375200 |
| O  | 1.40696800  | -2.23663000 | -0.44586800 |
| O  | 1.61485900  | -1.94433500 | -2.74595800 |
| C  | -0.30941800 | -1.01078000 | 1.83959400  |
| N  | -0.43003500 | -1.15132400 | 3.00234900  |
| Co | -0.09516000 | -0.79824200 | -0.03705600 |
| N  | -2.18446000 | -2.96786200 | -0.70027400 |

#### Mo-2'

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -2.14399100 | 0.80429400  | -0.59013800 |
| N | -2.73950100 | -0.97370000 | 0.42812300  |
| C | -1.28322700 | 1.76355100  | -1.25948700 |
| C | -3.45229500 | 1.01153800  | -0.19703300 |
| C | -3.83126800 | -0.12284700 | 0.44522300  |
| C | -1.68126900 | -0.42018400 | -0.21003100 |
| C | 0.76578900  | 1.09929300  | -0.04902300 |
| C | 0.14359800  | 3.28264000  | 0.15807600  |
| C | 1.24087200  | 3.08912000  | 0.92919800  |
| N | 1.60663200  | 1.76124800  | 0.78922900  |
| N | -0.12930300 | 2.06253700  | -0.43625200 |
| H | -0.94915100 | 1.34326800  | -2.21101000 |
| H | -1.83935200 | 2.68102200  | -1.44228000 |
| C | 2.70685700  | 1.14405900  | 1.50295000  |
| H | 3.45320700  | 1.90416900  | 1.73417900  |
| H | 2.35889500  | 0.68608600  | 2.43157200  |
| H | 3.15539000  | 0.37228500  | 0.87563700  |
| H | -4.76573800 | -0.39861700 | 0.90896500  |
| H | -3.98467300 | 1.92474900  | -0.41361000 |
| H | -0.44808200 | 4.16200900  | -0.04208700 |
| H | 1.80016200  | 3.76729500  | 1.55428700  |
| C | 2.45291900  | -1.25279400 | -1.06310100 |
| O | 3.58869300  | -1.42703100 | -1.30318900 |
| C | -2.72877500 | -2.29192200 | 1.03157700  |
| H | -3.48042000 | -2.92994100 | 0.56177300  |
| H | -1.74083400 | -2.73198800 | 0.89045100  |

|                |             |             |             |
|----------------|-------------|-------------|-------------|
| H              | -2.94109300 | -2.22000600 | 2.10037800  |
| O              | 1.17938800  | -1.83410300 | 2.19861700  |
| H              | 0.56983200  | -0.67495100 | -3.22742600 |
| H              | -0.16196200 | -0.54190900 | -3.11155700 |
| Mo             | 0.52952100  | -0.96018100 | -0.58123800 |
| N              | 0.91903500  | -1.47459600 | 1.08178400  |
| <b>Mo-TS3'</b> |             |             |             |
| N              | -1.09530700 | 2.00093500  | -0.75146900 |
| N              | -2.72596100 | 1.06303600  | 0.27938900  |
| C              | 0.20940500  | 2.18863000  | -1.34486700 |
| C              | -2.05789300 | 2.98118300  | -0.57409200 |
| C              | -3.08577500 | 2.38509800  | 0.07833400  |
| C              | -1.48841500 | 0.79826200  | -0.22217400 |
| C              | 1.34873000  | 0.72660800  | 0.27188800  |
| C              | 2.28454100  | 2.78179600  | -0.02767000 |
| C              | 3.04592800  | 2.10848900  | 0.87226000  |
| N              | 2.45654600  | 0.86773200  | 1.04274700  |
| N              | 1.26084600  | 1.92264100  | -0.37842500 |
| H              | 0.32262300  | 1.48837500  | -2.17964600 |
| H              | 0.29993800  | 3.21360600  | -1.69972200 |
| C              | 2.98035400  | -0.17183500 | 1.90737300  |
| H              | 3.31887700  | 0.26499400  | 2.84790600  |
| H              | 2.18880900  | -0.89415600 | 2.11141200  |
| H              | 3.82042500  | -0.68393700 | 1.42956300  |
| H              | -4.03662300 | 2.77177300  | 0.40986000  |
| H              | -1.92687100 | 3.98721400  | -0.94061100 |
| H              | 2.37323100  | 3.77472500  | -0.44003900 |
| H              | 3.93571900  | 2.39804400  | 1.40942500  |
| C              | -1.54518100 | -2.14401000 | -0.91099100 |
| O              | -2.35600000 | -2.85962000 | -1.37254700 |
| C              | -3.52666100 | 0.09470600  | 0.99845300  |
| H              | -3.50722600 | -0.86184900 | 0.47180800  |
| H              | -3.13545600 | -0.05562600 | 2.00828500  |
| H              | -4.55320700 | 0.45602900  | 1.05975500  |
| O              | -0.85860100 | -1.95723300 | 2.61291900  |
| H              | 0.61303800  | -0.92061800 | -1.88619200 |
| C              | 2.15400200  | -1.72874100 | -1.30251900 |
| O              | 1.73389900  | -2.39046500 | -0.38999200 |
| O              | 2.98305700  | -1.33935600 | -2.04807400 |
| N              | -0.65613900 | -1.42765800 | 1.55113400  |
| Mo             | -0.19824300 | -0.89697800 | -0.13571100 |
| <b>W-2'</b>    |             |             |             |
| N              | -2.29192100 | 0.63652300  | -0.67977200 |
| N              | -2.66997600 | -1.08638800 | 0.52637800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.51720300 | 1.63668000  | -1.39207200 |
| C | -3.59731200 | 0.75600300  | -0.24383600 |
| C | -3.83816200 | -0.34364700 | 0.51510500  |
| C | -1.69373900 | -0.49371600 | -0.20228900 |
| C | 0.48910600  | 1.31041900  | 0.00511100  |
| C | -0.40396000 | 3.41053000  | 0.01802800  |
| C | 0.62200000  | 3.38952500  | 0.90303100  |
| N | 1.15569000  | 2.11228400  | 0.87937300  |
| N | -0.46794100 | 2.14036200  | -0.52888700 |
| H | -1.06790000 | 1.17298400  | -2.27449300 |
| H | -2.16445400 | 2.45654500  | -1.69583800 |
| C | 2.24094100  | 1.66004900  | 1.72549600  |
| H | 2.78947200  | 2.52700200  | 2.09323000  |
| H | 1.85763600  | 1.08632000  | 2.57241900  |
| H | 2.91108900  | 1.02145000  | 1.14660600  |
| H | -4.72523700 | -0.66431100 | 1.03883100  |
| H | -4.22633900 | 1.58656700  | -0.52354000 |
| H | -1.06984400 | 4.20102400  | -0.29060400 |
| H | 1.03069500  | 4.16131200  | 1.53618800  |
| C | 2.53965600  | -0.75901400 | -0.80022700 |
| O | 3.70937200  | -0.74803200 | -0.94613400 |
| C | -2.49104500 | -2.30565100 | 1.29077200  |
| H | -3.32329100 | -2.98708700 | 1.10668200  |
| H | -1.55902500 | -2.78001500 | 0.98320800  |
| H | -2.44398400 | -2.08103400 | 2.35931200  |
| O | 1.07558000  | -1.56255200 | 2.37372200  |
| H | 0.62539100  | -1.52107800 | -3.03999200 |
| H | -0.11716300 | -1.41551000 | -2.96979700 |
| N | 0.89363000  | -1.21753700 | 1.22843100  |
| W | 0.57790900  | -0.75599000 | -0.46427400 |

#### W-TS3'

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.11041400 | 2.10721200 | -0.75971100 |
| N | -2.69714700 | 1.15762100 | 0.33322900  |
| C | 0.18108000  | 2.30291800 | -1.37867600 |
| C | -2.08113500 | 3.07535900 | -0.56319500 |
| C | -3.07967000 | 2.47237600 | 0.12720200  |
| C | -1.46936000 | 0.90259500 | -0.20169900 |
| C | 1.34902500  | 0.86726000 | 0.23831800  |
| C | 2.24291800  | 2.94148800 | -0.05487200 |
| C | 3.00148900  | 2.28990300 | 0.86333000  |
| N | 2.43832800  | 1.03711600 | 1.03111100  |
| N | 1.24715300  | 2.05816100 | -0.42224100 |
| H | 0.28980600  | 1.59114800 | -2.20504500 |
| H | 0.25667000  | 3.32319800 | -1.74943600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.96264100  | 0.01852700  | 1.92067800  |
| H | 3.32118100  | 0.48402800  | 2.83956900  |
| H | 2.16556900  | -0.68541100 | 2.16386700  |
| H | 3.78918600  | -0.51964000 | 1.44789200  |
| H | -4.02606500 | 2.84976900  | 0.48103400  |
| H | -1.97697900 | 4.07816700  | -0.94649400 |
| H | 2.31806200  | 3.93369900  | -0.47150300 |
| H | 3.87515300  | 2.60122000  | 1.41428700  |
| C | -1.51121000 | -2.03770000 | -0.83588200 |
| O | -2.32973600 | -2.78130900 | -1.24728000 |
| C | -3.46551700 | 0.18384500  | 1.07832900  |
| H | -3.47374500 | -0.76732400 | 0.54118800  |
| H | -3.02838800 | 0.02015600  | 2.06710600  |
| H | -4.48657400 | 0.54839700  | 1.19098800  |
| O | -0.65548500 | -1.76188200 | 2.66114600  |
| H | 0.68278900  | -0.91923100 | -1.86414800 |
| C | 2.20617100  | -1.62456200 | -1.21450200 |
| O | 1.77826700  | -2.25795800 | -0.28198400 |
| O | 3.05181200  | -1.25196400 | -1.94962400 |
| N | -0.53776800 | -1.25980700 | 1.56511800  |
| W | -0.16034000 | -0.75901900 | -0.14154200 |

#### Re-Cat

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.90974200  | 2.32788500  | 0.11408800  |
| N | 2.68815600  | 1.28420900  | -0.44622800 |
| C | -0.43762900 | 2.61916000  | 0.56150600  |
| C | 1.87313600  | 3.29523900  | -0.10140900 |
| C | 3.00071700  | 2.63026700  | -0.45313000 |
| C | 1.39638900  | 1.07068100  | -0.08559800 |
| C | -1.38580400 | 0.60920900  | -0.56886400 |
| C | -2.55622300 | 2.55117100  | -0.75608000 |
| C | -3.24654000 | 1.58941300  | -1.41629300 |
| N | -2.51579200 | 0.42319800  | -1.29901000 |
| N | -1.42697500 | 1.93519700  | -0.25080000 |
| H | -0.54909400 | 2.31445600  | 1.60487100  |
| H | -0.60491300 | 3.69113200  | 0.46818700  |
| C | -2.96471000 | -0.85257000 | -1.82353600 |
| H | -3.60821500 | -0.67482400 | -2.68497500 |
| H | -2.10540100 | -1.44730300 | -2.13407000 |
| H | -3.52914100 | -1.39898200 | -1.06345400 |
| H | 3.98467700  | 2.98498500  | -0.71670800 |
| H | 1.66363500  | 4.34759100  | 0.00891200  |
| H | -2.75209800 | 3.60104200  | -0.60505800 |
| H | -4.17452100 | 1.62708900  | -1.96467900 |
| C | -1.53496900 | 0.17879000  | 2.44853900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -0.30564700 | 0.10139400  | 2.06550500  |
| C  | -1.01208400 | -2.26888000 | 0.31643800  |
| O  | -1.71768900 | -3.19233500 | 0.44346600  |
| C  | 1.66145700  | -1.79205800 | 0.85001000  |
| O  | 2.53348300  | -2.41947200 | 1.31006300  |
| C  | 3.65937500  | 0.24399300  | -0.73153000 |
| H  | 4.12887100  | -0.10600900 | 0.19093600  |
| H  | 3.17120700  | -0.59554700 | -1.22636900 |
| H  | 4.42787200  | 0.64846500  | -1.39025500 |
| C  | 0.62820400  | -1.35470900 | -1.66924100 |
| O  | 0.87521800  | -1.71904600 | -2.75804000 |
| O  | -1.98323200 | 0.97890700  | 3.26522200  |
| H  | -2.22612300 | -0.56511900 | 1.96677500  |
| Re | 0.19843100  | -0.76445600 | 0.08913200  |

#### Re-1

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -1.09351600 | 2.20957300  | -0.49336400 |
| N | -2.59083700 | 1.09744400  | 0.54935800  |
| C | 0.11704100  | 2.52146200  | -1.22278900 |
| C | -2.06272400 | 3.12226100  | -0.12883500 |
| C | -3.01417000 | 2.41252400  | 0.52793100  |
| C | -1.40142900 | 0.94783300  | -0.08491900 |
| C | 1.47518200  | 0.83398700  | -0.04536600 |
| C | 2.35575000  | 2.92574400  | -0.14813200 |
| C | 3.24203200  | 2.13372100  | 0.50541500  |
| N | 2.68635900  | 0.86947900  | 0.56193600  |
| N | 1.28847600  | 2.11260700  | -0.47271900 |
| H | 0.10533700  | 1.99826400  | -2.18204200 |
| H | 0.16173600  | 3.59501000  | -1.39329500 |
| C | 3.36239300  | -0.27515100 | 1.14617500  |
| H | 4.07536000  | 0.07651700  | 1.89125400  |
| H | 2.63653400  | -0.92907700 | 1.62918200  |
| H | 3.89876800  | -0.83514700 | 0.37666700  |
| H | -3.94083000 | 2.71916000  | 0.98711400  |
| H | -1.98531200 | 4.17110900  | -0.36799600 |
| H | 2.38057600  | 3.97251500  | -0.40563000 |
| H | 4.20485100  | 2.35017400  | 0.94070500  |
| C | 1.30065200  | -2.16979500 | -0.56089200 |
| O | 2.08778500  | -3.02054000 | -0.68161100 |
| C | -1.48519100 | -2.05689600 | -0.58174200 |
| O | -2.33397900 | -2.84601600 | -0.70529100 |
| C | -3.35987100 | 0.01966100  | 1.14504800  |
| H | -3.93552800 | -0.50681100 | 0.38044300  |
| H | -2.69221500 | -0.68380800 | 1.64248800  |
| H | -4.04500500 | 0.43885200  | 1.88102700  |

|               |             |             |             |
|---------------|-------------|-------------|-------------|
| C             | -0.06538600 | -1.12728400 | 1.52388400  |
| O             | -0.08150700 | -1.34417400 | 2.67444600  |
| H             | 0.36869500  | -0.38809400 | -2.52034300 |
| H             | -0.38210000 | -0.49105400 | -2.58657800 |
| Re            | -0.04064400 | -0.76738500 | -0.32059300 |
| <b>Re-TS1</b> |             |             |             |
| N             | -1.26708700 | 2.26156000  | -0.38236400 |
| N             | -2.98668600 | 1.07617300  | 0.06775300  |
| C             | 0.09050400  | 2.62781600  | -0.72757000 |
| C             | -2.32385100 | 3.14465800  | -0.27887900 |
| C             | -3.41448500 | 2.38940500  | 0.00238900  |
| C             | -1.65489300 | 0.97248800  | -0.17362400 |
| C             | 1.11234100  | 0.80270800  | 0.57713200  |
| C             | 2.04882900  | 2.85959000  | 0.81476300  |
| C             | 2.78586300  | 1.98255100  | 1.54254000  |
| N             | 2.19465300  | 0.74347800  | 1.39195300  |
| N             | 1.03000700  | 2.12101400  | 0.24886300  |
| H             | 0.35528400  | 2.20804400  | -1.70235800 |
| H             | 0.16632400  | 3.71312300  | -0.76134000 |
| C             | 2.73946900  | -0.48073500 | 1.94644300  |
| H             | 3.42930600  | -0.22775700 | 2.75146700  |
| H             | 1.93432500  | -1.09697100 | 2.35022000  |
| H             | 3.26646600  | -1.02675900 | 1.15990300  |
| H             | -4.44546200 | 2.66031500  | 0.16684600  |
| H             | -2.20034600 | 4.20758500  | -0.41360300 |
| H             | 2.14494900  | 3.92223200  | 0.65709800  |
| H             | 3.65935700  | 2.12573200  | 2.15919300  |
| C             | 3.22773600  | 0.37185800  | -1.75504600 |
| O             | 3.34302600  | -0.78714100 | -1.33316000 |
| C             | 1.02983100  | -2.21938100 | -0.02810100 |
| O             | 1.70499300  | -3.15692100 | 0.11994900  |
| C             | -1.56146300 | -2.01102800 | -0.88655300 |
| O             | -2.32501200 | -2.79271700 | -1.30085700 |
| C             | -3.88034900 | -0.04351700 | 0.29750700  |
| H             | -4.79959500 | 0.32686900  | 0.75036000  |
| H             | -4.12346000 | -0.53880800 | -0.64569600 |
| H             | -3.41595400 | -0.76239800 | 0.97322300  |
| O             | -1.19034800 | -1.47540000 | 2.68223500  |
| O             | 2.23862700  | 0.92644400  | -2.33884700 |
| H             | 4.11137400  | 1.06445800  | -1.63339300 |
| H             | 0.95626300  | 0.07445100  | -2.13563000 |
| H             | 0.18132800  | -0.29413200 | -2.16046700 |
| Re            | -0.27149900 | -0.75568100 | -0.14681500 |
| C             | -0.83689900 | -1.19801100 | 1.59855200  |

**Re-2**

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -0.69603600 | 2.42159100  | -0.15792800 |
| N  | -2.68002700 | 1.67347500  | 0.10708900  |
| C  | 0.72294700  | 2.46002100  | -0.42960400 |
| C  | -1.50990100 | 3.53128300  | -0.02479900 |
| C  | -2.76796700 | 3.05376800  | 0.13854800  |
| C  | -1.40035100 | 1.25699800  | -0.08547600 |
| C  | 1.18026700  | 0.34209700  | 0.75754000  |
| C  | 2.60310200  | 2.06819500  | 1.18237300  |
| C  | 3.04702500  | 0.98902200  | 1.87227900  |
| N  | 2.16362000  | -0.04281500 | 1.61293300  |
| N  | 1.46543400  | 1.65392500  | 0.51655500  |
| H  | 0.91587000  | 2.07078000  | -1.43420400 |
| H  | 1.06860800  | 3.49017700  | -0.36101900 |
| C  | 2.32902200  | -1.38614800 | 2.13063400  |
| H  | 2.85105900  | -1.34002600 | 3.08673500  |
| H  | 1.35074300  | -1.84547000 | 2.27637700  |
| H  | 2.91284900  | -1.99626400 | 1.43586500  |
| H  | -3.70921100 | 3.56106800  | 0.28068500  |
| H  | -1.12095700 | 4.53682500  | -0.05620600 |
| H  | 2.97823700  | 3.07659400  | 1.10521000  |
| H  | 3.89116500  | 0.86440700  | 2.53226900  |
| C  | 3.61599600  | 0.44005700  | -1.87797100 |
| O  | 2.94197800  | -0.65599900 | -1.54592200 |
| C  | 0.50309400  | -2.39684800 | -0.35897600 |
| O  | 1.07401900  | -3.41091700 | -0.48835600 |
| C  | -1.95067300 | -1.46066800 | -1.22183600 |
| O  | -2.82239200 | -1.89178500 | -1.87379600 |
| C  | -3.83328400 | 0.80031600  | 0.20516700  |
| H  | -4.22588100 | 0.56862500  | -0.78822700 |
| H  | -3.55138400 | -0.12803700 | 0.70290700  |
| H  | -4.60980600 | 1.29830800  | 0.78607100  |
| C  | -1.24965200 | -1.29932800 | 1.51576300  |
| O  | -1.69402000 | -1.67144400 | 2.53485800  |
| O  | 3.13970600  | 1.51192800  | -2.18531000 |
| H  | 4.69892900  | 0.23441300  | -1.84434600 |
| H  | 1.97056500  | -0.45629800 | -1.54873500 |
| H  | 0.28458200  | -0.12894400 | -1.68548000 |
| Re | -0.48437800 | -0.73595000 | -0.17856100 |

**Re-3**

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.56298500 | 1.93128400 | -0.87959100 |
| N | -3.12919300 | 0.63135400 | -0.22723500 |
| C | -0.24398900 | 2.40756200 | -1.23332100 |
| C | -2.73832900 | 2.64455700 | -1.02348400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.73045700 | 1.81590700  | -0.61539800 |
| C  | -1.78080300 | 0.67687100  | -0.38965700 |
| C  | 0.86922000  | 1.10589900  | 0.53604000  |
| C  | 1.44967100  | 3.30436900  | 0.39258500  |
| C  | 2.17333400  | 2.75139500  | 1.39679600  |
| N  | 1.79951600  | 1.42142500  | 1.47454800  |
| N  | 0.66438500  | 2.28633300  | -0.11479700 |
| H  | 0.13828400  | 1.79884200  | -2.05968800 |
| H  | -0.30969300 | 3.45302300  | -1.52945400 |
| C  | 2.37793300  | 0.48127600  | 2.41330900  |
| H  | 2.69973400  | 1.01934500  | 3.30542700  |
| H  | 1.63134900  | -0.26340100 | 2.69111300  |
| H  | 3.24083500  | -0.02659400 | 1.97395800  |
| H  | -4.79801400 | 1.95861300  | -0.55685100 |
| H  | -2.75455000 | 3.65761800  | -1.39322000 |
| H  | 1.41246400  | 4.30876600  | 0.00131700  |
| H  | 2.90326600  | 3.17736800  | 2.06687700  |
| C  | 1.45273600  | -1.79047000 | 0.21297200  |
| O  | 2.45401600  | -2.39562600 | 0.29504200  |
| C  | -1.17013800 | -2.24648200 | -0.70314900 |
| O  | -1.76604800 | -3.13930100 | -1.17274400 |
| C  | -3.86444400 | -0.52232200 | 0.25255100  |
| H  | -4.09932100 | -1.20209700 | -0.57038000 |
| H  | -3.26581800 | -1.05355000 | 0.99347700  |
| H  | -4.79414700 | -0.18690300 | 0.71271300  |
| C  | -0.74454900 | -1.10645900 | 1.85256800  |
| O  | -1.08449500 | -1.34473200 | 2.95035900  |
| H  | 0.32932800  | -0.31573600 | -1.62614700 |
| C  | 3.40193000  | -0.27399600 | -1.95055900 |
| O  | 3.25835800  | -1.10729300 | -2.75763500 |
| O  | 3.57203500  | 0.56512600  | -1.15409200 |
| Re | -0.17225900 | -0.75109500 | 0.02780600  |

#### Re-TS2

|   |             |            |             |
|---|-------------|------------|-------------|
| N | 0.85307100  | 2.29538300 | 0.33448800  |
| N | 2.18167900  | 1.54056300 | -1.15924700 |
| C | -0.19462400 | 2.34001500 | 1.33301400  |
| C | 1.68235700  | 3.34659700 | -0.00695100 |
| C | 2.52736900  | 2.86351300 | -0.95100400 |
| C | 1.14493100  | 1.16421900 | -0.36637200 |
| C | -1.63738300 | 0.72300300 | 0.15847900  |
| C | -2.63424200 | 2.66212800 | 0.81098800  |
| C | -3.57687700 | 1.89524900 | 0.20943600  |
| N | -2.95050300 | 0.72679300 | -0.18523400 |
| N | -1.46439200 | 1.92894100 | 0.76983400  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.07565800  | 1.65982500  | 2.14560400  |
| H  | -0.28539900 | 3.35773900  | 1.70819500  |
| C  | -3.64288700 | -0.36855100 | -0.83567700 |
| H  | -4.44834000 | 0.03185100  | -1.45175100 |
| H  | -2.94482500 | -0.91717200 | -1.46768700 |
| H  | -4.06632800 | -1.04990700 | -0.09323900 |
| H  | 3.33213600  | 3.33414000  | -1.49334300 |
| H  | 1.59215100  | 4.32112000  | 0.44611300  |
| H  | -2.68338800 | 3.64322100  | 1.25649300  |
| H  | -4.62402800 | 2.07210200  | 0.02057900  |
| C  | -1.08759500 | -2.25458200 | 0.24161800  |
| O  | -1.73410000 | -3.18992200 | 0.51463400  |
| C  | 1.59693200  | -1.82087500 | -0.27315300 |
| O  | 2.54560600  | -2.50431500 | -0.30439400 |
| C  | 2.88635400  | 0.66871200  | -2.07926300 |
| H  | 3.70415900  | 0.15211000  | -1.57063900 |
| H  | 2.19587300  | -0.06865500 | -2.48892300 |
| H  | 3.29643800  | 1.26636000  | -2.89362200 |
| C  | -0.32699500 | -0.85816200 | -2.06026300 |
| O  | -0.53811900 | -0.97388400 | -3.20844200 |
| H  | 0.27745600  | -0.53264600 | 1.66401200  |
| C  | 1.25867600  | -0.80765800 | 2.80806700  |
| O  | 1.08454100  | -1.95208500 | 3.12000800  |
| O  | 1.82269500  | 0.23661600  | 3.00048100  |
| Re | 0.01091200  | -0.70619700 | -0.17350000 |