

Reaction Mechanism of low spin Iron (III)- and Cobalt (III) containing Nitrile Hydratases: A Quantum Mechanics Investigation

Tiziana Marino*, Mario Prejanò, Carmen Rizzuto, José Carlos Madrid Madrid, Nino Russo, Marirosa Toscano*

Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, 87036 Arcavacata di Rende (CS) (Italy)

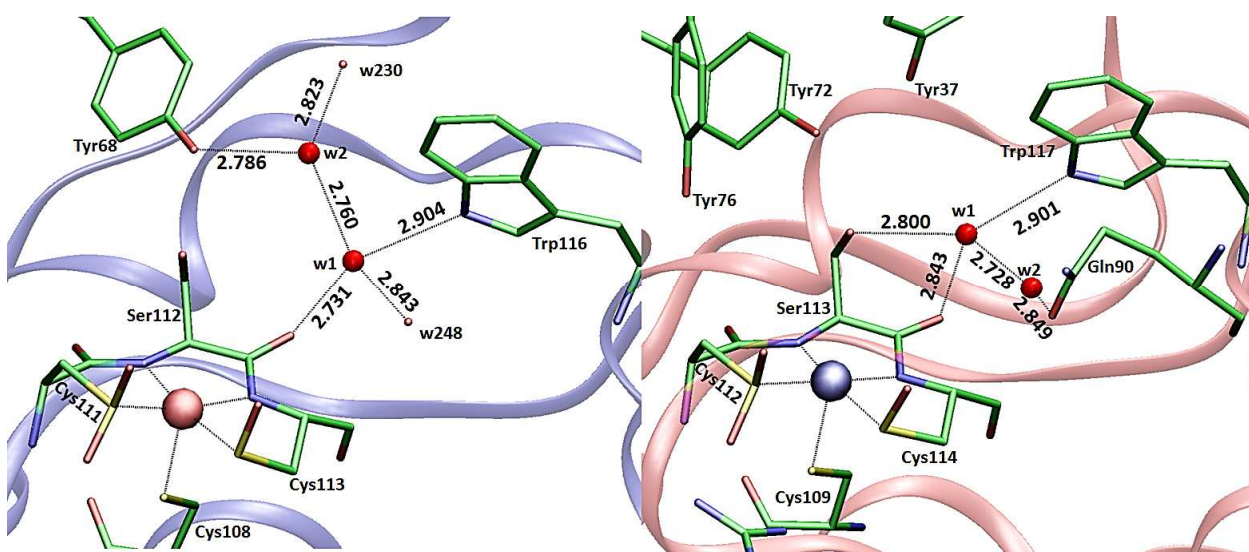


Figure S1. X ray hydrogen bonds network for water molecules explicitly considered in the model for the Co-NHase and Fe-NHase, on the left and on the right respectively.

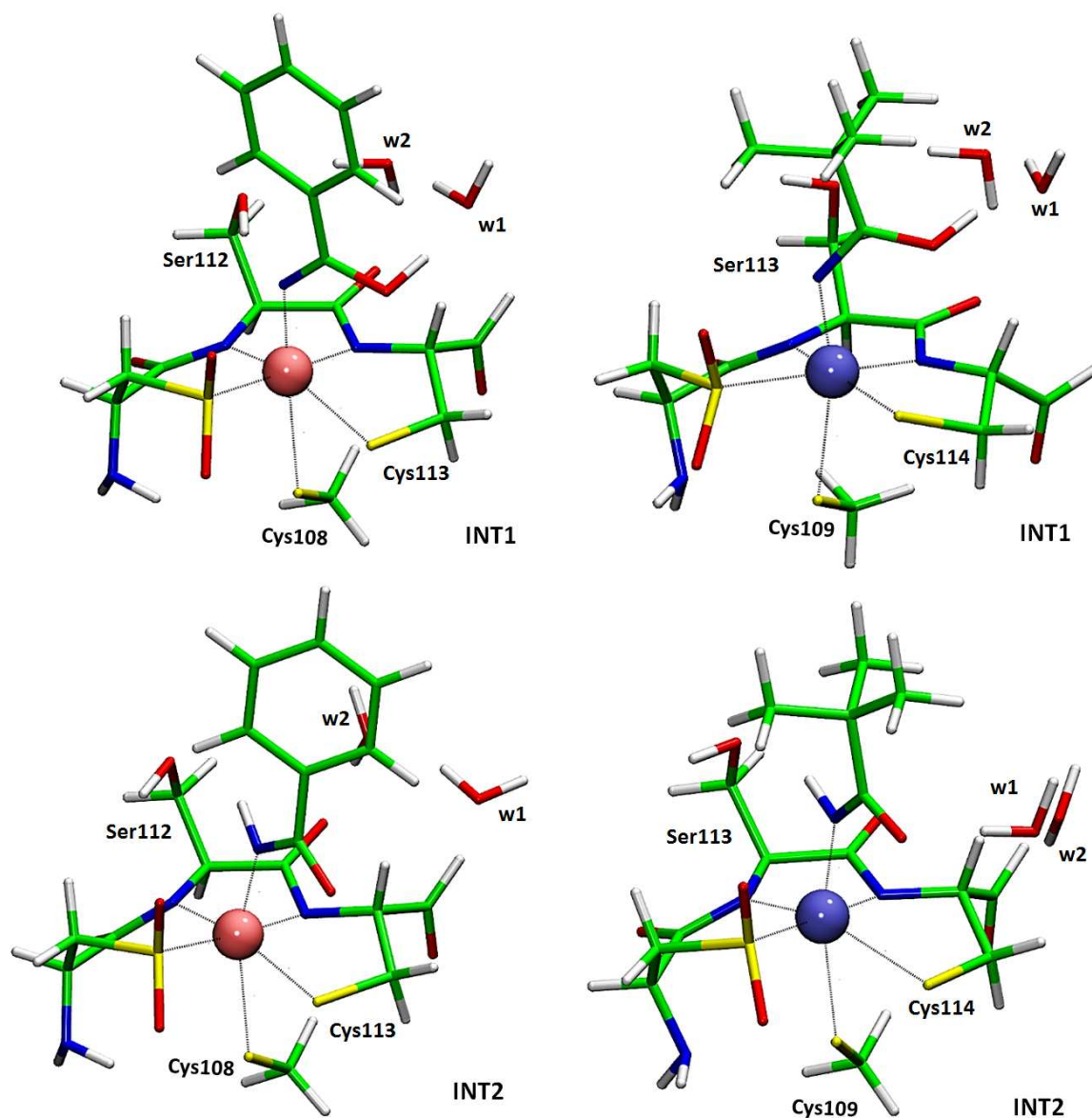


Figure S2. Optimized M06L structures of the two intermediates intercepted along potential energy surfaces for the Co-NHase and Fe-NHase. For clarity, only the amino acid residues of the inner coordination shell of the metal centre are retained

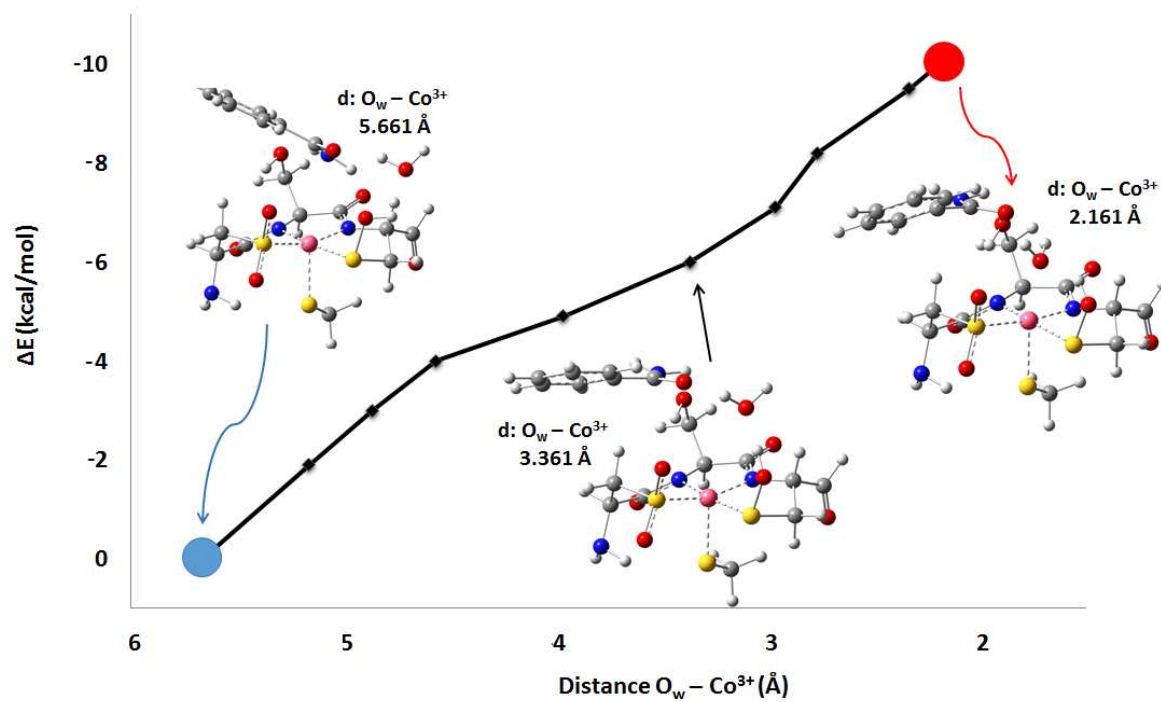


Figure S3. Potential energy scan for the approach of H_2O (w1) molecule to the EP complex of Co-NHase as a function of H_2O -Co distance.

Table S1. Cartesian coordinates for E CoNH

C	1.41200000	-4.99100000	-0.27500000
S	0.02500000	-3.92400000	-0.73600000
N	0.88400000	-2.35700000	-3.87200000
C	1.53800000	-1.34600000	-3.04600000
C	0.56400000	-0.26700000	-2.60900000
S	-0.66000000	-0.86500000	-1.43500000
C	2.44800000	-1.92400000	-1.95000000
O	3.45000000	-2.53200000	-2.34200000
O	-1.34900000	0.39000000	-0.90800000
O	-1.61500000	-1.71600000	-2.25900000
N	2.18700000	-1.66900000	-0.62500000
C	3.27300000	-2.13400000	0.25700000
C	2.74200000	-2.44200000	1.63900000
O	3.47700000	-2.58300000	2.62800000
C	4.35700000	-1.07300000	0.32300000
O	3.78200000	0.18200000	0.72100000
N	1.40800000	-2.56500000	1.66900000
C	0.76300000	-2.83700000	2.94300000
C	-0.56900000	-3.48900000	2.62600000
S	-1.43100000	-2.56400000	1.31000000
C	1.61000000	-3.79500000	3.79800000
O	1.66700000	-4.97800000	3.54400000
O	2.25600000	0.47900000	3.01900000
C	-6.15100000	5.04500000	3.70700000
C	-5.78000000	4.19400000	2.49800000
C	-6.02600000	4.95200000	1.19800000
C	-4.33500000	3.71700000	2.58400000
C	-4.14400000	1.68100000	-1.07500000
N	-3.89600000	0.75400000	0.00800000
C	-4.79300000	0.48600000	0.94700000
N	-6.02200000	1.05300000	0.86400000
N	-4.53300000	-0.39700000	1.91400000
C	9.61600000	3.76200000	-1.77900000
C	8.39400000	3.45500000	-0.96700000
C	7.58500000	2.35900000	-1.27000000
C	8.03300000	4.23900000	0.13700000
C	6.46400000	2.04400000	-0.50500000
C	6.91900000	3.94000000	0.91300000
C	6.12700000	2.83300000	0.59700000
O	5.04800000	2.56900000	1.38400000
C	-6.92100000	-1.58800000	-3.03600000
N	-6.03200000	-2.38800000	-2.21800000
C	-4.69800000	-2.21300000	-2.21600000
N	-4.15900000	-1.24200000	-2.96000000
N	-3.91200000	-2.95600000	-1.44100000
Co	0.42700000	-1.91500000	0.19000000
O	0.29800000	-0.05300000	1.32300000
O	-1.92300000	-1.20300000	2.26200000
H	5.09400000	-1.33300000	1.08600000
H	4.85000000	-0.97400000	-0.65000000
H	3.02800000	0.34600000	0.12900000
H	3.73500000	-3.04900000	-0.14000000
H	-5.53100000	5.94800000	3.74700000
H	-6.00000000	4.50200000	4.64500000
H	-6.43600000	3.30700000	2.50500000

H	-5.43200000	5.87300000	1.17000000
H	-5.73800000	4.36300000	0.31500000
H	-7.07500000	5.24100000	1.08400000
H	-3.65000000	4.57200000	2.64900000
H	-4.03700000	3.13900000	1.69800000
H	-4.15900000	3.09600000	3.46900000
H	-4.99800000	1.36900000	-1.68500000
H	-3.24800000	1.69200000	-1.69600000
H	-2.95600000	0.33500000	0.01100000
H	-5.16500000	-0.46800000	2.69400000
H	-3.56300000	-0.72200000	2.06000000
H	-6.60900000	1.02700000	1.68200000
H	-6.10900000	1.90300000	0.32600000
H	10.53400000	3.49100000	-1.24600000
H	9.61700000	3.21200000	-2.72400000
H	7.83500000	1.73200000	-2.12400000
H	8.64100000	5.10300000	0.39900000
H	5.84800000	1.18600000	-0.76200000
H	6.65200000	4.55000000	1.77000000
H	4.64200000	1.73800000	1.07700000
H	-6.76800000	-0.52400000	-2.83500000
H	-6.79000000	-1.77800000	-4.10800000
H	-6.39100000	-3.24300000	-1.82200000
H	-4.65300000	-0.92600000	-3.77900000
H	-3.12900000	-1.17900000	-2.94100000
H	-4.28900000	-3.58100000	-0.74900000
H	-2.89800000	-2.81300000	-1.50600000
H	1.53200000	-5.07000000	0.80800000
H	2.33400000	-4.62200000	-0.73300000
H	0.27900000	-2.92900000	-3.28500000
H	1.61100000	-2.98100000	-4.21300000
H	2.25000000	-0.83100000	-3.70400000
H	1.08000000	0.54800000	-2.09100000
H	0.00100000	0.12300000	-3.46300000
H	0.61500000	-1.90300000	3.51000000
H	-1.25300000	-3.54400000	3.47700000
H	-0.40700000	-4.49600000	2.22600000
H	2.09100000	-3.34400000	4.68600000
H	1.05700000	0.18400000	1.93300000
H	0.19500000	0.68600000	0.70100000
H	-1.18600000	-0.55500000	2.13100000
H	3.03200000	0.25700000	2.46900000
H	-4.30800000	2.70300000	-0.70500000
H	-7.94900000	-1.83200000	-2.77600000
H	9.69200000	4.82800000	-2.01500000
H	1.19800000	-5.98100000	-0.68700000
H	-7.19600000	5.36600000	3.67000000
H	2.43000000	1.37000000	3.33800000

Table S2. Cartesian coordinates for ES CoNH

C	0.56400000	-4.94000000	1.05900000
S	-0.63900000	-3.87500000	0.18000000
N	0.72700000	-3.60400000	-3.22100000
C	1.42600000	-2.40200000	-2.76000000
C	0.51900000	-1.16600000	-2.79700000
S	-0.86100000	-1.23400000	-1.62400000
C	2.25400000	-2.61900000	-1.47000000
O	3.29400000	-3.28000000	-1.60200000
O	-1.50100000	0.15100000	-1.65300000

O	-1.82700000	-2.27100000	-2.20300000
N	1.88000000	-2.05200000	-0.28600000
C	2.86600000	-2.23900000	0.80400000
C	2.19500000	-2.03500000	2.15200000
O	2.85100000	-1.87500000	3.20800000
C	4.01400000	-1.23800000	0.64000000
O	3.44400000	0.08400000	0.45600000
N	0.86800000	-2.03300000	2.09900000
C	0.13400000	-1.79900000	3.33800000
C	-1.29400000	-2.28900000	3.12100000
S	-1.89900000	-1.64100000	1.51300000
C	0.76200000	-2.53200000	4.54000000
O	0.66800000	-3.73200000	4.68200000
O	-2.24100000	-0.03400000	2.00500000
C	-5.71500000	6.65200000	1.01900000
C	-5.33900000	5.17000000	0.88000000
C	-3.97400000	5.00100000	0.19600000
C	-5.35600000	4.47100000	2.24900000
C	-3.98000000	1.71000000	-2.26400000
N	-3.89000000	1.18600000	-0.90800000
C	-4.84400000	1.32100000	0.00500000
N	-6.01900000	1.92000000	-0.32700000
N	-4.69000000	0.82700000	1.23800000
C	9.95300000	1.79500000	-2.33700000
C	8.56900000	1.97100000	-1.75600000
C	7.63500000	0.92700000	-1.78700000
C	8.18500000	3.16900000	-1.13400000
C	6.37000000	1.06400000	-1.21100000
C	6.92900000	3.32000000	-0.54600000
C	6.01700000	2.26000000	-0.57400000
O	4.79300000	2.43200000	0.02200000
C	-7.09700000	-1.66100000	-3.34500000
N	-6.31300000	-2.34700000	-2.31900000
C	-4.96400000	-2.33300000	-2.26900000
N	-4.26200000	-1.67500000	-3.20200000
N	-4.31000000	-2.92800000	-1.26900000
Co	0.07600000	-1.73300000	0.39500000
O	-0.31500000	1.52200000	3.03900000
O	2.30700000	0.93600000	3.00100000
H	4.62700000	-1.20300000	1.54200000
H	4.62300000	-1.50400000	-0.22700000
H	2.69500000	-0.07000000	-0.15000000
H	3.29600000	-3.24800000	0.78300000
H	-4.98600000	7.17600000	1.64800000
H	-6.70100000	6.77200000	1.48000000
H	-6.10100000	4.69500000	0.24100000
H	-3.18100000	5.47200000	0.78800000
H	-3.70200000	3.94400000	0.08200000
H	-3.96600000	5.46600000	-0.79700000
H	-4.64200000	4.94800000	2.93100000
H	-5.06300000	3.41600000	2.17000000
H	-6.34500000	4.52700000	2.71800000
H	-4.82200000	1.26800000	-2.81000000
H	-3.05700000	1.43300000	-2.77000000
H	-3.03000000	0.64800000	-0.72700000
H	-5.41500000	0.96100000	1.92600000
H	-3.76000000	0.51500000	1.56900000
H	-6.59900000	2.27500000	0.41900000
H	-6.06500000	2.45700000	-1.17900000
H	10.66800000	1.47800000	-1.56700000

H	9.96300000	1.03600000	-3.12500000
H	7.89500000	-0.01100000	-2.27100000
H	8.88600000	4.00000000	-1.10100000
H	5.65900000	0.24500000	-1.25700000
H	6.64600000	4.24600000	-0.05400000
H	4.36500000	1.55700000	0.12000000
H	-6.81000000	-0.60600000	-3.40000000
H	-6.98200000	-2.12500000	-4.33200000
H	-6.79300000	-3.00000000	-1.71700000
H	-4.66700000	-1.50000000	-4.10800000
H	-3.23200000	-1.72700000	-3.11000000
H	-4.79100000	-3.31400000	-0.47100000
H	-3.28000000	-2.93200000	-1.29900000
H	0.63300000	-4.69200000	2.11900000
H	1.54500000	-4.84500000	0.58800000
H	0.04400000	-3.91100000	-2.53100000
H	1.40900000	-4.35000000	-3.32900000
H	2.20100000	-2.19300000	-3.50800000
H	1.06900000	-0.26000000	-2.52900000
H	0.06100000	-1.05200000	-3.78400000
H	0.12800000	-0.72900000	3.57700000
H	-1.99400000	-1.94200000	3.88400000
H	-1.32500000	-3.37700000	3.05100000
H	1.23300000	-1.87300000	5.29300000
H	-0.49000000	2.03300000	3.83900000
H	0.66500000	1.32800000	3.02800000
H	2.55200000	0.11100000	3.46400000
H	2.71200000	0.80400000	2.12200000
H	-4.07100000	2.80400000	-2.26400000
H	-8.14900000	-1.71300000	-3.06400000
H	10.33000000	2.73000000	-2.76500000
H	0.21200000	-5.96900000	0.94400000
H	-5.73500000	7.15100000	0.04400000
H	-1.44900000	0.48100000	2.34400000
C	1.73600000	4.86800000	-0.00700000
C	1.70600000	3.51100000	0.31000000
C	0.56100000	2.76300000	-0.01800000
C	-0.54300000	3.36000000	-0.65800000
C	-0.49600000	4.71800000	-0.95900000
C	0.64000000	5.47000000	-0.63400000
H	2.62100000	5.44800000	0.23100000
H	2.56100000	3.04700000	0.78600000
H	-1.40100000	2.74900000	-0.91600000
H	-1.34000000	5.19200000	-1.44900000
H	0.67400000	6.52800000	-0.87800000
C	0.49900000	1.37100000	0.27200000
N	0.42500000	0.23400000	0.47800000

Table S3. Cartesian coordinates for TS1 CoNH

C	0.61800000	-4.63500000	1.96400000
S	-0.48300000	-3.82200000	0.78800000
N	0.86700000	-4.28600000	-2.54200000
C	1.52200000	-2.98000000	-2.50400000
C	0.53900000	-1.86200000	-2.81200000
S	-0.75300000	-1.64100000	-1.57400000
C	2.45800000	-2.77600000	-1.30000000
O	3.54900000	-3.36000000	-1.34800000
O	-1.43900000	-0.35000000	-1.92400000
O	-1.70700000	-2.82900000	-1.73300000

N	2.10000000	-1.95200000	-0.27900000
C	3.13900000	-1.75900000	0.75000000
C	2.51100000	-1.44100000	2.09000000
O	3.16900000	-1.01500000	3.05800000
C	4.06200000	-0.62300000	0.33700000
O	3.30600000	0.57900000	0.11700000
N	1.19400000	-1.67400000	2.12900000
C	0.45900000	-1.19500000	3.29100000
C	-0.88100000	-1.90700000	3.30500000
S	-1.54600000	-2.05600000	1.60600000
C	1.17700000	-1.51500000	4.61700000
O	1.32000000	-2.66100000	4.98500000
O	-1.90300000	0.49200000	1.72700000
C	-5.99800000	6.50200000	-0.48100000
C	-5.52900000	5.05800000	-0.36200000
C	-4.30900000	4.80500000	-1.24000000
C	-5.24300000	4.69800000	1.09200000
C	-4.09600000	1.04600000	-2.67600000
N	-3.80900000	0.84900000	-1.27000000
C	-4.66500000	1.13600000	-0.29500000
N	-5.88600000	1.64100000	-0.62800000
N	-4.38300000	0.84200000	0.97300000
C	9.82700000	1.56400000	-2.82600000
C	8.47400000	1.92000000	-2.28600000
C	7.40800000	1.01900000	-2.34000000
C	8.23400000	3.16400000	-1.68700000
C	6.16000000	1.33300000	-1.80800000
C	6.99800000	3.49100000	-1.14200000
C	5.95100000	2.56700000	-1.18800000
O	4.75300000	2.91100000	-0.63100000
C	-7.09900000	-2.57500000	-3.02100000
N	-6.28400000	-2.53100000	-1.81800000
C	-4.94100000	-2.61500000	-1.81100000
N	-4.24600000	-2.66000000	-2.94900000
N	-4.27200000	-2.62100000	-0.65700000
Co	0.30500000	-1.69300000	0.41900000
O	-0.40700000	1.87500000	3.87100000
O	2.20000000	1.65000000	2.87500000
H	4.77700000	-0.40400000	1.13500000
H	4.60800000	-0.90700000	-0.57000000
H	2.48900000	0.30600000	-0.33500000
H	3.74900000	-2.66800000	0.84900000
H	-5.21400000	7.18900000	-0.14000000
H	-6.88800000	6.69200000	0.12700000
H	-6.35200000	4.41500000	-0.71900000
H	-3.49300000	5.48800000	-0.97700000
H	-3.91200000	3.78900000	-1.11600000
H	-4.53200000	4.96400000	-2.30100000
H	-4.49600000	5.37700000	1.51800000
H	-4.83500000	3.68300000	1.19000000
H	-6.13800000	4.77700000	1.71800000
H	-5.00700000	0.51400000	-2.97700000
H	-3.25400000	0.63900000	-3.23400000
H	-2.90300000	0.41500000	-1.06600000
H	-5.01500000	1.20700000	1.67100000
H	-3.36200000	0.68700000	1.29600000
H	-6.39300000	2.11500000	0.10400000
H	-5.96000000	2.10800000	-1.52000000
H	10.55200000	1.39700000	-2.02100000
H	9.79200000	0.65000000	-3.42500000

H	7.55400000	0.04800000	-2.81000000
H	9.04100000	3.89300000	-1.63500000
H	5.33900000	0.62400000	-1.88200000
H	6.83100000	4.45400000	-0.66800000
H	4.22800000	2.10000000	-0.50300000
H	-6.74800000	-1.83100000	-3.74200000
H	-7.09600000	-3.56500000	-3.49000000
H	-6.74700000	-2.70500000	-0.94000000
H	-4.68500000	-2.95700000	-3.80500000
H	-3.22400000	-2.72200000	-2.86200000
H	-4.70100000	-2.31200000	0.19900000
H	-3.24900000	-2.68900000	-0.72000000
H	0.89800000	-3.99000000	2.80200000
H	1.52200000	-4.85700000	1.38800000
H	0.15000000	-4.36500000	-1.82600000
H	1.56300000	-5.00500000	-2.37600000
H	2.22200000	-2.97500000	-3.35000000
H	1.04200000	-0.89100000	-2.85200000
H	0.02200000	-2.04400000	-3.76000000
H	0.30000000	-0.11600000	3.21300000
H	-1.65000000	-1.36900000	3.86500000
H	-0.79500000	-2.92100000	3.71100000
H	1.44900000	-0.64700000	5.26800000
H	-0.53500000	2.69800000	4.35100000
H	0.50300000	1.92800000	3.50700000
H	2.64600000	0.87700000	3.26000000
H	2.48700000	1.60600000	1.95000000
H	-4.19600000	2.10900000	-2.92900000
H	-8.12300000	-2.32300000	-2.75500000
H	10.23600000	2.36000000	-3.45700000
H	0.14900000	-5.55600000	2.31300000
H	-6.23700000	6.76500000	-1.51500000
H	-1.66300000	0.90300000	2.57900000
C	-1.38900000	4.71700000	0.98300000
C	-1.45800000	3.32900000	1.04100000
C	-0.35100000	2.56300000	0.66100000
C	0.81700000	3.20900000	0.21300000
C	0.87600000	4.59400000	0.16000000
C	-0.22800000	5.35300000	0.54700000
H	-2.24800000	5.30800000	1.28800000
H	-2.35400000	2.83000000	1.39800000
H	1.67800000	2.61500000	-0.08100000
H	1.79000000	5.07400000	-0.17600000
H	-0.18000000	6.43700000	0.51500000
C	-0.29200000	1.12000000	0.69300000
N	0.37900000	0.19500000	0.34600000

Table S4. Cartesian coordinates for INT1 CoNH

C	0.44100000	-4.89800000	1.50700000
S	-0.63100000	-3.97300000	0.36500000
N	0.96700000	-3.83500000	-2.92400000
C	1.60500000	-2.54800000	-2.63600000
C	0.63400000	-1.38400000	-2.84900000
S	-0.74100000	-1.33200000	-1.67100000
C	2.45100000	-2.51700000	-1.33600000
O	3.58700000	-3.01200000	-1.42300000
O	-1.39700000	0.01600000	-1.90400000
O	-1.71200000	-2.46800000	-2.07300000
N	1.98300000	-1.95800000	-0.19400000

C	2.96500000	-1.83100000	0.90200000
C	2.24500000	-1.68100000	2.23400000
O	2.84500000	-1.41900000	3.29700000
C	3.89700000	-0.64000000	0.66400000
O	3.16400000	0.59500000	0.54900000
N	0.92400000	-1.86300000	2.14400000
C	0.11400000	-1.66200000	3.34400000
C	-1.18600000	-2.45500000	3.16500000
S	-1.76300000	-2.44300000	1.40800000
C	0.80100000	-2.17200000	4.64200000
O	0.93600000	-3.36000000	4.85400000
O	-1.33200000	0.75300000	1.78600000
C	-5.91900000	6.57600000	0.20400000
C	-5.33500000	5.15500000	0.19400000
C	-4.22400000	5.01300000	-0.85700000
C	-4.82600000	4.75800000	1.58900000
C	-4.10600000	1.34300000	-2.54200000
N	-3.69300000	1.06800000	-1.17200000
C	-4.44400000	1.26400000	-0.10300000
N	-5.72600000	1.70600000	-0.23900000
N	-3.98700000	0.95500000	1.12100000
C	9.82500000	1.57300000	-2.52300000
C	8.40000000	1.86400000	-2.09800000
C	7.41100000	0.87100000	-2.12300000
C	8.02500000	3.13600000	-1.63400000
C	6.10500000	1.12600000	-1.69100000
C	6.73000000	3.40200000	-1.18700000
C	5.76100000	2.39100000	-1.19800000
O	4.50000000	2.69500000	-0.74700000
C	-7.18000000	-2.15500000	-3.29400000
N	-6.30200000	-2.47700000	-2.16400000
C	-4.95400000	-2.45200000	-2.18600000
N	-4.27900000	-2.11400000	-3.29400000
N	-4.25100000	-2.72700000	-1.08400000
Co	0.19200000	-1.65900000	0.39300000
O	-0.21000000	1.71800000	3.92900000
O	2.30800000	1.34900000	3.24500000
H	4.58400000	-0.53600000	1.50700000
H	4.47000000	-0.82500000	-0.24700000
H	2.24700000	0.41000000	0.22200000
H	3.59300000	-2.72900000	0.95700000
H	-5.14600000	7.30700000	0.47100000
H	-6.73200000	6.66900000	0.93200000
H	-6.15500000	4.46900000	-0.07900000
H	-3.39900000	5.70300000	-0.64600000
H	-3.79300000	4.00400000	-0.86200000
H	-4.59400000	5.24000000	-1.86300000
H	-4.04100000	5.44800000	1.92200000
H	-4.38500000	3.75300000	1.58800000
H	-5.62700000	4.78900000	2.33600000
H	-4.99100000	0.75800000	-2.82000000
H	-3.27700000	1.04800000	-3.18300000
H	-2.74600000	0.64500000	-1.10700000
H	-4.54300000	1.21700000	1.92200000
H	-2.96800000	0.85100000	1.29700000
H	-6.16600000	2.12400000	0.56800000
H	-5.98400000	2.14400000	-1.11100000
H	10.46300000	1.37000000	-1.65300000
H	9.87600000	0.69900000	-3.17900000
H	7.65700000	-0.12200000	-2.49100000

H	8.76400000	3.93300000	-1.61000000
H	5.35300000	0.34500000	-1.75000000
H	6.45600000	4.38400000	-0.81300000
H	4.06500000	1.90300000	-0.36900000
H	-6.91000000	-1.18400000	-3.71900000
H	-7.13900000	-2.92300000	-4.07500000
H	-6.73200000	-2.90100000	-1.35400000
H	-4.71200000	-2.17300000	-4.20300000
H	-3.25300000	-2.12700000	-3.22800000
H	-4.68400000	-2.81400000	-0.17900000
H	-3.22000000	-2.71600000	-1.17300000
H	0.94600000	-4.22500000	2.20100000
H	1.17800000	-5.34500000	0.83200000
H	0.17000000	-4.02400000	-2.32400000
H	1.64500000	-4.58700000	-2.83900000
H	2.37100000	-2.41200000	-3.40800000
H	1.13200000	-0.42200000	-2.70600000
H	0.17500000	-1.43200000	-3.84100000
H	-0.11100000	-0.60300000	3.47600000
H	-2.02200000	-2.03300000	3.73000000
H	-1.06000000	-3.49900000	3.45900000
H	1.04400000	-1.40500000	5.40900000
H	-0.31700000	2.61100000	4.28000000
H	0.75900000	1.63000000	3.67500000
H	2.62600000	0.47800000	3.55100000
H	2.59300000	1.37300000	2.31100000
H	-4.30300000	2.41100000	-2.69500000
H	-8.20200000	-2.09300000	-2.92300000
H	10.26400000	2.42200000	-3.05800000
H	-0.11700000	-5.67700000	2.02800000
H	-6.31200000	6.85100000	-0.78000000
H	-1.08200000	1.19200000	2.65800000
C	-0.82900000	4.84100000	0.92300000
C	-1.01300000	3.47700000	1.15900000
C	-0.10600000	2.53300000	0.64800000
C	0.97800000	2.99100000	-0.12200000
C	1.17000000	4.35300000	-0.34500000
C	0.26700000	5.28500000	0.17800000
H	-1.53800000	5.55700000	1.32900000
H	-1.86600000	3.15200000	1.74500000
H	1.67700000	2.28400000	-0.54500000
H	2.03300000	4.67600000	-0.91800000
H	0.41800000	6.34700000	0.00900000
C	-0.28000000	1.07100000	0.90100000
N	0.43800000	0.19500000	0.34800000

Table S5. Cartesian coordinates for TS2 CoNH

C	0.47000000	-5.00700000	1.57800000
S	-0.63800000	-4.12700000	0.42700000
N	0.99800000	-3.98200000	-2.82200000
C	1.59500000	-2.66400000	-2.59000000
C	0.58100000	-1.54300000	-2.82700000
S	-0.79700000	-1.49900000	-1.64700000
C	2.45500000	-2.55000000	-1.30400000
O	3.63400000	-2.93600000	-1.40300000
O	-1.49500000	-0.18400000	-1.91900000
O	-1.72800000	-2.67900000	-2.02100000
N	1.94800000	-2.04700000	-0.15500000
C	2.92100000	-1.83500000	0.93300000

C	2.19300000	-1.69600000	2.26200000
O	2.78600000	-1.36700000	3.32000000
C	3.79100000	-0.60000000	0.67100000
O	3.00300000	0.60800000	0.57400000
N	0.88600000	-1.93200000	2.18200000
C	0.06500000	-1.76300000	3.38200000
C	-1.21200000	-2.59200000	3.19800000
S	-1.78100000	-2.57800000	1.44100000
C	0.76100000	-2.24900000	4.68300000
O	0.97100000	-3.42800000	4.87800000
O	-1.30700000	0.77700000	1.77200000
C	-6.21500000	6.27100000	0.19900000
C	-4.75000000	5.81800000	0.29600000
C	-3.78800000	6.96200000	-0.06000000
C	-4.43600000	5.26100000	1.69500000
C	-4.23700000	1.08300000	-2.51900000
N	-3.69500000	1.12400000	-1.16500000
C	-4.26900000	1.75500000	-0.14700000
N	-5.45300000	2.39900000	-0.34500000
N	-3.75100000	1.70100000	1.08300000
C	9.68200000	1.72100000	-2.42900000
C	8.23400000	1.96900000	-2.05500000
C	7.27900000	0.94300000	-2.09900000
C	7.80200000	3.23400000	-1.62400000
C	5.95000000	1.16200000	-1.71900000
C	6.48400000	3.46400000	-1.22800000
C	5.54900000	2.42200000	-1.26000000
O	4.26000000	2.69700000	-0.86900000
C	-7.20200000	-2.50600000	-3.27300000
N	-6.32100000	-2.76300000	-2.13000000
C	-4.97300000	-2.72500000	-2.15200000
N	-4.29800000	-2.44000000	-3.27500000
N	-4.26800000	-2.94200000	-1.03800000
Co	0.15100000	-1.77000000	0.42000000
O	-0.01300000	1.57400000	3.67600000
O	2.32100000	1.26000000	3.11700000
H	4.49800000	-0.46400000	1.49300000
H	4.34500000	-0.75800000	-0.25500000
H	2.07500000	0.38800000	0.24700000
H	3.60200000	-2.69300000	1.00800000
H	-6.42000000	7.07600000	0.91400000
H	-6.91200000	5.45200000	0.42300000
H	-4.58600000	5.01400000	-0.43700000
H	-3.89400000	7.79100000	0.65100000
H	-2.74700000	6.62600000	-0.03800000
H	-3.99400000	7.35400000	-1.06200000
H	-4.51000000	6.05000000	2.45200000
H	-3.42300000	4.84600000	1.73900000
H	-5.15100000	4.47900000	1.99600000
H	-5.24700000	0.65900000	-2.52900000
H	-3.57500000	0.44400000	-3.10000000
H	-2.77100000	0.67300000	-1.06900000
H	-4.11300000	2.33900000	1.77600000
H	-2.80100000	1.29500000	1.28800000
H	-5.79100000	3.01400000	0.38100000
H	-5.69900000	2.68700000	-1.28100000
H	9.78400000	0.83700000	-3.06700000
H	10.10800000	2.57500000	-2.96500000
H	7.57000000	-0.04600000	-2.44300000
H	8.51400000	4.05600000	-1.58700000

H	5.22600000	0.35700000	-1.79600000
H	6.16500000	4.44200000	-0.88100000
H	3.84400000	1.91600000	-0.45100000
H	-6.94400000	-1.55400000	-3.74500000
H	-7.15300000	-3.31100000	-4.01500000
H	-6.74600000	-3.14400000	-1.29700000
H	-4.73100000	-2.53600000	-4.18000000
H	-3.27200000	-2.43500000	-3.20600000
H	-4.70200000	-2.97500000	-0.12900000
H	-3.23800000	-2.90900000	-1.12500000
H	0.98600000	-4.31000000	2.23800000
H	1.19200000	-5.47100000	0.89900000
H	0.21400000	-4.17200000	-2.20700000
H	1.70000000	-4.70800000	-2.71900000
H	2.34600000	-2.52900000	-3.37700000
H	1.04700000	-0.56100000	-2.71500000
H	0.11900000	-1.63300000	-3.81500000
H	-0.20500000	-0.71400000	3.50500000
H	-2.05600000	-2.19400000	3.76800000
H	-1.05800000	-3.63500000	3.48400000
H	0.95000000	-1.48400000	5.47000000
H	-0.16500000	2.50100000	3.90200000
H	1.11200000	1.44100000	3.37500000
H	2.59600000	0.36400000	3.44300000
H	2.55500000	1.22200000	2.14700000
H	-4.25100000	2.07700000	-2.98400000
H	-8.22500000	-2.43700000	-2.90300000
H	10.29800000	1.55500000	-1.53600000
H	-0.06800000	-5.77200000	2.13800000
H	-6.45000000	6.64800000	-0.80200000
H	-0.70900000	1.23700000	2.83200000
C	-0.48800000	4.80400000	0.82000000
C	-0.75700000	3.46900000	1.13300000
C	-0.10100000	2.42300000	0.46000000
C	0.80800000	2.75500000	-0.55900000
C	1.08800000	4.08600000	-0.86500000
C	0.44200000	5.11700000	-0.17400000
H	-0.99200000	5.59700000	1.36400000
H	-1.47900000	3.23900000	1.90900000
H	1.30100000	1.96300000	-1.10800000
H	1.82800000	4.31000000	-1.62700000
H	0.66700000	6.15400000	-0.40600000
C	-0.34200000	0.98300000	0.84000000
N	0.39500000	0.08500000	0.31200000

Table S6. Cartesian coordinates for INT2 CoNH

C	0.77400000	-4.64500000	2.05200000
S	-0.25200000	-3.92100000	0.74300000
N	1.21100000	-4.11000000	-2.52800000
C	1.78000000	-2.76400000	-2.44000000
C	0.74400000	-1.70200000	-2.80300000
S	-0.57600000	-1.48900000	-1.57200000
C	2.62500000	-2.49600000	-1.16400000
O	3.72600000	-3.06100000	-1.12200000
O	-1.22900000	-0.17400000	-1.93700000
O	-1.54600000	-2.67400000	-1.77300000
N	2.18700000	-1.62300000	-0.20700000
C	3.17300000	-1.32100000	0.85300000
C	2.45100000	-1.04200000	2.16500000

O	2.98300000	-0.41900000	3.10600000
C	4.05100000	-0.14100000	0.42200000
O	3.24400000	0.90400000	-0.16300000
N	1.21200000	-1.55700000	2.20600000
C	0.36900000	-1.18400000	3.34700000
C	-0.90300000	-2.03500000	3.29300000
S	-1.45400000	-2.29400000	1.54300000
C	1.07800000	-1.44200000	4.70100000
O	1.34500000	-2.57100000	5.05700000
O	-1.97600000	0.25600000	1.32000000
C	-5.92700000	6.28300000	-1.02400000
C	-5.43800000	4.85200000	-0.76000000
C	-4.12900000	4.56200000	-1.51100000
C	-5.27400000	4.59800000	0.74600000
C	-3.95800000	0.73700000	-2.91500000
N	-3.76100000	0.69500000	-1.47100000
C	-4.68800000	0.99700000	-0.57200000
N	-5.92100000	1.40200000	-0.99000000
N	-4.45500000	0.80500000	0.73300000
C	9.96000000	1.38100000	-2.99700000
C	8.64400000	1.79900000	-2.37600000
C	7.46900000	1.06200000	-2.56700000
C	8.56200000	2.94900000	-1.57200000
C	6.25800000	1.44700000	-1.97800000
C	7.36700000	3.34200000	-0.97200000
C	6.20300000	2.58600000	-1.16600000
O	5.05700000	3.01500000	-0.55300000
C	-6.92500000	-2.92600000	-3.08800000
N	-6.11700000	-2.67900000	-1.89300000
C	-4.77000000	-2.69600000	-1.85900000
N	-4.05000000	-2.92600000	-2.96300000
N	-4.12100000	-2.46100000	-0.71300000
Co	0.38500000	-1.59000000	0.48500000
O	-0.74300000	1.56500000	4.74200000
O	1.57200000	1.97000000	3.25900000
H	4.55300000	0.29500000	1.28700000
H	4.79900000	-0.48300000	-0.30100000
H	2.73000000	0.46700000	-0.86200000
H	3.83200000	-2.18200000	1.02300000
H	-5.19200000	7.01300000	-0.66400000
H	-6.87500000	6.48300000	-0.51200000
H	-6.21300000	4.16800000	-1.14300000
H	-3.33500000	5.23900000	-1.17700000
H	-3.76600000	3.54400000	-1.32600000
H	-4.25000000	4.69900000	-2.59200000
H	-4.54100000	5.29100000	1.17400000
H	-4.89600000	3.58900000	0.94800000
H	-6.21900000	4.73700000	1.28400000
H	-4.80700000	0.11200000	-3.21600000
H	-3.04800000	0.34800000	-3.36700000
H	-2.82100000	0.39500000	-1.18100000
H	-5.07900000	1.24700000	1.39500000
H	-3.44900000	0.65500000	1.04700000
H	-6.52200000	1.83900000	-0.30500000
H	-5.99500000	1.81100000	-1.91100000
H	10.68800000	1.09200000	-2.23000000
H	9.83100000	0.52700000	-3.67000000
H	7.49100000	0.17000000	-3.18800000
H	9.45600000	3.54800000	-1.40800000
H	5.35700000	0.86600000	-2.15800000

H	7.31700000	4.22700000	-0.34600000
H	4.37400000	2.31700000	-0.56300000
H	-6.61200000	-2.26400000	-3.90100000
H	-6.86200000	-3.97000000	-3.41700000
H	-6.58900000	-2.69400000	-1.00000000
H	-4.45700000	-3.37200000	-3.77100000
H	-3.02500000	-2.87900000	-2.87000000
H	-4.56000000	-1.96900000	0.05200000
H	-3.09600000	-2.48800000	-0.76200000
H	1.25600000	-3.86500000	2.64300000
H	1.53400000	-5.21600000	1.50900000
H	0.43200000	-4.24500000	-1.89100000
H	1.93000000	-4.80100000	-2.33100000
H	2.53500000	-2.70300000	-3.23300000
H	1.19900000	-0.71100000	-2.87800000
H	0.23800000	-1.95100000	-3.74100000
H	0.09500000	-0.13100000	3.28600000
H	-1.74800000	-1.53500000	3.77200000
H	-0.76000000	-3.02200000	3.74000000
H	1.27100000	-0.56100000	5.34800000
H	-0.72100000	1.91800000	5.63900000
H	0.08500000	1.86700000	4.31000000
H	2.20500000	1.22100000	3.29700000
H	2.08500000	2.76000000	3.04700000
H	-4.11200000	1.76300000	-3.27000000
H	-7.96500000	-2.70100000	-2.84900000
H	10.40600000	2.19800000	-3.57600000
H	0.18100000	-5.31600000	2.67400000
H	-6.07700000	6.46200000	-2.09500000
H	1.01300000	0.87800000	0.51400000
C	-1.65700000	4.48100000	1.91000000
C	-1.61300000	3.08700000	1.94300000
C	-0.98200000	2.38800000	0.90400000
C	-0.41900000	3.08600000	-0.17400000
C	-0.47900000	4.48100000	-0.20900000
C	-1.09300000	5.17900000	0.83500000
H	-2.12000000	5.02500000	2.72800000
H	-2.00400000	2.53800000	2.79400000
H	0.04300000	2.53500000	-0.98700000
H	-0.04500000	5.02000000	-1.04600000
H	-1.12700000	6.26500000	0.81500000
C	-0.92300000	0.89600000	0.95700000
N	0.19100000	0.28700000	0.61500000

Table S7. Cartesian coordinates for TS3 CoNH

C	1.02700000	-5.07500000	0.49500000
S	-0.12400000	-3.91800000	-0.30300000
N	1.19800000	-3.36300000	-3.40600000
C	1.84000000	-2.19900000	-2.80100000
C	0.95500000	-0.96800000	-2.88700000
S	-0.43900000	-0.95400000	-1.72100000
C	2.47800000	-2.45400000	-1.41600000
O	3.27000000	-3.40200000	-1.35500000
O	-0.95400000	0.44900000	-1.83900000
O	-1.43700000	-2.00900000	-2.24500000
N	2.21900000	-1.57700000	-0.37400000
C	3.19800000	-1.70100000	0.73200000
C	2.49000000	-1.83700000	2.06500000
O	3.05200000	-1.67300000	3.15600000

C	4.17700000	-0.52800000	0.67900000
O	3.47000000	0.69800000	0.44400000
N	1.21800000	-2.26200000	1.92500000
C	0.46500000	-2.51800000	3.14700000
C	-0.69700000	-3.44500000	2.78500000
S	-1.42300000	-3.00100000	1.13800000
C	1.35000000	-3.19400000	4.22300000
O	1.66100000	-4.36400000	4.13800000
O	-2.04300000	1.05100000	0.62500000
C	-5.70000000	6.16300000	1.98300000
C	-5.08800000	4.92900000	1.30200000
C	-4.49500000	5.29400000	-0.06700000
C	-4.03200000	4.25600000	2.19200000
C	-3.79700000	1.77200000	-1.92800000
N	-4.35500000	1.51800000	-0.60600000
C	-5.59100000	1.78500000	-0.22600000
N	-6.42000000	2.48400000	-1.04200000
N	-6.05000000	1.29300000	0.93700000
C	10.11800000	2.47000000	-2.07600000
C	8.75300000	2.61100000	-1.43600000
C	7.71200000	1.72000000	-1.72600000
C	8.49200000	3.62900000	-0.50500000
C	6.46100000	1.82800000	-1.10800000
C	7.25300000	3.74800000	0.12600000
C	6.22900000	2.84000000	-0.16700000
O	5.02900000	2.99200000	0.47500000
C	-6.78100000	-1.56200000	-3.42000000
N	-5.97200000	-1.51000000	-2.20300000
C	-4.62900000	-1.65800000	-2.19100000
N	-3.94700000	-1.73100000	-3.34300000
N	-3.96000000	-1.71200000	-1.04100000
Co	0.35300000	-1.71500000	0.30400000
O	-4.43000000	-0.84500000	1.67400000
O	-2.10700000	-0.90000000	2.67400000
H	4.69500000	-0.42800000	1.63500000
H	4.91400000	-0.69500000	-0.11600000
H	2.82600000	0.49700000	-0.25700000
H	3.77500000	-2.62700000	0.62400000
H	-4.92900000	6.91900000	2.17400000
H	-6.15300000	5.90300000	2.94600000
H	-5.90400000	4.20700000	1.13800000
H	-3.69200000	6.03100000	0.04600000
H	-4.05900000	4.41600000	-0.55700000
H	-5.24900000	5.73000000	-0.73300000
H	-3.19900000	4.94200000	2.38500000
H	-3.61200000	3.36000000	1.71800000
H	-4.45400000	3.96400000	3.16000000
H	-4.44400000	1.34900000	-2.70300000
H	-2.81800000	1.29400000	-1.96700000
H	-3.66400000	1.21000000	0.08700000
H	-6.80000000	1.75700000	1.42600000
H	-5.47000000	0.59600000	1.43200000
H	-7.35900000	2.68400000	-0.73400000
H	-6.01500000	3.15400000	-1.68100000
H	10.07000000	1.87600000	-2.99400000
H	10.54300000	3.44700000	-2.33000000
H	7.87400000	0.92500000	-2.45000000
H	9.27600000	4.34300000	-0.26200000
H	5.66400000	1.13600000	-1.36400000
H	7.06600000	4.53300000	0.85100000

H	4.47700000	2.19200000	0.36400000
H	-6.46400000	-0.78800000	-4.12500000
H	-6.73400000	-2.54500000	-3.90400000
H	-6.44200000	-1.63800000	-1.31800000
H	-4.40800000	-1.91600000	-4.21900000
H	-2.92300000	-1.80000000	-3.27900000
H	-4.32600000	-1.41200000	-0.13200000
H	-2.94900000	-1.83100000	-1.13500000
H	1.40400000	-4.68300000	1.43900000
H	1.85900000	-5.12900000	-0.21800000
H	0.27400000	-3.53600000	-3.02300000
H	1.78200000	-4.18700000	-3.29400000
H	2.72200000	-1.97200000	-3.41900000
H	1.50700000	-0.05900000	-2.64400000
H	0.49600000	-0.87100000	-3.87500000
H	0.08100000	-1.58600000	3.57700000
H	-1.54100000	-3.35400000	3.46800000
H	-0.37500000	-4.48700000	2.74000000
H	1.61600000	-2.56000000	5.08900000
H	-4.85900000	-1.51300000	2.22500000
H	-3.46000000	-0.77700000	2.06500000
H	-2.10100000	-0.66600000	3.61100000
H	-1.06300000	-0.44400000	2.07700000
H	-3.66700000	2.84500000	-2.11700000
H	-7.81900000	-1.36200000	-3.15000000
H	10.82400000	1.97300000	-1.39900000
H	0.54400000	-6.04600000	0.61100000
H	-6.47200000	6.62500000	1.35800000
H	0.69500000	0.26000000	1.81500000
C	-0.19200000	4.70300000	-0.22000000
C	-0.81200000	3.47900000	0.00700000
C	-0.11400000	2.43200000	0.63700000
C	1.21200000	2.64400000	1.04600000
C	1.83800000	3.87100000	0.81400000
C	1.13700000	4.90000000	0.18000000
H	-0.73600000	5.50200000	-0.71600000
H	-1.83400000	3.31000000	-0.30700000
H	1.78900000	1.86300000	1.52900000
H	2.87300000	4.01100000	1.10800000
H	1.62600000	5.85100000	-0.00700000
C	-0.83200000	1.14800000	0.83300000
N	-0.16800000	0.00600000	1.33800000

Table S8. Cartesian coordinates for EP CoNH

C	0.91700000	-5.09900000	-0.14700000
S	-0.22800000	-3.87600000	-0.87400000
N	1.38100000	-2.13600000	-3.72700000
C	1.89500000	-1.20900000	-2.71800000
C	0.88500000	-0.10600000	-2.38900000
S	-0.54400000	-0.73100000	-1.46400000
C	2.53900000	-1.89900000	-1.49200000
O	3.57800000	-2.52900000	-1.68100000
O	-1.22600000	0.48900000	-0.87200000
O	-1.40000000	-1.43400000	-2.52200000
N	1.99700000	-1.69500000	-0.23100000
C	2.90800000	-2.06000000	0.86900000
C	2.10400000	-2.30700000	2.13200000
O	2.61800000	-2.38500000	3.25400000
C	3.92700000	-0.92100000	1.06000000

O	3.23400000	0.34000000	0.88200000
N	0.78000000	-2.45900000	1.88900000
C	-0.07800000	-2.86800000	3.00800000
C	-1.33500000	-3.49900000	2.40500000
S	-1.93400000	-2.49500000	0.99000000
C	0.64000000	-3.89300000	3.91500000
O	0.75500000	-5.05500000	3.58400000
O	-1.31200000	2.11100000	2.18400000
C	-6.02600000	5.72300000	2.76300000
C	-5.23800000	4.83800000	1.78300000
C	-4.23900000	5.67000000	0.96400000
C	-4.52300000	3.69300000	2.51700000
C	-3.69800000	2.13400000	-1.69900000
N	-3.80500000	1.22100000	-0.57000000
C	-4.90500000	1.06100000	0.15000000
N	-6.00600000	1.80800000	-0.13000000
N	-4.97700000	0.11000000	1.09100000
C	10.15300000	2.70200000	-0.30400000
C	8.66000000	2.51700000	-0.45500000
C	7.89200000	1.92600000	0.55600000
C	7.99700000	2.90900000	-1.63000000
C	6.51700000	1.72500000	0.40700000
C	6.62600000	2.71300000	-1.79800000
C	5.88100000	2.11500000	-0.77700000
O	4.53200000	1.94400000	-0.97400000
C	-6.48600000	-0.82400000	-4.09200000
N	-5.78100000	-1.77000000	-3.23400000
C	-4.45400000	-1.70400000	-3.01000000
N	-3.72400000	-0.75200000	-3.60400000
N	-3.86000000	-2.55200000	-2.16600000
Co	0.16200000	-1.97700000	0.21500000
O	-1.60100000	0.10800000	3.71200000
O	-2.73800000	-1.27100000	1.85200000
H	4.34200000	-0.94700000	2.06900000
H	4.72400000	-0.99900000	0.31500000
H	2.52000000	0.09000000	0.25400000
H	3.45700000	-2.98300000	0.64700000
H	-5.34700000	6.19600000	3.48200000
H	-6.75800000	5.13700000	3.33200000
H	-5.96700000	4.39800000	1.08100000
H	-3.48200000	6.11700000	1.61900000
H	-3.70600000	5.05300000	0.23000000
H	-4.73900000	6.48300000	0.42600000
H	-3.82700000	4.09100000	3.26400000
H	-3.92500000	3.07100000	1.84100000
H	-5.23800000	3.04900000	3.04600000
H	-4.44800000	1.90500000	-2.46400000
H	-2.70000000	2.00400000	-2.11400000
H	-2.93300000	0.71800000	-0.34700000
H	-5.71500000	0.15000000	1.77900000
H	-4.13700000	-0.43900000	1.34000000
H	-6.78400000	1.77300000	0.51200000
H	-5.87500000	2.70500000	-0.57600000
H	10.48900000	3.64000000	-0.75800000
H	10.45100000	2.71300000	0.75000000
H	8.37200000	1.61800000	1.48200000
H	8.56500000	3.37600000	-2.43200000
H	5.94000000	1.27700000	1.21200000
H	6.12400000	3.01400000	-2.71200000
H	4.15900000	1.42100000	-0.23600000

H	-6.29700000	0.20200000	-3.76300000
H	-6.20500000	-0.93200000	-5.14700000
H	-6.27000000	-2.59900000	-2.93000000
H	-4.05400000	-0.31500000	-4.45000000
H	-2.71100000	-0.75600000	-3.39100000
H	-4.38900000	-3.17400000	-1.57400000
H	-2.84100000	-2.48400000	-2.06000000
H	0.79500000	-5.19000000	0.93400000
H	1.94900000	-4.82500000	-0.38000000
H	0.64400000	-2.72000000	-3.33800000
H	2.13600000	-2.75400000	-4.01500000
H	2.74600000	-0.68900000	-3.17500000
H	1.31900000	0.68100000	-1.76700000
H	0.47800000	0.33000000	-3.30600000
H	-0.33500000	-1.99100000	3.61500000
H	-2.16400000	-3.57600000	3.11300000
H	-1.10700000	-4.48800000	2.00400000
H	1.01500000	-3.50800000	4.87800000
H	-2.03700000	0.22100000	4.56600000
H	-1.57900000	1.00300000	3.22500000
H	-2.20600000	-0.81100000	2.58100000
H	0.51900000	0.67800000	3.05600000
H	-3.79900000	3.18000000	-1.38500000
H	-7.55600000	-1.01400000	-4.00700000
H	10.70500000	1.88800000	-0.79200000
H	0.69000000	-6.05500000	-0.62700000
H	-6.56500000	6.51900000	2.23800000
H	1.73200000	1.13800000	1.91700000
C	-0.53100000	4.35500000	-1.24300000
C	-0.80400000	3.59600000	-0.10700000
C	0.22800000	2.91200000	0.55200000
C	1.54000000	3.02100000	0.06900000
C	1.81300000	3.76700000	-1.07900000
C	0.77600000	4.43200000	-1.73900000
H	-1.33400000	4.89000000	-1.74300000
H	-1.81000000	3.51600000	0.28700000
H	2.36900000	2.54900000	0.58200000
H	2.83500000	3.81400000	-1.44000000
H	0.98700000	5.01900000	-2.62800000
C	-0.14100000	2.06900000	1.72600000
N	0.78400000	1.25100000	2.26500000

Table S9. Cartesian coordinates for E+P CoNH

C	-1.54100000	-5.04600000	0.67000000
S	-0.21000000	-3.86800000	1.11000000
N	-1.46500000	-1.76700000	3.85000000
C	-1.98000000	-0.88300000	2.80300000
C	-0.91500000	0.09900000	2.30800000
S	0.42400000	-0.69800000	1.38100000
C	-2.78500000	-1.60600000	1.69700000
O	-3.88000000	-2.06700000	2.02800000
O	1.18500000	0.44000000	0.72200000
O	1.26600000	-1.40100000	2.45300000
N	-2.31800000	-1.62400000	0.39900000
C	-3.33000000	-2.06400000	-0.58800000
C	-2.64600000	-2.66600000	-1.80600000
O	-3.25100000	-2.89800000	-2.86500000
C	-4.16100000	-0.83000000	-0.99000000
O	-3.25500000	0.29800000	-1.12300000

N	-1.33900000	-2.90700000	-1.61500000
C	-0.57000000	-3.40500000	-2.75300000
C	0.72900000	-3.98800000	-2.20800000
S	1.46500000	-2.80000000	-1.01700000
C	-1.34700000	-4.48200000	-3.53900000
O	-1.47300000	-5.61000000	-3.11400000
O	0.47100000	2.16600000	-1.58200000
C	6.46500000	4.32300000	-4.01200000
C	5.85300000	3.64900000	-2.77700000
C	5.94300000	4.56800000	-1.54900000
C	4.40200000	3.21700000	-3.03800000
C	3.97700000	1.69800000	1.00000000
N	3.75900000	0.75300000	-0.08600000
C	4.71600000	0.33600000	-0.90100000
N	5.98400000	0.80300000	-0.73900000
N	4.47400000	-0.59300000	-1.83400000
C	-9.76600000	3.79400000	0.06200000
C	-8.28900000	3.46800000	0.09100000
C	-7.73800000	2.52700000	-0.79100000
C	-7.42500000	4.07200000	1.01700000
C	-6.38200000	2.19200000	-0.74900000
C	-6.06800000	3.74700000	1.07600000
C	-5.54400000	2.80000000	0.19200000
O	-4.20200000	2.49900000	0.27400000
C	6.52200000	-1.23000000	3.68300000
N	5.63400000	-2.18100000	3.01900000
C	4.31400000	-1.96800000	2.84200000
N	3.74400000	-0.85000000	3.31100000
N	3.56500000	-2.84000000	2.16200000
Co	-0.51100000	-2.04300000	-0.15800000
O	-0.33500000	-0.31400000	-1.73000000
O	1.93900000	-1.60600000	-2.15700000
H	-4.64900000	-0.99300000	-1.95200000
H	-4.90300000	-0.61100000	-0.21500000
H	-2.57300000	0.07700000	-0.44800000
H	-4.00300000	-2.81800000	-0.16600000
H	5.91500000	5.23700000	-4.26500000
H	6.42900000	3.66200000	-4.88500000
H	6.44700000	2.74500000	-2.57100000
H	5.37800000	5.49200000	-1.72100000
H	5.52000000	4.09700000	-0.65300000
H	6.97900000	4.85100000	-1.33000000
H	3.78000000	4.08900000	-3.27400000
H	3.95400000	2.72600000	-2.16700000
H	4.33300000	2.52900000	-3.88700000
H	4.75700000	1.34200000	1.68200000
H	3.03600000	1.77500000	1.54200000
H	2.79000000	0.41300000	-0.16000000
H	5.15500000	-0.77000000	-2.55700000
H	3.51900000	-0.95400000	-1.97900000
H	6.66700000	0.58600000	-1.45000000
H	6.11000000	1.70600000	-0.30500000
H	-9.95600000	4.81900000	0.39900000
H	-10.17900000	3.68900000	-0.94600000
H	-8.37600000	2.04600000	-1.52800000
H	-7.82000000	4.81000000	1.71100000
H	-5.97600000	1.46900000	-1.45200000
H	-5.41100000	4.21600000	1.80200000
H	-4.00300000	1.72500000	-0.29500000
H	6.44200000	-0.24500000	3.21400000

H	6.31000000	-1.14700000	4.75600000
H	5.98900000	-3.10500000	2.82000000
H	4.17300000	-0.34300000	4.06900000
H	2.72700000	-0.75600000	3.14700000
H	3.97100000	-3.61300000	1.65800000
H	2.55600000	-2.65000000	2.09000000
H	-1.51100000	-5.31800000	-0.38600000
H	-2.51100000	-4.60800000	0.91300000
H	-0.80900000	-2.44000000	3.46000000
H	-2.24400000	-2.29300000	4.23800000
H	-2.74200000	-0.25200000	3.27700000
H	-1.33700000	0.83500000	1.62000000
H	-0.42600000	0.60000000	3.14900000
H	-0.35000000	-2.58300000	-3.45200000
H	1.48100000	-4.17000000	-2.98000000
H	0.53800000	-4.90800000	-1.65200000
H	-1.72500000	-4.15700000	-4.52300000
H	-1.16200000	-0.32200000	-2.23900000
H	-0.05400000	0.64600000	-1.63300000
H	1.14000000	-1.01900000	-2.25100000
H	-1.96900000	2.20600000	-1.12600000
H	4.22800000	2.69500000	0.62400000
H	7.54800000	-1.58000000	3.56600000
H	-10.33100000	3.12300000	0.72100000
H	-1.38300000	-5.93300000	1.28900000
H	7.51100000	4.60000000	-3.84000000
H	-1.93000000	3.30400000	0.18000000
C	2.64300000	5.12100000	0.53400000
C	1.85700000	4.30500000	-0.28000000
C	0.71900000	3.67600000	0.24500000
C	0.38700000	3.85200000	1.59600000
C	1.18700000	4.65200000	2.41400000
C	2.31200000	5.29300000	1.88300000
H	3.50800000	5.62800000	0.11700000
H	2.10600000	4.15100000	-1.32400000
H	-0.47500000	3.34400000	2.01900000
H	0.93000000	4.78000000	3.46100000
H	2.92200000	5.93000000	2.51700000
C	-0.08200000	2.80200000	-0.66000000
N	-1.41000000	2.70200000	-0.44300000

Table S10. Cartesian coordinates for E FeNH

C	3.86300000	-3.89300000	1.90500000
O	3.10800000	-2.94200000	2.18100000
N	5.12500000	-3.94100000	2.38200000
S	-4.01200000	-1.72100000	-1.98900000
N	-5.10800000	1.53700000	-2.27000000
C	-3.86400000	2.17000000	-1.84200000
C	-3.54800000	2.15900000	-0.32700000
S	-3.48800000	0.47600000	0.33800000
C	-2.70300000	1.68800000	-2.74300000
O	-2.49500000	2.33600000	-3.77600000
O	-2.70900000	0.59900000	1.68500000
O	-4.94500000	0.07100000	0.60400000
N	-1.92600000	0.62000000	-2.38400000
C	-0.83500000	0.34000000	-3.34800000
C	-0.31800000	-1.07200000	-3.14800000
O	0.64400000	-1.52500000	-3.82500000
C	0.33300000	1.34500000	-3.26900000

O	0.96200000	1.36900000	-1.97500000
N	-0.93800000	-1.75500000	-2.19700000
C	-0.48000000	-3.12500000	-1.94700000
C	-1.54700000	-3.85700000	-1.13000000
S	-2.22800000	-2.78000000	0.19100000
C	-0.22800000	-3.90300000	-3.25900000
O	-1.13900000	-4.30100000	-3.95500000
O	-0.92700000	-2.84600000	1.27300000
C	6.23100000	-4.12400000	-1.97000000
C	5.10300000	-3.43000000	-2.35300000
C	6.73600000	-3.44100000	-0.80300000
N	4.87800000	-2.36100000	-1.50400000
C	5.87300000	-2.33100000	-0.55400000
C	7.84300000	-3.64200000	0.04600000
C	6.10200000	-1.41700000	0.48300000
C	8.07000000	-2.74200000	1.08600000
C	7.21200000	-1.63600000	1.29500000
C	6.25600000	1.88100000	2.26400000
C	5.18100000	1.26500000	2.92000000
C	6.01400000	2.39700000	0.98000000
C	3.91500000	1.16600000	2.33200000
C	4.75500000	2.31400000	0.37800000
C	3.69700000	1.69700000	1.05800000
O	2.43300000	1.58200000	0.52800000
N	-3.38900000	-1.49200000	3.36100000
C	-2.62200000	-2.15200000	4.22100000
N	-3.16500000	-2.73600000	5.31400000
N	-1.30700000	-2.25100000	3.97800000
C	0.80700000	6.77200000	-2.94900000
C	-0.19900000	5.88000000	-3.35300000
C	1.39000000	6.56100000	-1.69200000
C	-0.60700000	4.81600000	-2.54800000
C	1.00200000	5.49500000	-0.87100000
C	0.00500000	4.62000000	-1.30700000
O	-0.40400000	3.53200000	-0.54700000
C	1.20400000	5.63700000	3.11200000
C	1.33300000	4.27900000	2.79700000
C	-0.10200000	6.15800000	3.18500000
C	0.20900000	3.45900000	2.58000000
C	-1.22500000	5.36500000	2.97500000
C	-1.08100000	3.99900000	2.68600000
O	-2.23600000	3.29000000	2.50800000
N	-8.02400000	-3.26600000	1.66500000
C	-7.37300000	-2.16800000	1.23200000
N	-7.60800000	-0.97500000	1.80900000
N	-6.46900000	-2.23500000	0.25800000
Fe	-2.18700000	-0.77300000	-1.10600000
H	5.80200000	-4.55800000	1.95400000
H	5.50600000	-3.07400000	2.74100000
H	1.10000000	1.03200000	-3.98000000
H	-0.02100000	2.34200000	-3.53200000
H	0.31800000	1.71900000	-1.33300000
H	-1.21600000	0.40800000	-4.37500000
H	4.44900000	-3.60400000	-3.19700000
H	4.11600000	-1.69200000	-1.59800000
H	8.52300000	-4.47300000	-0.12400000
H	8.93100000	-2.87700000	1.73500000
H	5.44600000	-0.56900000	0.64700000
H	7.42600000	-0.93400000	2.09600000
H	6.82400000	2.87300000	0.43300000

H	5.33000000	0.84400000	3.91200000
H	4.59600000	2.72400000	-0.61700000
H	3.09800000	0.66900000	2.84600000
H	2.39800000	1.92900000	-0.37800000
H	-2.95100000	-0.79600000	2.72900000
H	-2.60700000	-3.32900000	5.90800000
H	-4.04400000	-2.40800000	5.68500000
H	-0.68500000	-2.63100000	4.67600000
H	-1.01800000	-2.32100000	2.99300000
H	2.16500000	7.23700000	-1.33900000
H	-0.68200000	6.01800000	-4.31700000
H	1.46100000	5.35400000	0.10400000
H	-1.38900000	4.14500000	-2.88500000
H	-0.05600000	3.62300000	0.35800000
H	-0.24000000	7.21300000	3.41200000
H	2.32000000	3.83100000	2.71600000
H	-2.22500000	5.78100000	3.03400000
H	0.35400000	2.40400000	2.35200000
H	-2.10700000	2.34400000	2.31400000
H	-7.89800000	-4.11000000	1.12500000
H	-6.14300000	-3.11700000	-0.11300000
H	-5.87500000	-1.41500000	0.05600000
H	-8.43200000	-0.81500000	2.36700000
H	-7.08000000	-0.16700000	1.49200000
H	-5.90900000	1.95400000	-1.80500000
H	-5.10700000	0.53600000	-2.08900000
H	-3.94000000	3.23100000	-2.09900000
H	-2.56800000	2.60400000	-0.13200000
H	-4.31200000	2.68300000	0.25400000
H	0.46700000	-3.10600000	-1.39400000
H	-1.15900000	-4.75100000	-0.63600000
H	-2.39400000	-4.12500000	-1.76300000
H	0.82600000	-4.13200000	-3.49600000
C	7.63000000	1.98800000	2.90100000
H	8.39200000	1.50300000	2.28000000
H	7.93000000	3.03400000	3.02700000
H	7.64800000	1.51500000	3.88800000
C	2.39700000	6.53400000	3.39200000
H	2.37100000	7.43400000	2.76700000
H	2.40400000	6.86200000	4.43800000
H	3.34000000	6.01400000	3.19800000
C	1.24200000	7.90600000	-3.85600000
H	0.37900000	8.46100000	-4.23900000
H	1.89100000	8.61300000	-3.33000000
H	1.79700000	7.52700000	-4.72300000
C	6.85400000	-5.29400000	-2.67700000
H	7.85300000	-5.04200000	-3.05500000
H	6.97100000	-6.15900000	-2.01200000
H	6.24500000	-5.60800000	-3.53000000
C	3.42400000	-5.05200000	1.03200000
H	3.84900000	-6.00100000	1.37000000
H	2.33500000	-5.11100000	1.02800000
H	3.77500000	-4.86700000	0.00900000
C	-4.84500000	-1.54900000	3.31100000
H	-5.31000000	-1.08300000	4.19000000
H	-5.12900000	-0.97900000	2.43200000
H	-5.18800000	-2.58500000	3.21900000
C	-8.91900000	-3.33400000	2.83000000
H	-9.87000000	-2.82400000	2.64200000
H	-9.12800000	-4.38400000	3.03300000

H	-8.43300000	-2.90100000	3.71000000
C	-3.66800000	-2.00400000	-3.76600000
H	-4.59900000	-2.34100000	-4.22700000
H	-3.36500000	-1.05700000	-4.21600000
H	-2.89100000	-2.75500000	-3.90500000
O	-0.60500000	-0.00900000	0.09400000
H	-1.00100000	0.24800000	0.94900000
H	0.22100000	-0.50900000	0.28100000
H	-0.07200000	-2.50000000	0.85400000
O	1.34300000	-1.87800000	0.50400000
H	2.02000000	-2.22700000	1.14400000
H	1.80300000	-1.64900000	-0.34900000

Table S11. Cartesian coordinates for ES FeNH

C	-3.09300000	-4.75200000	-1.99100000
O	-1.91300000	-4.65300000	-2.38500000
N	-4.13100000	-4.50800000	-2.81400000
S	4.50500000	-0.80500000	2.11300000
N	4.87500000	2.51200000	1.94700000
C	3.49900000	2.70800000	1.50500000
C	3.19500000	2.48400000	0.01600000
S	3.43900000	0.78500000	-0.56000000
C	2.51000000	2.01400000	2.47100000
O	2.28700000	2.58000000	3.54600000
O	2.66900000	0.75500000	-1.90000000
O	4.95300000	0.63400000	-0.81000000
N	1.84100000	0.87000000	2.10000000
C	0.79300000	0.47300000	3.06800000
C	0.54300000	-1.02100000	2.97100000
O	-0.47300000	-1.56400000	3.49200000
C	-0.48600000	1.32400000	2.98900000
O	-1.02700000	1.44300000	1.66800000
N	1.53000000	-1.67700000	2.37700000
C	1.48800000	-3.13700000	2.35600000
C	2.84100000	-3.65000000	1.85600000
S	3.35300000	-2.73000000	0.34900000
C	1.22100000	-3.70600000	3.76400000
O	2.03200000	-3.62000000	4.66000000
O	2.42700000	-3.57700000	-0.78600000
C	-6.10200000	-4.30300000	2.40500000
C	-5.11300000	-3.40200000	2.72500000
C	-6.51100000	-3.98400000	1.05900000
N	-4.90300000	-2.52100000	1.67200000
C	-5.74000000	-2.86200000	0.63100000
C	-7.44700000	-4.54800000	0.17300000
C	-5.90100000	-2.28900000	-0.63600000
C	-7.60000000	-3.99200000	-1.09600000
C	-6.84000000	-2.86600000	-1.49100000
C	-6.62800000	1.99500000	-1.75000000
C	-5.66700000	2.85500000	-2.30700000
C	-6.34900000	1.45000000	-0.48800000
C	-4.48300000	3.16600000	-1.63700000
C	-5.17100000	1.75900000	0.20400000
C	-4.23100000	2.62300000	-0.37100000
O	-3.05500000	2.97700000	0.22900000
N	3.17800000	-1.55400000	-3.16500000
C	2.46800000	-2.60100000	-3.54800000
N	3.01900000	-3.57400000	-4.30400000
N	1.15900000	-2.67700000	-3.23100000

C	-1.09600000	6.89200000	2.94100000
C	-0.02700000	6.04800000	3.27500000
C	-1.77600000	6.64600000	1.74100000
C	0.37100000	5.00700000	2.43700000
C	-1.40300000	5.59900000	0.89500000
C	-0.31900000	4.79500000	1.24400000
O	0.09200000	3.73500000	0.43600000
C	-1.57800000	5.64100000	-3.17600000
C	-1.36100000	4.42100000	-3.83100000
C	-0.53600000	6.13300000	-2.37300000
C	-0.16200000	3.71200000	-3.69300000
C	0.65800000	5.43000000	-2.20800000
C	0.85100000	4.20400000	-2.86200000
O	2.05100000	3.57200000	-2.66200000
N	8.00100000	-2.78600000	-1.70800000
C	7.37300000	-1.62500000	-1.42500000
N	7.51200000	-0.56800000	-2.25100000
N	6.58600000	-1.50300000	-0.36400000
Fe	2.49800000	-0.60000000	1.07600000
H	-5.07900000	-4.44300000	-2.46300000
H	-3.94000000	-4.18600000	-3.75300000
H	-1.24400000	0.83500000	3.60500000
H	-0.27400000	2.31600000	3.39700000
H	-0.51300000	2.12600000	1.19900000
H	1.16900000	0.62500000	4.09200000
H	-4.56300000	-3.28700000	3.64900000
H	-4.11000000	-1.90000000	1.60900000
H	-8.04700000	-5.40100000	0.47700000
H	-8.33000000	-4.41000000	-1.78300000
H	-5.33700000	-1.41300000	-0.93700000
H	-7.00500000	-2.42700000	-2.47200000
H	-7.06500000	0.77500000	-0.02500000
H	-5.84800000	3.29400000	-3.28600000
H	-4.98600000	1.33300000	1.18700000
H	-3.74300000	3.82500000	-2.08000000
H	-2.82200000	2.42300000	0.99500000
H	2.73000000	-0.74200000	-2.68600000
H	2.55400000	-4.46000000	-4.42500000
H	3.93700000	-3.46700000	-4.70300000
H	0.62200000	-3.48800000	-3.50900000
H	0.88100000	-2.30100000	-2.33200000
H	-2.62300000	7.27000000	1.46600000
H	0.51200000	6.20400000	4.20700000
H	-1.96200000	5.39200000	-0.01000000
H	1.19300000	4.36100000	2.72100000
H	-0.21000000	3.90100000	-0.47100000
H	-0.66300000	7.07600000	-1.84700000
H	-2.13800000	4.01400000	-4.47500000
H	1.44600000	5.81200000	-1.56700000
H	-0.01000000	2.78400000	-4.23700000
H	2.00400000	2.60100000	-2.73100000
H	7.95200000	-3.50800000	-1.00300000
H	6.29100000	-2.30500000	0.17600000
H	5.97500000	-0.66400000	-0.28700000
H	8.29400000	-0.49900000	-2.88400000
H	7.01600000	0.28700000	-2.01800000
H	5.50200000	3.13900000	1.45100000
H	5.18200000	1.55500000	1.79600000
H	3.27100000	3.76800000	1.66800000
H	2.15000000	2.71300000	-0.19600000

H	3.83000000	3.10100000	-0.62700000
H	0.69300000	-3.50000000	1.69700000
H	2.80800000	-4.70400000	1.57000000
H	3.61400000	-3.49500000	2.60700000
H	0.25800000	-4.23200000	3.90800000
C	-7.93400000	1.71200000	-2.46600000
H	-8.34100000	0.73500000	-2.18300000
H	-8.69000000	2.46600000	-2.21600000
H	-7.80600000	1.72500000	-3.55300000
C	-2.88000000	6.40700000	-3.30700000
H	-3.45000000	6.38300000	-2.37000000
H	-2.69900000	7.45900000	-3.55100000
H	-3.51500000	5.98400000	-4.09200000
C	-1.48000000	8.03900000	3.84200000
H	-0.81200000	8.89700000	3.69600000
H	-2.50100000	8.38100000	3.64500000
H	-1.41700000	7.75600000	4.89800000
C	-6.69000000	-5.36500000	3.28900000
H	-7.75300000	-5.17500000	3.48300000
H	-6.61800000	-6.35800000	2.82900000
H	-6.17700000	-5.40600000	4.25500000
C	-3.42300000	-5.12800000	-0.56500000
H	-4.46700000	-5.41400000	-0.42400000
H	-2.76500000	-5.94200000	-0.25400000
H	-3.22400000	-4.26100000	0.07300000
C	4.62600000	-1.43200000	-3.28700000
H	4.93900000	-1.31100000	-4.33300000
H	4.90700000	-0.54200000	-2.73200000
H	5.12500000	-2.30400000	-2.85100000
C	8.77300000	-3.07000000	-2.92300000
H	9.73100000	-2.53800000	-2.93100000
H	8.97700000	-4.14000000	-2.95200000
H	8.19600000	-2.80300000	-3.81400000
C	4.15900000	-0.86200000	3.91200000
H	5.12000000	-0.96200000	4.42100000
H	3.69200000	0.07900000	4.21100000
H	3.51000000	-1.69900000	4.17200000
H	1.45300000	-3.55800000	-0.57100000
O	-0.24100000	-3.56700000	-0.56100000
H	-0.78700000	-4.12900000	-1.15800000
H	-0.78500000	-3.38400000	0.23600000
O	-1.80800000	-3.01200000	1.71500000
H	-2.24300000	-3.73400000	2.18500000
H	-1.33600000	-2.47400000	2.41600000
N	0.84700000	-0.74000000	-0.10700000
C	-0.15600000	-0.59200000	-0.66500000
C	-1.41700000	-0.27700000	-1.36100000
C	-1.31300000	1.20800000	-1.76900000
H	-2.21300000	1.48900000	-2.32300000
H	-1.24600000	1.86100000	-0.90200000
H	-0.44300000	1.36500000	-2.40800000
C	-1.60100000	-1.13900000	-2.62900000
H	-1.61000000	-2.20600000	-2.40100000
H	-2.56900000	-0.87300000	-3.06600000
H	-0.82900000	-0.93100000	-3.37300000
C	-2.58900000	-0.53200000	-0.39000000
H	-3.50200000	-0.15200000	-0.85400000
H	-2.69300000	-1.60100000	-0.19300000
H	-2.42900000	-0.00900000	0.55400000

Table S12. Cartesian coordinates for TS1 FeNH

C	-2.34500000	-5.00300000	-1.89900000
O	-1.10800000	-5.14100000	-1.99900000
N	-3.09500000	-4.56800000	-2.92800000
S	4.24200000	-0.68500000	2.37100000
N	4.81300000	2.25600000	2.09200000
C	3.64900000	2.93900000	1.49200000
C	3.48400000	2.64700000	-0.00100000
S	3.45500000	0.87500000	-0.39300000
C	2.42500000	2.63100000	2.37900000
O	2.13400000	3.48000000	3.23100000
O	2.85100000	0.75400000	-1.77900000
O	4.95300000	0.46100000	-0.40700000
N	1.74200000	1.45700000	2.23700000
C	0.62200000	1.28300000	3.18900000
C	0.38900000	-0.19700000	3.43500000
O	-0.50200000	-0.60100000	4.21900000
C	-0.67800000	1.93200000	2.69100000
O	-1.18900000	1.28400000	1.50500000
N	1.17400000	-0.98500000	2.70700000
C	0.90300000	-2.41900000	2.70900000
C	2.17600000	-3.18300000	2.31600000
S	3.26900000	-2.21900000	1.18500000
C	0.45600000	-2.90700000	4.11200000
O	1.25900000	-3.08200000	5.00800000
O	1.04400000	-2.65900000	-0.61300000
C	-5.73100000	-4.56300000	2.42700000
C	-4.84900000	-3.57200000	2.79700000
C	-6.03600000	-4.32000000	1.03900000
N	-4.60300000	-2.71400000	1.74200000
C	-5.31500000	-3.15000000	0.64800000
C	-6.81600000	-4.99000000	0.07900000
C	-5.37300000	-2.64000000	-0.65300000
C	-6.86200000	-4.49800000	-1.22500000
C	-6.15000000	-3.32800000	-1.58600000
C	-6.68600000	1.44600000	-2.02000000
C	-5.81400000	2.37000000	-2.62200000
C	-6.24000000	0.81100000	-0.85100000
C	-4.56100000	2.66100000	-2.08000000
C	-4.98400000	1.08800000	-0.29200000
C	-4.14500000	2.02300000	-0.90600000
O	-2.90300000	2.35500000	-0.41900000
N	3.62600000	-1.86200000	-2.84900000
C	3.27500000	-3.13800000	-3.14800000
N	4.02400000	-3.76900000	-4.12700000
N	2.33200000	-3.73300000	-2.46800000
C	-1.60200000	6.97900000	2.51900000
C	-0.28400000	6.49800000	2.47600000
C	-2.53700000	6.38400000	1.66200000
C	0.08600000	5.45700000	1.62600000
C	-2.18600000	5.33500000	0.80500000
C	-0.87100000	4.86000000	0.79900000
O	-0.46900000	3.80000000	0.02400000
C	-2.01800000	5.52000000	-3.37100000
C	-1.70600000	4.26900000	-3.91600000
C	-1.03200000	6.14300000	-2.58400000
C	-0.47300000	3.64600000	-3.67500000
C	0.19700000	5.54000000	-2.33600000
C	0.47600000	4.27400000	-2.86600000
O	1.69100000	3.71100000	-2.54400000

N	7.89900000	-2.64000000	-2.14100000
C	7.17600000	-1.66800000	-1.55000000
N	7.44600000	-0.37300000	-1.76700000
N	6.15500000	-1.97400000	-0.74400000
Fe	2.22700000	-0.12300000	1.32400000
H	-4.07900000	-4.36700000	-2.80100000
H	-2.64400000	-4.31500000	-3.79600000
H	-1.44800000	1.81800000	3.45600000
H	-0.50600000	2.99100000	2.49500000
H	-0.46400000	1.22400000	0.85500000
H	0.86600000	1.76800000	4.14100000
H	-4.38400000	-3.39800000	3.75900000
H	-3.86800000	-2.00400000	1.75800000
H	-7.37700000	-5.88100000	0.35000000
H	-7.46900000	-5.00300000	-1.97000000
H	-4.84700000	-1.72900000	-0.91600000
H	-6.24100000	-2.93600000	-2.59600000
H	-6.87800000	0.08100000	-0.36100000
H	-6.12200000	2.87900000	-3.53200000
H	-4.67000000	0.58700000	0.62000000
H	-3.89600000	3.38000000	-2.54600000
H	-2.66800000	1.91500000	0.42000000
H	2.98700000	-1.29400000	-2.29800000
H	3.69100000	-4.67900000	-4.41400000
H	4.36000000	-3.20600000	-4.89700000
H	2.05000000	-4.64700000	-2.80600000
H	1.62000000	-3.13900000	-1.44300000
H	-3.56600000	6.73600000	1.66500000
H	0.46700000	6.93200000	3.13100000
H	-2.92800000	4.87700000	0.15900000
H	1.09700000	5.06800000	1.64200000
H	-1.22800000	3.47700000	-0.49100000
H	-1.24000000	7.11100000	-2.13500000
H	-2.43400000	3.76000000	-4.54300000
H	0.93000000	6.01400000	-1.69200000
H	-0.26000000	2.67600000	-4.11400000
H	1.71900000	2.76600000	-2.75400000
H	7.74200000	-3.58100000	-1.80900000
H	5.71700000	-2.88100000	-0.80900000
H	5.55600000	-1.18200000	-0.43900000
H	8.31200000	-0.07100000	-2.18600000
H	6.79100000	0.32300000	-1.40900000
H	5.11000000	2.75600000	2.92500000
H	5.59400000	2.20700000	1.44400000
H	3.74100000	4.03100000	1.55800000
H	2.54500000	3.06400000	-0.37900000
H	4.31300000	3.05900000	-0.58700000
H	0.09800000	-2.62100000	1.99300000
H	1.94700000	-4.09100000	1.75200000
H	2.77200000	-3.44300000	3.19300000
H	-0.61200000	-3.15600000	4.23000000
C	-8.06500000	1.18000000	-2.59800000
H	-8.46800000	0.22600000	-2.24300000
H	-8.77200000	1.96700000	-2.30700000
H	-8.03900000	1.15300000	-3.69300000
C	-3.35800000	6.19100000	-3.61000000
H	-3.83900000	6.45900000	-2.66200000
H	-3.24100000	7.11300000	-4.19000000
H	-4.04000000	5.53500000	-4.16000000
C	-1.98900000	8.07800000	3.48300000

H	-1.36300000	8.96800000	3.34900000
H	-3.03200000	8.38100000	3.34700000
H	-1.87000000	7.75200000	4.52300000
C	-6.26800000	-5.66100000	3.29400000
H	-7.35800000	-5.59300000	3.39900000
H	-6.04800000	-6.65200000	2.87600000
H	-5.83500000	-5.61900000	4.29800000
C	-3.07000000	-5.28800000	-0.60800000
H	-4.14900000	-5.38400000	-0.73300000
H	-2.67600000	-6.21100000	-0.17500000
H	-2.89700000	-4.46700000	0.09500000
C	4.67200000	-1.11100000	-3.51800000
H	4.38400000	-0.80400000	-4.53400000
H	4.84700000	-0.20800000	-2.93700000
H	5.59200000	-1.69700000	-3.58000000
C	8.92600000	-2.45100000	-3.17300000
H	9.85900000	-2.05800000	-2.75300000
H	9.13300000	-3.42000000	-3.62700000
H	8.55900000	-1.77700000	-3.95300000
C	3.97100000	-1.08000000	4.13300000
H	4.21700000	-0.14300000	4.64400000
H	2.93600000	-1.34700000	4.33400000
H	4.66100000	-1.86600000	4.44400000
H	0.46900000	-3.34700000	-0.19600000
O	-0.00500000	-4.88800000	0.42000000
H	-0.39000000	-5.17300000	-0.45300000
H	-0.70400000	-5.02100000	1.07000000
O	-2.24800000	-1.21700000	2.10400000
H	-1.92000000	-1.20700000	3.02200000
H	-1.92100000	-0.35500000	1.77200000
N	0.80700000	-0.26300000	0.09500000
C	0.33700000	-1.02200000	-0.70700000
C	-0.69100000	-0.98900000	-1.81400000
C	-0.76000000	0.47900000	-2.28600000
H	-1.50200000	0.56900000	-3.08500000
H	-1.05900000	1.15500000	-1.48600000
H	0.21600000	0.79600000	-2.66300000
C	-0.30300000	-1.87800000	-3.00900000
H	-0.30800000	-2.93700000	-2.75500000
H	-1.02900000	-1.70700000	-3.81100000
H	0.68700000	-1.61500000	-3.39400000
C	-2.05200000	-1.43300000	-1.24600000
H	-2.78800000	-1.44500000	-2.05500000
H	-2.00400000	-2.42800000	-0.80000000
H	-2.40400000	-0.74100000	-0.47800000

Table S13. Cartesian coordinates for INT1 FeNH

C	-2.74600000	-4.58600000	-1.91300000
O	-1.52000000	-4.47700000	-1.74000000
N	-3.43500000	-3.77300000	-2.74700000
S	4.97400000	0.03400000	2.21600000
N	4.86800000	2.63700000	1.87800000
C	3.53200000	3.05600000	1.43000000
C	3.31800000	2.85500000	-0.07000000
S	3.83800000	1.22100000	-0.68400000
C	2.49900000	2.39300000	2.36700000
O	2.16900000	3.05800000	3.36900000
O	3.26600000	1.10900000	-2.07800000
O	5.38100000	1.30700000	-0.71700000

N	2.04800000	1.15400000	2.09900000
C	1.14000000	0.60500000	3.11800000
C	1.16500000	-0.90700000	3.05600000
O	0.41600000	-1.61300000	3.76600000
C	-0.29600000	1.15000000	3.09000000
O	-1.01100000	0.82200000	1.89200000
N	2.09700000	-1.42400000	2.23900000
C	2.24200000	-2.88300000	2.22100000
C	3.56600000	-3.23100000	1.53500000
S	3.86600000	-2.14900000	0.07500000
C	2.26500000	-3.43500000	3.66200000
O	3.12800000	-3.12400000	4.45900000
O	0.65600000	-2.31700000	-0.34300000
C	-5.93900000	-5.08800000	2.32400000
C	-4.94700000	-4.48700000	3.06500000
C	-6.08600000	-4.28400000	1.13500000
N	-4.46900000	-3.36000000	2.41900000
C	-5.15300000	-3.20600000	1.23500000
C	-6.91400000	-4.36200000	0.00000000
C	-5.05300000	-2.21400000	0.25100000
C	-6.81200000	-3.37900000	-0.98500000
C	-5.89700000	-2.30800000	-0.85400000
C	-7.22000000	1.19600000	-2.02100000
C	-6.10800000	1.63000000	-2.76200000
C	-7.04900000	1.02200000	-0.64000000
C	-4.87500000	1.89100000	-2.15500000
C	-5.82600000	1.27600000	-0.01600000
C	-4.73900000	1.71400000	-0.77600000
O	-3.50600000	1.98000000	-0.21500000
N	3.04300000	-1.82000000	-3.07700000
C	2.66200000	-3.08600000	-3.25200000
N	3.15300000	-3.77700000	-4.31400000
N	1.85200000	-3.69800000	-2.39100000
C	-2.14800000	6.29900000	2.95200000
C	-0.87800000	5.70500000	3.00800000
C	-3.03900000	5.84500000	1.97200000
C	-0.50800000	4.69000000	2.12600000
C	-2.69000000	4.82400000	1.08200000
C	-1.42300000	4.24400000	1.17200000
O	-1.02800000	3.21000000	0.34300000
C	-2.52100000	5.43800000	-3.03900000
C	-2.02300000	4.37900000	-3.81000000
C	-1.68900000	5.95000000	-2.03000000
C	-0.74400000	3.85300000	-3.59500000
C	-0.41400000	5.43500000	-1.79900000
C	0.06300000	4.38000000	-2.58300000
O	1.32700000	3.91400000	-2.30400000
N	7.95100000	-2.25500000	-2.16000000
C	7.35400000	-1.11300000	-1.75800000
N	7.20500000	-0.07400000	-2.59600000
N	6.88500000	-1.00300000	-0.51500000
Fe	2.85000000	-0.27600000	0.95800000
H	-4.44100000	-3.71600000	-2.65900000
H	-2.95700000	-2.96100000	-3.11400000
H	-0.83800000	0.68800000	3.92100000
H	-0.27500000	2.22900000	3.24400000
H	-0.85700000	1.52900000	1.23800000
H	1.51400000	0.86300000	4.12100000
H	-4.54300000	-4.77700000	4.02600000
H	-3.72300000	-2.74900000	2.74400000

H	-7.63400000	-5.17000000	-0.10000000
H	-7.46600000	-3.41600000	-1.85200000
H	-4.36300000	-1.38500000	0.35600000
H	-5.87100000	-1.52500000	-1.60600000
H	-7.88100000	0.66900000	-0.03600000
H	-6.20600000	1.77800000	-3.83500000
H	-5.71900000	1.12400000	1.05600000
H	-4.02500000	2.24400000	-2.73100000
H	-3.52900000	1.85100000	0.74400000
H	2.66300000	-1.29700000	-2.29100000
H	2.86500000	-4.73400000	-4.45300000
H	3.48700000	-3.28400000	-5.12800000
H	1.28000000	-4.47600000	-2.69100000
H	1.52000000	-3.20600000	-1.54700000
H	-4.02900000	6.28900000	1.90000000
H	-0.16300000	6.03100000	3.75800000
H	-3.39200000	4.48500000	0.32700000
H	0.47400000	4.23900000	2.19600000
H	-1.71700000	3.05000000	-0.32300000
H	-2.04800000	6.75900000	-1.39800000
H	-2.63800000	3.96000000	-4.60400000
H	0.20600000	5.82000000	-0.99600000
H	-0.37900000	3.03400000	-4.21100000
H	1.50700000	3.07800000	-2.75700000
H	8.18500000	-2.90900000	-1.42600000
H	6.52500000	-1.82500000	-0.04000000
H	6.33900000	-0.14700000	-0.32200000
H	7.78500000	0.03900000	-3.41200000
H	6.63600000	0.71000000	-2.26900000
H	5.13600000	3.06100000	2.76100000
H	5.59700000	2.72200000	1.17600000
H	3.39300000	4.13000000	1.61000000
H	2.26100000	2.94500000	-0.32400000
H	3.88800000	3.57700000	-0.66500000
H	1.39700000	-3.33000000	1.69400000
H	3.57100000	-4.27300000	1.20200000
H	4.38500000	-3.08300000	2.24300000
H	1.48500000	-4.17600000	3.91400000
C	-8.56700000	0.94800000	-2.67100000
H	-9.03100000	0.03400000	-2.28500000
H	-9.25800000	1.77500000	-2.47100000
H	-8.47600000	0.85000000	-3.75700000
C	-3.88300000	6.04300000	-3.30500000
H	-4.36600000	6.36100000	-2.37500000
H	-3.80400000	6.92600000	-3.95100000
H	-4.54900000	5.33000000	-3.80200000
C	-2.52400000	7.40300000	3.90900000
H	-2.05700000	8.35400000	3.62400000
H	-3.60600000	7.56300000	3.93300000
H	-2.19600000	7.17400000	4.92900000
C	-6.73700000	-6.30500000	2.69500000
H	-7.80400000	-6.06800000	2.79200000
H	-6.64900000	-7.09400000	1.93700000
H	-6.40000000	-6.72100000	3.64900000
C	-3.54100000	-5.62600000	-1.16700000
H	-4.45300000	-5.92400000	-1.69000000
H	-2.90900000	-6.49700000	-0.98700000
H	-3.84900000	-5.21000000	-0.20000000
C	4.18100000	-1.20700000	-3.75500000
H	3.98200000	-1.07000000	-4.82500000

H	4.32100000	-0.22500000	-3.31000000
H	5.08000000	-1.81800000	-3.62400000
C	8.44100000	-2.54800000	-3.50900000
H	9.37000000	-2.01100000	-3.73500000
H	8.63400000	-3.61900000	-3.57600000
H	7.68000000	-2.29000000	-4.25100000
C	4.51100000	0.07500000	3.97400000
H	5.41600000	0.16500000	4.57800000
H	3.84600000	0.91900000	4.16800000
H	3.99700000	-0.86200000	4.21200000
H	-0.14000000	-2.78500000	0.09600000
O	-1.01000000	-3.70200000	0.92100000
H	-1.47800000	-4.20100000	0.23200000
H	-1.62100000	-3.12900000	1.43400000
O	-2.05500000	-1.75000000	2.53600000
H	-1.30200000	-1.82000000	3.16300000
H	-1.91900000	-0.86000000	2.15300000
N	1.41900000	-0.14700000	-0.25900000
C	0.56200000	-0.99600000	-0.65000000
C	-0.56900000	-0.57300000	-1.61100000
C	-0.42100000	0.90700000	-1.98300000
H	-1.29000000	1.23900000	-2.55700000
H	-0.31600000	1.53900000	-1.10300000
H	0.48000000	1.05500000	-2.58600000
C	-0.49400000	-1.41800000	-2.90300000
H	-0.60300000	-2.48400000	-2.69300000
H	-1.30100000	-1.10000000	-3.57400000
H	0.44600000	-1.24800000	-3.43700000
C	-1.93100000	-0.82700000	-0.93300000
H	-2.73800000	-0.53200000	-1.61100000
H	-2.06800000	-1.88100000	-0.68500000
H	-2.03300000	-0.23100000	-0.02700000

Table S14. Cartesian coordinates for TS2 FeNH

C	2.77500000	-4.95100000	2.15000000
O	1.62000000	-4.54900000	1.93500000
N	3.39200000	-4.68900000	3.32900000
S	-5.55800000	0.49900000	-2.21200000
N	-4.95100000	3.05300000	-1.90000000
C	-3.56100000	3.33500000	-1.51600000
C	-3.32500000	3.16100000	-0.00700000
S	-4.04100000	1.64100000	0.74300000
C	-2.58500000	2.55200000	-2.43400000
O	-1.98200000	3.20900000	-3.30100000
O	-3.43900000	1.59500000	2.13700000
O	-5.56100000	1.97700000	0.78800000
N	-2.41800000	1.22000000	-2.23900000
C	-1.45600000	0.58200000	-3.11400000
C	-1.64500000	-0.94800000	-3.17700000
O	-0.82200000	-1.66500000	-3.78900000
C	0.01200000	0.95300000	-2.65800000
O	0.26200000	0.73000000	-1.32100000
N	-2.73500000	-1.41400000	-2.55000000
C	-2.94200000	-2.85900000	-2.49700000
C	-4.26900000	-3.15200000	-1.76200000
S	-4.49500000	-2.15100000	-0.21500000
C	-3.01900000	-3.45500000	-3.91400000
O	-3.83900000	-3.08800000	-4.73100000
O	-1.28600000	-2.41700000	0.90100000

C	5.67900000	-5.43800000	-2.46100000
C	4.49300000	-5.00700000	-3.00900000
C	5.97200000	-4.52400000	-1.38600000
N	4.03100000	-3.87900000	-2.34900000
C	4.91600000	-3.56500000	-1.33900000
C	7.01400000	-4.45000000	-0.44200000
C	4.88600000	-2.55200000	-0.36900000
C	6.98000000	-3.44800000	0.52400000
C	5.92500000	-2.51000000	0.56000000
C	7.83700000	0.72500000	1.72400000
C	6.65500000	1.01500000	2.41900000
C	7.79000000	0.73500000	0.32200000
C	5.45900000	1.28700000	1.74900000
C	6.60600000	1.00400000	-0.36500000
C	5.43900000	1.26700000	0.35500000
O	4.22800000	1.49800000	-0.27200000
N	-3.41400000	-1.89400000	3.20800000
C	-3.15800000	-3.15200000	3.55800000
N	-3.29800000	-3.54500000	4.84400000
N	-2.80200000	-4.02500000	2.61000000
C	2.90800000	6.20900000	-2.92000000
C	1.61400000	5.66400000	-2.96600000
C	3.83800000	5.63800000	-2.03700000
C	1.25200000	4.59100000	-2.16200000
C	3.49900000	4.56100000	-1.22300000
C	2.19900000	4.03300000	-1.28400000
O	1.79800000	2.98100000	-0.53000000
C	3.43100000	5.45700000	3.06300000
C	2.77800000	4.45500000	3.79300000
C	2.68900000	6.11100000	2.06600000
C	1.44600000	4.10700000	3.53600000
C	1.36300000	5.77800000	1.79600000
C	0.73600000	4.76500000	2.52700000
O	-0.56500000	4.45900000	2.20300000
N	-7.83800000	-1.55100000	2.64900000
C	-7.34400000	-0.41200000	2.12500000
N	-7.11800000	0.65900000	2.90600000
N	-7.06200000	-0.33200000	0.82500000
Fe	-3.35300000	-0.23200000	-1.08100000
H	4.36300000	-4.91900000	3.47500000
H	2.93800000	-4.07300000	3.98900000
H	0.70600000	0.39200000	-3.29800000
H	0.08500000	2.03000000	-2.88600000
H	-0.67900000	0.47300000	-0.61000000
H	-1.52500000	0.97000000	-4.14000000
H	3.93100000	-5.42000000	-3.83700000
H	3.12400000	-3.44800000	-2.50500000
H	7.83000000	-5.16600000	-0.46500000
H	7.78100000	-3.37700000	1.25500000
H	4.08300000	-1.82200000	-0.31900000
H	5.93100000	-1.72800000	1.31200000
H	8.68900000	0.51200000	-0.24700000
H	6.66200000	1.02400000	3.50600000
H	6.58900000	0.98400000	-1.45200000
H	4.54800000	1.50800000	2.29600000
H	4.33200000	1.42600000	-1.23100000
H	-3.38300000	-1.69900000	2.21000000
H	-2.91700000	-4.42700000	5.14900000
H	-3.51100000	-2.86800000	5.56100000
H	-2.49300000	-4.95300000	2.85300000

H	-2.42900000	-3.59600000	1.75500000
H	4.84400000	6.04600000	-1.98400000
H	0.88000000	6.08200000	-3.65100000
H	4.22200000	4.13900000	-0.53200000
H	0.25900000	4.15900000	-2.21900000
H	2.56100000	2.58300000	-0.07300000
H	3.16100000	6.89300000	1.47500000
H	3.31400000	3.93200000	4.58300000
H	0.81100000	6.28100000	1.00800000
H	0.96700000	3.32400000	4.12000000
H	-0.88400000	3.72100000	2.73900000
H	-8.11100000	-2.26400000	1.98800000
H	-6.74600000	-1.16400000	0.32500000
H	-6.60700000	0.55200000	0.53800000
H	-7.58700000	0.77900000	3.78900000
H	-6.61800000	1.44700000	2.48600000
H	-5.24100000	3.54100000	-2.74100000
H	-5.62200000	3.16200000	-1.14400000
H	-3.32100000	4.38300000	-1.73800000
H	-2.25500000	3.14400000	0.21700000
H	-3.78700000	3.97600000	0.56200000
H	-2.10800000	-3.33700000	-1.96800000
H	-4.32600000	-4.20900000	-1.49000000
H	-5.10500000	-2.92200000	-2.42500000
H	-2.31600000	-4.27900000	-4.14300000
C	9.12400000	0.42000000	2.45300000
H	9.66400000	-0.40700000	1.98100000
H	9.79700000	1.28700000	2.45600000
H	8.93700000	0.14800000	3.49600000
C	4.87000000	5.84200000	3.34600000
H	5.42100000	6.03500000	2.42000000
H	4.92700000	6.75400000	3.95300000
H	5.39500000	5.05100000	3.89100000
C	3.28100000	7.37900000	-3.78600000
H	2.81900000	8.30700000	-3.42200000
H	4.36200000	7.53700000	-3.80500000
H	2.94100000	7.23800000	-4.81800000
C	6.50700000	-6.61700000	-2.87500000
H	7.51500000	-6.31600000	-3.18700000
H	6.62600000	-7.33500000	-2.05300000
H	6.04700000	-7.14900000	-3.71300000
C	3.55500000	-5.74500000	1.14000000
H	4.26600000	-6.42600000	1.61700000
H	2.86300000	-6.32500000	0.52700000
H	4.12700000	-5.08700000	0.48000000
C	-3.68400000	-0.79200000	4.12400000
H	-2.91100000	-0.73200000	4.89800000
H	-3.65900000	0.13400000	3.54200000
H	-4.66700000	-0.89600000	4.59900000
C	-8.04100000	-1.80900000	4.07000000
H	-8.92200000	-1.29100000	4.46500000
H	-8.19000000	-2.88100000	4.20700000
H	-7.15900000	-1.50900000	4.64400000
C	-5.22100000	0.38000000	-3.99900000
H	-6.10700000	0.69100000	-4.55500000
H	-4.37000000	1.01400000	-4.25900000
H	-4.96700000	-0.65500000	-4.24300000
H	-0.38900000	-3.15100000	0.30200000
O	0.68900000	-3.66400000	-0.72000000
H	1.34400000	-3.96300000	-0.04700000

H	1.17600000	-3.22400000	-1.45600000
O	1.34800000	-1.87100000	-2.06200000
H	0.70300000	-2.05200000	-2.78700000
H	1.28600000	-0.91300000	-1.93800000
N	-1.51500000	-0.31400000	-0.01900000
C	-0.86800000	-1.12100000	0.72600000
C	0.38000000	-0.70500000	1.55600000
C	0.39400000	0.82300000	1.75900000
H	1.21000000	1.08800000	2.44000000
H	0.56000000	1.35600000	0.82100000
H	-0.55000000	1.16700000	2.19500000
C	0.30600000	-1.38700000	2.94300000
H	0.35500000	-2.47400000	2.86800000
H	1.15400000	-1.04400000	3.54700000
H	-0.60900000	-1.10300000	3.47500000
C	1.69000000	-1.13000000	0.85600000
H	2.54400000	-0.83600000	1.47800000
H	1.74400000	-2.21000000	0.71700000
H	1.78700000	-0.60900000	-0.09900000

Table S15. Cartesian coordinates for INT2 FeNH

C	-1.00400000	4.98600000	2.30400000
O	0.15100000	4.70000000	2.67500000
N	-2.08800000	4.57600000	2.98600000
S	3.75100000	0.14800000	-2.80800000
N	3.41800000	-2.56700000	-3.25400000
C	2.20400000	-3.06400000	-2.57300000
C	2.35600000	-3.16600000	-1.05600000
S	2.90100000	-1.63600000	-0.22500000
C	1.00300000	-2.22900000	-3.05700000
O	0.33900000	-2.70400000	-3.98800000
O	2.54200000	-1.84500000	1.22300000
O	4.44900000	-1.65500000	-0.44400000
N	0.73100000	-1.02200000	-2.48900000
C	-0.40300000	-0.31000000	-3.11800000
C	-0.22200000	1.18600000	-2.93200000
O	-1.11300000	1.99800000	-3.26100000
C	-1.77500000	-0.78000000	-2.61900000
O	-1.82400000	-0.83600000	-1.18600000
N	0.98000000	1.51000000	-2.46200000
C	1.22800000	2.92700000	-2.22700000
C	2.73800000	3.16600000	-2.08700000
S	3.61100000	1.73500000	-1.30900000
C	0.72900000	3.76500000	-3.42400000
O	1.25200000	3.68700000	-4.51600000
O	2.07600000	1.18800000	1.56700000
C	-3.93400000	6.15800000	-2.17400000
C	-3.09800000	5.46300000	-3.01500000
C	-4.15400000	5.30100000	-1.03700000
N	-2.77400000	4.23000000	-2.47300000
C	-3.41800000	4.09900000	-1.26800000
C	-4.90100000	5.42400000	0.14600000
C	-3.42700000	3.03300000	-0.36300000
C	-4.90800000	4.36600000	1.05400000
C	-4.17900000	3.18200000	0.79900000
C	-6.63000000	0.29400000	2.62100000
C	-5.87100000	-0.65200000	3.32600000
C	-6.27500000	0.53600000	1.28700000
C	-4.80000000	-1.32600000	2.73500000

C	-5.21000000	-0.12900000	0.67800000
C	-4.46100000	-1.06200000	1.40400000
O	-3.39600000	-1.72800000	0.85900000
N	4.09300000	0.20600000	3.22700000
C	4.13100000	0.66500000	4.47400000
N	4.91500000	0.03300000	5.39300000
N	3.45200000	1.75600000	4.81500000
C	-3.97600000	-5.85200000	-3.11000000
C	-2.66600000	-5.54300000	-3.50300000
C	-4.44700000	-5.28800000	-1.91700000
C	-1.83400000	-4.74200000	-2.72100000
C	-3.63800000	-4.47100000	-1.12500000
C	-2.32300000	-4.22400000	-1.52200000
O	-1.46000000	-3.46200000	-0.73600000
C	-3.37500000	-5.08200000	3.00000000
C	-2.52900000	-4.23600000	3.73200000
C	-2.82500000	-5.71600000	1.87800000
C	-1.21400000	-3.98400000	3.33500000
C	-1.51300000	-5.47500000	1.46600000
C	-0.70700000	-4.57300000	2.17000000
O	0.54600000	-4.32200000	1.67000000
N	8.51800000	-0.13400000	1.01200000
C	7.40600000	-0.67500000	0.47600000
N	7.10100000	-1.96600000	0.65800000
N	6.56200000	0.07200000	-0.24400000
Fe	1.86300000	0.09700000	-1.44300000
H	-3.00800000	4.63900000	2.56600000
H	-1.94800000	3.92500000	3.74500000
H	-2.52300000	-0.05800000	-2.95500000
H	-1.99700000	-1.76600000	-3.03600000
H	-1.47000000	-1.72600000	-0.96300000
H	-0.39200000	-0.49300000	-4.20100000
H	-2.70600000	5.75400000	-3.98100000
H	-2.21200000	3.49800000	-2.90200000
H	-5.47900000	6.32400000	0.34100000
H	-5.51300000	4.43300000	1.95500000
H	-2.87800000	2.12100000	-0.57300000
H	-4.22500000	2.36400000	1.50800000
H	-6.82800000	1.27300000	0.71000000
H	-6.11700000	-0.86500000	4.36400000
H	-4.94700000	0.09300000	-0.35300000
H	-4.20900000	-2.04800000	3.28800000
H	-3.15600000	-1.32700000	-0.00100000
H	3.32100000	0.53000000	2.60600000
H	4.94700000	0.39200000	6.33400000
H	5.07000000	-0.95900000	5.29700000
H	3.38400000	2.01800000	5.78600000
H	3.16400000	2.46500000	4.09400000
H	-5.46700000	-5.48700000	-1.59700000
H	-2.28100000	-5.94300000	-4.43800000
H	-4.01300000	-4.02400000	-0.21000000
H	-0.82900000	-4.50000000	-3.04300000
H	-1.75800000	-3.53100000	0.18700000
H	-3.43800000	-6.39200000	1.28900000
H	-2.90400000	-3.75600000	4.63300000
H	-1.11400000	-5.95100000	0.57700000
H	-0.58300000	-3.32600000	3.92400000
H	0.91200000	-3.49000000	2.00700000
H	8.76700000	0.79000000	0.68900000
H	6.57600000	1.07800000	-0.17100000

H	5.67000000	-0.37800000	-0.52300000
H	7.78900000	-2.63200000	0.96800000
H	6.18400000	-2.28600000	0.33000000
H	3.43300000	-2.90700000	-4.21100000
H	4.25900000	-2.88800000	-2.78200000
H	1.95500000	-4.08000000	-2.90800000
H	1.39900000	-3.43200000	-0.59700000
H	3.10200000	-3.91700000	-0.77400000
H	0.73100000	3.25900000	-1.31200000
H	2.93900000	3.99100000	-1.40200000
H	3.21200000	3.35200000	-3.05200000
H	-0.08000000	4.48800000	-3.21100000
C	-7.79900000	1.02000000	3.25900000
H	-7.83400000	2.06900000	2.94600000
H	-8.75500000	0.56500000	2.97300000
H	-7.73800000	0.99400000	4.35100000
C	-4.83200000	-5.26200000	3.37600000
H	-5.25000000	-6.17000000	2.93100000
H	-4.96200000	-5.32400000	4.46100000
H	-5.42800000	-4.41100000	3.02400000
C	-4.83300000	-6.78800000	-3.93300000
H	-4.62400000	-7.83500000	-3.68400000
H	-5.89900000	-6.61700000	-3.75600000
H	-4.64500000	-6.66500000	-5.00400000
C	-4.53100000	7.51800000	-2.38400000
H	-5.62700000	7.47500000	-2.40100000
H	-4.25000000	8.21200000	-1.58300000
H	-4.20200000	7.95400000	-3.33200000
C	-1.24500000	5.81200000	1.06200000
H	-0.88800000	5.24400000	0.19700000
H	-2.29400000	6.05700000	0.89800000
H	-0.64900000	6.72500000	1.12900000
C	5.03700000	-0.79100000	2.73400000
H	4.83900000	-1.78900000	3.14500000
H	4.89100000	-0.86900000	1.66400000
H	6.06300000	-0.49300000	2.97100000
C	9.44000000	-0.79000000	1.94800000
H	10.10000000	-1.50300000	1.44200000
H	10.05300000	-0.02100000	2.41700000
H	8.87500000	-1.30500000	2.73000000
C	3.32000000	0.87100000	-4.42700000
H	4.18400000	1.38600000	-4.84700000
H	3.06900000	-0.00300000	-5.03400000
H	2.44900000	1.52300000	-4.35400000
O	2.93400000	3.80000000	3.19000000
H	2.10200000	4.24000000	3.43100000
H	2.85200000	3.75400000	2.21600000
O	1.76200000	3.86900000	0.65400000
H	1.12700000	4.27400000	1.28200000
H	1.74900000	2.91400000	0.86600000
N	0.63800000	0.41400000	-0.00600000
C	0.92800000	0.74000000	1.24000000
C	-0.17900000	0.58500000	2.31200000
C	-0.34200000	-0.91800000	2.60400000
H	-1.10800000	-1.06600000	3.37000000
H	-0.66400000	-1.46800000	1.71600000
H	0.60300000	-1.34500000	2.95300000
C	0.23200000	1.31600000	3.59800000
H	0.40500000	2.38000000	3.41600000
H	-0.56300000	1.21300000	4.34600000

H	1.14700000	0.89400000	4.01800000
C	-1.52100000	1.15200000	1.81100000
H	-2.27300000	1.07700000	2.60400000
H	-1.43300000	2.20200000	1.52500000
H	-1.91100000	0.59200000	0.96000000
H	-0.32100000	0.14200000	-0.21200000

Table S16. Cartesian coordinates for TS3 FeNH

C	-0.90500000	4.49000000	2.80000000
O	0.07400000	3.89400000	3.27200000
N	-2.17000000	4.15600000	3.14600000
S	3.87000000	0.15200000	-2.92700000
N	3.29700000	-2.64000000	-3.35600000
C	2.07400000	-2.95600000	-2.59200000
C	2.29700000	-3.00400000	-1.08800000
S	2.96700000	-1.49300000	-0.31700000
C	0.97000000	-2.00100000	-3.08000000
O	0.32100000	-2.39700000	-4.06000000
O	2.61700000	-1.68200000	1.13500000
O	4.50600000	-1.58500000	-0.53200000
N	0.75800000	-0.78800000	-2.48700000
C	-0.30100000	-0.01100000	-3.17800000
C	-0.05900000	1.47100000	-2.98100000
O	-0.89400000	2.33700000	-3.32400000
C	-1.73600000	-0.44300000	-2.84100000
O	-1.96300000	-0.53600000	-1.43300000
N	1.16600000	1.74300000	-2.52400000
C	1.56900000	3.14600000	-2.47200000
C	3.10200000	3.20400000	-2.46400000
S	3.82300000	1.81500000	-1.48400000
C	1.05600000	3.91400000	-3.71400000
O	1.52200000	3.71500000	-4.81700000
O	2.04100000	0.79900000	2.18000000
C	-3.42800000	6.44400000	-1.52000000
C	-2.63200000	5.77200000	-2.42200000
C	-3.87600000	5.45400000	-0.57400000
N	-2.55900000	4.42700000	-2.10000000
C	-3.32400000	4.20100000	-0.97900000
C	-4.70600000	5.49900000	0.56200000
C	-3.60300000	3.00900000	-0.29700000
C	-4.97200000	4.31500000	1.25100000
C	-4.42700000	3.08200000	0.82200000
C	-6.68800000	0.47800000	2.69600000
C	-5.62700000	-0.15700000	3.35900000
C	-6.71400000	0.40300000	1.29400000
C	-4.61500000	-0.81900000	2.65600000
C	-5.71300000	-0.25500000	0.57700000
C	-4.64900000	-0.85500000	1.25900000
O	-3.62400000	-1.49300000	0.60300000
N	4.24700000	-0.29400000	3.31500000
C	4.32200000	0.36000000	4.47700000
N	5.08200000	-0.17500000	5.48400000
N	3.72700000	1.53300000	4.65400000
C	-4.32100000	-5.34400000	-3.40400000
C	-3.01400000	-5.00100000	-3.78500000
C	-4.75700000	-4.92800000	-2.13800000
C	-2.15800000	-4.30100000	-2.93200000
C	-3.92100000	-4.21700000	-1.27100000
C	-2.61400000	-3.92500000	-1.66800000

O	-1.73200000	-3.24600000	-0.83500000
C	-3.84700000	-5.06300000	2.73700000
C	-3.02100000	-4.19100000	3.45900000
C	-3.26500000	-5.76800000	1.67100000
C	-1.67200000	-4.01600000	3.13100000
C	-1.92400000	-5.60100000	1.32300000
C	-1.12200000	-4.71500000	2.05000000
O	0.18700000	-4.57300000	1.64800000
N	8.43200000	-0.85500000	1.76800000
C	7.35300000	-1.10000000	0.99500000
N	7.03700000	-2.34500000	0.61700000
N	6.55400000	-0.10200000	0.59900000
Fe	2.03200000	0.31300000	-1.52800000
H	-2.96800000	4.48500000	2.61400000
H	-2.30300000	3.33600000	3.72100000
H	-2.41300000	0.31800000	-3.23700000
H	-1.94500000	-1.40200000	-3.32200000
H	-1.63900000	-1.41800000	-1.16400000
H	-0.20100000	-0.16200000	-4.26300000
H	-2.12200000	6.15300000	-3.29700000
H	-2.04300000	3.71300000	-2.61100000
H	-5.14600000	6.43800000	0.88500000
H	-5.63000000	4.33100000	2.11700000
H	-3.20500000	2.06100000	-0.64300000
H	-4.66600000	2.17700000	1.36800000
H	-7.52300000	0.88300000	0.74800000
H	-5.58200000	-0.12800000	4.44500000
H	-5.74600000	-0.29100000	-0.50900000
H	-3.79400000	-1.30400000	3.17400000
H	-3.44500000	-1.07100000	-0.25900000
H	3.48300000	-0.01600000	2.68400000
H	5.08600000	0.29400000	6.37800000
H	5.17900000	-1.17800000	5.53200000
H	3.76900000	1.96400000	5.56700000
H	3.31200000	2.15300000	3.89300000
H	-5.77000000	-5.15700000	-1.81700000
H	-2.65100000	-5.28700000	-4.76900000
H	-4.27500000	-3.89200000	-0.29900000
H	-1.15700000	-4.03000000	-3.24900000
H	-2.10700000	-3.21900000	0.06000000
H	-3.87600000	-6.44500000	1.08000000
H	-3.43600000	-3.63000000	4.29200000
H	-1.49700000	-6.12500000	0.47500000
H	-1.05700000	-3.33100000	3.70700000
H	0.59800000	-3.81800000	2.08900000
H	8.69500000	0.11400000	1.87500000
H	6.57100000	0.79100000	1.07000000
H	5.69200000	-0.36900000	0.09200000
H	7.68600000	-3.11000000	0.70700000
H	6.14500000	-2.48100000	0.13000000
H	3.22200000	-3.01600000	-4.29700000
H	4.12600000	-3.02900000	-2.91500000
H	1.68600000	-3.94900000	-2.85500000
H	1.34600000	-3.18100000	-0.57700000
H	2.99900000	-3.79600000	-0.80500000
H	1.16100000	3.63200000	-1.57700000
H	3.49100000	4.11000000	-1.99800000
H	3.49700000	3.13400000	-3.47800000
H	0.30000000	4.69700000	-3.53100000
C	-7.75700000	1.23700000	3.45300000

H	-7.71600000	2.31000000	3.22600000
H	-8.76100000	0.88900000	3.18300000
H	-7.64200000	1.11900000	4.53400000
C	-5.30500000	-5.25500000	3.09700000
H	-5.92700000	-5.34000000	2.19900000
H	-5.45200000	-6.17000000	3.68400000
H	-5.68300000	-4.41600000	3.68800000
C	-5.21500000	-6.15900000	-4.31400000
H	-5.06700000	-7.23400000	-4.15000000
H	-6.27300000	-5.94200000	-4.13500000
H	-5.00300000	-5.95700000	-5.36900000
C	-3.81800000	7.89400000	-1.53900000
H	-4.90200000	8.01100000	-1.65800000
H	-3.53800000	8.40100000	-0.60700000
H	-3.33300000	8.42400000	-2.36500000
C	-0.78000000	5.64200000	1.82100000
H	-1.38800000	5.46500000	0.92700000
H	-1.13900000	6.56700000	2.28400000
H	0.26700000	5.76500000	1.54500000
C	4.90300000	-1.57000000	3.06100000
H	4.47400000	-2.38200000	3.66500000
H	4.73200000	-1.82500000	2.02200000
H	5.97500000	-1.49800000	3.27000000
C	9.31400000	-1.86400000	2.37600000
H	9.95100000	-2.35000000	1.62900000
H	9.95200000	-1.35900000	3.10100000
H	8.72100000	-2.61700000	2.90400000
C	3.36000000	0.72800000	-4.58500000
H	4.21400000	1.18900000	-5.08400000
H	3.07300000	-0.19100000	-5.10100000
H	2.51000000	1.40700000	-4.54100000
O	2.85800000	3.45000000	3.04700000
H	1.91100000	3.68400000	3.14100000
H	2.95500000	3.25700000	2.07700000
O	2.83000000	3.08800000	0.38000000
H	2.54900000	3.99000000	0.17100000
H	1.84800000	2.17300000	0.22200000
N	1.13600000	1.22400000	0.14300000
C	1.04000000	0.77300000	1.47900000
C	-0.30900000	0.29200000	2.01300000
C	-0.42100000	-1.19700000	1.61400000
H	-1.41700000	-1.56400000	1.86400000
H	-0.26000000	-1.33900000	0.54300000
H	0.34000000	-1.77400000	2.14300000
C	-0.32500000	0.43100000	3.54500000
H	-0.23500000	1.48100000	3.83800000
H	-1.26800000	0.03100000	3.93300000
H	0.50100000	-0.12200000	4.00100000
C	-1.47700000	1.08200000	1.40100000
H	-2.40600000	0.81000000	1.90800000
H	-1.34100000	2.15900000	1.51600000
H	-1.61800000	0.84200000	0.34600000
H	0.21500000	1.45700000	-0.22000000

Table S17. Cartesian coordinates for EP FeNH

C	-2.83400000	-4.40300000	-1.82000000
O	-1.61100000	-4.19900000	-1.93900000
N	-3.74100000	-3.87100000	-2.66500000
S	3.71000000	-2.30200000	2.45700000

N	4.29300000	0.71300000	3.74300000
C	3.30600000	1.58800000	3.12600000
C	3.54200000	1.98900000	1.65600000
S	3.49200000	0.58300000	0.48100000
C	1.87300000	1.06900000	3.37700000
O	1.23300000	1.58200000	4.29900000
O	2.73200000	1.15400000	-0.71900000
O	4.96900000	0.30000000	0.11300000
N	1.34000000	0.09900000	2.56100000
C	-0.05800000	-0.23900000	2.88700000
C	-0.43700000	-1.52600000	2.19000000
O	-1.57900000	-2.01300000	2.25800000
C	-1.06200000	0.86500000	2.49800000
O	-0.91100000	1.25900000	1.12500000
N	0.57000000	-2.08900000	1.48900000
C	0.24300000	-3.34200000	0.80100000
C	1.53700000	-3.95400000	0.27000000
S	2.68400000	-2.66300000	-0.33500000
C	-0.41100000	-4.34400000	1.77300000
O	0.16200000	-4.73000000	2.77100000
O	0.63800000	-0.52800000	-3.76800000
C	-5.91800000	-4.75000000	2.43300000
C	-4.75500000	-4.30000000	3.01900000
C	-6.10600000	-3.94100000	1.25500000
N	-4.21500000	-3.25500000	2.28700000
C	-5.02800000	-3.00600000	1.20600000
C	-7.06800000	-3.92400000	0.22900000
C	-4.91100000	-2.05500000	0.18700000
C	-6.94800000	-2.98800000	-0.79800000
C	-5.88500000	-2.05500000	-0.81000000
C	-6.36300000	2.04000000	-1.70500000
C	-5.54200000	2.97100000	-2.36000000
C	-5.84900000	1.41800000	-0.55900000
C	-4.25900000	3.25700000	-1.90400000
C	-4.56100000	1.69400000	-0.08800000
C	-3.75300000	2.60900000	-0.77200000
O	-2.46300000	2.88700000	-0.40700000
N	3.75000000	-0.60000000	-3.24000000
C	3.77200000	0.73100000	-3.31000000
N	4.83900000	1.41800000	-2.81400000
N	2.78500000	1.38000000	-3.93700000
C	-1.13800000	6.38800000	3.98100000
C	-0.04000000	5.56500000	4.27800000
C	-1.75100000	6.22700000	2.72900000
C	0.46500000	4.65200000	3.35000000
C	-1.27000000	5.30800000	1.79000000
C	-0.13900000	4.55000000	2.09800000
O	0.41400000	3.65900000	1.17000000
C	-1.32400000	5.72600000	-2.33300000
C	-1.07200000	4.63500000	-3.17700000
C	-0.31100000	6.08800000	-1.42900000
C	0.11600000	3.90300000	-3.09700000
C	0.89100000	5.37500000	-1.34900000
C	1.09700000	4.26200000	-2.17300000
O	2.30100000	3.55600000	-2.12700000
N	7.97300000	-3.09400000	-1.12300000
C	7.36200000	-2.00900000	-0.61400000
N	7.65700000	-0.78400000	-1.07800000
N	6.45300000	-2.10900000	0.36000000
Fe	2.16700000	-1.13400000	1.36800000

H	-4.72200000	-3.86400000	-2.41600000
H	-3.43000000	-3.19600000	-3.34900000
H	-2.07100000	0.46100000	2.61800000
H	-0.93000000	1.72800000	3.15300000
H	-0.25900000	1.99000000	1.12000000
H	-0.17100000	-0.39900000	3.96800000
H	-4.26900000	-4.64200000	3.92200000
H	-3.34200000	-2.77300000	2.48200000
H	-7.89800000	-4.62600000	0.24100000
H	-7.69600000	-2.95300000	-1.58600000
H	-4.09400000	-1.34200000	0.17700000
H	-5.83500000	-1.31300000	-1.60100000
H	-6.45600000	0.69300000	-0.02400000
H	-5.91100000	3.47600000	-3.25100000
H	-4.18400000	1.18900000	0.79700000
H	-3.62300000	3.95400000	-2.43200000
H	-2.14300000	2.26800000	0.28500000
H	2.82100000	-1.01700000	-3.26500000
H	4.74800000	2.42600000	-2.87600000
H	5.11500000	1.11300000	-1.88100000
H	2.57900000	2.31800000	-3.58900000
H	1.97500000	0.81000000	-4.19400000
H	-2.62600000	6.82100000	2.48000000
H	0.43500000	5.63700000	5.25300000
H	-1.77100000	5.16700000	0.83800000
H	1.29700000	4.00500000	3.60400000
H	0.19200000	3.97700000	0.27700000
H	-0.46000000	6.93800000	-0.76900000
H	-1.82100000	4.33400000	-3.90400000
H	1.67400000	5.68200000	-0.66200000
H	0.27400000	3.04900000	-3.74700000
H	2.31100000	2.87500000	-1.42100000
H	7.75000000	-3.98200000	-0.69600000
H	6.09100000	-3.00100000	0.66600000
H	5.87100000	-1.28600000	0.57400000
H	8.37500000	-0.62700000	-1.76700000
H	7.12900000	0.01000000	-0.73400000
H	5.20100000	1.16100000	3.81300000
H	4.38900000	-0.18000000	3.26400000
H	3.32400000	2.52800000	3.68500000
H	2.75600000	2.67000000	1.31300000
H	4.52800000	2.44300000	1.52200000
H	-0.45300000	-3.14500000	-0.02100000
H	1.36100000	-4.66500000	-0.54200000
H	2.09100000	-4.44300000	1.07600000
H	-1.40900000	-4.72200000	1.49700000
C	-7.75500000	1.74900000	-2.21500000
H	-8.11800000	0.78000000	-1.85600000
H	-8.47000000	2.51000000	-1.87900000
H	-7.78500000	1.73600000	-3.31000000
C	-2.65000000	6.46100000	-2.36400000
H	-3.29700000	6.12500000	-1.54500000
H	-2.50800000	7.54100000	-2.25100000
H	-3.18400000	6.28600000	-3.30300000
C	-1.62200000	7.43100000	4.96700000
H	-1.06400000	8.36900000	4.84800000
H	-2.68300000	7.65900000	4.82100000
H	-1.48600000	7.09700000	6.00000000
C	-6.83500000	-5.82800000	2.93200000
H	-7.83100000	-5.42800000	3.16100000

H	-6.96900000	-6.62200000	2.18700000
H	-6.44300000	-6.28900000	3.84400000
C	-3.37000000	-5.26900000	-0.70900000
H	-4.43700000	-5.48000000	-0.80000000
H	-2.80500000	-6.20400000	-0.69000000
H	-3.21400000	-4.75400000	0.24200000
C	4.82200000	-1.40400000	-2.66500000
H	4.87000000	-1.29000000	-1.58300000
H	4.62400000	-2.44800000	-2.90900000
H	5.77600000	-1.10600000	-3.10600000
C	8.93900000	-3.10000000	-2.23500000
H	9.86000000	-2.57300000	-1.96400000
H	9.19000000	-4.13700000	-2.45400000
H	8.50000000	-2.65400000	-3.13300000
C	2.84600000	-2.69800000	4.02900000
H	3.53300000	-3.27300000	4.65400000
H	2.58000000	-1.76800000	4.53400000
H	1.95400000	-3.29000000	3.81300000
O	0.58600000	-3.46600000	-3.31900000
H	-0.29400000	-3.73200000	-2.95600000
H	0.43300000	-2.69900000	-3.89700000
O	1.88400000	-2.06400000	-1.65900000
H	1.40700000	-2.76000000	-2.24100000
H	1.13900000	0.39000000	-1.47600000
N	0.15700000	0.35700000	-1.74100000
C	-0.21200000	-0.15500000	-2.92000000
C	-1.71800000	-0.20200000	-3.23200000
C	-2.14200000	1.23100000	-3.63000000
H	-3.21500000	1.25400000	-3.83900000
H	-1.94400000	1.94000000	-2.82500000
H	-1.60800000	1.55800000	-4.53000000
C	-1.97800000	-1.15000000	-4.41300000
H	-1.71500000	-2.18400000	-4.16600000
H	-3.04100000	-1.11800000	-4.67800000
H	-1.39700000	-0.86200000	-5.29300000
C	-2.52300000	-0.66200000	-2.00000000
H	-3.58200000	-0.73400000	-2.25900000
H	-2.18500000	-1.64000000	-1.64600000
H	-2.46100000	0.04700000	-1.17100000
H	-0.51100000	0.60800000	-1.02300000

Table S18. Cartesian coordinates for E+P FeNH

C	3.95000000	-4.31600000	1.23600000
O	2.72400000	-4.14300000	1.28500000
N	4.74500000	-4.11200000	2.31900000
S	-5.57500000	-2.04700000	-1.23000000
N	-5.96700000	1.36000000	-0.56100000
C	-4.85900000	2.32300000	-0.62600000
C	-4.01400000	2.23400000	0.65500000
S	-3.84000000	0.48700000	1.20400000
C	-4.00000000	2.09500000	-1.88600000
O	-3.86900000	3.04600000	-2.67000000
O	-2.46200000	0.47100000	1.94800000
O	-4.98500000	0.31400000	2.21400000
N	-3.38000000	0.89200000	-2.05000000
C	-2.45800000	0.85000000	-3.20000000
C	-2.11300000	-0.58400000	-3.59500000
O	-1.39800000	-0.80700000	-4.58100000
C	-1.16000000	1.66100000	-2.97200000

O	-0.58000000	1.42400000	-1.66200000
N	-2.62400000	-1.55300000	-2.79700000
C	-2.18500000	-2.90200000	-3.14200000
C	-2.83300000	-3.93900000	-2.22000000
S	-2.76700000	-3.45000000	-0.46200000
C	-2.56900000	-3.24200000	-4.59800000
O	-3.72700000	-3.27000000	-4.96000000
O	0.69100000	-0.10300000	1.62500000
C	7.50800000	-3.40500000	-2.74400000
C	6.87100000	-2.18700000	-2.72400000
C	7.83300000	-3.70800000	-1.37000000
N	6.77800000	-1.71300000	-1.42000000
C	7.37500000	-2.62000000	-0.57100000
C	8.45900000	-4.79800000	-0.73900000
C	7.55300000	-2.58400000	0.81600000
C	8.62200000	-4.77800000	0.64400000
C	8.18100000	-3.67700000	1.41400000
C	6.99500000	2.60600000	1.01800000
C	5.77600000	3.29300000	1.13000000
C	7.23500000	1.90000000	-0.16900000
C	4.81900000	3.26100000	0.11600000
C	6.28800000	1.85900000	-1.20000000
C	5.06900000	2.52800000	-1.04800000
O	4.05200000	2.46700000	-1.97200000
N	-2.41800000	-2.22600000	2.76500000
C	-1.39300000	-3.07200000	2.64100000
N	-1.61800000	-4.41200000	2.70200000
N	-0.13900000	-2.62800000	2.53200000
C	0.05700000	6.96400000	-2.77500000
C	-1.15600000	6.27100000	-2.92100000
C	0.90400000	6.57900000	-1.72700000
C	-1.51400000	5.22900000	-2.06600000
C	0.56900000	5.52800000	-0.86400000
C	-0.63900000	4.85500000	-1.04600000
O	-1.00400000	3.76700000	-0.25000000
C	1.15900000	5.44000000	3.08500000
C	1.24400000	4.13800000	2.58300000
C	-0.08400000	5.84400000	3.61000000
C	0.15000000	3.25400000	2.60800000
C	-1.18000000	4.98900000	3.64400000
C	-1.07200000	3.67600000	3.15400000
O	-2.17500000	2.88900000	3.23600000
N	-7.35200000	-3.71000000	1.85600000
C	-7.12200000	-2.48300000	2.35900000
N	-7.07600000	-2.31200000	3.70000000
N	-6.93000000	-1.43700000	1.56500000
Fe	-3.52400000	-0.89300000	-1.16000000
H	5.75200000	-4.15800000	2.24600000
H	4.33000000	-3.77300000	3.17500000
H	-0.42800000	1.36000000	-3.72400000
H	-1.37200000	2.72400000	-3.07100000
H	-0.78600000	2.20700000	-1.10500000
H	-2.93700000	1.30400000	-4.07700000
H	6.47200000	-1.61200000	-3.54800000
H	6.40200000	-0.81900000	-1.14200000
H	8.81300000	-5.64200000	-1.32300000
H	9.11000000	-5.61100000	1.14100000
H	7.22000000	-1.73300000	1.40300000
H	8.35900000	-3.67100000	2.48600000
H	8.17700000	1.37400000	-0.30000000

H	5.56700000	3.86100000	2.03300000
H	6.50700000	1.32500000	-2.12300000
H	3.87700000	3.79300000	0.20900000
H	4.36600000	2.09800000	-2.80900000
H	-2.25200000	-1.22000000	2.61500000
H	-0.85100000	-5.01000000	2.42700000
H	-2.52000000	-4.74200000	2.38900000
H	0.57700000	-3.25400000	2.17200000
H	0.06900000	-1.63200000	2.38600000
H	1.84700000	7.09900000	-1.58000000
H	-1.84000000	6.55200000	-3.71800000
H	1.23800000	5.24000000	-0.05800000
H	-2.45600000	4.70400000	-2.18900000
H	-0.53800000	3.79800000	0.60700000
H	-0.19200000	6.85300000	4.00200000
H	2.18300000	3.78900000	2.16300000
H	-2.13100000	5.31300000	4.05400000
H	0.25400000	2.23100000	2.25400000
H	-2.06200000	1.99800000	2.83500000
H	-7.24800000	-3.80300000	0.85200000
H	-6.79200000	-1.60400000	0.55700000
H	-6.31700000	-0.66000000	1.89400000
H	-7.32600000	-3.04900000	4.33900000
H	-7.04100000	-1.37200000	4.06800000
H	-6.55800000	1.43800000	-1.38500000
H	-6.55000000	1.53900000	0.25300000
H	-5.19200000	3.36500000	-0.72000000
H	-3.01600000	2.64800000	0.50500000
H	-4.48700000	2.73300000	1.50600000
H	-1.09100000	-2.96000000	-3.05900000
H	-2.35300000	-4.91600000	-2.32100000
H	-3.90100000	-4.03200000	-2.43600000
H	-1.73900000	-3.48700000	-5.28500000
C	8.01300000	2.65800000	2.13700000
H	8.83000000	1.95100000	1.97000000
H	8.45200000	3.65900000	2.22300000
H	7.55200000	2.42200000	3.10300000
C	2.34500000	6.38500000	3.09900000
H	2.10600000	7.33300000	2.60400000
H	2.65100000	6.62000000	4.12500000
H	3.20900000	5.94800000	2.58600000
C	0.41900000	8.08600000	-3.72500000
H	-0.32900000	8.88700000	-3.69600000
H	1.39000000	8.52500000	-3.47600000
H	0.46900000	7.72600000	-4.76000000
C	7.83200000	-4.24900000	-3.94700000
H	8.91400000	-4.39500000	-4.04700000
H	7.37400000	-5.24300000	-3.87400000
H	7.47000000	-3.78000000	-4.86700000
C	4.67300000	-4.75100000	-0.02800000
H	5.68400000	-5.11800000	0.15900000
H	4.07800000	-5.52100000	-0.52400000
H	4.74400000	-3.89400000	-0.70500000
C	-3.81000000	-2.61000000	3.02200000
H	-3.87600000	-3.26900000	3.89400000
H	-4.36100000	-1.69200000	3.21600000
H	-4.25700000	-3.10300000	2.14900000
C	-7.62900000	-4.91000000	2.64900000
H	-8.53500000	-4.78400000	3.25200000
H	-7.79800000	-5.73900000	1.96200000

H	-6.78400000	-5.16700000	3.29700000
C	-6.10600000	-1.54500000	-2.92400000
H	-6.07100000	-0.45800000	-3.01000000
H	-5.43400000	-1.99400000	-3.65800000
H	-7.12700000	-1.89600000	-3.08900000
O	-1.11100000	-3.33000000	-0.22400000
H	-0.91600000	-2.36500000	-0.31800000
O	-1.46300000	-0.65700000	-0.30900000
H	-1.06100000	0.06300000	-0.87800000
H	-1.44100000	-0.27300000	0.59900000
N	2.01100000	0.86500000	0.07900000
C	1.83600000	0.21500000	1.24800000
C	3.07900000	-0.04600000	2.12600000
C	3.35700000	1.24900000	2.92400000
H	4.21600000	1.09200000	3.58600000
H	3.59700000	2.08000000	2.26000000
H	2.49600000	1.52700000	3.53800000
C	2.77900000	-1.18300000	3.11700000
H	2.60500000	-2.12700000	2.59500000
H	3.64100000	-1.31200000	3.78100000
H	1.91100000	-0.95100000	3.73700000
C	4.31300000	-0.42200000	1.27900000
H	5.13700000	-0.69200000	1.94700000
H	4.10600000	-1.28400000	0.63600000
H	4.66900000	0.40800000	0.66200000
H	1.21500000	1.04800000	-0.52500000
H	2.91500000	1.15900000	-0.25700000