

Supporting Information for Mechanism of Fe(II)-PNP Complexes Catalyzed in the N-formylation of Amines with CO₂ and H₂: The Superior Performance of N-H Ligand Methylated Complexes

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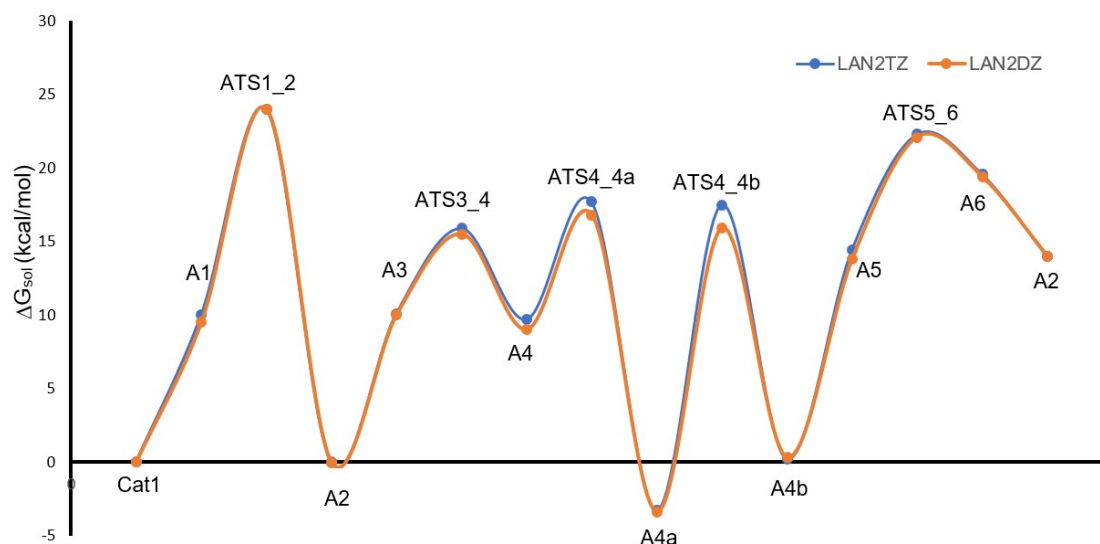


Figure S1 Potential energy surfaces of **Cat1** for CO_2 hydrogenation. The Gibbs free energies based on LAN2TZ and LAN2DZ basis sets are presented in blue and red, respectively.

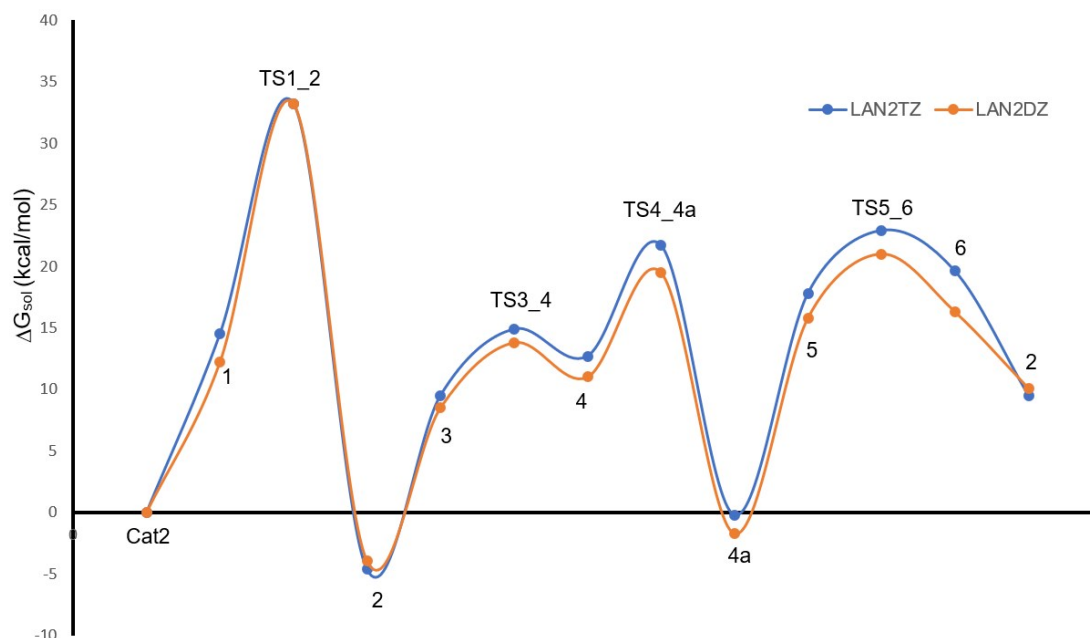


Figure S2 Potential energy surfaces of **Cat2** for CO_2 hydrogenation. The Gibbs free energies based on LAN2TZ and LAN2DZ basis sets are presented in blue and red, respectively.

According to Figure S1 and Figure S2, the energy differences between the two

basis sets of optimized structures are very small, and the trends of the two sets of Gibbs energy profiles are the same. Therefore, changes of basis sets not going to affect our final conclusions.

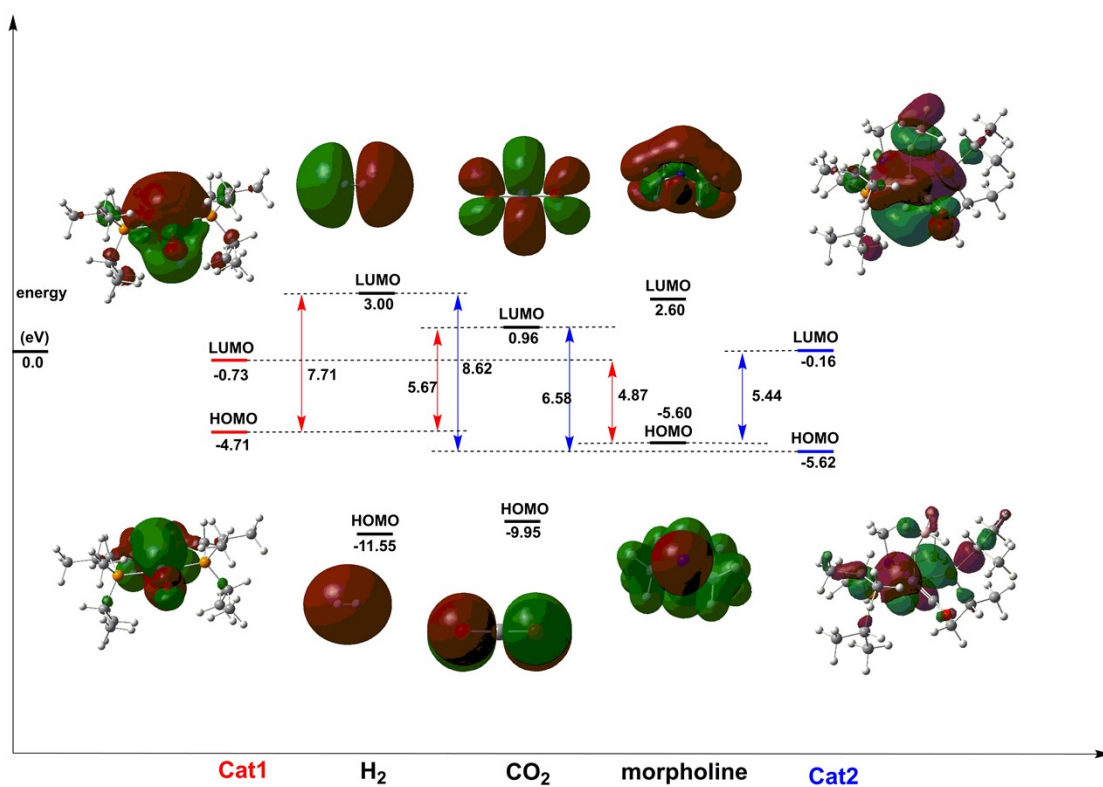


Figure S3 The HOMOs and LUMOs of **Cat1**, **Cat2**, H₂, CO₂ and morpholine.

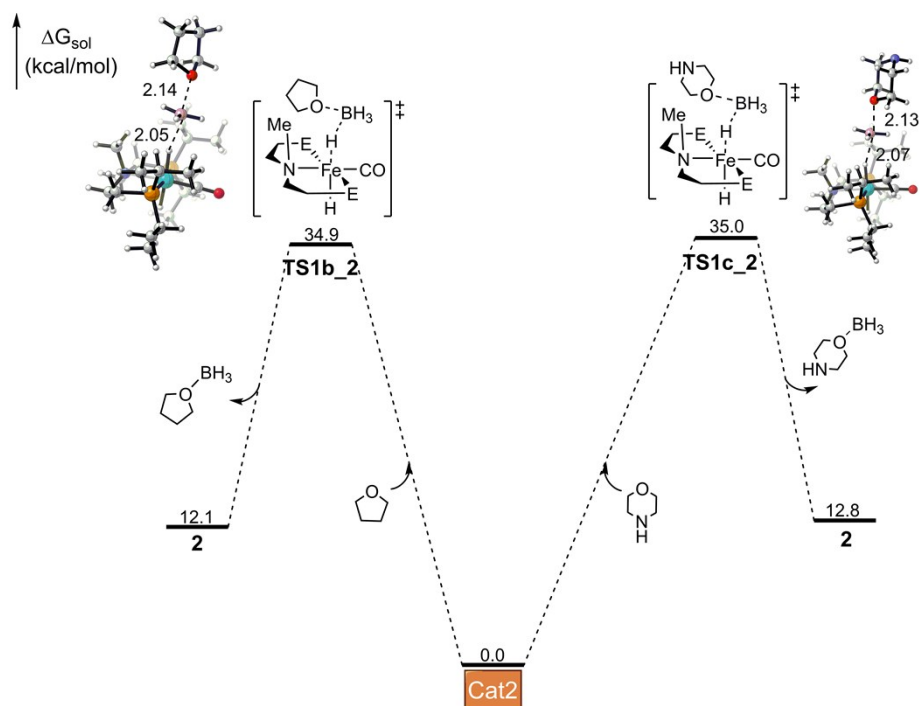


Figure S4 Thermodynamics of the reaction of **Cat2** with morpholine and THF, respectively.

Complexes	Relative Free Energies (kcal/mol)		
	Cat2+H ₂ +CO ₂	TS1_2	2
pyrrolidine	0.0	31.5	-5.5
N-methylpiperazine	0.0	31.3	-4.4
piperidine	0.0	30.9	-5.4

Figure S5 Reaction free energy of different nucleophilic amines with **Cat2**.

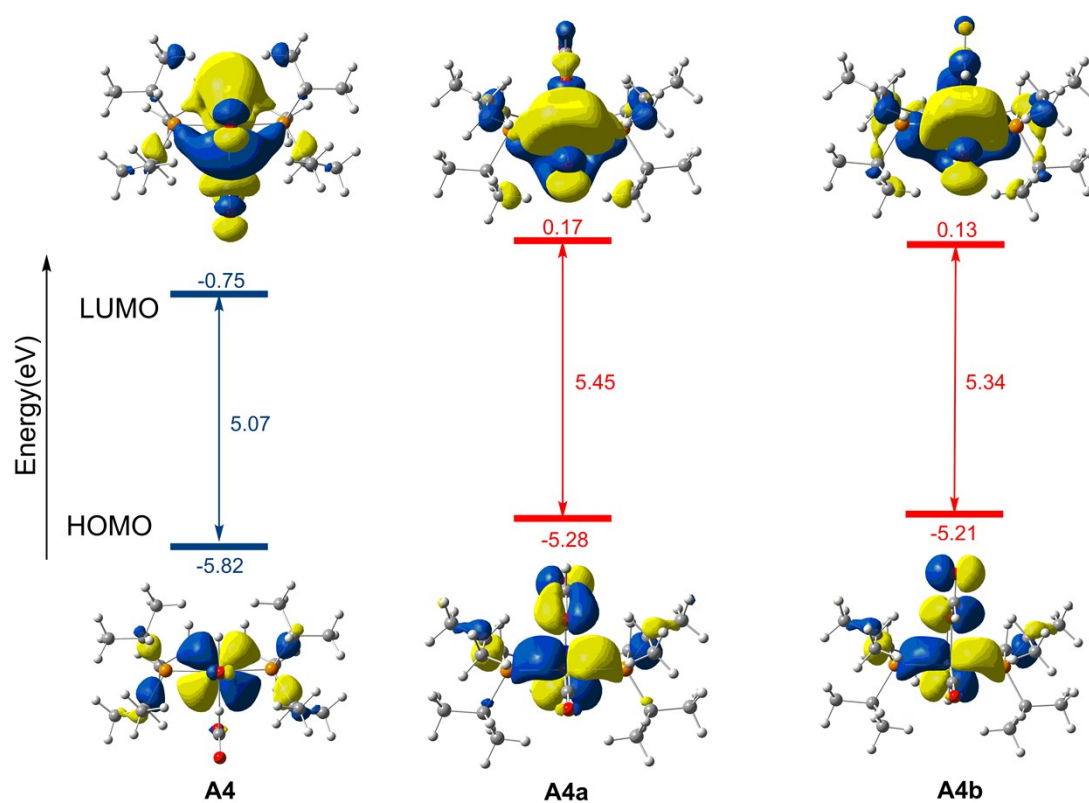


Figure S6 The HOMOs and LUMOs of **A4**, **4a** and **4b**.

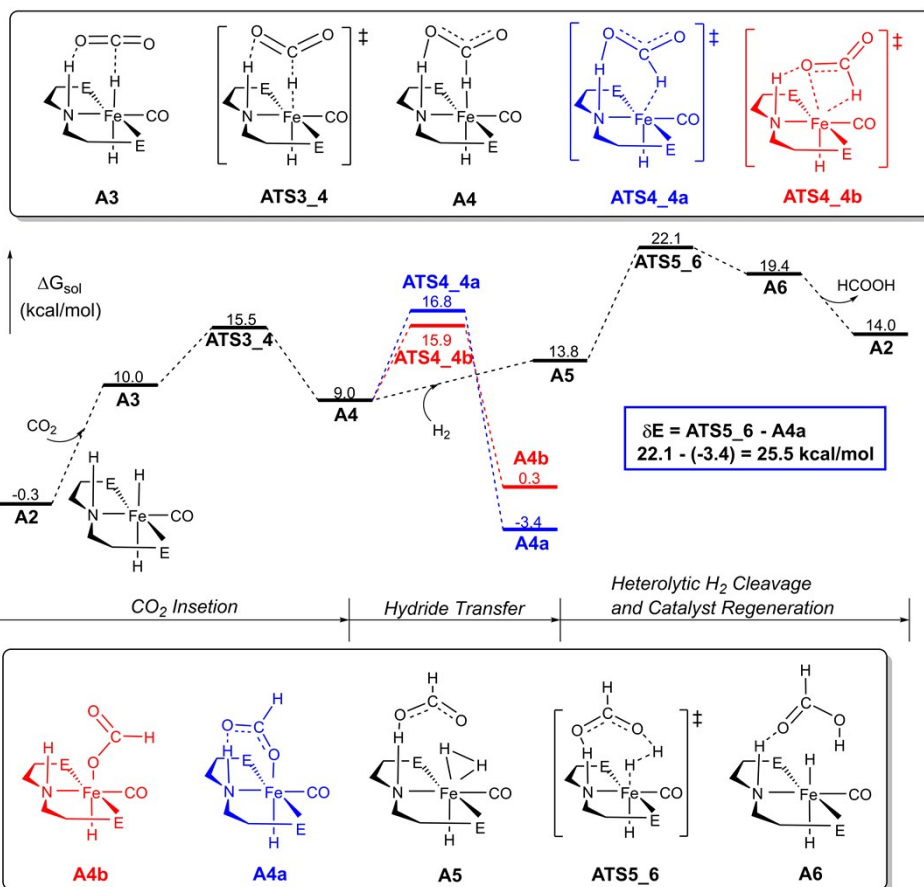


Figure S7 Reaction free energy profile for **Cat1** complex catalyzed CO_2 hydrogenation step via ligand assisted mechanism, along with optimized structures. δE denotes the energetic span of the cycle.

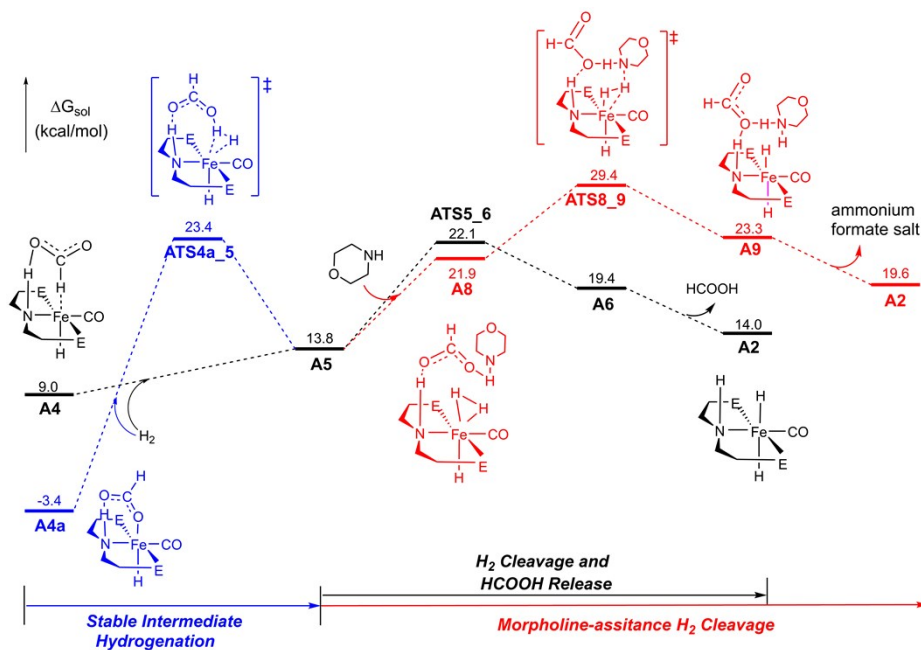


Figure S8 Reaction free energy profile for **Cat1** complex catalyzed for H_2 activation step, along with optimized structures.

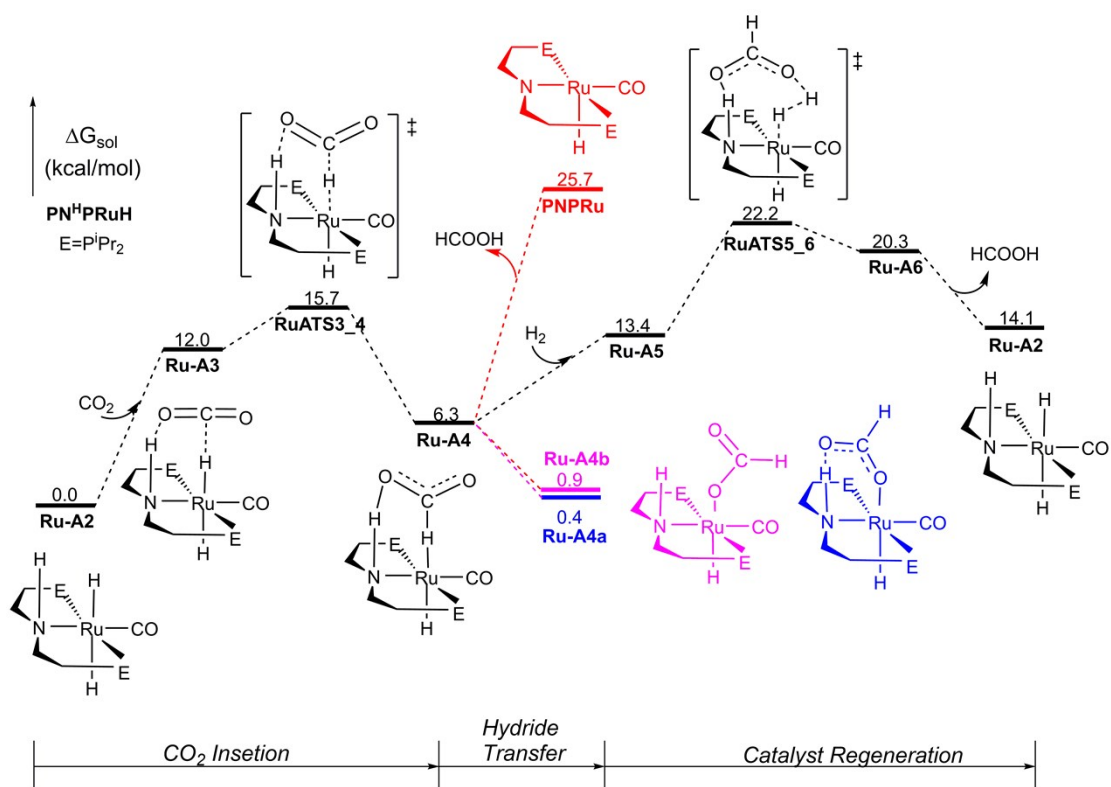


Figure S9 Reaction free energy profile for Ru-PNHp complex catalyzed CO₂ hydrogenation step, along with optimized structures.

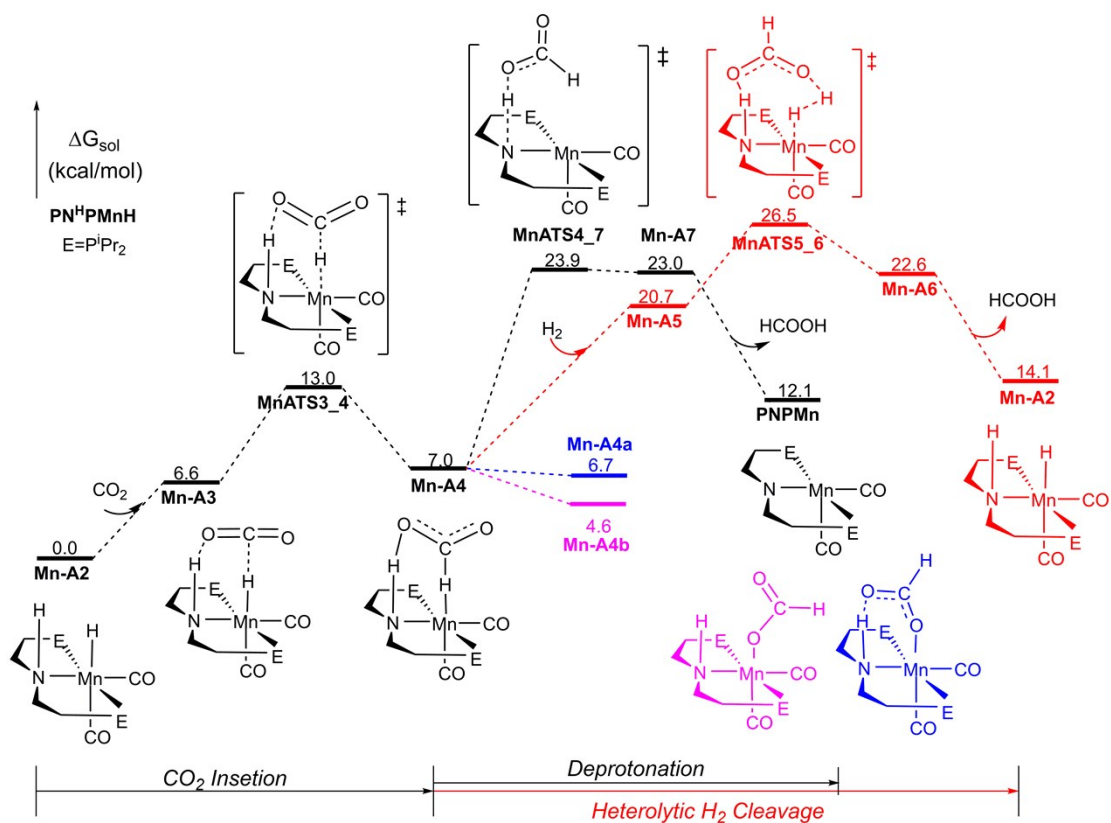


Figure S10 Reaction free energy profile for Mn-PNHp complex catalyzed CO₂ hydrogenation step, along with optimized structures.

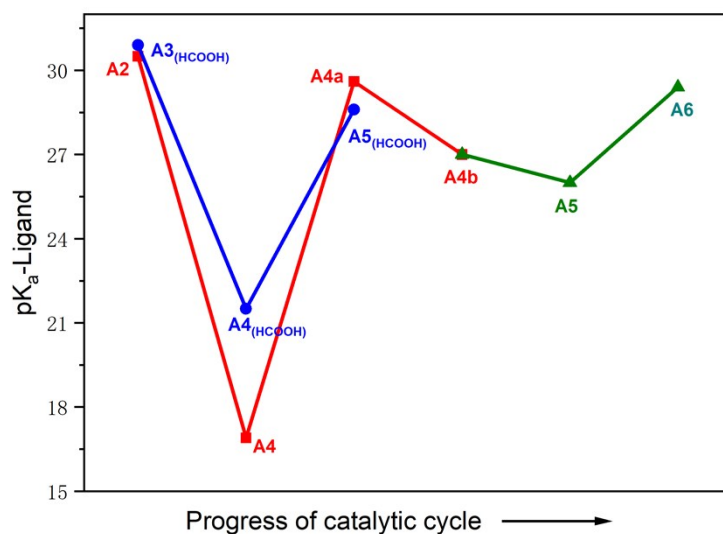
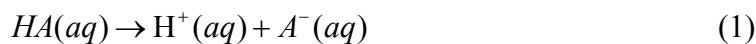


Figure S11 Calculated variation of the pKa-ligand value along the catalytic cycle for CO₂ hydrogenation and HCOOH hydrogenation for the **Cat1**. The free energy of solvation in water were calculated with M05-2X/6-31G* level.

The calculation method of pKa

Using the direct approach, given the proton dissociation reaction shown in **eq 1**, the pKa of molecule HA was calculated according to **eq 2**. The free energy difference in the 1 M standard state, ΔG_{aq} , was calculated directly from the aqueous Gibbs free energies of the acid and conjugate base with **eq 3**.



$$pKa = \frac{\Delta G_{aq}}{2.303RT} \quad (2)$$

$$\Delta G_{aq} = \Delta G_{gas} + \Delta \Delta G_{solv} \quad (3)$$

Among this, ΔG_{gas} was calculated in **eq 4**, ΔG_{solv} was calculated in **eq 5**,

$$\Delta G_{gas} = G_{gas}(H^+) + G_{gas}(A^-) - G_{gas}(HA) \quad (4)$$

$$\Delta \Delta G_{solv} = \Delta G_{solv}(H^+) + \Delta G_{solv}(A^-) - \Delta G_{solv}(HA) \quad (5)$$

ΔG_{solv} is the solvation free energy. The gas-phase free energy ($G_{gas}(H^+) = 6.28$ kcal/mol) and the experimentally measured hydration free energy ($\Delta G_{aq,solv}(H^+) = 265.9$ kcal/mol) were taken from the literature. Finally, ΔG_{aq} was calculated in **eq 6**.

$$\begin{aligned} \Delta G_{aq} &= -6.28 + G_{gas}(HA) - 264.01 + \Delta G_{solv}(A^-) - \Delta G_{solv}(HA) \\ &= G_{gas}(A^-) - G_{gas}(HA) + \Delta G_{solv}(A^-) - \Delta G_{solv}(HA) - 270.29 \end{aligned} \quad (6)$$

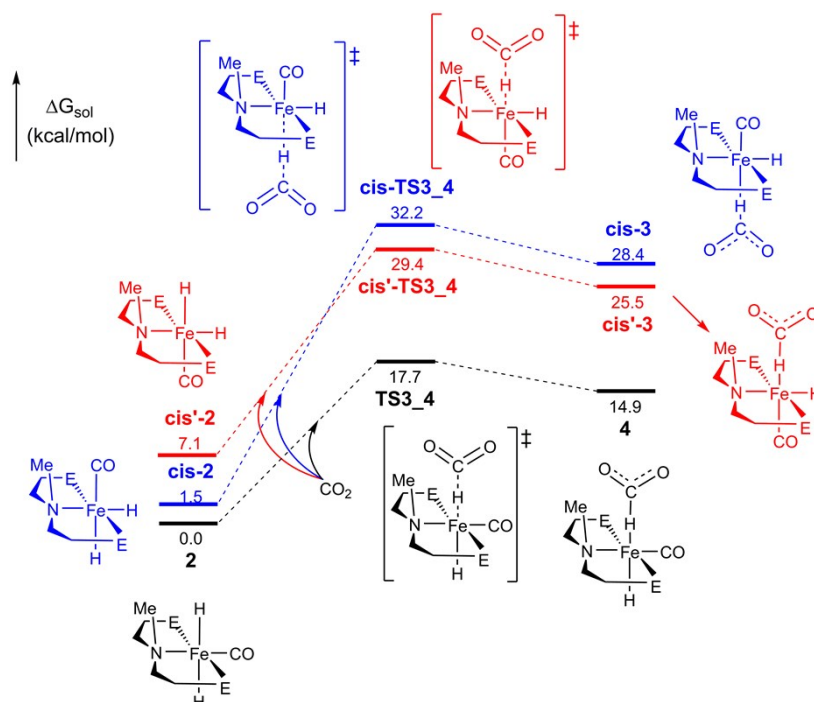


Figure S12 Comparison of barriers for CO₂ insertion promoted by **2** and other two cis isomers.

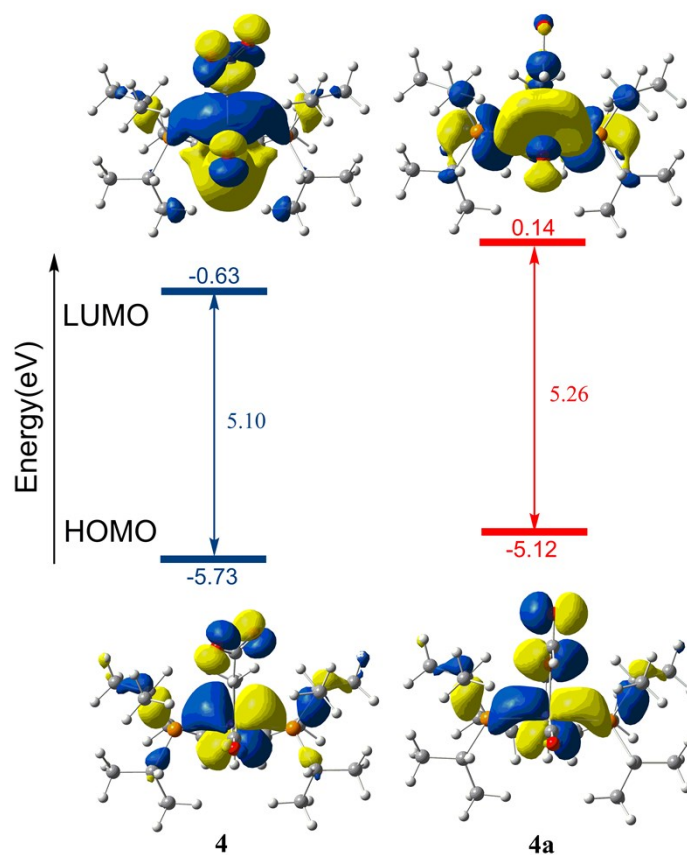


Figure S13 The HOMOs and LUMOs of **4** and **4a**.

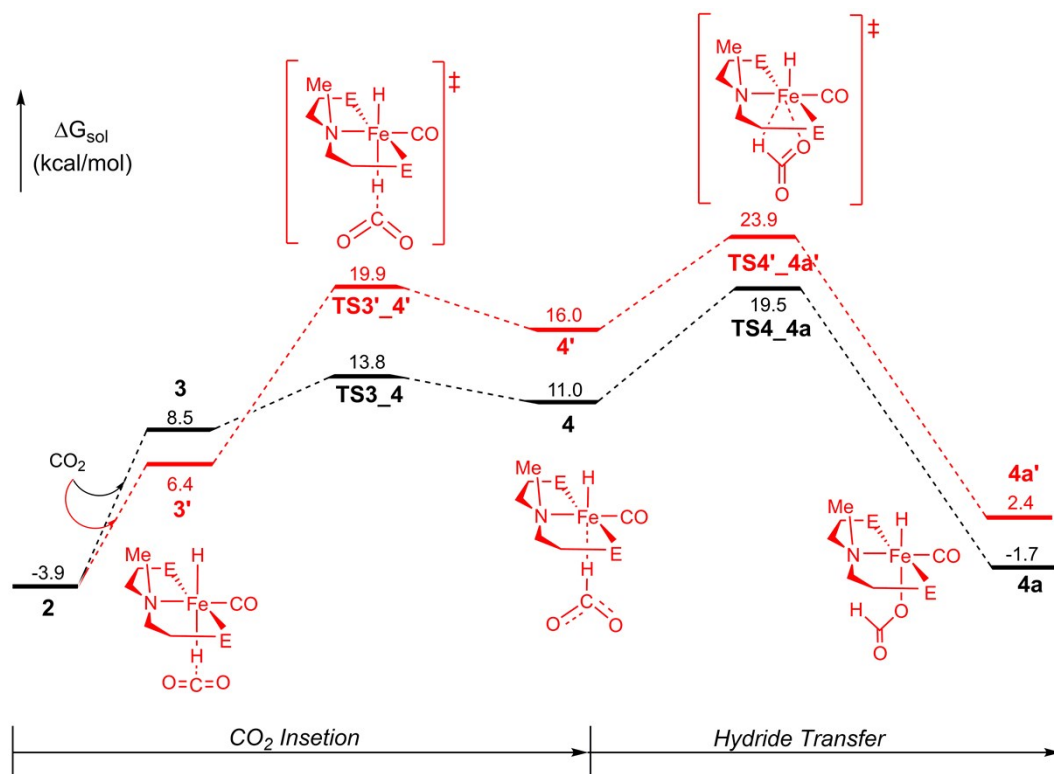


Figure S14 Free energy profile for CO₂ coordination with the H site beneath Fe, along with optimized structures.

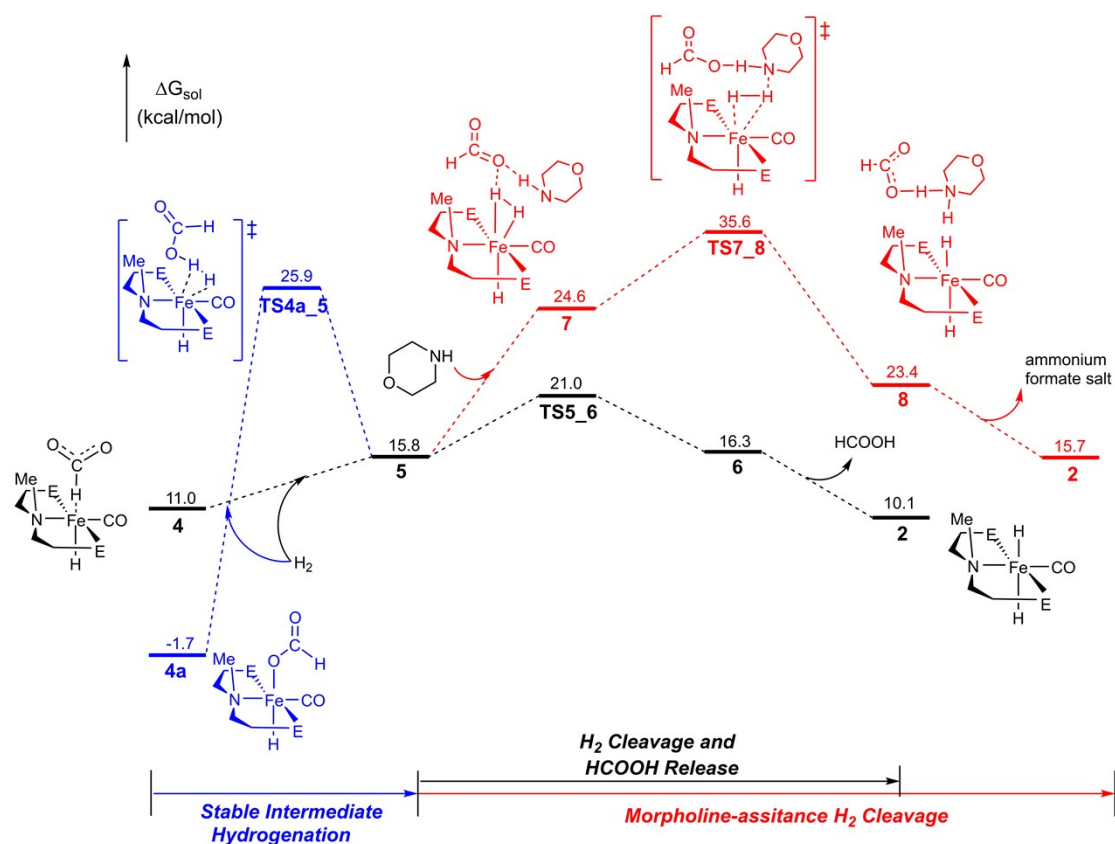


Figure S15 Reaction free energy profile for Cat2 complex catalysed for H₂ activation step, along with optimized structures.

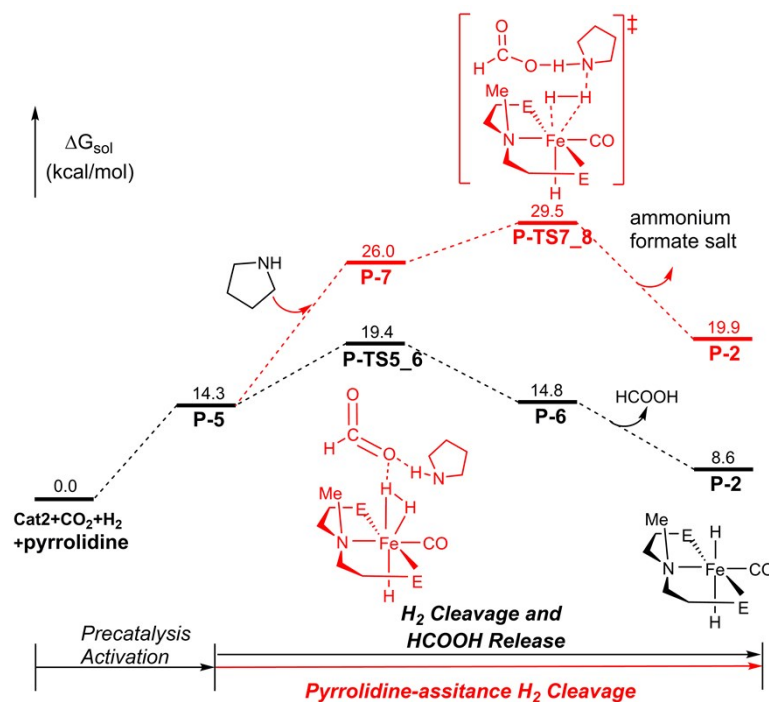


Figure S16 Free energy profile for heterolytic H₂ cleavage step by using pyrrolidine, along with optimized structures.

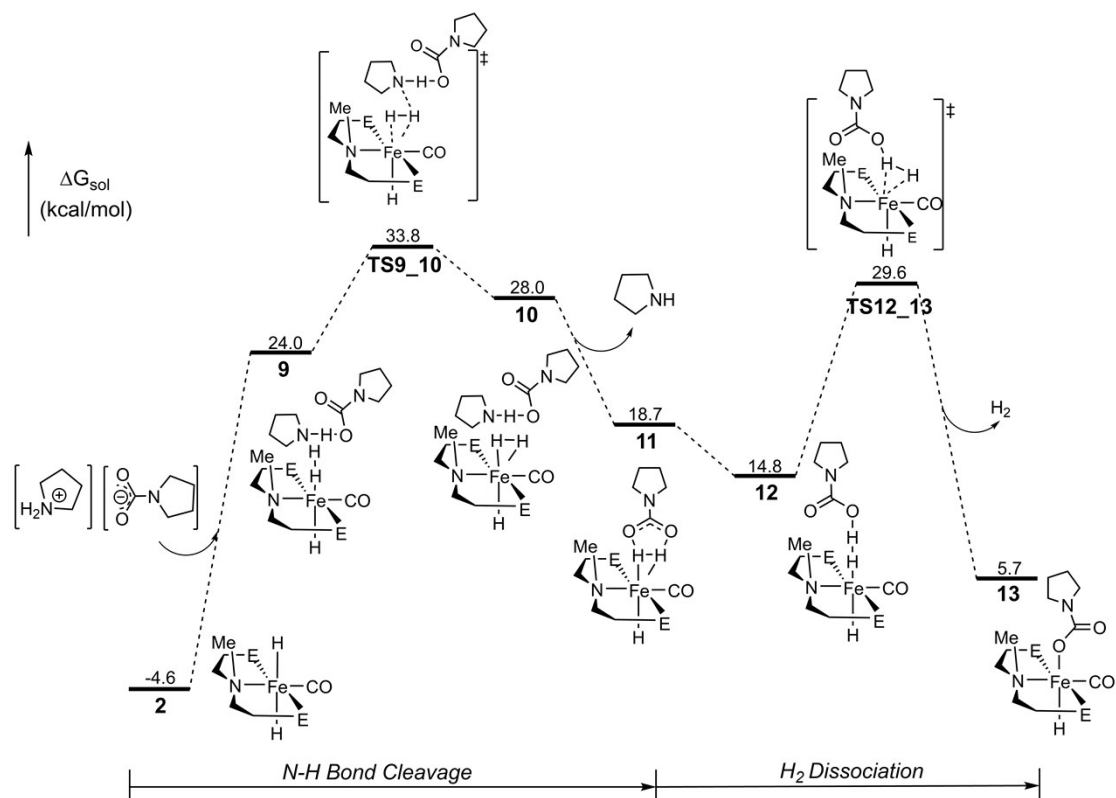


Figure S17 Free energy profile of carbamate complex formation step, along with optimized structures.

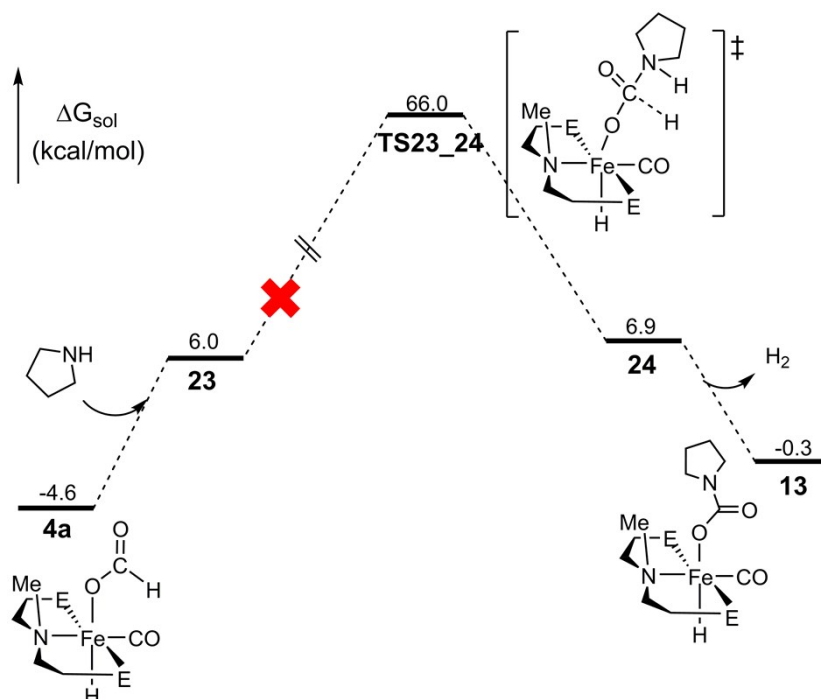


Figure S18 Free energy profile of amine thermal condensation to formamide step, along with optimized structures.

Figure S19 Two possible ways to form CO.

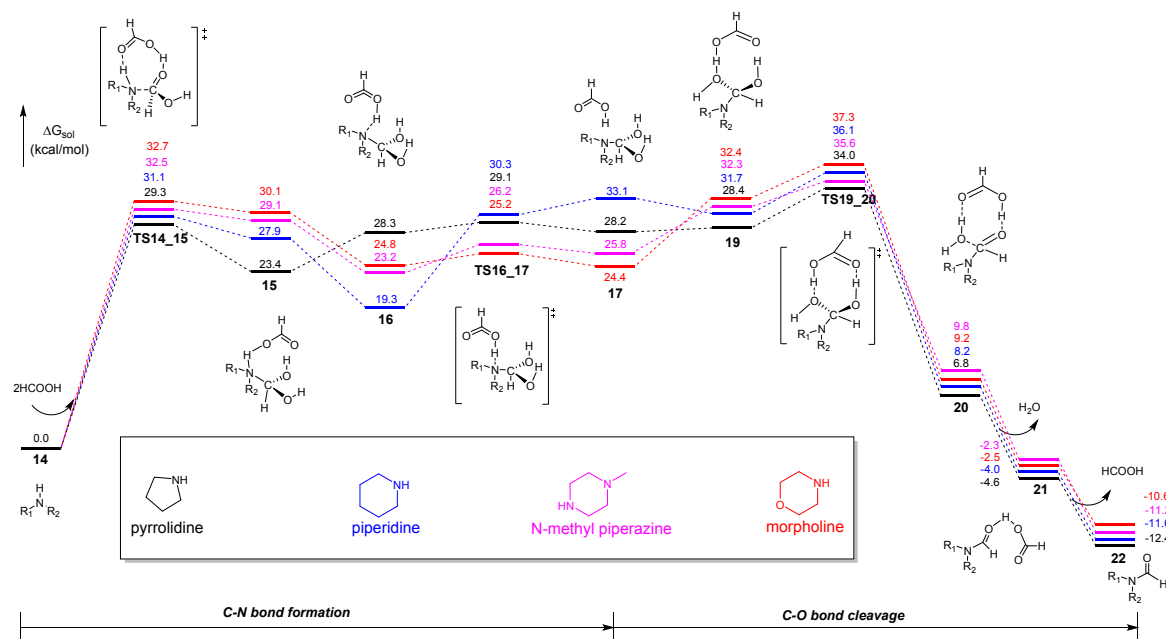
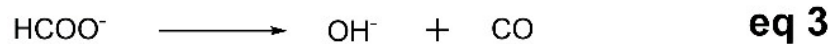
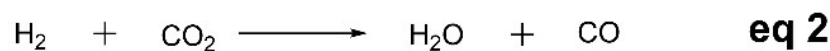


Figure S20 Free energy profile of amine thermal condensation to formamide step by different nucleophilic amines, along with optimized structures.

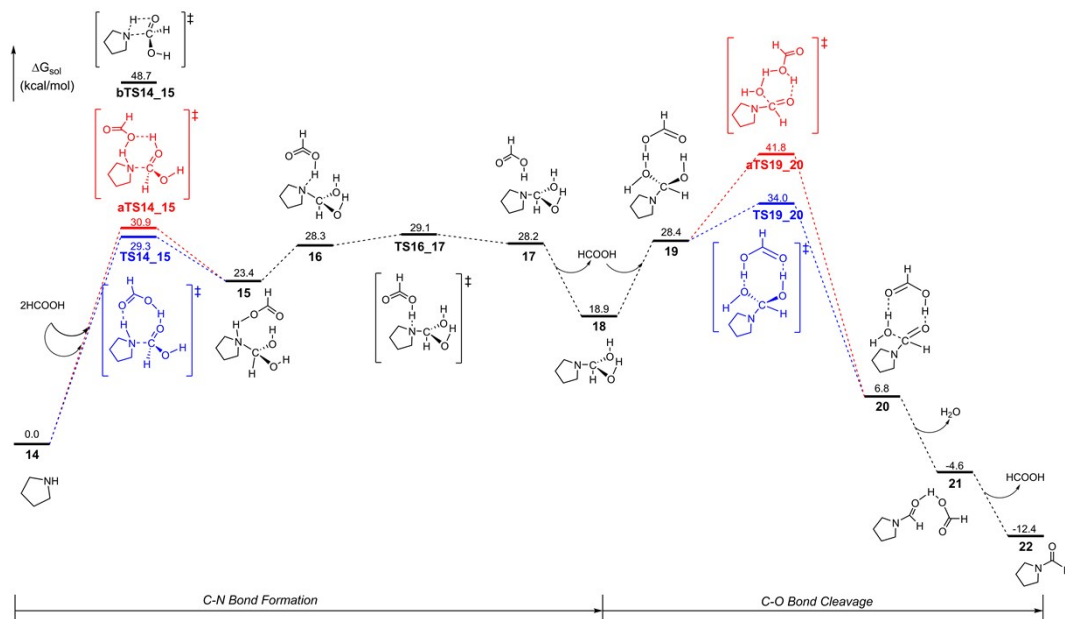


Figure 21 Free energy profile of pyrrolidine thermal condensation to formamide step, along with optimized structures.

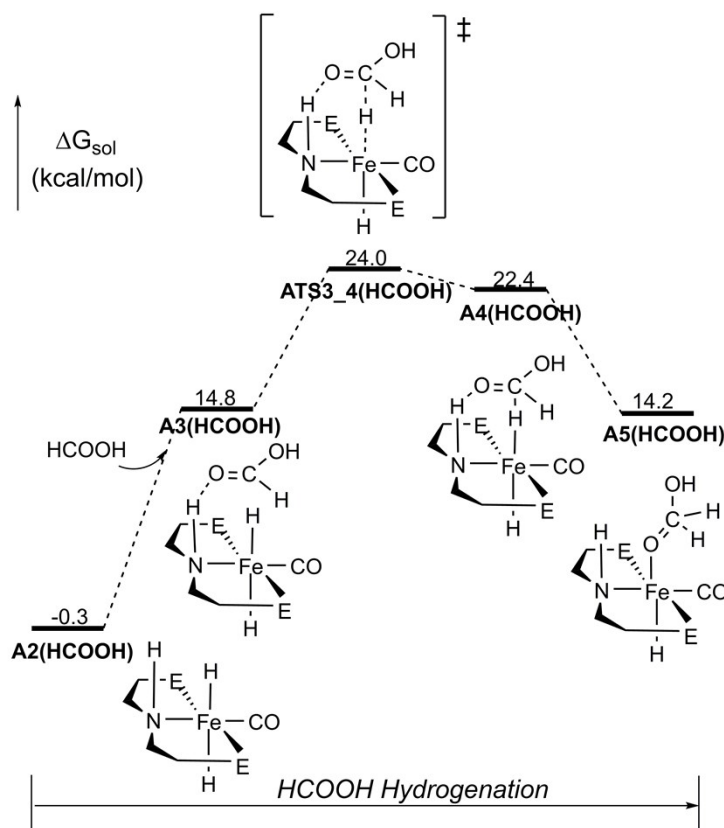


Figure 22 Reaction free energy profile for **Cat1** complex catalysed HCOOH hydrogenation step.

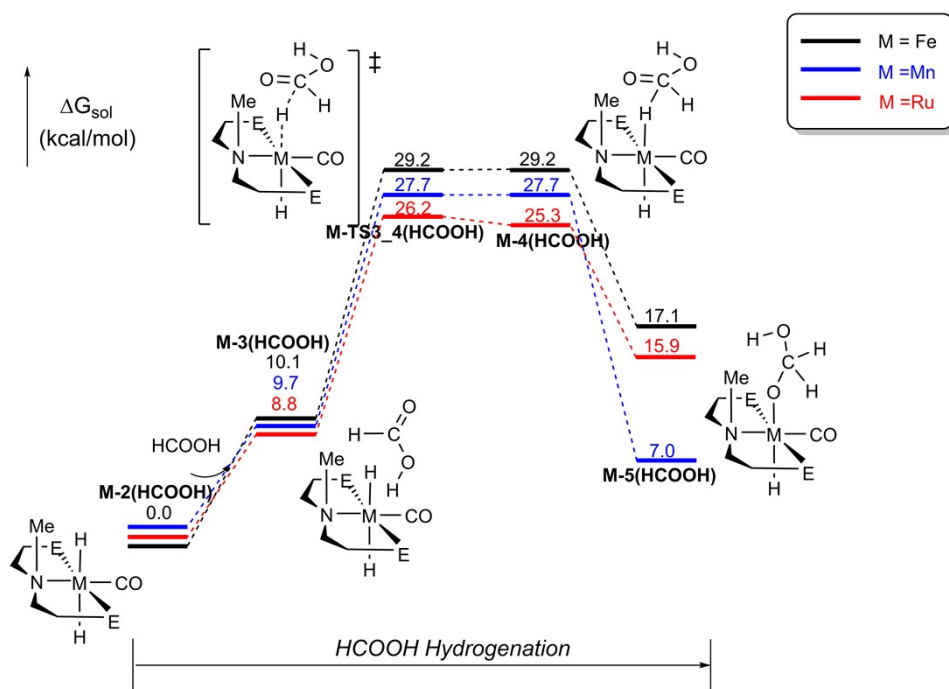


Figure 23 Reaction free energy profile for Cat2-like complex catalysed HCOOH hydrogenation step.

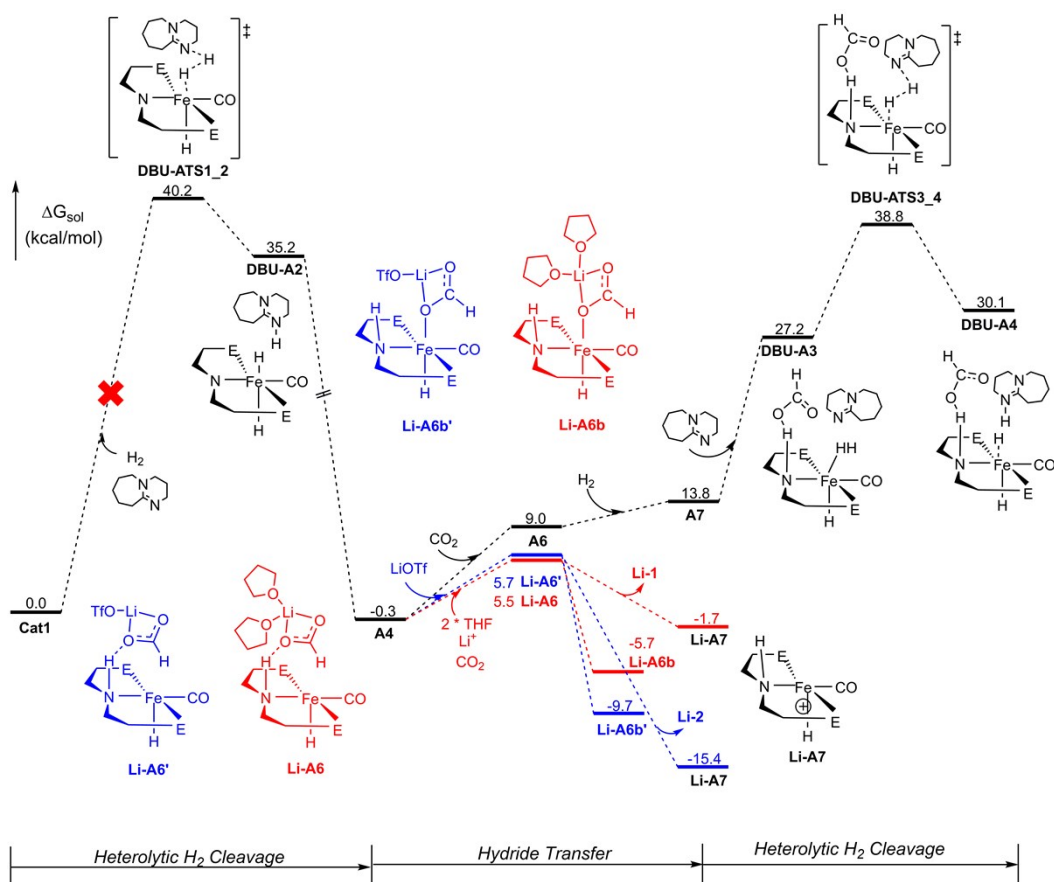


Figure 24 Reaction free energy profile for Cat1 catalysed CO₂ hydrogenation step via Lewis acid and DBU, along with optimized structures.

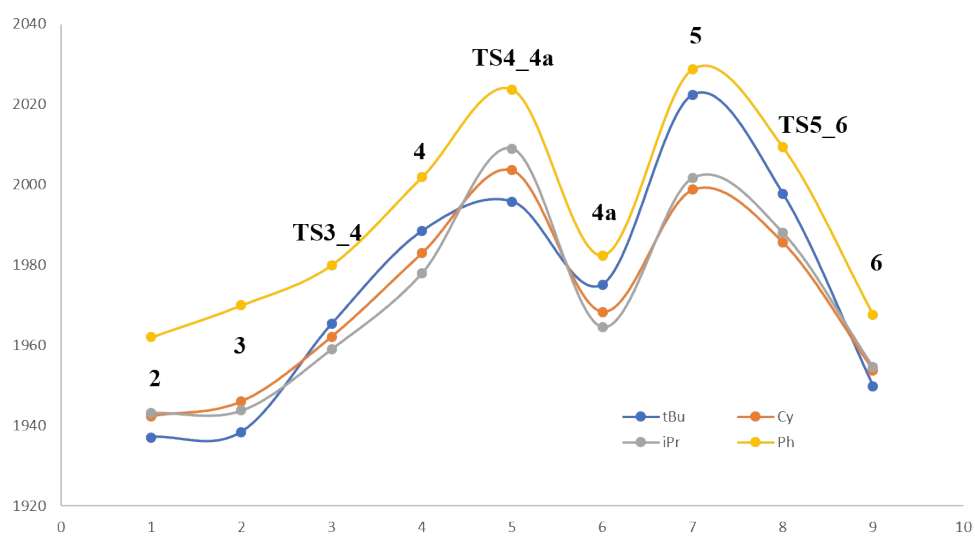


Figure 25 The CO stretching frequencies of different ligand PNP catalysts in CO₂ hydrogenation reaction.

Cartesian coordinates of all the structures

Atom X Y Z Atom X Y Z

CO₂

C 0.00000000 0.00000000 0.00000000
O 0.00000000 0.00000000 1.16895200
O 0.00000000 0.00000000 -1.16895200

H₂

H 0.00000000 0.00000000 0.37167300
H 0.00000000 0.00000000 -0.37167300

Morpholine

C 1.17917900 -0.74740900 0.20040500
C 1.20856600 0.72238600 -0.22024700
C -1.20856900 0.72238200 -0.22024600
C -1.17917600 -0.74741400 0.20040300
H 2.08965900 1.21795800 0.20293100
H 1.23062000 -0.82204700 1.30096600
H 2.02859500 -1.29837200 -0.21766400
H -2.08966200 1.21794700 0.20293500
H -1.28870000 0.77747700 -1.31391700
H -1.23061900 -0.82205400 1.30096400
H -2.02859000 -1.29838000 -0.21766800
H 1.28869300 0.77747900 -1.31391900
O 0.00000400 -1.39687800 -0.27647500
N -0.00000300 1.45618500 0.18592800
H -0.00000200 1.53205100 1.20378100

Pyrrolidine(14)

C 0.77737600 1.02802500 -0.07033300
C -0.77737100 1.02803500 -0.07030200
C -1.15834300 -0.45282500 0.19465400
C 1.15833700 -0.45282300 0.19467900
H 1.16363900 1.35576200 -1.04124200
H 1.19698500 1.69789800 0.68687000
H -1.16367300 1.35583700 -1.04117200
H -1.19693500 1.69786700 0.68696100
H -1.33777200 -0.60776800 1.26667400
H -2.05711700 -0.77404300 -0.33967000
H 1.33772000 -0.60773800 1.26671100
H 2.05713000 -0.77405700 -0.33960100
N 0.00000200 -1.27355300 -0.20234900
H 0.00001400 -1.33135900 -1.22127600

N-methyl piperazine

C 0.29851200 1.20519300 0.18106600
C -1.18086500 1.20679200 -0.22019100
C -1.18084100 -1.20679100 -0.22019700
C 0.29854000 -1.20519000 0.18107600
H -1.67960400 2.08571000 0.20232900
H 0.37583600 1.27934200 1.28610300
H 0.80259500 2.08485300 -0.23766600
H -1.67956200 -2.08573300 0.20228700
H -1.25164900 -1.27866400 -1.31337000
H 0.37585700 -1.27932800 1.28611600
H 0.80263800 -2.08484300 -0.23765000
H -1.25170200 1.27866900 -1.31335600
N 0.96431300 0.00000300 -0.31914600
C 2.38505700 0.00001200 -0.00355200
H 2.59160000 0.00000700 1.08438000
H 2.86225300 -0.88692600 -0.43458100
H 2.86222800 0.88696700 -0.43456900
N -1.90389700 -0.00002300 0.20195900
H -1.95582600 0.00000300 1.22107500

Piperidine

C 1.17917900 -0.74740900 0.20040500
C 1.20856600 0.72238600 -0.22024700
C -1.20856900 0.72238200 -0.22024600
C -1.17917600 -0.74741400 0.20040300
H 2.08965900 1.21795800 0.20293100
H 1.23062000 -0.82204700 1.30096600
H 2.02859500 -1.29837200 -0.21766400
H -2.08966200 1.21794700 0.20293500
H -1.28870000 0.77747700 -1.31391700
H -1.23061900 -0.82205400 1.30096400
H -2.02859000 -1.29838000 -0.21766800
H 1.28869300 0.77747900 -1.31391900
O 0.00000400 -1.39687800 -0.27647500
N -0.00000300 1.45618500 0.18592800
H -0.00000200 1.53205100 1.20378100

Cat1

Fe 0.00000600 0.03981300 -0.10803600

H 0.00000100 -0.27445300 1.34418300
 P 2.26811700 -0.11890600 -0.20550700
 P -2.26808700 -0.11901100 -0.20554200
 O -0.00043800 2.76388200 0.93655300
 N 0.00005600 -1.59344300 -1.04785600
 C -0.00003900 1.69567500 0.45890800
 C 2.46696900 -1.61134500 -1.29341500
 H 2.58821900 -1.23244600 -2.31417300
 H 3.35696800 -2.20099400 -1.05089400
 C 1.18744800 -2.44139300 -1.20450100
 H 1.09692400 -3.05707700 -2.11569900
 H 1.26149500 -3.16029800 -0.36849500
 C -1.18729700 -2.44144700 -1.20452100
 H -1.26132400 -3.16035800 -0.36851800
 H -1.09672800 -3.05712400 -2.11571900
 C -2.46685600 -1.61145700 -1.29345700
 H -3.35683300 -2.20114600 -1.05095200
 H -2.58810400 -1.23256100 -2.31421600
 C 3.23023400 -0.51039100 1.36186700
 H 4.28092200 -0.60742500 1.06214000
 C 2.77648500 -1.84716800 1.96761200
 H 3.32967300 -2.03876400 2.89524700
 H 2.95957200 -2.69226900 1.29781600
 H 1.70943500 -1.82885900 2.21154700
 C 3.11164800 0.61752400 2.39727700
 H 2.07208400 0.75211400 2.71395400
 H 3.47621500 1.57618300 2.01862400
 H 3.70247100 0.36954900 3.28759000
 C 3.29319100 1.15234400 -1.15972400
 H 2.87503400 1.04244800 -2.16977600
 C 3.07435700 2.61257900 -0.74126700
 H 3.44714200 2.81705700 0.26739200
 H 2.01989000 2.89312200 -0.77657800
 H 3.61757000 3.27354000 -1.42788600
 C 4.79049500 0.81382000 -1.22904800
 H 5.28685500 1.47845200 -1.94650900
 H 4.97469100 -0.21497600 -1.55490100
 H 5.28383000 0.95589200 -0.26145900
 C -3.23021500 -0.51051300 1.36182100
 H -4.28087100 -0.60776700 1.06205200
 C -2.77625100 -1.84714100 1.96773400
 H -1.70921500 -1.82860800 2.21171600
 H -2.95915600 -2.69235100 1.29802800
 H -3.32944400 -2.03873200 2.89536700

C -3.11188700 0.61753900 2.39711000
 H -3.70271900 0.36956200 3.28741800
 H -3.47660000 1.57609100 2.01832500
 H -2.07236500 0.75234900 2.71383300
 C -3.29316800 1.15222500 -1.15976000
 H -2.87498400 1.04236300 -2.16980500
 C -4.79046500 0.81368100 -1.22911900
 H -5.28382300 0.95573600 -0.26154000
 H -4.97464000 -0.21511400 -1.55498800
 H -5.28681800 1.47831500 -1.94658400
 C -3.07435700 2.61244700 -0.74124400
 H -3.61753900 3.27343300 -1.42786100
 H -2.01988500 2.89299000 -0.77649900
 H -3.44718300 2.81688600 0.26740900

A1

Fe 0.00001100 -0.08780700 -0.19199400
 H 0.00002000 0.64177700 1.10571100
 P -2.25789600 0.15385900 -0.21925100
 P 2.25792800 0.15378900 -0.21926700
 O 0.00018000 -2.49119400 1.46895300
 N 0.00002400 1.70756000 -1.16995800
 C -0.00000800 -1.56995100 0.75567400
 C -2.45785100 1.73949300 -1.16495700
 H -2.56809000 1.46765500 -2.22093400
 H -3.35094300 2.29813600 -0.86557000
 C -1.17194600 2.54204300 -0.96852900
 H -1.17546400 3.39132800 -1.67993000
 H -1.18958800 3.01027900 0.04035400
 C 1.17204100 2.54199000 -0.96858000
 H 1.18973600 3.01024200 0.04029400
 H 1.17557600 3.39126200 -1.67999600
 C 2.45791000 1.73938200 -1.16503100
 H 3.35103300 2.29800400 -0.86570000
 H 2.56809300 1.46749800 -2.22100300
 C -3.24350700 0.40655700 1.36177800
 H -4.27731400 0.55862800 1.02722200
 C -2.80397600 1.66551100 2.12378200
 H -3.42170300 1.77949600 3.02295600
 H -2.91748200 2.57626000 1.52934300
 H -1.75870200 1.59608800 2.44129900
 C -3.20241600 -0.81788500 2.28784500
 H -2.18486700 -1.01463100 2.63915900
 H -3.57568600 -1.72588800 1.80687000

H	-3.82735600	-0.63290400	3.16987400	N	0.00000000	-1.42425400	-1.33311700
C	-3.25163400	-1.06949500	-1.26018500	C	3.16089100	1.47600500	-0.85033100
H	-2.86502900	-0.85067700	-2.26544900	C	4.45331000	1.20988900	-1.63943600
C	-2.93455800	-2.54381500	-0.96845800	C	3.36829400	2.58014100	0.19882000
H	-3.29290600	-2.86000600	0.01600400	H	2.40922400	1.83772400	-1.56413500
H	-1.86057800	-2.74495600	-1.01568900	H	4.32999600	0.43496900	-2.40135500
H	-3.42610800	-3.18074400	-1.71383900	H	4.75183500	2.12909900	-2.15890600
C	-4.76559900	-0.81162500	-1.27147700	H	5.28550200	0.91871400	-0.99392700
H	-5.24366100	-1.44109300	-2.03182800	H	2.44157500	2.83595700	0.71947300
H	-5.00982500	0.22938000	-1.50732800	H	4.11052600	2.29107800	0.95004000
H	-5.22656800	-1.05974300	-0.30958000	H	3.73474700	3.49103200	-0.28905000
C	3.24355900	0.40654000	1.36174600	C	3.22184000	-0.56542400	1.40582500
H	4.27742100	0.55824200	1.02719300	C	4.74544000	-0.66600700	1.23228200
C	2.80437300	1.66579900	2.12344100	C	2.67044100	-1.88559800	1.96940400
H	1.75906000	1.59677300	2.44091300	H	3.00416000	0.22673700	2.13472100
H	2.91819300	2.57637600	1.52879800	H	5.21031900	0.29883400	1.01985400
H	3.42208600	1.77979800	3.02262200	H	5.19351000	-1.04458600	2.15926800
C	3.20207900	-0.81766700	2.28810700	H	5.01817700	-1.36303200	0.43207000
H	3.82694600	-0.63260500	3.17017000	H	1.58921800	-1.84863600	2.12029900
H	3.57521400	-1.72586900	1.80740800	H	2.89536300	-2.72913800	1.30716600
H	2.18444300	-1.01410300	2.63934100	H	3.14350800	-2.09413300	2.93637100
C	3.25159600	-1.06963700	-1.26018600	P	-2.26734200	-0.01770600	-0.12198700
H	2.86527400	-0.85052900	-2.26549500	C	-1.20253800	-2.23615900	-1.36364200
C	4.76563000	-0.81215000	-1.27108800	C	-2.45327900	-1.35314000	-1.40211700
H	5.22632200	-1.06056000	-0.30913300	H	-1.25427000	-2.91091600	-0.48679900
H	5.01017300	0.22883800	-1.50669000	H	-1.20676500	-2.89462100	-2.25227100
H	5.24370400	-1.44159700	-2.03144800	H	-2.51137600	-0.85133200	-2.37442100
C	2.93405400	-2.54393500	-0.96884300	H	-3.37082500	-1.93663100	-1.27653000
H	3.42559000	-3.18083600	-1.71425800	C	0.00000200	1.57755100	1.03654900
H	1.86002800	-2.74476900	-1.01635500	O	0.00000600	2.46347300	1.79643300
H	3.29210000	-2.86044600	0.01562400	C	-3.16086600	1.47607200	-0.85024500
H	-0.39308000	-0.84836800	-1.73657800	C	-3.36836200	2.58008700	0.19901700
H	0.39307300	-0.84775200	-1.73689600	C	-4.45322300	1.21001500	-1.63947100

ATSI_2

Fe	0.00000000	0.18184700	-0.00635800	H	-2.44168600	2.83584600	0.71977600
H	0.00000500	-0.64779900	1.24737400	H	-3.73477700	3.49103200	-0.28877900
C	1.20251800	-2.23619000	-1.36359200	H	-4.11065500	2.29093400	0.95014300
C	2.45328200	-1.35320400	-1.40205400	H	-4.32979400	0.43527300	-2.40155200
H	1.20675200	-2.89467100	-2.25220700	H	-5.28542800	0.91862400	-0.99407700
H	1.25420800	-2.91093000	-0.48673200	H	-4.75179800	2.12930900	-2.15876300
H	2.51142400	-0.85143200	-2.37437400	C	-3.22186600	-0.56547500	1.40578200
H	3.37081000	-1.93671200	-1.27641600	C	-2.67043700	-1.88563500	1.96936500
P	2.26734300	-0.01771500	-0.12198100	C	-4.74545600	-0.66611600	1.23218100
				H	-3.00424100	0.22668500	2.13469700

H -1.58922300 -1.84862700 2.12031500
H -3.14354400 -2.09420900 2.93630400
H -2.89528600 -2.72917300 1.30710000
H -5.21036500 0.29870300 1.01971600
H -5.01813400 -1.36316700 0.43197300
H -5.19354800 -1.04469400 2.15915600
H -0.00000200 0.93400500 -1.54463300
H 0.00000800 0.01641900 -1.71178900

A2

Fe 0.00000000 0.14194300 0.05139300
H -0.00000100 -0.95159500 1.15061400
C 1.22881700 -2.27392800 -1.32407700
C 2.46172500 -1.37239000 -1.37397200
H 1.24108800 -2.98851400 -2.16010600
H 1.20031100 -2.84547900 -0.39249200
H 2.53635700 -0.91152900 -2.36567100
H 3.37699000 -1.95208900 -1.21793800
P 2.25293200 0.00151300 -0.12781700
N 0.00000300 -1.44647700 -1.36793600
C 3.10233100 1.48366600 -0.93044300
C 4.42955700 1.25626600 -1.67202200
C 3.19795700 2.66090600 0.05234700
H 2.34881500 1.74793100 -1.68198600
H 4.38822700 0.40525400 -2.35874900
H 4.65845100 2.14445000 -2.27447900
H 5.27229900 1.10107700 -0.99475100
H 2.23090900 2.88285000 0.51315100
H 3.91991200 2.46764000 0.85360600
H 3.52962600 3.56343300 -0.47476500
C 3.28628900 -0.50209200 1.37365400
C 4.80894300 -0.51992100 1.17090700
C 2.82237700 -1.85200400 1.94521200
H 3.04468000 0.27235100 2.11387300
H 5.21726900 0.47402500 0.97926000
H 5.29447100 -0.90013300 2.07843600
H 5.10434400 -1.17825300 0.34584400
H 1.74586800 -1.87181600 2.12771000
H 3.07384900 -2.68003400 1.27209100
H 3.33418200 -2.04131500 2.89641200
P -2.25293000 0.00152800 -0.12782600
C -1.22884200 -2.27388700 -1.32414400
C -2.46171700 -1.37230500 -1.37405500
H -1.20038800 -2.84546600 -0.39257600

H -1.24110600 -2.98844800 -2.16019400
H -2.53628900 -0.91139300 -2.36573600
H -3.37701000 -1.95197700 -1.21809000
C 0.00000200 1.35690000 1.28062900
O 0.00003400 2.13275900 2.15691600
C -3.10233100 1.48373100 -0.93035500
C -3.19799700 2.66089100 0.05252700
C -4.42953600 1.25636600 -1.67198100
H -2.34880400 1.74806800 -1.68186200
H -2.23096300 2.88281100 0.51337200
H -3.52966500 3.56345500 -0.47452100
H -3.91996700 2.46755000 0.85375300
H -4.38817000 0.40542200 -2.35879000
H -5.27228800 1.10109200 -0.99474200
H -4.65844100 2.14460200 -2.27435800
C -3.28629300 -0.50216500 1.37361300
C -2.82237600 -1.85209900 1.94511800
C -4.80894500 -0.52000000 1.17085000
H -3.04469900 0.27224500 2.11387100
H -1.74587000 -1.87191000 2.12762800
H -3.33419100 -2.04145200 2.89630500
H -3.07383700 -2.68010300 1.27196100
H -5.21728100 0.47395100 0.97924800
H -5.10433000 -1.17829600 0.34575300
H -5.29447800 -0.90026000 2.07835700
H -0.00000800 1.14212000 -1.17437900
H 0.00003600 -0.95076200 -2.25926100

A1a

Fe 0.02909900 -0.33516900 -0.06513200
H 0.08176600 -1.83593000 -0.11412700
P -2.21380600 -0.67237100 0.12610700
P 2.29688200 -0.50396400 0.17268200
O 0.06562500 -0.39133400 -2.97993500
N 0.01556900 -0.38497900 1.97539500
C 0.04667300 -0.32298800 -1.81176300
C -2.45146300 -0.54745200 1.96397300
H -2.65630200 0.50760400 2.17656800
H -3.30677200 -1.12737900 2.32614900
C -1.14153600 -0.97222800 2.63275200
H -1.18161300 -0.67471200 3.70083200
H -1.09559200 -2.08247500 2.65140700
C 1.20046800 -0.87988600 2.65572200
H 1.24892400 -1.99035300 2.67108800

H 1.19473300 -0.58429300 3.72510900
C 2.47987000 -0.34097500 2.01405900
H 3.37928400 -0.82945800 2.40320600
H 2.57290000 0.73303400 2.21768900
C -2.90871000 -2.35717900 -0.37433000
H -3.99948300 -2.23852600 -0.36541800
C -2.55113800 -3.47610200 0.61503700
H -2.99936000 -4.41830300 0.27528700
H -2.92363900 -3.28287900 1.62460000
H -1.46842200 -3.62662900 0.67193600
C -2.47302300 -2.76276000 -1.79214200
H -1.39432000 -2.94294100 -1.82793900
H -2.71219100 -2.00879400 -2.54582700
H -2.97881300 -3.69224700 -2.08174500
C -3.49984700 0.55179500 -0.52743000
H -3.11728600 1.50849000 -0.15093300
C -3.53948700 0.64491800 -2.06056200
H -4.00753800 -0.23879700 -2.50644600
H -2.54398100 0.75688500 -2.49923600
H -4.13692000 1.51304600 -2.36522900
C -4.91491600 0.36088200 0.04102100
H -5.56281200 1.18062100 -0.29372500
H -4.92992700 0.35803200 1.13481100
H -5.37216500 -0.57194100 -0.30596700
C 3.15679700 -2.11727400 -0.30051800
H 4.23142400 -1.90392200 -0.24719700
C 2.85696400 -3.26486100 0.67534400
H 1.78894000 -3.50413300 0.69202100
H 3.17455300 -3.04231000 1.69755100
H 3.39472900 -4.16504600 0.35250300
C 2.81681000 -2.55300200 -1.73481900
H 3.40512700 -3.44038100 -1.99931400
H 3.03361500 -1.78209000 -2.47822600
H 1.75866200 -2.81689200 -1.82219000
C 3.47852000 0.84321100 -0.44470200
H 3.02772000 1.75719600 -0.03314700
C 4.90578800 0.75323000 0.11805900
H 5.44319400 -0.11820100 -0.27097300
H 4.92132700 0.70024600 1.21055900
H 5.47787700 1.64195700 -0.17639300
C 3.50234000 0.99403800 -1.97326000
H 4.02741000 1.91663200 -2.24960200
H 2.49794600 1.04039000 -2.40366400
H 4.03558200 0.16645300 -2.45230900

C -0.32247000 4.06356700 1.42326600
C -0.67997700 2.59159400 1.25160500
C -0.13487300 2.78680400 -1.09868000
C 0.18258300 4.26405700 -0.86235200
H -0.45675700 1.99936500 2.14294000
H 0.73677200 4.16628200 1.71918800
H -0.93715100 4.52407800 2.20369300
H 0.50156100 2.39062700 -1.89479800
H -1.17752500 2.67870200 -1.41599200
H 1.26367200 4.38619800 -0.67098400
H -0.07182300 4.85884400 -1.74588700
H -1.75128700 2.50919100 1.04415700
O -0.56575500 4.80086000 0.22453200
N 0.05372200 1.97436000 0.12439900
H 1.04103000 2.02596900 0.37052800

ATS1a_2a

Fe -0.01437300 -0.16424100 -0.17980600
H -0.01307800 -1.66239800 -0.02938900
P -2.25361900 -0.56246100 0.16263700
P 2.23513300 -0.55440800 0.06904000
O -0.02489200 -0.41811400 -3.07760600
N 0.01976900 0.24517500 1.86355600
C -0.02665300 -0.30610900 -1.91501200
C -2.47336600 0.04174500 1.91524400
H -2.76187400 1.09621200 1.84671800
H -3.28312600 -0.47677600 2.44034000
C -1.15298900 -0.10005600 2.67903900
H -1.19304800 0.52766100 3.58660400
H -1.05259100 -1.13601900 3.03508600
C 1.23655600 -0.07767900 2.62123400
H 1.17679500 -1.11733600 2.97509600
H 1.30697700 0.54773700 3.52851100
C 2.51565100 0.09307800 1.79731700
H 3.36476800 -0.38393400 2.29718300
H 2.76371900 1.15484600 1.69648700
C -2.79719100 -2.37083500 0.20730900
H -3.86964000 -2.33971600 0.42782700
C -2.13151800 -3.19297600 1.31900300
H -2.50674500 -4.22336000 1.28001500
H -2.35667000 -2.80431700 2.31631600
H -1.04486200 -3.22856000 1.20008000
C -2.60161100 -3.05042400 -1.15655200
H -1.54195000 -3.08383700 -1.43035600

H -3.14125400 -2.54201200 -1.96077200
H -2.97072600 -4.08254300 -1.11461800
C -3.70737600 0.28663500 -0.72496800
H -3.68216900 1.29959400 -0.30969800
C -3.49280100 0.41514200 -2.24015400
H -3.49920400 -0.55751700 -2.74227900
H -2.54660800 0.90814700 -2.47589600
H -4.30069500 1.01306700 -2.67997700
C -5.09756400 -0.28503500 -0.40520100
H -5.86725600 0.39290800 -0.79431300
H -5.27059800 -0.39104300 0.67097300
H -5.26153100 -1.26056200 -0.87429200
C 2.80690700 -2.35906900 0.09235400
H 3.89956300 -2.30785500 0.01312100
C 2.47198400 -3.10132400 1.39424000
H 1.39162400 -3.14724000 1.56324200
H 2.94024400 -2.64742700 2.27202300
H 2.83925300 -4.13308800 1.32733700
C 2.27527300 -3.15834100 -1.10950200
H 2.76567100 -4.13933800 -1.14047900
H 2.45795900 -2.66931600 -2.06935900
H 1.19810100 -3.32437500 -1.01906200
C 3.62842800 0.27733000 -0.91642300
H 3.31748200 1.32463700 -0.96495400
C 5.00566900 0.23304100 -0.23536800
H 5.38938000 -0.78882200 -0.14221100
H 4.99468500 0.68225100 0.76185100
H 5.73015000 0.79399300 -0.83891100
C 3.72207600 -0.22823500 -2.36478100
H 4.40740400 0.41332500 -2.93193000
H 2.75483400 -0.20847300 -2.87493100
H 4.11795000 -1.24736200 -2.41712700
C -1.19095600 4.21821000 0.31598300
C -1.20031000 2.79649300 -0.25379900
C 1.16664600 2.80757800 -0.24430200
C 1.13767700 4.23027600 0.32317300
H -2.09441000 2.29813400 0.12002700
H -1.24452500 4.17641600 1.41900600
H -2.05455400 4.78708300 -0.04742000
H 2.06237700 2.32076700 0.14273200
H 1.27750500 2.87795500 -1.34194400
H 1.18516300 4.18960300 1.42648000
H 1.99762900 4.80771600 -0.03533500
H -1.29991200 2.86909300 -1.35183900

O -0.02904100 4.93962000 -0.08091400
N -0.01461600 2.02279200 0.11370900
H -0.00304000 1.38090500 1.27413900

A2a

Fe -0.06345900 -0.26246000 -0.07890400
H -0.16915900 -1.80120900 -0.06834900
P -2.34272800 -0.40437600 0.12784800
P 2.18826500 -0.68286100 0.13177300
O -0.09173000 -0.30912900 -2.98113700
N -0.07498500 -0.35476100 2.05291100
C -0.08035800 -0.27204100 -1.81475600
C -2.57059200 -0.31754100 1.97954900
H -2.71577700 0.73782400 2.23384500
H -3.46088100 -0.85605600 2.32103200
C -1.32446900 -0.86511500 2.67346800
H -1.34405200 -0.62059900 3.74529100
H -1.29623500 -1.95411600 2.58703500
C 1.10510800 -1.01509000 2.66264800
H 0.97042300 -2.09307100 2.54616500
H 1.14579100 -0.80122700 3.74073400
C 2.38706100 -0.55499300 1.97992400
H 3.25015800 -1.10915900 2.36042700
H 2.55638300 0.50655300 2.19328300
C -3.20034500 -2.01289700 -0.36988600
H -4.27137700 -1.82224800 -0.23819500
C -2.83161200 -3.20760000 0.52165400
H -3.36804200 -4.09848100 0.17207500
H -3.11084700 -3.05261700 1.56812900
H -1.75998500 -3.42608500 0.47747600
C -2.94428200 -2.35588600 -1.84537000
H -1.88915600 -2.59250300 -2.01412900
H -3.22147500 -1.54362700 -2.52278500
H -3.53275200 -3.23685000 -2.12985600
C -3.52924500 0.95085200 -0.45200600
H -3.22299100 1.79454000 0.17708400
C -3.29430700 1.36907400 -1.91033200
H -3.58138800 0.58356100 -2.61711100
H -2.24691900 1.62365700 -2.09139500
H -3.89871400 2.25392200 -2.14511100
C -5.01718300 0.68459400 -0.17774200
H -5.59347500 1.59979200 -0.36144900
H -5.20690800 0.38334200 0.85792400
H -5.42574900 -0.08860500 -0.83684500

C	2.86084400	-2.38581000	-0.34544400	H	3.37103300	-0.01379500	-2.10645000
H	3.95138800	-2.27057200	-0.38401800	P	2.25042700	-0.30158200	0.11338500
C	2.54267300	-3.48748000	0.67558800	N	-0.00000600	0.03554400	-1.54938000
H	1.46309100	-3.64355500	0.77072500	C	3.29581500	0.81757500	1.21003400
H	2.95106000	-3.27561800	1.66802000	C	4.62508200	1.32415600	0.62818500
H	2.98202000	-4.43457500	0.33883000	C	3.48910800	0.20340500	2.60627000
C	2.36946300	-2.81290700	-1.73860200	H	2.63680000	1.68864900	1.32017600
H	2.85962100	-3.74928300	-2.03268400	H	4.49612900	1.80871400	-0.34417400
H	2.58480900	-2.07152200	-2.51182400	H	5.05522400	2.07072600	1.30759600
H	1.28898300	-2.98570700	-1.73011800	H	5.36323900	0.52668300	0.51218600
C	3.54027700	0.48952100	-0.46820800	H	2.54583400	-0.13945400	3.04190200
H	3.12237300	1.47242400	-0.22459200	H	4.17880700	-0.64669400	2.58119200
C	4.88156700	0.34927800	0.26938100	H	3.91503600	0.95095000	3.28580700
H	5.32850600	-0.64183500	0.13182300	C	3.01919900	-2.01854400	0.16384600
H	4.79027600	0.53212100	1.34347600	C	4.52568800	-2.09133400	-0.12522400
H	5.59600600	1.08257400	-0.12523300	C	2.24800000	-2.97865600	-0.75664500
C	3.75521600	0.42028400	-1.98845300	H	2.84592800	-2.34100800	1.19854000
H	4.38957300	1.25469600	-2.31094100	H	5.12264600	-1.57134900	0.62722500
H	2.81880400	0.48094800	-2.55036600	H	4.84763200	-3.14024700	-0.12801400
H	4.26498100	-0.50405300	-2.28103200	H	4.77293900	-1.67352300	-1.10774600
C	0.00320900	3.99471700	1.31550400	H	1.17003800	-2.92379600	-0.58515500
C	-0.64731200	2.66675100	0.90797500	H	2.44049300	-2.76230800	-1.81315700
C	0.67772000	2.57191900	-0.99254600	H	2.57117400	-4.00979700	-0.57001500
C	1.32249400	3.91434000	-0.62357100	P	-2.25047100	-0.30160400	0.11340600
H	-1.01708700	2.18572100	1.82451200	C	-1.19763900	-0.00530500	-2.40052700
H	0.85078200	3.79515100	1.99625000	C	-2.46267300	0.34509000	-1.61111000
H	-0.71067700	4.64900700	1.83222800	H	-1.30713100	-1.00170200	-2.86133600
H	1.39524700	2.00651400	-1.59538800	H	-1.09116400	0.70191200	-3.23874200
H	-0.18045700	2.80672500	-1.66630500	H	-2.54581900	1.43461800	-1.52100100
H	2.26593700	3.73386700	-0.07701100	H	-3.37108000	-0.01374900	-2.10643200
H	1.55192900	4.50611900	-1.51894000	C	-0.00001000	0.67122400	1.81026000
H	-1.54956500	2.93960500	0.31319000	O	-0.00001500	1.30393800	2.79475900
O	0.45477800	4.71959800	0.17430900	C	-3.29574600	0.81767200	1.21002300
N	0.27715100	1.81284300	0.18177200	C	-3.48862700	0.20377900	2.60643500
H	0.00731100	0.64287000	2.25049100	C	-4.62514100	1.32409300	0.62834300
A1b				H	-2.63673500	1.68879400	1.31982600
Fe	0.00000100	-0.18761300	0.30365600	H	-2.54516200	-0.13872000	3.04193400
H	-0.00003300	-1.45380400	1.13348600	H	-3.91460800	0.95137000	3.28588800
C	1.19759600	-0.00504900	-2.40056600	H	-4.17808400	-0.64653400	2.58175300
C	2.46267300	0.34515900	-1.61112200	H	-4.49639200	1.80836600	-0.34418900
H	1.09104100	0.70242400	-3.23855200	H	-5.36332500	0.52659300	0.51273500
H	1.30710700	-1.00130800	-2.86168000	H	-5.05512800	2.07086000	1.30763600
H	2.54599800	1.43467100	-1.52100800	C	-3.01940800	-2.01850600	0.16396300
				C	-2.24809700	-2.97888800	-0.75614500

C -4.52582800 -2.09115300 -0.12550300
H -2.84644600 -2.34078800 1.19876600
H -1.17017100 -2.92413600 -0.58439800
H -2.57144500 -4.00995400 -0.56939500
H -2.44029800 -2.76272700 -1.81274800
H -5.12295600 -1.57093600 0.62664800
H -4.77275400 -1.67351300 -1.10817800
H -4.84791000 -3.14002400 -0.12817900
C 0.00002500 3.41843200 -1.38813700
O 0.00007600 3.56215800 -0.22765800
O -0.00004400 3.32297500 -2.55438800

ATS1b_2b

Fe 0.00170400 -0.25423000 0.18926000
H 0.00421400 -1.64423600 -0.29931000
C 1.19276800 0.97635200 -2.25118500
C 2.46818600 1.02408200 -1.40688800
H 1.13352700 1.89424600 -2.86004200
H 1.25101400 0.14074700 -2.97063400
H 2.57771800 2.01927200 -0.96165800
H 3.36488700 0.84124000 -2.00799600
P 2.27765300 -0.18157500 -0.00844400
N -0.00073700 0.85252200 -1.40809600
C 3.23306700 0.57870500 1.43133500
C 4.52891000 1.33136600 1.08536900
C 3.46516000 -0.43362000 2.56522900
H 2.50982800 1.32104300 1.79462300
H 4.38628300 2.07235800 0.29361900
H 4.87950600 1.87042200 1.97425100
H 5.33227600 0.65801900 0.77567600
H 2.54248400 -0.93051800 2.87496000
H 4.18644500 -1.20558300 2.27873800
H 3.87088100 0.08282800 3.44316900
C 3.16130900 -1.76165200 -0.52200400
C 4.68744400 -1.65623600 -0.66556400
C 2.55279000 -2.33497400 -1.81346500
H 2.93198400 -2.45734100 0.29591100
H 5.18673300 -1.42284800 0.27706500
H 5.08718600 -2.61605400 -1.01563700
H 4.97351300 -0.89744200 -1.40244900
H 1.46450000 -2.41383000 -1.75631600
H 2.80802500 -1.71791600 -2.68199400
H 2.95830800 -3.33725000 -1.99536400
P -2.27350300 -0.19416600 -0.01365200

C -1.18562800 0.94463000 -2.26702500
C -2.47145300 0.97927300 -1.43814100
H -1.21917900 0.09996800 -2.97736500
H -1.13629000 1.85694500 -2.88489000
H -2.60419600 1.97930100 -1.01038100
H -3.35768100 0.76956000 -2.04595900
C 0.00137600 -0.98530700 1.77196500
O 0.00152300 -1.54602600 2.79864100
C -3.23616800 0.60709500 1.39812700
C -3.40891600 -0.34448000 2.59266300
C -4.56342200 1.29567800 1.03702300
H -2.53454400 1.39493900 1.70350200
H -2.45832200 -0.76816000 2.92523100
H -3.84103600 0.20136400 3.43972200
H -4.08578400 -1.17312700 2.35963000
H -4.46201900 1.99102800 0.19884100
H -5.35157300 0.58036900 0.78926300
H -4.91107300 1.87732000 1.89982200
C -3.13376100 -1.79888800 -0.48812000
C -2.54390100 -2.36485600 -1.79156500
C -4.66506900 -1.73689100 -0.59123500
H -2.86351000 -2.48140000 0.32842900
H -1.45263100 -2.41342100 -1.76297200
H -2.92608700 -3.37918800 -1.95618000
H -2.83976000 -1.76108400 -2.65662000
H -5.14496100 -1.51441300 0.36406300
H -4.99268300 -0.99000100 -1.32281700
H -5.04647400 -2.70927200 -0.92691100
C -0.03548200 2.92133000 -0.14146200
O 0.01666700 2.50456700 0.96750500
O -0.09396100 3.66782400 -1.05164800

A2b

Fe -0.00002300 -0.30418200 -0.01290100
H 0.00027300 -0.85951200 -1.41250900
C 1.22018300 2.18097500 -1.24143300
C 2.48718900 1.68637900 -0.54161400
H 1.20550800 3.27844800 -1.26588100
H 1.17257600 1.81270500 -2.26991300
H 2.64041600 2.25235500 0.38226500
H 3.36575800 1.85812300 -1.17095800
P 2.28622400 -0.11270400 -0.08160800
N -0.00005300 1.68171700 -0.54976700
C 3.10714500 -0.26781900 1.60512800

C 4.40853700 0.51605800 1.84007600
 C 3.25894100 -1.73982600 2.01919900
 H 2.32961500 0.17931200 2.23735000
 H 4.32646000 1.56733700 1.54975500
 H 4.64827500 0.49581600 2.91044900
 H 5.26046800 0.08454000 1.30837500
 H 2.31591300 -2.28778400 1.94223700
 H 4.00626200 -2.26069100 1.41102500
 H 3.58878800 -1.79761300 3.06303200
 C 3.27154900 -1.10710300 -1.33536000
 C 4.79457700 -0.91808500 -1.27591200
 C 2.75710400 -0.84981000 -2.76169200
 H 3.03627800 -2.14792700 -1.07517000
 H 5.22271400 -1.27131600 -0.33565500
 H 5.26549200 -1.49014900 -2.08467700
 H 5.07942600 0.13139500 -1.41067700
 H 1.67924900 -1.00913100 -2.84452400
 H 2.98170000 0.17180900 -3.08955100
 H 3.25659500 -1.53255500 -3.45887300
 P -2.28621600 -0.11275000 -0.08178900
 C -1.22013100 2.18088500 -1.24174500
 C -2.48726800 1.68621100 -0.54220500
 H -1.17224200 1.81257300 -2.27019700
 H -1.20553500 3.27835500 -1.26622200
 H -2.64081900 2.25232700 0.38153700
 H -3.36569400 1.85777800 -1.17179800
 C -0.00004900 -1.97329800 0.47488600
 O -0.00010400 -3.12010200 0.69159800
 C -3.10697600 -0.26731000 1.60509500
 C -3.25836400 -1.73914100 2.01993500
 C -4.40857700 0.51628400 1.83984300
 H -2.32947600 0.18034700 2.23699100
 H -2.31523300 -2.28693600 1.94313300
 H -3.58807600 -1.79645500 3.06383800
 H -4.00566200 -2.26045400 1.41211300
 H -4.32698000 1.56739800 1.54879100
 H -5.26047500 0.08409400 1.30862700
 H -4.64805900 0.49664500 2.91028300
 C -3.27152100 -1.10758600 -1.33517900
 C -2.75724300 -0.85052900 -2.76161300
 C -4.79455400 -0.91878200 -1.27558100
 H -3.03607000 -2.14831700 -1.07478700
 H -1.67935000 -1.00959500 -2.84448600
 H -3.25662200 -1.53355100 -3.45859800

H -2.98210800 0.17096700 -3.08967500
 H -5.22250800 -1.27195300 -0.33521600
 H -5.07957900 0.13063500 -1.41046100
 H -5.26549700 -1.49102800 -2.08420300
 C -0.00015600 2.09568800 0.91764400
 O 0.00043400 1.03795400 1.63218800
 O -0.00073600 3.27857000 1.22523100

Cat2

Fe 0.00577900 0.19879100 -0.08084000
 H 0.04155500 1.65180400 0.86259200
 H 0.01187400 -1.12695200 -0.76482600
 B -0.11637500 2.89679400 1.06115000
 H -0.90766100 2.97393400 1.98712500
 H 0.97965200 3.32116100 1.38402300
 H -0.53345400 3.43562700 0.05538500
 C -1.21814300 -1.79821100 1.83571500
 C -2.49456500 -1.00079200 1.57327700
 H -1.26538600 -2.28177400 2.82291700
 H -1.11573000 -2.58360500 1.08491700
 H -2.68454200 -0.29244000 2.38441800
 H -3.35433100 -1.67727800 1.53379300
 P -2.28280500 -0.03356200 -0.00249800
 N 0.01652900 -0.95542400 1.75756200
 C -3.30795700 1.52979400 0.21884300
 C -4.62967800 1.41180200 0.99488700
 C -3.49567900 2.26276800 -1.11984000
 H -2.62916000 2.13985900 0.82357200
 H -4.50116000 0.92734300 1.96731500
 H -5.01796900 2.41975600 1.18739200
 H -5.40118200 0.86659800 0.44595200
 H -2.54832300 2.39526700 -1.65053800
 H -4.18883900 1.73751800 -1.78549000
 H -3.91027100 3.26081500 -0.93701200
 C -3.11223700 -1.04926200 -1.36150900
 C -4.63559000 -1.20496000 -1.22447400
 C -2.46850000 -2.43521700 -1.52893000
 H -2.90329400 -0.47128200 -2.27148600
 H -5.16659900 -0.25500000 -1.30337600
 H -5.00691500 -1.85136100 -2.02907500
 H -4.91509700 -1.67684800 -0.27567800
 H -1.38935500 -2.37488000 -1.68363300
 H -2.65591300 -3.07135200 -0.65625600
 H -2.91008000 -2.93763400 -2.39761600

C	0.08600000	-0.09103400	2.96318500	H	2.34757700	-1.61298900	2.11679200
H	0.11341600	-0.70415100	3.87577300	H	3.33087600	-0.17551800	2.36929400
H	0.97484400	0.53664400	2.92808600	P	2.33881300	-0.28820600	0.08552700
H	-0.77837100	0.56953800	3.00061700	N	-0.10367600	-0.21981200	1.96864800
P	2.29139800	-0.04741300	-0.01240300	C	3.19175100	-1.80663000	-0.61983200
C	1.19365000	-1.88117100	1.74503600	C	4.51610600	-2.23155300	0.03679400
C	2.51010400	-1.15620600	1.46899700	C	3.29208800	-1.77092300	-2.15324000
H	1.00787800	-2.61729500	0.96061000	H	2.45349300	-2.57373200	-0.37090300
H	1.24651400	-2.41557500	2.70564500	H	4.46351500	-2.22349200	1.12979800
H	2.80185800	-0.53881900	2.32271600	H	4.74224500	-3.26125000	-0.26642500
H	3.31289100	-1.88510600	1.31864600	H	5.36078000	-1.61086900	-0.26757900
C	0.00079900	0.92602500	-1.66123300	H	2.33463500	-1.52942500	-2.62102300
O	-0.00266400	1.34397400	-2.74758500	H	4.03355000	-1.04998800	-2.51006900
C	3.31914100	1.48278000	0.36562500	H	3.59413700	-2.75879400	-2.51973700
C	3.42984400	2.38747600	-0.87151800	C	3.38044600	1.25603100	-0.29041500
C	4.68014200	1.28981600	1.05457100	C	4.87475800	1.01090500	-0.55481300
H	2.66255400	1.99468600	1.07786700	C	3.25745800	2.34058900	0.79512300
H	2.45342600	2.58067600	-1.32543000	H	2.92177400	1.64583200	-1.20513500
H	3.85623900	3.35576600	-0.58490300	H	5.06062900	0.33097800	-1.38670400
H	4.08289500	1.95456500	-1.63704400	H	5.34350600	1.96950600	-0.80819200
H	4.62007900	0.63522900	1.92949400	H	5.38771600	0.62408000	0.33152000
H	5.44231800	0.88700400	0.38377500	H	2.23200300	2.61974200	1.03353800
H	5.03921500	2.26507800	1.40610100	H	3.75559900	2.03423800	1.72138300
C	3.10496000	-0.93889800	-1.46384900	H	3.76170700	3.24723900	0.44164300
C	2.47419100	-2.31772100	-1.71634000	C	-0.47641900	-1.54189300	2.53661100
C	4.63318800	-1.07579100	-1.37941900	H	-0.58249400	-1.46500000	3.62738500
H	2.86326500	-0.29859000	-2.32218400	H	-1.41706600	-1.89205100	2.11600300
H	1.39012700	-2.26055000	-1.83213700	H	0.28697700	-2.28055600	2.29943000
H	2.89353200	-2.74631600	-2.63420200	P	-2.38137400	-0.09039000	0.02222000
H	2.69706700	-3.01651100	-0.90169700	C	-1.12511100	0.80439100	2.36571700
H	5.14298900	-0.11159200	-1.41424400	C	-2.51493200	0.53074800	1.78183700
H	4.94795100	-1.59917900	-0.46958700	H	-0.76097600	1.76730900	2.00400400
H	4.99181200	-1.66369900	-2.23312000	H	-1.18324800	0.84417700	3.46346000
1a							
C	0.24953100	2.69206400	-0.37821700	H	-3.06523400	-0.19627300	2.38201200
O	0.70044800	2.88117800	-1.49481400	H	-3.09409700	1.45898100	1.80662700
O	-0.06790000	3.32781000	0.61896000	C	-0.03417100	-0.17104200	-1.94985200
Fe	-0.02515500	-0.22575700	-0.17592600	O	-0.07757900	-0.13518100	-3.10203200
H	0.03491500	1.44001900	-0.17164900	C	-3.28952200	-1.74759500	-0.03110900
C	1.21096500	0.19013000	2.56209300	C	-3.63178700	-2.12515000	-1.48197800
C	2.39690200	-0.53645000	1.92797900	C	-4.49664600	-1.93257700	0.90194800
H	1.18596000	0.00884800	3.64568300	H	-2.51610700	-2.44478700	0.29864600
H	1.30941700	1.26566900	2.41398900	H	-2.77653100	-2.00174000	-2.15377700
				H	-3.92928700	-3.17887100	-1.52209700
				H	-4.46508800	-1.53292400	-1.87389100

H	-4.23230700	-1.82121600	1.95729500	H	-1.00847700	-4.39542100	-0.75595500
H	-5.32137300	-1.24931200	0.68669000	C	2.97172100	-2.57057000	-1.42416200
H	-4.87750800	-2.95374600	0.77803700	C	3.48133200	-4.01679900	-1.32263900
C	-3.40871300	1.05641700	-1.06716100	C	4.15904500	-1.61597700	-1.62812900
C	-2.75578000	2.42688700	-1.27869300	H	2.32345500	-2.49160400	-2.30681800
C	-4.86693200	1.21973300	-0.60918000	H	2.67722300	-4.75139200	-1.39064000
H	-3.40883200	0.54008400	-2.03496900	H	4.17501800	-4.21642900	-2.14849500
H	-1.79015100	2.34551400	-1.77806600	H	4.02866200	-4.19078600	-0.38937600
H	-3.40473500	3.03723000	-1.91772400	H	3.83901000	-0.57783500	-1.73842800
H	-2.61470700	2.97078300	-0.33998100	H	4.86877900	-1.67165300	-0.79435800
H	-5.42546000	0.28301600	-0.64128000	H	4.70365800	-1.90272900	-2.53550900
H	-4.93689200	1.62751700	0.40504200	C	1.42168300	0.29424100	2.95312600
H	-5.37445900	1.92468900	-1.27808800	H	2.04801600	0.46949000	3.83993600
H	0.56818300	-3.07007400	-1.69112800	H	0.59279000	1.00057100	2.95686200
B	0.02678500	-3.10308200	-0.61082500	H	0.99869200	-0.70718300	3.00518700
H	-1.09925700	-3.54063600	-0.66441200	P	0.71616200	2.40956800	-0.02365400
H	0.69622400	-3.64349000	0.24786200	C	2.81370700	1.82703700	1.68468800
H	-0.10505400	-1.89092000	-0.16043300	C	1.76655700	2.90975800	1.43167300
I				H	3.55454900	1.83853900	0.88323100
Fe	1.03896700	0.13669700	-0.08095200	H	3.33855700	2.01726900	2.63299600
H	-0.34161500	-0.21371700	0.90028900	H	1.11184100	3.03050400	2.29907500
H	2.28348400	0.47453300	-0.83236300	H	2.26138900	3.87312900	1.27147500
B	-1.50553700	-0.62963900	1.19057300	C	0.26870600	-0.06889500	-1.62707800
H	-1.34396500	-1.44373600	2.08402700	O	-0.17970300	-0.19251300	-2.69400600
H	-2.12484100	0.34178600	1.58673700	C	-1.00547700	3.03548800	0.40388100
H	-2.01902700	-1.12911100	0.20706600	C	-1.97182000	2.85229000	-0.77677200
C	3.36413200	-0.52174600	1.74708800	C	-1.13032800	4.43132900	1.03618000
C	2.91613500	-1.96276500	1.51275900	H	-1.29626200	2.30615200	1.16848000
H	3.88776400	-0.43448100	2.71082500	H	-1.95906200	1.82637100	-1.15605200
H	4.05928900	-0.22298300	0.96074400	H	-2.99621400	3.07259200	-0.45428800
H	2.32576300	-2.33142500	2.35628500	H	-1.73930000	3.52623400	-1.60839700
H	3.79038700	-2.61646200	1.42693000	H	-0.42694500	4.58407300	1.86020000
P	1.84762600	-2.01602100	-0.01159100	H	-0.98524600	5.23912800	0.31585000
N	2.22601200	0.45016500	1.71397600	H	-2.14017000	4.54276200	1.45035900
C	0.60308600	-3.39536900	0.29283900	C	1.35701500	3.39261000	-1.50218500
C	1.09436900	-4.65671900	1.02176300	C	2.86885900	3.19316600	-1.70347900
C	-0.16106600	-3.74236700	-0.99505000	C	1.03094800	4.89428000	-1.49670400
H	-0.10361500	-2.88955100	0.95947000	H	0.84345600	2.93106600	-2.35542500
H	1.62421400	-4.42529400	1.95076900	H	3.14427300	2.13773700	-1.75440800
H	0.22549300	-5.26937200	1.29277400	H	3.17510800	3.67015500	-2.64175400
H	1.74891500	-5.27762300	0.40582500	H	3.44526100	3.66290100	-0.89808800
H	-0.56369800	-2.85093200	-1.48436000	H	-0.04002700	5.09044300	-1.57260700
H	0.46789500	-4.27398300	-1.71717500	H	1.40994300	5.39326700	-0.59796100
				H	1.51059900	5.37174400	-2.35993200

C -6.13107700 0.42316000 -0.47731700
 C -6.05461500 0.14005800 1.02453400
 C -5.66157600 -2.19091100 0.51560100
 C -5.74628000 -1.84764400 -0.97287800
 H -5.63703700 1.00695500 1.54949100
 H -5.13644200 0.72187800 -0.85150100
 H -6.83540000 1.23426900 -0.69466600
 H -4.95864000 -3.01734100 0.67058600
 H -6.65071500 -2.52538500 0.85832800
 H -4.73587600 -1.63880000 -1.36529700
 H -6.17244400 -2.67630300 -1.54959000
 H -7.07253400 -0.02120800 1.40571900
 O -6.59648800 -0.72113100 -1.19341500
 N -5.25007800 -1.04768900 1.34205300
 H -4.27057500 -0.84003400 1.14520700

TS1_2

Fe 1.15349900 0.05221100 -0.18720900
 H -0.44610100 -0.06680900 0.04910500
 H 2.67991300 0.16187900 -0.31832700
 B -2.23912900 -0.33336600 -0.00398500
 H -2.15476700 -1.09050500 0.92515500
 H -2.43755500 0.83230100 0.19830900
 H -2.18248800 -0.74819600 -1.12808100
 C 2.36713600 -1.09260400 2.35068500
 C 1.81651500 -2.40683500 1.79950400
 H 2.45296200 -1.14295000 3.44731100
 H 3.36554100 -0.91630100 1.94656100
 H 0.88238700 -2.67876000 2.29949100
 H 2.52679500 -3.21754700 1.99318900
 P 1.46039300 -2.19274300 -0.01936800
 N 1.52852800 0.08488200 1.97093800
 C -0.02077000 -3.31398700 -0.32923600
 C -0.05727300 -4.68413900 0.36881800
 C -0.33205900 -3.43299800 -1.82967000
 H -0.81637100 -2.70712300 0.11440300
 H 0.17101500 -4.61817500 1.43696300
 H -1.06910300 -5.10067100 0.28226100
 H 0.62789600 -5.40877100 -0.07655700
 H -0.38478800 -2.45341500 -2.31191700
 H 0.41463300 -4.03421500 -2.35972400
 H -1.30344100 -3.92218500 -1.97022600
 C 2.94070100 -2.94482500 -0.93053000
 C 3.04662000 -4.47739800 -0.90195800

C 4.27283200 -2.33363700 -0.46480600
 H 2.77532600 -2.62854200 -1.96927100
 H 2.21176100 -4.96797700 -1.40521500
 H 3.96337300 -4.78744400 -1.41895500
 H 3.10685500 -4.86460600 0.12150100
 H 4.25541900 -1.24217100 -0.49184100
 H 4.52421500 -2.65132300 0.55398700
 H 5.08125100 -2.67951100 -1.12014400
 C 0.27668500 0.06398700 2.76536000
 H 0.49923800 0.11224400 3.84260100
 H -0.35721000 0.90575700 2.49298700
 H -0.28408500 -0.84479100 2.55632200
 P 1.15410000 2.32391400 -0.00684000
 C 2.30252500 1.31931500 2.30401300
 C 1.63390100 2.58811300 1.77860300
 H 3.28589000 1.20741800 1.84399300
 H 2.44091600 1.38305000 3.39479700
 H 0.73253700 2.82032800 2.35203200
 H 2.31086800 3.44066900 1.89699600
 C 0.98231600 0.04613400 -1.90501400
 O 0.89927500 0.04580600 -3.07133800
 C -0.49914500 3.21485300 -0.18120700
 C -0.93122900 3.28769300 -1.65360200
 C -0.69288700 4.56241200 0.53344100
 H -1.16007000 2.49100000 0.30787600
 H -0.89051500 2.30783600 -2.13779600
 H -1.96539600 3.64598100 -1.72177000
 H -0.30713000 3.97921100 -2.23072200
 H -0.35635000 4.54065100 1.57436300
 H -0.18156800 5.38725200 0.03218200
 H -1.76288900 4.80610300 0.54646100
 C 2.41672200 3.29667600 -1.02634800
 C 3.85378600 2.81969100 -0.76047400
 C 2.34818500 4.82563700 -0.89146700
 H 2.16178500 3.02915200 -2.06081200
 H 3.95578100 1.73957500 -0.88094700
 H 4.53729300 3.31121100 -1.46314200
 H 4.18297500 3.08597900 0.25127100
 H 1.41600100 5.24002800 -1.27918700
 H 2.46200300 5.14889500 0.14951000
 H 3.16730900 5.27957100 -1.46302700
 C -6.66323000 -0.14086400 -1.10208800
 C -5.14687400 0.04864700 -1.11869200
 C -5.12285200 -0.37102500 1.26930100

C -6.64088200 -0.54688900 1.21876200
H -4.72759600 -0.28963900 -2.07165600
H -6.91228600 -1.19052700 -1.33701600
H -7.14623000 0.49797400 -1.84889200
H -4.68848600 -1.01343900 2.04239400
H -4.88390600 0.66935000 1.52182200
H -6.88944600 -1.61475600 1.08878300
H -7.10673600 -0.20064900 2.14746300
H -4.90981900 1.11356300 -1.00600800
O -7.21608400 0.22074900 0.16299500
N -4.48542400 -0.67580800 -0.02152300
H -4.55195800 -1.67791300 -0.19788400

2

Fe 0.00001500 -0.19960100 0.05943200
H 0.00001900 -0.73565200 -1.42384000
H 0.00002300 0.44096300 1.47475800
C -1.21080100 2.55133500 -0.10898900
C -2.49992100 1.79620900 -0.43517400
H -1.26050800 3.57957200 -0.50086000
H -1.08134000 2.60574600 0.97324000
H -2.75171300 1.89140100 -1.49481700
H -3.33464200 2.22817400 0.12630900
P -2.25373000 -0.01199200 -0.02995700
N 0.00002900 1.86596300 -0.65279000
C -3.08567000 -0.93949800 -1.44916600
C -4.42363400 -0.41575400 -1.99627700
C -3.15121800 -2.44465700 -1.14729800
H -2.33289300 -0.80000600 -2.23467300
H -4.41145200 0.66293600 -2.18089700
H -4.63160200 -0.90343000 -2.95698500
H -5.26641800 -0.63374200 -1.33656400
H -2.17596000 -2.83884700 -0.84663100
H -3.87151100 -2.66994000 -0.35286900
H -3.46997500 -2.99283000 -2.04194500
C -3.28089000 -0.32826100 1.52368000
C -4.80368200 -0.20797800 1.35814900
C -2.80866900 0.55703700 2.68833000
H -3.04237500 -1.36926900 1.77888000
H -5.21504700 -0.97669900 0.70136500
H -5.28929400 -0.32265400 2.33532600
H -5.09664500 0.77216900 0.96428200
H -1.73276400 0.47189100 2.85494700
H -3.04467800 1.61301200 2.50943900

H -3.32580900 0.25944300 3.60837400
C 0.00004300 1.98070600 -2.13195000
H 0.00005700 3.03750500 -2.44066900
H 0.87730100 1.48715900 -2.54669000
H -0.87721800 1.48717700 -2.54670600
P 2.25375900 -0.01203100 -0.02993300
C 1.21086300 2.55131100 -0.10897100
C 2.49997600 1.79616700 -0.43514800
H 1.08139200 2.60571800 0.97325700
H 1.26059100 3.57954900 -0.50083400
H 2.75177600 1.89135500 -1.49478900
H 3.33469900 2.22812000 0.12634000
C 0.00000200 -1.76810700 0.77989500
O -0.00009700 -2.80986200 1.31306200
C 3.08567900 -0.93954500 -1.44915800
C 3.15151300 -2.44466700 -1.14716500
C 4.42346300 -0.41562500 -1.99654600
H 2.33276900 -0.80025500 -2.23457200
H 2.17636200 -2.83899000 -0.84632800
H 3.47023700 -2.99286700 -2.04180900
H 3.87195200 -2.66976100 -0.35281700
H 4.41107600 0.66305000 -2.18123800
H 5.26640500 -0.63343500 -1.33698000
H 4.63133100 -0.90333100 -2.95726000
C 3.28085900 -0.32830900 1.52374900
C 2.80842400 0.55682800 2.68843400
C 4.80364900 -0.20782200 1.35838100
H 3.04245200 -1.36936500 1.77885200
H 1.73251700 0.47151200 2.85496000
H 3.32553400 0.25923500 3.60849500
H 3.04429300 1.61285200 2.50964600
H 5.21519200 -0.97649800 0.70165900
H 5.09652600 0.77236100 0.96453700
H 5.28916600 -0.32242100 2.33561500

Morpholine-BH₃ (N site)

B 2.56968700 -0.00002800 -0.06974200
H 3.04024700 1.00763200 0.42187700
H 2.65514100 0.00008100 -1.28208200
H 3.04021900 -1.00760500 0.42192000
C -1.20155700 -1.17245400 0.18229600
C 0.27677800 -1.22444600 -0.18290800
C 0.27677200 1.22445800 -0.18291300
C -1.20156800 1.17245000 0.18230000

H 0.76198300 -2.09551900 0.26237700
H -1.32271100 -1.22139200 1.27739300
H -1.72098700 -2.02977200 -0.25440200
H 0.76204300 2.09548200 0.26239900
H 0.40814300 1.26440000 -1.26713000
H -1.32273500 1.22142800 1.27741000
H -1.72103800 2.02974900 -0.25440400
H 0.40816400 -1.26439100 -1.26712600
O -1.82716000 -0.00000800 -0.32968700
N 0.99222600 0.00000600 0.29666500
H 0.93224900 0.00002300 1.31866300

THF

C -1.13422100 -0.46866800 0.15785300
O 0.00000000 -1.20790800 -0.29506300
C 1.13422000 -0.46866900 0.15785300
C 0.77692500 1.01632000 -0.05094700
C -0.77692500 1.01632000 -0.05094700
H -2.00514500 -0.80131100 -0.41429700
H -1.32269400 -0.67642900 1.22439000
H 1.32269300 -0.67643000 1.22439000
H 2.00514500 -0.80131300 -0.41429600
H 1.19933200 1.64657900 0.73666700
H 1.16446300 1.37688500 -1.00794700
H -1.19933100 1.64657900 0.73666700
H -1.16446300 1.37688600 -1.00794700

TS1b_2

Fe -0.98556000 0.23315600 -0.20073800
H 0.52428900 -0.30877600 -0.08835700
H -2.44507400 0.73714500 -0.20759300
B 2.49214000 -0.83524000 -0.28759200
H 2.67560200 -0.29573200 0.76749600
H 2.16522700 -1.98479200 -0.31445500
H 2.54831400 -0.20736600 -1.30286000
C -1.48677000 1.67431500 2.41493000
C -0.49945400 2.69241300 1.84444100
H -1.49592300 1.72437700 3.51495400
H -2.49330500 1.90213400 2.05964100
H 0.48489200 2.58403700 2.30788200
H -0.84303500 3.70823800 2.06653500
P -0.32844100 2.39875900 0.00889800
N -1.17993700 0.27693600 1.98304000
C 1.47704500 2.77818200 -0.37984400

C 2.15291400 3.94642200 0.35610100
C 1.70952100 2.85242000 -1.89741400
H 1.94920800 1.85399900 -0.03049100
H 2.01496300 3.89354400 1.44037500
H 3.23366400 3.90992000 0.16806500
H 1.79975900 4.92414900 0.01993700
H 1.28300100 1.98973100 -2.41710600
H 1.28208200 3.76058100 -2.33605200
H 2.78562600 2.86356900 -2.10850100
C -1.37199900 3.74803400 -0.80845900
C -0.83654500 5.18186200 -0.67136700
C -2.83308200 3.69688000 -0.33261500
H -1.35620700 3.47093700 -1.87094400
H 0.11722000 5.32594400 -1.18205400
H -1.55249000 5.88417900 -1.11647300
H -0.71016600 5.47040600 0.37850500
H -3.25695600 2.69457000 -0.42226900
H -2.92286300 4.01690000 0.71230000
H -3.43927900 4.38345100 -0.93564200
C 0.04097800 -0.18728500 2.68729400
H -0.10580900 -0.15542600 3.77813700
H 0.28454400 -1.20535700 2.38857300
H 0.89040400 0.43859100 2.42155400
P -1.83503000 -1.86777000 -0.02902400
C -2.33029500 -0.59063700 2.38069100
C -2.22998900 -1.99774300 1.79155800
H -3.23535400 -0.10349200 2.01386300
H -2.39137300 -0.63952100 3.47934800
H -1.43223400 -2.56639200 2.27778600
H -3.16171600 -2.54405000 1.97288200
C -0.94992400 0.24954700 -1.92662300
O -0.96348300 0.27811700 -3.09577600
C -0.64316900 -3.29496700 -0.33926200
C -0.35095500 -3.44767500 -1.84001200
C -0.92287100 -4.65312900 0.32522300
H 0.26236800 -2.88510400 0.12178200
H -0.04877400 -2.49770800 -2.29045800
H 0.46879800 -4.16017500 -1.99172600
H -1.22046200 -3.82632900 -2.38914500
H -1.18859700 -4.56097900 1.38286500
H -1.71814700 -5.21298100 -0.17198600
H -0.01519900 -5.26785100 0.27420900
C -3.44612900 -2.27016000 -0.93559300
C -4.58550500 -1.33207700 -0.50595700

C -3.91668100 -3.72949200 -0.85037200
 H -3.20658700 -2.04665600 -1.98373900
 H -4.30224200 -0.28076800 -0.58903300
 H -5.46088300 -1.50459000 -1.14348200
 H -4.89453500 -1.52611700 0.52811200
 H -3.22833000 -4.42003800 -1.34059100
 H -4.04999600 -4.05671400 0.18711200
 H -4.88819600 -3.82970700 -1.35026900
 C 5.45752600 -0.24091600 -0.33718100
 O 4.56372300 -1.36363800 -0.41637600
 C 5.00395300 -2.29483100 0.59122200
 C 6.54238300 -2.16277500 0.64637100
 C 6.83963100 -0.87363200 -0.16507100
 H 5.33651400 0.34455000 -1.25108900
 H 5.19090600 0.38712700 0.52591100
 H 4.54608000 -2.03173800 1.55453700
 H 4.65096100 -3.28519000 0.29535800
 H 6.88446900 -2.08122400 1.68165700
 H 7.03592900 -3.03105200 0.20251200
 H 7.53753000 -0.20185700 0.34189900
 H 7.26143700 -1.12398200 -1.14282500

THF-BH₃

B 2.28019200 -0.00778400 0.13125700
 H 2.31395800 0.16112200 1.33550800
 H 2.75038900 0.91900900 -0.49002100
 H 2.71658300 -1.08364700 -0.21207500
 C -0.06906800 -1.19159900 0.11981500
 O 0.74228100 -0.03869100 -0.28624000
 C -0.04012900 1.20581200 -0.13723500
 C -1.44375000 0.74849200 0.26257200
 C -1.48690400 -0.72963000 -0.16333000
 H 0.27503400 -2.03933100 -0.47302600
 H 0.11025900 -1.38240800 1.18314800
 H 0.45315000 1.82206900 0.61587400
 H 0.00155400 1.70418300 -1.10764900
 H -1.57414400 0.83259000 1.34538700
 H -2.21497700 1.35165800 -0.22167000
 H -2.22209300 -1.31079100 0.39801100
 H -1.70981500 -0.82444700 -1.23078700

TS1c_2

Fe -1.17287900 0.11817000 -0.18852200
 H 0.34860400 -0.16509300 0.24577800

H -2.65611100 0.40251600 -0.50217100
 B 2.39390200 -0.43988800 0.32412700
 H 2.37182200 0.19507400 1.33988500
 H 2.21338700 -1.62109900 0.35794800
 H 2.49243200 0.11882300 -0.72906000
 C -2.33740700 1.61721000 2.17408200
 C -1.41485500 2.73769400 1.69529400
 H -2.54788900 1.72793600 3.24932100
 H -3.28679900 1.67306800 1.63877700
 H -0.52020600 2.80058400 2.32088500
 H -1.92720800 3.70213000 1.77773700
 P -0.88729500 2.36938000 -0.05585700
 N -1.77085000 0.25915700 1.91499100
 C 0.88271000 3.00837100 -0.17251800
 C 1.23824600 4.32393700 0.53969900
 C 1.37133400 3.00583500 -1.62948400
 H 1.41480800 2.20288200 0.34406400
 H 0.88903300 4.35095000 1.57646800
 H 2.33017800 4.43138800 0.56624900
 H 0.84108800 5.20380600 0.02872100
 H 1.19457100 2.04242000 -2.11508400
 H 0.88479300 3.78446900 -2.22727900
 H 2.45069600 3.19755100 -1.66062100
 C -1.95688500 3.48852300 -1.14479000
 C -1.66646500 4.99415300 -1.04756900
 C -3.45583100 3.23930800 -0.91046600
 H -1.71834700 3.15372200 -2.16309900
 H -0.66985200 5.25637100 -1.40697400
 H -2.38831900 5.54537000 -1.66319000
 H -1.76948900 5.36279100 -0.02070200
 H -3.70969000 2.17986800 -0.98633600
 H -3.77168100 3.59894600 0.07607600
 H -4.03976900 3.78895300 -1.65842500
 C -0.64429700 0.02109300 2.85151100
 H -0.98716800 0.09078300 3.89559600
 H -0.21358900 -0.96379900 2.68091100
 H 0.14529900 0.75123900 2.68305800
 P -1.75196800 -2.07463800 0.00907800
 C -2.84671300 -0.74448800 2.17800400
 C -2.45005500 -2.15327700 1.73871400
 H -3.72516400 -0.42025100 1.61735300
 H -3.10394600 -0.73593500 3.24887200
 H -1.68662400 -2.56669800 2.40327700
 H -3.31650700 -2.81957500 1.80168400

C -0.79905200 0.02363200 -1.87156400
 O -0.57393200 -0.03600200 -3.01800700
 C -0.34515900 -3.33010200 0.02024800
 C 0.19699200 -3.55902600 -1.39885600
 C -0.54663700 -4.65697600 0.76988400
 H 0.41451700 -2.75887800 0.56533500
 H 0.41784700 -2.61533100 -1.90575400
 H 1.12860000 -4.13599500 -1.35582000
 H -0.50846300 -4.12230800 -2.01993100
 H -0.95521800 -4.51642400 1.77521100
 H -1.20050400 -5.35094800 0.23708900
 H 0.42579100 -5.15257200 0.88537600
 C -3.10339600 -2.76099800 -1.12331900
 C -4.40656300 -1.95415400 -1.00589500
 C -3.40976500 -4.25940500 -0.97514600
 H -2.69554600 -2.59162300 -2.12894000
 H -4.24221000 -0.88649500 -1.16353100
 H -5.12363200 -2.30704600 -1.75675000
 H -4.87440000 -2.08846200 -0.02313800
 H -2.56534400 -4.89097900 -1.25636000
 H -3.70783200 -4.51807600 0.04729300
 H -4.24635900 -4.52646600 -1.63296300
 C 5.20754000 0.54210700 0.49540200
 C 6.70106100 0.30966000 0.72055700
 C 6.49665400 -1.85048100 -0.33288200
 C 5.00654300 -1.58843700 -0.54535800
 H 7.23079300 1.26786600 0.67781200
 H 5.03774300 1.06910600 -0.45628400
 H 4.76372200 1.13071600 1.30287600
 H 6.87781200 -2.47713600 -1.14681600
 H 6.63066900 -2.40513600 0.60503500
 H 4.82896700 -1.13621000 -1.53328600
 H 4.42042600 -2.50850200 -0.47440600
 H 6.84974300 -0.10780500 1.72493600
 O 4.50148400 -0.71131500 0.47796600
 N 7.29250600 -0.61777700 -0.25312900
 H 7.28878700 -0.17080200 -1.17006600

Morpholine-BH₃ (O site)

B -2.55689200 0.00012800 -0.04351600
 H -2.92795600 -1.01181000 -0.59178200
 H -2.92801300 1.01228700 -0.59132300
 H -2.75970000 -0.00018000 1.15442800
 C -0.28745700 -1.21649000 0.22729800

C 1.16434100 -1.20328800 -0.23396200
 C 1.16470700 1.20308300 -0.23402200
 C -0.28701500 1.21670600 0.22734700
 H 1.66221200 -2.09008100 0.17117100
 H -0.37397400 -1.24558900 1.32012900
 H -0.85178400 -2.04323700 -0.20474000
 H 1.66290000 2.08978400 0.17094300
 H 1.19253300 1.27759600 -1.32799400
 H -0.37340000 1.24558300 1.32017400
 H -0.85130300 2.04351700 -0.20459500
 H 1.19223600 -1.27796700 -1.32793200
 O -0.96018100 0.00011500 -0.24261700
 N 1.89796500 -0.00019800 0.16703700
 H 2.00894100 -0.00014900 1.18080900

TS1_2 (Pyrrolidine)

Fe -0.92821400 0.24843900 -0.19390800
 H 0.57128300 -0.36549600 -0.09698100
 H -2.35691400 0.81799600 -0.18952900
 B 2.27791600 -0.93429700 -0.26065800
 H 2.59998100 -0.23161200 0.65860900
 H 1.94518500 -2.06744300 -0.05090000
 H 2.34835200 -0.53023900 -1.38765100
 C -1.32027100 1.70583500 2.43503000
 C -0.29827400 2.67787300 1.84572500
 H -1.30407600 1.75370500 3.53507700
 H -2.32218300 1.98364400 2.10241600
 H 0.69199200 2.51629800 2.28058300
 H -0.58375900 3.70763500 2.08573500
 P -0.18896000 2.38912900 0.00564200
 N -1.08992800 0.29640700 1.99394800
 C 1.61438700 2.71905800 -0.43469600
 C 2.34206600 3.86784000 0.28252100
 C 1.80868500 2.78772300 -1.95795300
 H 2.07220900 1.78307400 -0.09794800
 H 2.21254800 3.83248200 1.36849700
 H 3.41872200 3.78719900 0.08513000
 H 2.02471700 4.85497400 -0.06173400
 H 1.34683300 1.93671200 -2.46626100
 H 1.39345600 3.70628000 -2.38653700
 H 2.87882700 2.77156800 -2.19703700
 C -1.21367100 3.77217800 -0.77951100
 C -0.62738900 5.18723200 -0.65471900
 C -2.66289300 3.77023900 -0.26576200

H -1.23601000 3.49797200 -1.84260800
H 0.31374500 5.30180800 -1.19522800
H -1.33353300 5.91425700 -1.07492700
H -0.45776500 5.46704300 0.39133100
H -3.12936400 2.78749400 -0.35910000
H -2.71432000 4.07824800 0.78522000
H -3.25652800 4.48889000 -0.84341800
C 0.11871100 -0.22972900 2.67512100
H -0.01259400 -0.20196200 3.76795100
H 0.31186900 -1.25488600 2.36425400
H 0.99216600 0.35995100 2.40535300
P -1.93093300 -1.78373800 -0.02475600
C -2.27344100 -0.51549400 2.41223000
C -2.26103900 -1.91905800 1.80662800
H -3.16213600 0.02084900 2.07506300
H -2.30863600 -0.57384900 3.51142200
H -1.46789800 -2.52780200 2.25056500
H -3.20688300 -2.42588800 2.02295500
C -0.91238700 0.25940700 -1.92030400
O -0.93969700 0.28352100 -3.08917300
C -0.88912200 -3.30656200 -0.39924600
C -0.60680800 -3.43757200 -1.90385700
C -1.30298800 -4.64941500 0.22541200
H 0.05319400 -3.00752800 0.07370700
H -0.21897600 -2.50455600 -2.32305900
H 0.14717300 -4.21527900 -2.07556700
H -1.50138700 -3.72118300 -2.46961900
H -1.53002000 -4.56353500 1.29267100
H -2.16753400 -5.09991100 -0.26664700
H -0.47098900 -5.35892300 0.13072500
C -3.60710900 -1.98628900 -0.88014100
C -4.66414000 -1.04534600 -0.27886100
C -4.17196700 -3.41340900 -0.95088600
H -3.40204500 -1.64499900 -1.90342600
H -4.31116100 -0.01321600 -0.22693500
H -5.56819700 -1.06599400 -0.89921600
H -4.95622900 -1.36422900 0.72859500
H -3.53994100 -4.08781700 -1.53178000
H -4.31458400 -3.84742500 0.04516900
H -5.15493900 -3.39003700 -1.43776500
C 6.48704100 -2.27033900 0.79899500
C 6.81464400 -1.16690300 -0.24655700
C 5.43789900 -0.56558000 -0.60798400
C 4.93563800 -2.31943000 0.84173100

H 6.90230800 -3.23478200 0.49029000
H 6.90201500 -2.04109500 1.78532300
H 7.27823600 -1.60736700 -1.13573800
H 7.50515100 -0.41045500 0.13922300
H 5.19522100 0.26931400 0.06136400
H 5.36917900 -0.20267300 -1.63656000
H 4.55911400 -1.76641700 1.71076900
H 4.52934200 -3.33271200 0.89153500
N 4.44996400 -1.63396100 -0.37132800
H 4.48004500 -2.28572300 -1.15418100

Pyrrolidine-BH₃

B 2.31830500 -0.00080300 0.08047300
H 2.36945500 0.03586200 1.29573700
H 2.80847100 0.99123100 -0.42554300
H 2.81098100 -1.02016400 -0.36538300
C -1.51685300 0.76901600 0.04553900
C -1.49762600 -0.77951300 -0.08317300
C -0.04271400 -1.16924800 0.19459900
C -0.03137100 1.19114200 0.09482500
H -2.03371000 1.22694200 -0.80171000
H -2.03035900 1.09305000 0.95416600
H -1.77986400 -1.08335300 -1.09645900
H -2.18470600 -1.27034500 0.61017600
H 0.16416300 -1.24139800 1.26566400
H 0.28708500 -2.08838700 -0.29169500
H 0.28725000 1.43426300 1.11068500
H 0.22426700 2.02678100 -0.55768600
N 0.75773800 -0.01517600 -0.32380600
H 0.71265700 -0.06262000 -1.34441600

TS1_2 (N-methyl piperazine)

Fe -1.39203500 0.09728700 -0.18473900
H 0.14581800 -0.15718700 0.25227900
H -2.87412100 0.35183100 -0.51272900
B 1.94756700 -0.33742200 0.30656600
H 1.96494500 0.36753400 1.28051900
H 1.83535900 -1.52465400 0.43725700
H 2.09136800 0.13480500 -0.78597700
C -2.56606300 1.58412200 2.18303200
C -1.65269800 2.70994100 1.69983600
H -2.76588800 1.68871700 3.26085000
H -3.52145600 1.63973600 1.65861700
H -0.74587600 2.76444900 2.30848100

H -2.16208700 3.67397500 1.80376500
P -1.15786100 2.35951100 -0.06371600
N -1.99925300 0.22856500 1.91161700
C 0.58712000 3.05214700 -0.23094500
C 0.92604200 4.35995400 0.50321200
C 1.02493500 3.10121800 -1.70361800
H 1.16239700 2.25184900 0.24547200
H 0.63062500 4.33967000 1.55673200
H 2.01264500 4.51219400 0.47805500
H 0.46651000 5.23778400 0.04300400
H 0.84283800 2.15325100 -2.21705000
H 0.51214100 3.89349900 -2.25983700
H 2.10080200 3.30500400 -1.76324700
C -2.28591200 3.44823800 -1.12454100
C -2.04106800 4.96186500 -1.02006300
C -3.77262400 3.15282200 -0.86812600
H -2.05357900 3.12739300 -2.14899900
H -1.05795300 5.25869600 -1.38906900
H -2.78758800 5.49474200 -1.62215900
H -2.14250200 5.31914400 0.01093500
H -3.99737500 2.08733600 -0.94898600
H -4.08333500 3.49598400 0.12585500
H -4.38408000 3.69093800 -1.60239800
C -0.87019000 -0.01765300 2.84219200
H -1.21107100 0.03609200 3.88788900
H -0.43573500 -0.99839200 2.65692000
H -0.08411800 0.71792600 2.68176900
P -1.96520600 -2.10074000 0.00344200
C -3.07590200 -0.77634100 2.16768100
C -2.67794400 -2.18410700 1.72686700
H -3.95175100 -0.45061200 1.60389100
H -3.33747700 -0.77012200 3.23747600
H -1.92106000 -2.60147800 2.39639700
H -3.54607600 -2.84907500 1.77976200
C -0.98137700 -0.00456100 -1.85743200
O -0.71555900 -0.07422300 -2.99402700
C -0.56100900 -3.35876500 0.02195200
C -0.00734700 -3.58635600 -1.39321000
C -0.77096800 -4.68689100 0.76727000
H 0.19757100 -2.79107700 0.57292000
H 0.22708200 -2.64282600 -1.89390700
H 0.91931300 -4.17062100 -1.34289900
H -0.71059800 -4.14141200 -2.02396600
H -1.18700800 -4.54824500 1.76981500

H -1.42187100 -5.37839600 0.22768800
H 0.19964900 -5.18472000 0.88867000
C -3.30750100 -2.78012000 -1.14449100
C -4.61418000 -1.97873600 -1.03015000
C -3.61078600 -4.28047900 -1.01085000
H -2.89274500 -2.60136200 -2.14562600
H -4.45218200 -0.90960900 -1.17920100
H -5.32468900 -2.32871600 -1.78853600
H -5.08833300 -2.12155600 -0.05162300
H -2.76239500 -4.90782800 -1.28936600
H -3.91773400 -4.54789600 0.00666600
H -4.44053900 -4.54414600 -1.67859000
C 6.42883300 0.50756000 0.74666200
C 4.91762700 0.69153100 0.58163000
C 4.77895900 -1.47267800 -0.49274300
C 6.29151400 -1.64628100 -0.32655300
H 4.51567500 1.28657500 1.40751200
H 6.63667900 0.07998500 1.74984200
H 6.92840500 1.48293100 0.70198900
H 4.27815500 -2.44436700 -0.44217700
H 4.56593600 -1.03592300 -1.47557800
H 6.49357300 -2.21005600 0.60817900
H 6.68972300 -2.24319300 -1.15588800
H 4.71532600 1.23003800 -0.35196400
N 6.96230900 -0.34429600 -0.31815500
C 8.40769400 -0.48557200 -0.21941900
H 8.73547500 -0.97691600 0.71728800
H 8.78175400 -1.08179200 -1.05881600
H 8.88213700 0.50073500 -0.26484300
N 4.19362200 -0.58632800 0.52373400
H 4.25519400 -1.04150400 1.43412100

N-methyl piperazine-BH₃

B -3.01923900 -0.00000700 -0.07923400
H -3.49251500 1.00707500 0.41166200
H -3.49249800 -1.00715500 0.41152900
H -3.10508500 0.00010400 -1.29189300
C 0.74690900 1.19956900 0.19394100
C -0.72806300 1.22440700 -0.19033100
C -0.72804200 -1.22441900 -0.19034000
C 0.74692500 -1.19955300 0.19394300
H -1.23053300 2.09189400 0.24127500
H 0.84191600 1.27194000 1.29654800
H 1.23299000 2.08490600 -0.22935000

H -1.23048400 -2.09190600 0.24128600
H -0.84624500 -1.25432800 -1.27621700
H 0.84192100 -1.27192500 1.29655100
H 1.23302400 -2.08489300 -0.22933700
H -0.84624800 1.25431100 -1.27621100
N 1.40029600 0.00000500 -0.32701500
C 2.83112700 0.00000300 -0.05162700
H 3.06712600 -0.00002800 1.02911500
H 3.29292100 -0.88667000 -0.49789800
H 3.29289600 0.88671400 -0.49784100
N -1.44238100 -0.00001000 0.28759400
H -1.38154000 -0.00000800 1.30938800

TS1_2 (Piperidine)

Fe -1.12953600 0.12076900 -0.17747900
H 0.39530800 -0.16712700 0.29686000
H -2.59630500 0.40358500 -0.54771600
B 2.17934800 -0.42452600 0.35387000
H 2.23449200 0.28140700 1.32624400
H 2.02368500 -1.60611200 0.48990800
H 2.33959600 0.03877800 -0.74016900
C -2.34224900 1.65621100 2.13772900
C -1.38897000 2.75777600 1.67766100
H -2.57870500 1.77500000 3.20663700
H -3.27635300 1.72613600 1.57771900
H -0.50396600 2.80092400 2.31839900
H -1.88245000 3.73254900 1.75387600
P -0.83998700 2.37936900 -0.06410900
N -1.79469500 0.28668100 1.89891900
C 0.92877900 3.02212500 -0.17007100
C 1.27628400 4.32153800 0.57465700
C 1.41878200 3.05688200 -1.62669100
H 1.46604300 2.20783200 0.32667300
H 0.96033400 4.30324500 1.62215300
H 2.36573100 4.45440500 0.57135000
H 0.84147400 5.20885900 0.10906900
H 1.23004300 2.11219800 -2.14375900
H 0.94610500 3.86061200 -2.20163100
H 2.50091400 3.23295100 -1.64909900
C -1.89626300 3.49149700 -1.17386400
C -1.61545000 4.99897100 -1.07106400
C -3.39852700 3.23748000 -0.96870000
H -1.63611300 3.15695000 -2.18713400
H -0.61143700 5.26760100 -1.40415700

H -2.32416400 5.54557600 -1.70574900
H -1.74826100 5.36728500 -0.04748100
H -3.64777800 2.17714700 -1.04671900
H -3.73488900 3.59882900 0.01040500
H -3.96944900 3.78313900 -1.72951900
C -0.69903400 0.02986000 2.86529300
H -1.06562900 0.11791500 3.89984700
H -0.29009000 -0.96761800 2.71529000
H 0.11281900 0.73805600 2.70969300
P -1.76960200 -2.05896300 0.00778500
C -2.90009900 -0.69158000 2.13555800
C -2.52640000 -2.11131000 1.71307900
H -3.75462800 -0.34874200 1.54969000
H -3.18659200 -0.67183800 3.19876800
H -1.79597300 -2.54318200 2.40264800
H -3.41184900 -2.75396700 1.75017200
C -0.67792500 -0.00340600 -1.83830900
O -0.38621900 -0.08934500 -2.96728500
C -0.41315100 -3.36415000 0.07406100
C 0.18747500 -3.60961800 -1.31912500
C -0.69432400 -4.68610700 0.80816600
H 0.34347600 -2.82264800 0.65395800
H 0.47942900 -2.67529300 -1.80646500
H 1.08725000 -4.23048400 -1.23305300
H -0.51088400 -4.13490200 -1.97999300
H -1.14979700 -4.53614000 1.79173300
H -1.34066600 -5.35818200 0.23918400
H 0.25552000 -5.21161100 0.97018700
C -3.10555100 -2.69671800 -1.17225000
C -4.40035600 -1.87482300 -1.06700400
C -3.43862000 -4.19300400 -1.06693100
H -2.67114300 -2.50997000 -2.16353800
H -4.21793200 -0.80563800 -1.18965700
H -5.10054200 -2.19564100 -1.84749400
H -4.89720600 -2.03119800 -0.10191600
H -2.59733300 -4.83225700 -1.33968800
H -3.76864200 -4.46975600 -0.05921900
H -4.26108800 -4.43097200 -1.75312300
C 6.70034400 0.31041100 0.71302800
C 5.18268700 0.50315600 0.57460400
C 4.93618500 -1.67822300 -0.50079000
C 6.44533000 -1.94595800 -0.39862100
H 4.78778700 1.10824100 1.39747000
H 6.91987100 -0.11373400 1.70339500

H 7.20236700 1.28521200 0.66785000
H 4.36677500 -2.61127900 -0.43632500
H 4.70416000 -1.22646200 -1.47446200
H 6.64856300 -2.51050400 0.52274700
H 6.76569700 -2.57913600 -1.23560000
H 4.96090600 1.04110800 -0.35687700
N 4.43174200 -0.76223300 0.53549200
H 4.50606600 -1.21836400 1.44408000
C 7.23564300 -0.62833800 -0.37906400
H 8.30427200 -0.82288700 -0.22913400
H 7.13910600 -0.13575600 -1.35706600

Piperidine-BH₃

B 2.58789100 -0.00004800 0.06671100
H 3.06022400 1.00663200 -0.42643200
H 3.05991900 -1.00651100 -0.42706600
H 2.68444800 -0.00025200 1.27912900
C -1.16545000 1.25971400 -0.21219300
C 0.30821800 1.23639000 0.19248400
C 0.30837000 -1.23628300 0.19251300
C -1.16523500 -1.25983100 -0.21219400
H 0.85241200 2.09130800 -0.21367000
H -1.23921700 1.34102500 -1.30535400
H -1.62611300 2.16292000 0.20283500
H 0.85286400 -2.09102200 -0.21353000
H 0.41997300 -1.25078200 1.28099900
H -1.23915300 -1.34129000 -1.30536200
H -1.62590400 -2.16308100 0.20276700
H 0.41989700 1.25109800 1.28094600
N 1.00833800 0.00014900 -0.28666700
H 0.94059700 0.00009300 -1.30763100
C -1.89913200 -0.00009800 0.26583400
H -2.93292300 -0.00014100 -0.09630800
H -1.94546800 -0.00015200 1.36312800

A3

Fe -0.00008100 -0.41585500 0.21097100
H 0.00004100 1.14357400 0.43994900
H -0.00016800 -1.93249600 -0.15368000
C 1.22852900 -0.54668300 -2.55565600
C 2.46270200 -0.00752600 -1.83352900
H 1.23563300 -0.24192200 -3.61248400
H 1.20409100 -1.63885300 -2.51799400
H 2.53729100 1.07365300 -1.99535800

H 3.37762500 -0.45730100 -2.23170300
P 2.25350700 -0.29750200 -0.00008500
N -0.00000200 -0.05890400 -1.88435800
C 3.06433700 1.20716700 0.80251800
C 4.36858500 1.74709900 0.19391900
C 3.18428000 1.01954300 2.32299100
H 2.28397800 1.95787600 0.62906100
H 4.30707900 1.87118100 -0.89172400
H 4.57851200 2.73603800 0.62059900
H 5.23104600 1.11323800 0.41065600
H 2.23155600 0.72196900 2.77092200
H 3.93372800 0.26352100 2.58178200
H 3.49333100 1.96064500 2.79338500
C 3.32321800 -1.79855000 0.41798500
C 4.84202700 -1.60771000 0.28422000
C 2.88005300 -3.03738900 -0.37727900
H 3.08796700 -1.98205000 1.47495300
H 5.23909100 -0.88410500 0.99887500
H 5.34895900 -2.56216600 0.47384900
H 5.12653800 -1.28576400 -0.72418500
H 1.80857600 -3.22372800 -0.27837300
H 3.11563900 -2.93580100 -1.44346200
H 3.41722300 -3.91985000 -0.00967300
P -2.25365800 -0.29710300 -0.00007100
C -1.22880800 -0.54595100 -2.55568600
C -2.46269600 -0.00635200 -1.83340200
H -1.20489500 -1.63814100 -2.51824000
H -1.23580600 -0.24098100 -3.61245400
H -2.53666800 1.07492800 -1.99483500
H -3.37785800 -0.45547700 -2.23176100
C -0.00012100 -0.82364600 1.88967100
O -0.00015900 -1.15185700 3.01304300
C -3.06430700 1.20728700 0.80324300
C -3.18478400 1.01870400 2.32355600
C -4.36821500 1.74792200 0.19453900
H -2.28372300 1.95793300 0.63055800
H -2.23224700 0.72068700 2.77159400
H -3.49380900 1.95956700 2.79444400
H -3.93444100 0.26265600 2.58166100
H -4.30613200 1.87309100 -0.89094700
H -5.23083800 1.11390900 0.41018600
H -4.57828400 2.73645400 0.62209000
C -3.32368400 -1.79812300 0.41730200
C -2.88048900 -3.03683800 -0.37813600

C -4.84243300 -1.60703100 0.28315800
H -3.08876300 -1.98192000 1.47429200
H -1.80909000 -3.22343200 -0.27887400
H -3.41798500 -3.91928400 -0.01096900
H -3.11564500 -2.93491600 -1.44438200
H -5.23959500 -0.88349200 0.99782300
H -5.12662700 -1.28487600 -0.72527100
H -5.34955600 -2.56144800 0.47247800
H 0.00029900 0.95941200 -1.95052000
C 0.00092900 3.85994000 -0.68306900
O 0.00092800 3.36250200 -1.74361100
O 0.00092600 4.39937400 0.35272500

ATS3_4

Fe -0.00304400 -0.21835500 -0.22209200
H -0.00194500 1.37209900 -0.03015200
H -0.01363500 -1.75586200 -0.28114300
C -1.21915900 -1.05401500 2.42544300
C -2.47607300 -0.40695800 1.84521500
H -1.22962700 -0.99453800 3.52352700
H -1.16208700 -2.10933100 2.14598100
H -2.59490500 0.60130300 2.25718700
H -3.36981200 -0.97498500 2.12147900
P -2.26509100 -0.23620700 -0.00187900
N -0.00663900 -0.39105200 1.88457100
C -3.15266400 1.37633300 -0.41316400
C -4.50375600 1.65834400 0.26499000
C -3.22191000 1.60221300 -1.93144100
H -2.43382600 2.10063700 -0.01221200
H -4.48135400 1.46811000 1.34235300
H -4.75648000 2.71728900 0.12883300
H -5.32128500 1.07441600 -0.16307400
H -2.23806200 1.51204500 -2.40095300
H -3.89852500 0.89225200 -2.41938400
H -3.59875700 2.61031100 -2.14152800
C -3.23960000 -1.65213400 -0.78494300
C -4.77085200 -1.54558700 -0.72544500
C -2.79099400 -3.00962200 -0.21984500
H -2.93097400 -1.61133200 -1.83804200
H -5.15472900 -0.69296300 -1.28868200
H -5.21471300 -2.44899400 -1.16217800
H -5.13739900 -1.47139400 0.30463100
H -1.70671700 -3.13410800 -0.26413600
H -3.11215500 -3.13426300 0.82091100

H -3.25173900 -3.81766000 -0.80024000
P 2.26045800 -0.22766100 -0.00550300
C 1.23103300 -0.98962400 2.44297800
C 2.46199400 -0.30726700 1.84738300
H 1.21831800 -2.05369700 2.19242500
H 1.23626600 -0.90119700 3.53908400
H 2.52513200 0.72235500 2.21656000
H 3.37927700 -0.81988800 2.15383700
C -0.00066300 -0.18774200 -1.95163100
O 0.00087200 -0.23631100 -3.11971900
C 3.15300800 1.35435500 -0.51672200
C 3.31942600 1.43029000 -2.04310800
C 4.45625400 1.71904800 0.21338100
H 2.40657700 2.10742000 -0.24055200
H 2.37053400 1.27290400 -2.56456900
H 3.69010200 2.42264500 -2.32617700
H 4.03955000 0.69430600 -2.41612100
H 4.35339800 1.67830800 1.30201000
H 5.29621000 1.08017700 -0.06898900
H 4.73240500 2.74905900 -0.04523500
C 3.25356300 -1.67186100 -0.70953300
C 2.73976300 -3.02026300 -0.17961700
C 4.77736900 -1.59232300 -0.53080400
H 3.02574300 -1.62716900 -1.78338900
H 1.66110200 -3.12713300 -0.31234600
H 3.23487200 -3.83736000 -0.71766900
H 2.97070400 -3.14577600 0.88480900
H 5.22068100 -0.74588800 -1.05830500
H 5.06094100 -1.52630300 0.52591800
H 5.23972200 -2.50280200 -0.93215200
H -0.03369300 0.58817600 2.17645600
C 0.00297400 3.03342900 0.87991600
O -0.08813900 2.67471800 2.00898900
O 0.09448000 3.77681000 -0.03351900

A4

Fe -0.00005900 -0.13571200 -0.20400600
H -0.00029400 1.57757600 0.17140400
H -0.00007600 -1.60335200 -0.41292600
C -1.22455000 -1.06329700 2.39573300
C -2.46979400 -0.37014200 1.84280800
H -1.22042800 -1.01481100 3.49385200
H -1.20289000 -2.11828600 2.10880600
H -2.53636400 0.64059100 2.25866500

H -3.38080300 -0.90484200 2.12850000
 P -2.28038300 -0.19174300 -0.00086800
 N -0.00005000 -0.42203300 1.85363400
 C -3.17927500 1.40230300 -0.45206700
 C -4.47291100 1.71948800 0.31591800
 C -3.37467300 1.52122900 -1.97255600
 H -2.44062500 2.16011600 -0.16701900
 H -4.33279000 1.68361600 1.40022900
 H -4.79273400 2.73852500 0.06621300
 H -5.29541900 1.04776200 0.05901600
 H -2.43639500 1.38207400 -2.51803200
 H -4.10181200 0.79732300 -2.35454400
 H -3.74938900 2.52220100 -2.21566900
 C -3.21627600 -1.62133600 -0.79191600
 C -4.74020700 -1.59917800 -0.59637400
 C -2.65064900 -2.97956600 -0.34488600
 H -2.99932500 -1.50344800 -1.86201000
 H -5.21291700 -0.73725200 -1.07078900
 H -5.17673800 -2.49895300 -1.04691800
 H -5.01515800 -1.60176700 0.46443700
 H -1.57131600 -3.04683300 -0.49888300
 H -2.86118400 -3.17159000 0.71324800
 H -3.12814200 -3.77975300 -0.92224400
 P 2.28027800 -0.19181300 -0.00089400
 C 1.22444800 -1.06332100 2.39571700
 C 2.46968900 -0.37016300 1.84278500
 H 1.20277100 -2.11830600 2.10878400
 H 1.22033600 -1.01484100 3.49383700
 H 2.53621100 0.64058700 2.25860900
 H 3.38070700 -0.90483400 2.12850000
 C -0.00007200 -0.03675800 -1.93938200
 O -0.00010800 -0.08702800 -3.10342400
 C 3.17930800 1.40213300 -0.45217000
 C 3.37469600 1.52098100 -1.97266600
 C 4.47298700 1.71920100 0.31579100
 H 2.44074400 2.16003700 -0.16714800
 H 2.43640000 1.38188400 -2.51812500
 H 3.74948900 2.52191400 -2.21582200
 H 4.10177100 0.79700400 -2.35464200
 H 4.33285300 1.68343300 1.40010300
 H 5.29540000 1.04733900 0.05894300
 H 4.79295100 2.73817400 0.06600700
 C 3.21609900 -1.62148400 -0.79189300
 C 2.65053800 -2.97969200 -0.34471200

C 4.74004700 -1.59928700 -0.59647800
 H 2.99905900 -1.50368100 -1.86198000
 H 1.57118900 -3.04698500 -0.49858200
 H 3.12798100 -3.77990700 -0.92207400
 H 2.86119800 -3.17164700 0.71341000
 H 5.21270900 -0.73739300 -1.07100100
 H 5.01508300 -1.60178100 0.46431100
 H 5.17655600 -2.49909300 -1.04698200
 H -0.00001100 0.57186800 2.16028800
 C 0.00025100 2.58388100 0.81351000
 O 0.00057600 2.38827600 2.04538800
 O 0.00039700 3.58793600 0.10308800

ATS4_4a

Fe 0.00002700 -0.10021400 0.22092500
 H 0.00010300 3.91012500 -0.42385700
 H 0.00002000 -1.60597100 0.20030600
 C 1.22310400 -0.76428400 -2.47717700
 C 2.46995500 -0.13643200 -1.85109500
 H 1.23209000 -0.61098200 -3.56660200
 H 1.19937600 -1.84307000 -2.29485000
 H 2.54415700 0.91074200 -2.16242700
 H 3.37834300 -0.64582400 -2.18848700
 P 2.27867300 -0.14864800 0.00235700
 N -0.00000900 -0.17526800 -1.88628200
 C 3.16150300 1.39774900 0.60973700
 C 4.45768900 1.80877300 -0.10619900
 C 3.33719300 1.37419300 2.13702200
 H 2.40186100 2.15518100 0.38763600
 H 4.34239700 1.84300300 -1.19363800
 H 4.74298100 2.81732400 0.21889600
 H 5.29662100 1.14663300 0.12215100
 H 2.39597100 1.16108200 2.65303400
 H 4.07562100 0.63126700 2.45662500
 H 3.68724900 2.35354500 2.48432300
 C 3.23351500 -1.64598100 0.63077800
 C 4.75815700 -1.58067100 0.45148900
 C 2.69298000 -2.95211600 0.02569000
 H 3.00770400 -1.65805000 1.70562000
 H 5.21504300 -0.76733500 1.01847300
 H 5.20754700 -2.51672200 0.80566500
 H 5.03872800 -1.46543800 -0.60169500
 H 1.61292600 -3.04915700 0.15630500
 H 2.91802500 -3.02070600 -1.04479400

H 3.17497700 -3.80707300 0.51445800
P -2.27864200 -0.14878300 0.00236400
C -1.22292500 -0.76487500 -2.47701500
C -2.46996100 -0.13723900 -1.85108500
H -1.19882800 -1.84360300 -2.29437700
H -1.23198000 -0.61187300 -3.56648500
H -2.54449700 0.90982100 -2.16272300
H -3.37820000 -0.64700700 -2.18830600
C -0.00002200 -0.30103800 1.94905700
O -0.00007500 -0.55739700 3.08692100
C -3.16154400 1.39780400 0.60910100
C -3.33687700 1.37488500 2.13643200
C -4.45794200 1.80837000 -0.10671400
H -2.40205100 2.15524600 0.38650700
H -2.39543700 1.16234900 2.65228600
H -3.68723600 2.35425300 2.48338900
H -4.07494600 0.63181900 2.45655100
H -4.34303900 1.84181000 -1.19421900
H -5.29683800 1.14644800 0.12241200
H -4.74305200 2.81717200 0.21775300
C -3.23334000 -1.64596200 0.63136500
C -2.69280000 -2.95223200 0.02656300
C -4.75800700 -1.58076900 0.45224000
H -3.00742400 -1.65773800 1.70618500
H -1.61274500 -3.04921200 0.15719200
H -3.17478200 -3.80707700 0.51554300
H -2.91786100 -3.02107900 -1.04389900
H -5.21484000 -0.76731300 1.01909600
H -5.03871400 -1.46579300 -0.60093500
H -5.20730400 -2.51675600 0.80669700
H -0.00029400 0.84195300 -2.09209100
C -0.00017100 2.84450800 -0.75144600
O -0.00079200 2.62398500 -1.98159100
O 0.00013800 2.01013700 0.21078700

ATS4_4b

Fe -0.03297800 -0.15812000 0.20986300
H 0.00934100 2.53974300 0.46649900
H -0.04976200 -1.61589900 0.39486100
C 1.20046700 -0.85177700 -2.48620500
C 2.44286100 -0.22285700 -1.85387200
H 1.18764400 -0.65624300 -3.56736000
H 1.20305200 -1.93622900 -2.34670000
H 2.51868800 0.82849700 -2.15234700

H 3.35140100 -0.72691700 -2.19827200
P 2.26017300 -0.24275600 -0.00139900
N -0.03761900 -0.32206700 -1.86139900
C 3.20970500 1.26043200 0.60924900
C 4.54774700 1.56658300 -0.08470800
C 3.35231800 1.24908500 2.13992600
H 2.52601100 2.07689500 0.34459200
H 4.45015000 1.61265200 -1.17341500
H 4.90044400 2.55076400 0.24742100
H 5.32901700 0.84153200 0.15558900
H 2.38954600 1.11731900 2.64289400
H 4.02658700 0.45939100 2.48784600
H 3.76823200 2.20630700 2.47500700
C 3.11075000 -1.79759500 0.63319600
C 4.64262300 -1.80942300 0.51713300
C 2.52850300 -3.06361700 -0.01789100
H 2.84056000 -1.81259700 1.69738900
H 5.11664600 -1.03344600 1.12085400
H 5.02337900 -2.77569700 0.86994700
H 4.97471500 -1.68980400 -0.52010600
H 1.43906800 -3.10329800 0.05588300
H 2.80595600 -3.13316000 -1.07559000
H 2.93516000 -3.94918800 0.48412000
P -2.32021700 -0.17158400 -0.01287100
C -1.24825200 -0.96598700 -2.43343400
C -2.51290700 -0.32761500 -1.85723400
H -1.20203100 -2.03177900 -2.19139500
H -1.24277000 -0.87037600 -3.52830900
H -2.62078000 0.68817100 -2.24790100
H -3.40357500 -0.89391900 -2.14563200
C -0.04103800 -0.13199100 1.95087500
O -0.04936100 -0.24140500 3.11011600
C -3.16096500 1.44534400 0.43688800
C -3.23349800 1.63327200 1.96024200
C -4.51077500 1.75165800 -0.23376900
H -2.42882500 2.15378600 0.03060700
H -2.25736600 1.51099300 2.43919600
H -3.58855300 2.64445200 2.19100900
H -3.93022600 0.92777700 2.42637200
H -4.48617300 1.59856500 -1.31671800
H -5.33076300 1.15599900 0.17469600
H -4.75836000 2.80652500 -0.06279500
C -3.25407800 -1.60180800 0.77439500
C -2.75188100 -2.95127800 0.23460000

C -4.78490800 -1.52806800 0.67321300
H -2.97239600 -1.53714800 1.83365300
H -1.66809100 -3.05585200 0.32773100
H -3.22002700 -3.76649100 0.79829400
H -3.02230100 -3.08721700 -0.81861600
H -5.19722200 -0.67163500 1.21027700
H -5.12392000 -1.47797600 -0.36749000
H -5.22208100 -2.43219700 1.11444400
H -0.10573400 0.69344700 -2.04595600
C 0.22169600 2.90318600 -0.58909500
O -0.54148300 2.41311600 -1.48090200
O 1.15416500 3.71324900 -0.71474000

A4a

Fe 0.00002700 -0.10021400 0.22092500
H 0.00010300 3.91012500 -0.42385700
H 0.00002000 -1.60597100 0.20030600
C 1.22310400 -0.76428400 -2.47717700
C 2.46995500 -0.13643200 -1.85109500
H 1.23209000 -0.61098200 -3.56660200
H 1.19937600 -1.84307000 -2.29485000
H 2.54415700 0.91074200 -2.16242700
H 3.37834300 -0.64582400 -2.18848700
P 2.27867300 -0.14864800 0.00235700
N -0.00000900 -0.17526800 -1.88628200
C 3.16150300 1.39774900 0.60973700
C 4.45768900 1.80877300 -0.10619900
C 3.33719300 1.37419300 2.13702200
H 2.40186100 2.15518100 0.38763600
H 4.34239700 1.84300300 -1.19363800
H 4.74298100 2.81732400 0.21889600
H 5.29662100 1.14663300 0.12215100
H 2.39597100 1.16108200 2.65303400
H 4.07562100 0.63126700 2.45662500
H 3.68724900 2.35354500 2.48432300
C 3.23351500 -1.64598100 0.63077800
C 4.75815700 -1.58067100 0.45148900
C 2.69298000 -2.95211600 0.02569000
H 3.00770400 -1.65805000 1.70562000
H 5.21504300 -0.76733500 1.01847300
H 5.20754700 -2.51672200 0.80566500
H 5.03872800 -1.46543800 -0.60169500
H 1.61292600 -3.04915700 0.15630500
H 2.91802500 -3.02070600 -1.04479400

H 3.17497700 -3.80707300 0.51445800
P -2.27864200 -0.14878300 0.00236400
C -1.22292500 -0.76487500 -2.47701500
C -2.46996100 -0.13723900 -1.85108500
H -1.19882800 -1.84360300 -2.29437700
H -1.23198000 -0.61187300 -3.56648500
H -2.54449700 0.90982100 -2.16272300
H -3.37820000 -0.64700700 -2.18830600
C -0.00002200 -0.30103800 1.94905700
O -0.00007500 -0.55739700 3.08692100
C -3.16154400 1.39780400 0.60910100
C -3.33687700 1.37488500 2.13643200
C -4.45794200 1.80837000 -0.10671400
H -2.40205100 2.15524600 0.38650700
H -2.39543700 1.16234900 2.65228600
H -3.68723600 2.35425300 2.48338900
H -4.07494600 0.63181900 2.45655100
H -4.34303900 1.84181000 -1.19421900
H -5.29683800 1.14644800 0.12241200
H -4.74305200 2.81717200 0.21775300
C -3.23334000 -1.64596200 0.63136500
C -2.69280000 -2.95223200 0.02656300
C -4.75800700 -1.58076900 0.45224000
H -3.00742400 -1.65773800 1.70618500
H -1.61274500 -3.04921200 0.15719200
H -3.17478200 -3.80707700 0.51554300
H -2.91786100 -3.02107900 -1.04389900
H -5.21484000 -0.76731300 1.01909600
H -5.03871400 -1.46579300 -0.60093500
H -5.20730400 -2.51675600 0.80669700
H -0.00029400 0.84195300 -2.09209100
C -0.00017100 2.84450800 -0.75144600
O -0.00079200 2.62398500 -1.98159100
O 0.00013800 2.01013700 0.21078700

A4b

Fe -0.00001300 -0.08322800 -0.16070500
H 0.00006500 2.96745000 -0.66725000
H -0.00003600 -1.49766400 -0.70904500
C -1.22397600 -1.59375700 2.18470200
C -2.47031900 -0.80405900 1.79005900
H -1.22120600 -1.78662800 3.26694000
H -1.19842200 -2.56001300 1.67434000
H -2.55238000 0.08884500 2.41956700

H -3.37514900 -1.39928800 1.94908900
 P -2.28890100 -0.22192800 0.02779300
 N -0.00006500 -0.85458200 1.79161800
 C -3.21180200 1.41688500 -0.02525000
 C -4.52929200 1.52313300 0.76018100
 C -3.37229400 1.92100900 -1.46876700
 H -2.48662700 2.06994100 0.47294600
 H -4.43092300 1.17814300 1.79362600
 H -4.83554000 2.57593800 0.79970300
 H -5.34490900 0.96559500 0.29415100
 H -2.42563100 1.91017600 -2.01697900
 H -4.09578400 1.32268800 -2.03285000
 H -3.73731200 2.95468600 -1.46133100
 C -3.22219600 -1.46054700 -1.04272600
 C -4.75026600 -1.45744000 -0.88324800
 C -2.68193700 -2.88793700 -0.85101800
 H -2.97785600 -1.14484400 -2.06567800
 H -5.20319400 -0.51726300 -1.20316100
 H -5.18253900 -2.25412300 -1.50111200
 H -5.05173900 -1.64963100 0.15257800
 H -1.59768400 -2.93947000 -0.97399700
 H -2.93716300 -3.28064500 0.13981000
 H -3.14111400 -3.55309500 -1.59167200
 P 2.28886100 -0.22175600 0.02779600
 C 1.22426000 -1.59269800 2.18540800
 C 2.47020900 -0.80250800 1.79051200
 H 1.19944000 -2.55930000 1.67567300
 H 1.22137200 -1.78488900 3.26776500
 H 2.55152300 0.09095200 2.41932900
 H 3.37536400 -1.39704800 1.95027600
 C -0.00010800 0.40894400 -1.82842300
 O -0.00020700 0.63162200 -2.97373000
 C 3.21190800 1.41694900 -0.02652100
 C 3.37270900 1.91982400 -1.47043600
 C 4.52926400 1.52367900 0.75907100
 H 2.48676000 2.07055600 0.47098600
 H 2.42606600 1.90893800 -2.01867800
 H 3.73812800 2.95336300 -1.46380400
 H 4.09598900 1.32076300 -2.03399700
 H 4.43063200 1.17955200 1.79277700
 H 5.34490400 0.96565600 0.29366700
 H 4.83563700 2.57647900 0.79779100
 C 3.22216200 -1.46112800 -1.04186600
 C 2.68161100 -2.88833400 -0.84962100

C 4.75021000 -1.45823300 -0.88211400
 H 2.97806800 -1.14583900 -2.06501000
 H 1.59736500 -2.93972200 -0.97273600
 H 3.14076600 -3.55389600 -1.58992500
 H 2.93662000 -3.28067400 0.14141000
 H 5.20340600 -0.51836100 -1.20253700
 H 5.05146700 -1.64982900 0.15388300
 H 5.18242400 -2.25539700 -1.49939800
 H -0.00057300 0.04697000 2.27744400
 C 0.00008500 2.88068300 0.44705700
 O 0.00006200 1.67139600 0.89576600
 O 0.00012100 3.90890500 1.12628400

A5

Fe -0.05451400 -0.33841500 0.18448700
 H 0.76753300 5.01750900 -0.14285500
 H -0.10179900 -1.53543100 -0.69637900
 C 1.17085700 0.43596900 -2.44306600
 C 2.44923000 0.58701900 -1.62246200
 H 1.19841300 1.11194700 -3.30931300
 H 1.06888800 -0.58623700 -2.81899300
 H 2.60032300 1.64268900 -1.37558300
 H 3.32455600 0.24711600 -2.18462500
 P 2.22859100 -0.32200000 -0.01542300
 N -0.01885400 0.73993100 -1.60788700
 C 3.12314300 0.73103300 1.25864100
 C 4.49947300 1.29339000 0.86511800
 C 3.16331000 0.03211500 2.62624900
 H 2.43830700 1.58576200 1.32645300
 H 4.48865400 1.77036800 -0.11942900
 H 4.78844600 2.06211700 1.59233100
 H 5.28518600 0.53447900 0.86547900
 H 2.17106600 -0.30272300 2.94630700
 H 3.82853400 -0.83879300 2.62237500
 H 3.53790300 0.72615500 3.38772800
 C 3.10195600 -1.98161100 -0.16516900
 C 4.63487800 -1.92026100 -0.24257000
 C 2.54005400 -2.79898000 -1.34052100
 H 2.82501400 -2.49809700 0.76342900
 H 5.08058300 -1.52560200 0.67242900
 H 5.03172900 -2.93221500 -0.38937900
 H 4.98002500 -1.31029500 -1.08473400
 H 1.45128600 -2.88145400 -1.29865200
 H 2.81426400 -2.35521300 -2.30439600

H 2.96070000 -3.81088900 -1.31566700
 P 2.33081200 -0.15001700 0.00617700
 C -1.25476000 0.58199200 -2.41452500
 C -2.48592900 0.85030300 -1.55289100
 H -1.27341800 -0.43662600 -2.81321100
 H -1.23363500 1.27526800 -3.26707000
 H -2.49831800 1.90530400 -1.25920400
 H -3.40959500 0.64718400 -2.10365000
 C -0.07849300 -1.53190200 1.45962600
 O -0.09747700 -2.41042800 2.22100500
 C -3.12297900 0.90228100 1.35118900
 C -3.25093800 0.11277600 2.66338200
 C -4.42525600 1.63845500 0.99688900
 H -2.35105500 1.66847300 1.49728200
 H -2.30666000 -0.35936400 2.95374600
 H -3.54656000 0.78639900 3.47587700
 H -4.01314900 -0.67070600 2.59262900
 H -4.34246700 2.20334800 0.06360300
 H -5.28096100 0.96514900 0.91055600
 H -4.65474900 2.35832200 1.79201300
 C -3.34909400 -1.71486700 -0.20974300
 C -2.87040600 -2.52724000 -1.42497000
 C -4.87061800 -1.51330900 -0.27421100
 H -3.11459200 -2.29418400 0.69332600
 H -1.79395100 -2.71354900 -1.39862400
 H -3.38475300 -3.49502700 -1.43967600
 H -3.10865500 -2.01759700 -2.36549500
 H -5.27833300 -1.11530900 0.65688900
 H -5.16042600 -0.84413400 -1.09181400
 H -5.35616900 -2.47974900 -0.45625000
 H 0.04559300 1.76182200 -1.37342000
 C 0.58945800 3.90995400 -0.19842900
 O 0.15277200 3.49449100 -1.30740900
 O 0.84771200 3.25820900 0.84263200
 H 0.17334800 1.34664100 0.93117100
 H -0.17583600 0.82580400 1.41699400

AT55_6

Fe -0.03804400 -0.33465900 0.19345800
 H 0.64512200 4.94218900 -0.33142400
 H -0.06139300 -1.65679500 -0.51888800
 C 1.19232900 0.15930300 -2.50975600
 C 2.45486600 0.43531000 -1.69638700
 H 1.21235300 0.73395300 -3.44680500

H 1.12190400 -0.90104000 -2.76807400
 H 2.57385200 1.51626500 -1.56683600
 H 3.34751600 0.06467400 -2.21023900
 P 2.23818900 -0.30308500 -0.00095500
 N -0.01500100 0.51632400 -1.72165100
 C 3.13161500 0.88839200 1.15168200
 C 4.48848300 1.44541500 0.68928400
 C 3.20877300 0.32750500 2.57985800
 H 2.42536800 1.72749100 1.16120700
 H 4.46028000 1.81992300 -0.33833500
 H 4.76390500 2.29015500 1.33286400
 H 5.29313300 0.70968400 0.75850500
 H 2.22923200 0.00696800 2.94740000
 H 3.89251000 -0.52602000 2.64651700
 H 3.58201900 1.09921400 3.26328200
 C 3.15903800 -1.94727700 0.00933400
 C 4.68909500 -1.84964800 -0.08655000
 C 2.62212500 -2.89549500 -1.07553300
 H 2.89899500 -2.37617800 0.98596600
 H 5.13032300 -1.36816500 0.78807700
 H 5.11546800 -2.85808900 -0.15367900
 H 5.00926500 -1.30118100 -0.97960000
 H 1.53866200 -3.01946300 -1.01390600
 H 2.87069000 -2.53626300 -2.08076100
 H 3.08628000 -3.88179200 -0.95849900
 P 2.30940300 -0.19059000 -0.00161600
 C -1.24355900 0.23874800 -2.50811600
 C -2.48703000 0.57676800 -1.68909500
 H -1.23510200 -0.82146400 -2.77678600
 H -1.23374400 0.82195600 -3.44011000
 H -2.54972600 1.66153400 -1.55083400
 H -3.39971700 0.25985700 -2.20385800
 C -0.05692600 -1.27697300 1.65331800
 O -0.07145400 -1.98967600 2.57552300
 C -3.13464600 1.03097000 1.17262100
 C -3.29613100 0.42793900 2.57689100
 C -4.42745000 1.71166700 0.69562900
 H -2.36213600 1.80708800 1.23411900
 H -2.36033300 0.00060200 2.94996500
 H -3.60725400 1.20724900 3.28226700
 H -4.06050300 -0.35628700 2.59751200
 H -4.31827900 2.16734000 -0.29273400
 H -5.27851800 1.02796000 0.66044300
 H -4.68439600 2.51695900 1.39488700

C -3.32787800 -1.77519100 -0.00476500
C -2.82481800 -2.75896900 -1.07394300
C -4.84762200 -1.58826800 -0.13366900
H -3.11395700 -2.21391700 0.97894200
H -1.75233000 -2.94732100 -0.98676800
H -3.34979400 -3.71513200 -0.96397800
H -3.02816400 -2.39050700 -2.08593400
H -5.28120600 -1.07778300 0.72868200
H -5.11547100 -1.02723300 -1.03593800
H -5.33038000 -2.57058900 -0.20671100
H 0.02710600 1.54303000 -1.57570000
C 0.42994100 3.85116500 -0.37729600
O 0.23503900 3.34680400 -1.49859800
O 0.41517200 3.28060800 0.76727800
H 0.12852700 1.91406800 0.79534600
H -0.07904700 1.08898700 1.04595100

A6

Fe 0.01240200 -0.36594400 0.19023000
H -0.17053200 5.11058800 -0.43562600
H 0.02327700 -1.75332600 -0.46814200
C 1.22833400 0.06258700 -2.54591900
C 2.47517100 0.41134400 -1.73417600
H 1.23717800 0.59824500 -3.50647200
H 1.19533300 -1.00930200 -2.75878400
H 2.57009200 1.50021900 -1.65674000
H 3.37988300 0.04328600 -2.22874800
P 2.27000600 -0.26018600 -0.00551100
N 0.00262700 0.40070600 -1.78094700
C 3.12655200 1.01213000 1.09246300
C 4.46008100 1.60607100 0.61028200
C 3.21958700 0.51937300 2.54479300
H 2.38337000 1.81824100 1.07006500
H 4.41709800 1.94574200 -0.42896000
H 4.70542700 2.48081900 1.22569400
H 5.29219700 0.90437400 0.70130300
H 2.25153900 0.17589000 2.92093200
H 3.93685500 -0.30156000 2.65273500
H 3.55675300 1.33542900 3.19493000
C 3.27155000 -1.85839000 0.07401100
C 4.79937800 -1.70408200 0.01760000
C 2.80881800 -2.86158200 -0.99547500
H 3.00117700 -2.27164000 1.05499900
H 5.19981800 -1.18152000 0.88852800

H 5.26538800 -2.69704000 -0.00725700
H 5.12568900 -1.17113600 -0.88274800
H 1.72950400 -3.02597900 -0.96409800
H 3.07821700 -2.52539600 -2.00354600
H 3.30663800 -3.82476900 -0.83154000
P -2.24760900 -0.29605600 0.00015800
C -1.21690500 0.03384400 -2.54275600
C -2.46796100 0.36530100 -1.73044500
H -1.16386900 -1.03852000 -2.74897600
H -1.23717900 0.56376200 -3.50630300
H -2.57883800 1.45271100 -1.65667100
H -3.36766600 -0.01876600 -2.22189400
C 0.01913400 -1.15208900 1.73036100
O 0.02335800 -1.74396600 2.73866000
C -3.12153000 0.96620300 1.09579000
C -3.20241900 0.47666800 2.54997300
C -4.46630500 1.53607900 0.61551900
H -2.39254900 1.78507400 1.06802200
H -2.22815600 0.14937200 2.92450000
H -3.55088000 1.28909700 3.19868300
H -3.90630100 -0.35527200 2.66217300
H -4.43147500 1.87391800 -0.42466000
H -5.28604500 0.82038800 0.71015500
H -4.72497000 2.40807200 1.22940200
C -3.22301900 -1.90999200 0.08799400
C -2.74756100 -2.90951500 -0.97934800
C -4.75317200 -1.78021400 0.03467500
H -2.94391500 -2.31521200 1.06984900
H -1.66570700 -3.05671300 -0.95088900
H -3.22956700 -3.87988500 -0.81064600
H -3.02528000 -2.58092800 -1.98767900
H -5.15936800 -1.25812800 0.90314000
H -5.08996600 -1.25861400 -0.86846300
H -5.20337200 -2.78059800 0.01776600
H -0.01286900 1.42029200 -1.66514600
C -0.12813700 4.01103200 -0.49310500
O -0.14457500 3.41565400 -1.56017200
O -0.05776500 3.47467600 0.70852300
H -0.02757500 2.44548600 0.66006900
H 0.00613500 1.11701100 0.77247400

ATS4a_5

Fe -0.04468100 -0.36310200 0.17279000
H 0.69570000 4.95366300 -0.33415400

H -0.09356600 -1.63695500 -0.55845300
 C 1.18028600 0.32983700 -2.47249700
 C 2.45413000 0.53463300 -1.65623400
 H 1.19020600 0.98347000 -3.35591500
 H 1.10513500 -0.70345300 -2.82435100
 H 2.58174500 1.60092000 -1.44474400
 H 3.33800600 0.19472200 -2.20490200
 P 2.24654400 -0.32043800 -0.01701900
 N -0.01807300 0.62345500 -1.64388700
 C 3.11141000 0.80137800 1.21638600
 C 4.47606800 1.37622700 0.80040400
 C 3.17097800 0.16267800 2.61211300
 H 2.40301800 1.63973800 1.24286700
 H 4.46194500 1.80063900 -0.20773300
 H 4.74287600 2.18809500 1.48817600
 H 5.27837300 0.63561100 0.84449000
 H 2.19193600 -0.19277000 2.94760000
 H 3.86689200 -0.68336400 2.64453300
 H 3.52120000 0.90090900 3.34305500
 C 3.14543100 -1.96905400 -0.11048300
 C 4.67651300 -1.88074200 -0.19254100
 C 2.59608400 -2.82956700 -1.26089400
 H 2.87641500 -2.46008400 0.83399100
 H 5.11465300 -1.44703700 0.70837000
 H 5.09398300 -2.88857200 -0.30750600
 H 5.00750600 -1.29079000 -1.05453600
 H 1.51046700 -2.94321200 -1.20676500
 H 2.84820600 -2.40153800 -2.23775600
 H 3.04550200 -3.82835400 -1.21639700
 P -2.33123800 -0.16713300 -0.00144700
 C -1.24904500 0.44152600 -2.45540800
 C -2.48489200 0.74908400 -1.61308300
 H -1.26886400 -0.59049200 -2.81767200
 H -1.21822000 1.10302800 -3.33237400
 H -2.49929500 1.81838800 -1.37695100
 H -3.40684500 0.51499700 -2.15429000
 C -0.06865100 -1.38771000 1.58520800
 O -0.09117700 -2.16728000 2.44993500
 C -3.13107600 0.95481500 1.28084900
 C -3.28581400 0.23236800 2.62826100
 C -4.42327700 1.68008700 0.87086300
 H -2.35754000 1.72349500 1.40264900
 H -2.35420800 -0.24141400 2.95278600
 H -3.57935400 0.94986000 3.40294000

H -4.06049100 -0.54079600 2.58606200
 H -4.31949000 2.20847700 -0.08115200
 H -5.27924300 1.00591100 0.79338200
 H -4.66588300 2.43086700 1.63282100
 C -3.34432000 -1.74444500 -0.14338500
 C -2.85856800 -2.61187700 -1.31754500
 C -4.86563200 -1.54893900 -0.22773900
 H -3.11285100 -2.27953500 0.78725500
 H -1.78353100 -2.80334000 -1.27508000
 H -3.37746500 -3.57705200 -1.29349400
 H -3.08651900 -2.14401800 -2.28200200
 H -5.28149600 -1.10575000 0.67904700
 H -5.14995800 -0.92143600 -1.07953100
 H -5.34851000 -2.52411100 -0.36540700
 H 0.02675100 1.65222600 -1.41995100
 C 0.52440300 3.84261400 -0.34747700
 O 0.06395300 3.38861800 -1.43220500
 O 0.81280400 3.22630100 0.70571300
 H 0.04438100 1.72606300 1.99592500
 H -0.17175100 1.18441500 2.46849900

ATS4_7

P 2.20895400 -0.54722000 -0.23283100
 N 0.07535500 0.66019800 -1.69447600
 C -1.14339900 0.81962600 -2.51945100
 C 1.26381500 0.51873700 -2.57879800
 C 2.22858700 -0.56407100 -2.08301600
 H 3.22946300 -0.45117000 -2.51414100
 H 1.84471200 -1.54437200 -2.37903100
 C -2.35909400 1.09552100 -1.63808700
 H -3.29272400 1.01877300 -2.20454600
 P -2.29282800 -0.08321100 -0.20450900
 C -0.08288100 -0.70765200 1.74040500
 O -0.13672900 -1.01062300 2.86527200
 C 3.13388100 -2.09514500 0.30356400
 H 4.19167500 -1.89106600 0.09800500
 C 2.97198600 -2.37084300 1.80780400
 H 3.63500600 -3.19314300 2.10176000
 H 3.22227300 -1.50835100 2.43089000
 H 1.94726600 -2.67222100 2.04476100
 C 2.72406600 -3.33556300 -0.50610900
 H 2.99467500 -3.25598300 -1.56262000
 H 3.23843600 -4.21629900 -0.10349800
 H 1.64671900 -3.52274100 -0.44043800

C -3.14507000 -1.61775100 -0.88674000
H -2.61211000 -1.75433300 -1.83760800
C -2.90898100 -2.88397800 -0.04833300
H -3.26514500 -3.76120300 -0.60174000
H -1.84804500 -3.03101900 0.17006700
H -3.45084600 -2.85704900 0.90160300
C -4.63711600 -1.42392000 -1.19900300
H -5.01976100 -2.30600000 -1.72631600
H -5.23104500 -1.30658900 -0.28699100
H -4.82442100 -0.55612400 -1.83862800
H -1.01694900 1.64873500 -3.23390200
H -1.31207300 -0.08499200 -3.12399800
H -2.30059500 2.10990200 -1.23234800
H 1.79114000 1.48283600 -2.65365900
H 0.94845100 0.26575500 -3.59931700
C -3.45304100 0.68320800 1.06543300
H -4.36711300 0.94260300 0.51532300
C -2.85575800 1.97318700 1.64993400
H -3.58302900 2.43831100 2.32587000
H -1.95237900 1.76326300 2.23265900
H -2.60253900 2.71469200 0.88701400
C -3.82346200 -0.28392800 2.20137900
H -4.44384200 0.24013800 2.93825100
H -4.39463300 -1.14605100 1.84975300
H -2.93531300 -0.65284200 2.72441100
C 3.30265500 0.92154900 0.21862100
H 2.82571500 1.73197800 -0.34756000
C 4.76316800 0.81321500 -0.24291100
H 5.27143600 1.77245200 -0.08623400
H 5.31370700 0.05812400 0.32824700
H 4.85266600 0.56757600 -1.30549800
C 3.22112200 1.29398900 1.70789800
H 3.66110800 2.28512700 1.86786400
H 2.19006700 1.32671600 2.07223100
H 3.77770800 0.58692000 2.33130000
H 0.26364200 2.01687000 -1.18807100
H 0.15131000 2.16876400 0.90898200
C 0.33220600 3.15344300 0.41364100
O 0.42579300 4.17104900 1.07935500
O 0.42191300 3.07952400 -0.89063400
Fe -0.02241200 -0.25970600 0.05250700
H -0.11521200 -1.69788500 -0.27590600

A7

P 2.20668500 -0.56555000 -0.22324400
N 0.06346600 0.54438900 -1.71972500
C -1.14598600 0.73154200 -2.54794600
C 1.24824500 0.40038900 -2.60207800
C 2.23193400 -0.64755700 -2.07105900
H 3.23118500 -0.53377300 -2.50544300
H 1.86242600 -1.64269400 -2.33380000
C -2.36341700 1.03204900 -1.67739700
H -3.29584800 0.93174600 -2.24227200
P -2.29584100 -0.09676400 -0.20352400
C -0.07325800 -0.58210400 1.76688300
O -0.11964000 -0.80188000 2.91221700
C 3.13139600 -2.09000300 0.37534200
H 4.19137900 -1.88849900 0.17871400
C 2.94664800 -2.31525900 1.88552000
H 3.60374400 -3.12787800 2.21729500
H 3.18849000 -1.43221700 2.48268500
H 1.91772400 -2.60711700 2.11626200
C 2.73872000 -3.35869600 -0.39751300
H 3.02289900 -3.31256000 -1.45245900
H 3.25220800 -4.22280400 0.04085000
H 1.66150600 -3.54950100 -0.33977000
C -3.15399100 -1.65215800 -0.83149200
H -2.62331000 -1.82233100 -1.77835800
C -2.91991500 -2.88990700 0.04890200
H -3.28665300 -3.78347500 -0.47041700
H -1.85828900 -3.03648100 0.26402100
H -3.45337200 -2.82579900 1.00197800
C -4.64637400 -1.46621400 -1.14678800
H -5.03029400 -2.36226500 -1.64910100
H -5.23872900 -1.32395300 -0.23727100
H -4.83495300 -0.61629800 -1.80958900
H -0.99986300 1.55634600 -3.26443400
H -1.33163300 -0.16912400 -3.15564300
H -2.31320700 2.06034200 -1.30684900
H 1.76011000 1.37006000 -2.71741300
H 0.93512000 0.10431100 -3.61273400
C -3.46013400 0.72020400 1.03091800
H -4.37457300 0.94916100 0.46803700
C -2.87227800 2.03983800 1.55616600
H -3.60598300 2.53384600 2.20400400
H -1.97230700 1.86205900 2.15429800
H -2.61756100 2.74474200 0.75957300
C -3.82728200 -0.19456000 2.21031200

H -4.45101400 0.35996200 2.92160800
H -4.39384700 -1.07474300 1.89847200
H -2.93749000 -0.53486200 2.74968300
C 3.30532800 0.91572700 0.17509900
H 2.83168000 1.70723400 -0.42000700
C 4.76553600 0.78719300 -0.28335300
H 5.27499800 1.75110300 -0.16352800
H 5.31551400 0.05421200 0.31640200
H 4.85428800 0.50046200 -1.33559000
C 3.22874100 1.34329000 1.64962600
H 3.67759100 2.33571200 1.77297700
H 2.19892500 1.39848900 2.01456600
H 3.78030500 0.65529200 2.29846800
H 0.29094600 2.05557400 -1.19911900
H 0.10293700 2.21960300 0.87174900
C 0.34185600 3.17919500 0.36267400
O 0.47502100 4.21803000 0.97945900
O 0.45734600 3.06320600 -0.94748700
Fe -0.02597900 -0.26848300 0.04879700
H -0.12292600 -1.73200400 -0.14340700

A8

H -0.28714600 -0.46289300 -0.17040400
H -1.17522100 1.03684900 -2.45629400
C -1.83075300 1.86379700 -2.16753600
C -1.84331700 2.08325000 -0.64785200
H -2.84492100 1.61110800 -2.49815500
H -1.51801200 2.75700200 -2.71838100
P -0.13888000 2.17806500 0.13263200
C -2.78560400 3.23105900 -0.25717200
H -2.22143200 1.16082100 -0.19284100
Fe 1.27795900 0.41091900 -0.19182100
C -0.52195100 1.98640800 1.94077100
C 0.46754500 3.94447700 -0.07570700
H -2.81559600 3.39888200 0.82443600
H -2.50794800 4.17406100 -0.74087300
H -3.80403100 2.98192900 -0.57728400
P 2.77642100 -1.32316000 -0.06854500
C 1.60139000 0.74935400 -1.88041000
C 0.67647000 1.34054100 2.62972900
H -1.38493400 1.31511200 1.99657900
H -0.78638800 2.93455800 2.41945100
C 0.94500500 4.22447500 -1.50835800
C 1.56491800 4.31300900 0.93360800

H -0.40761400 4.57251500 0.13263800
C 2.80758800 -1.66439900 1.75778800
C 2.18629300 -2.93757900 -0.84063500
C 4.54279400 -0.99186700 -0.62242600
O 1.89401500 1.00424900 -2.97517200
N 1.12958500 0.14157200 1.87936700
H 1.51619500 2.03928500 2.68426500
H 0.41426700 1.05424700 3.65813700
H 0.18376400 4.00165500 -2.26045300
H 1.20666800 5.28459200 -1.60828300
H 1.83885800 3.63939900 -1.74661500
H 2.44586900 3.67241300 0.81971000
H 1.88247100 5.34857500 0.76229500
H 1.21981600 4.24596500 1.96932300
C 2.36610900 -0.40253500 2.49418500
H 2.08458000 -2.46409500 1.94703200
H 3.78632800 -2.00900700 2.10555600
C 2.78559900 -4.24347100 -0.29335400
C 2.25707700 -2.88247500 -2.37428400
H 1.12674200 -2.92651400 -0.55253300
C 5.48203100 -2.20718200 -0.60222600
C 5.16169000 0.17075400 0.17154100
H 4.42605100 -0.66241600 -1.66318600
H 2.18640700 -0.63042100 3.55432500
H 3.13894200 0.36992500 2.44418300
H 2.77144700 -4.28707900 0.79942900
H 2.18803800 -5.08714700 -0.65933000
H 3.81309000 -4.40581100 -0.62619100
H 1.74762300 -2.00236000 -2.77854300
H 3.29242200 -2.86893300 -2.73134700
H 1.77379800 -3.76907100 -2.80047200
H 5.17528200 -2.98129800 -1.30805800
H 6.49233700 -1.88841700 -0.88581200
H 5.54995700 -2.65646500 0.39470600
H 4.53405300 1.06485900 0.14894800
H 5.33317600 -0.10488600 1.21822600
H 6.13522500 0.42697700 -0.26190200
H 2.40273900 1.34746400 0.08628900
H 0.19955000 -0.83573900 -0.67030200
C -1.83053400 -1.79203400 1.76943200
O -0.71842400 -1.91445600 2.34646100
O -2.19957900 -0.88774200 0.97385400
H 0.39138300 -0.59178600 2.00314000
H -2.58285700 -2.59131300 1.99586400

C -5.55266800 -2.60815600 -1.01332600
 C -5.01117100 -1.29732700 -1.58811400
 C -5.88514700 -0.14236100 0.34469300
 C -6.40903800 -1.48070200 0.87043900
 H -4.09421000 -1.48985000 -2.15765500
 H -4.76736100 -3.10541400 -0.41756300
 H -5.86573700 -3.29561600 -1.80743000
 H -5.60385600 0.50256500 1.18562100
 H -6.69474000 0.36007200 -0.20370900
 H -5.66131100 -1.93482100 1.54386800
 H -7.34048800 -1.35172500 1.43352400
 H -5.75535500 -0.88662800 -2.28542900
 O -6.70502100 -2.37586000 -0.20177600
 N -4.73288300 -0.29531500 -0.55230200
 H -3.91874300 -0.59414000 -0.00356800

ATS8_9

H -1.10651500 -0.53324300 -0.65624700
 H -1.06100200 1.59707200 -2.73664600
 C -1.51074100 2.56698700 -2.50629100
 C -1.70961100 2.76028700 -0.99532900
 H -2.48069600 2.61585700 -3.01574200
 H -0.87889300 3.34679600 -2.94281900
 P -0.14920200 2.45587700 0.01441600
 C -2.42361400 4.08427300 -0.68581300
 H -2.35147000 1.94305800 -0.64333700
 Fe 0.95195300 0.47299500 -0.23468400
 C -0.81769400 2.28689900 1.74187600
 C 0.79729100 4.08333700 0.01336100
 H -2.58907000 4.22806500 0.38682600
 H -1.86476400 4.94719300 -1.06296800
 H -3.40573200 4.09560400 -1.17339200
 P 2.09804500 -1.49985700 -0.01871900
 C 1.57764200 0.81165600 -1.82746600
 C 0.12012300 1.38282400 2.53681800
 H -1.80288900 1.81151500 1.67031300
 H -0.94507200 3.25338300 2.24034800
 C 1.51304600 4.33781100 -1.32150200
 C 1.79649900 4.18462600 1.17563200
 H 0.03672600 4.86051900 0.15674100
 C 1.74263200 -1.94982600 1.75049500
 C 1.43055300 -2.94661400 -1.02282400
 C 3.97112500 -1.44549800 -0.21245200
 O 2.05961300 1.04920200 -2.85997900

N 0.41508200 0.13882100 1.77566100
 H 1.07073800 1.88462200 2.73623300
 H -0.33540600 1.12080900 3.50099200
 H 0.83048500 4.34086500 -2.17535400
 H 2.00706400 5.31637800 -1.29289700
 H 2.28486700 3.58404500 -1.50574700
 H 2.56130600 3.40332000 1.11674900
 H 2.30749800 5.15389300 1.12931400
 H 1.31148500 4.11963200 2.15361200
 C 1.41424600 -0.67304300 2.51995700
 H 0.86971900 -2.61049600 1.75233900
 H 2.56555500 -2.49491400 2.22339800
 C 1.68960400 -4.36463100 -0.48749000
 C 1.81074800 -2.82219200 -2.50663300
 H 0.35164600 -2.76491300 -0.94247200
 C 4.68726100 -2.80395300 -0.16972800
 C 4.60639800 -0.48447100 0.80643600
 H 4.11013200 -1.01294100 -1.21182000
 H 1.01754700 -0.92348000 3.51227400
 H 2.30992600 -0.06052500 2.65434200
 H 1.44509700 -4.46431600 0.57413100
 H 1.05417600 -5.07262300 -1.03377200
 H 2.72445200 -4.68455100 -0.62708200
 H 1.54732000 -1.84290900 -2.91733700
 H 2.88278400 -2.97914600 -2.66685300
 H 1.27828700 -3.58125500 -3.09148300
 H 4.40401900 -3.45290100 -1.00074500
 H 5.77025600 -2.64344100 -0.23658600
 H 4.49676000 -3.33976200 0.76689700
 H 4.14087900 0.50375100 0.78603000
 H 4.53498500 -0.87907400 1.82625100
 H 5.67171400 -0.36404900 0.57772400
 H 2.16639800 1.17048900 0.28957400
 H -0.35768900 -0.36000200 -0.98430100
 C -2.85946800 -0.67786800 2.97338800
 O -1.77422200 -1.30055600 2.81607200
 O -3.49480900 0.02226100 2.14218600
 H -0.46212200 -0.41432200 1.81942800
 H -3.32363500 -0.76463400 3.99214600
 C -4.04728300 -3.12753100 -0.06344400
 C -2.63814600 -2.53923300 -0.13387500
 C -3.52338000 -0.77099900 -1.54688300
 C -4.90241200 -1.42500300 -1.43683900
 H -2.11727000 -2.69884600 0.81400400

H -4.57049800 -2.72991000 0.82179600
H -4.01121600 -4.21893600 0.02073300
H -3.63249800 0.31541200 -1.62716900
H -3.02823200 -1.12875100 -2.45960100
H -5.46508800 -0.97201500 -0.60346000
H -5.47629600 -1.27678400 -2.35799800
H -2.08104500 -3.03348000 -0.94129700
O -4.79252800 -2.83325300 -1.24494400
N -2.66314600 -1.08916100 -0.39628600
H -2.98502200 -0.60410600 0.46057100

A9

H -1.85189000 -0.68187800 -0.40829400
H -0.99455400 1.66628500 -2.68470400
C -1.40023800 2.64853200 -2.42829700
C -1.47548200 2.85262500 -0.90874300
H -2.40277800 2.72551900 -2.86723100
H -0.78056400 3.40924700 -2.91354500
P 0.14273600 2.46278700 -0.01557900
C -2.09327400 4.21400600 -0.55681200
H -2.12980800 2.06873900 -0.50409400
Fe 1.08276300 0.41779600 -0.23711800
C -0.42232500 2.44522400 1.76309800
C 1.17132000 4.03954500 -0.15446200
H -2.14577200 4.38223500 0.52360200
H -1.53207700 5.04238300 -1.00195200
H -3.11688900 4.27177500 -0.94722000
P 1.98752400 -1.65480800 -0.00889200
C 1.57707700 0.60792000 -1.88365800
C 0.46531500 1.48296000 2.54897600
H -1.45778800 2.08771100 1.77006600
H -0.41575300 3.44112400 2.21731400
C 1.84745300 4.16549700 -1.52826900
C 2.22228700 4.15824600 0.95956400
H 0.46199600 4.86747100 -0.03386700
C 1.64250300 -2.03709700 1.78268700
C 1.13145200 -3.04028000 -0.96790000
C 3.84677900 -1.89786600 -0.24104800
O 1.94726800 0.72860300 -2.98640300
N 0.59320800 0.19449000 1.82616600
H 1.47073800 1.89634000 2.66680100
H 0.04689200 1.31084800 3.55086700
H 1.13240400 4.15753300 -2.35536400
H 2.40276000 5.10994500 -1.58359300

H 2.56074200 3.35144600 -1.69079600
H 2.94503000 3.33719900 0.91559500
H 2.77544900 5.09787100 0.83913100
H 1.77668200 4.16940300 1.95852700
C 1.51775500 -0.71747200 2.54132800
H 0.69133600 -2.57781200 1.83289600
H 2.40565600 -2.68010400 2.23320000
C 1.15890000 -4.45692200 -0.37137300
C 1.55656800 -3.04228600 -2.44524200
H 0.09288800 -2.69102000 -0.92939500
C 4.35605700 -3.33887400 -0.08078700
C 4.65128600 -0.95670000 0.66986400
H 4.01694000 -1.58184600 -1.27884000
H 1.15574600 -0.89948100 3.56329900
H 2.48838000 -0.21855600 2.60903200
H 0.82571800 -4.47771400 0.67054000
H 0.47580400 -5.09927700 -0.94182300
H 2.14856800 -4.91684700 -0.41783800
H 1.47614000 -2.04932200 -2.89752200
H 2.58759200 -3.38893000 -2.57318100
H 0.91219100 -3.71988100 -3.01825200
H 3.97567400 -4.00848800 -0.85460400
H 5.45085800 -3.35020000 -0.15142700
H 4.09006700 -3.75731400 0.89654200
H 4.32221200 0.08012300 0.57592200
H 4.56742800 -1.25058400 1.72288300
H 5.71354500 -1.00724000 0.40223000
H 2.40797300 1.05790100 0.24568400
H -0.31889900 -0.24089800 -0.62624800
C -2.95157900 -0.14326600 2.84507500
O -1.94750200 -0.88838400 2.78519500
O -3.66237900 0.28872900 1.88273000
H -0.33470200 -0.24556300 1.87638100
H -3.28371000 0.19013800 3.85758600
C -4.42232400 -2.81279900 0.06822600
C -2.95355700 -2.40705600 0.02042700
C -3.61909400 -0.58764400 -1.51822100
C -5.05249000 -1.09391300 -1.39975000
H -2.46704800 -2.56236900 0.98547500
H -4.92095900 -2.31688100 0.91542300
H -4.50354800 -3.89405500 0.20647100
H -3.59386800 0.49850900 -1.63174300
H -3.11811300 -1.04678500 -2.37530000
H -5.58053800 -0.55048600 -0.60075400

H -5.58262900 -0.92091500 -2.34017600
H -2.42528600 -2.96029900 -0.76106900
O -5.08831500 -2.49594200 -1.15153300
N -2.85606700 -0.94835100 -0.28802400
H -3.20488100 -0.38867800 0.59047700

Ru-A2

H -0.00001800 1.22078800 -1.30985500
H 0.00000100 -0.90448200 1.34693300
C 1.23443600 -2.36448500 -1.20897800
C 2.47662000 -1.47692500 -1.30529700
H 1.25801400 -3.13105300 -1.99728600
H 1.19535800 -2.87447500 -0.24342300
H 2.54873300 -1.05946200 -2.31627900
H 3.38048100 -2.07234100 -1.13921500
P 2.35455100 -0.03006300 -0.12343800
N -0.00000200 -1.54995200 -1.32428400
C 3.24371400 1.36109400 -1.03641700
C 4.56165000 1.03618300 -1.75902800
C 3.37292000 2.60684900 -0.14768300
H 2.49571800 1.58542100 -1.80636400
H 4.49006800 0.13668400 -2.37849600
H 4.81524700 1.86844000 -2.42754600
H 5.40092200 0.90663300 -1.07235500
H 2.41104600 2.88912500 0.29073600
H 4.08885500 2.45625100 0.66790000
H 3.72908100 3.45628700 -0.74254100
C 3.38221700 -0.49350800 1.39401400
C 4.90649500 -0.50536400 1.20547300
C 2.91965600 -1.83252400 1.99038800
H 3.12582500 0.29772900 2.11083200
H 5.30918000 0.48616100 0.99047800
H 5.38431400 -0.85695200 2.12833900
H 5.21504900 -1.18385100 0.40236300
H 1.83994100 -1.85820600 2.15368000
H 3.19422000 -2.67468100 1.34454400
H 3.41299900 -1.99146400 2.95658900
P -2.35455500 -0.03004600 -0.12342200
C -1.23446400 -2.36445200 -1.20901100
C -2.47662400 -1.47686000 -1.30534000
H -1.19542400 -2.87445500 -0.24346100
H -1.25805100 -3.13100900 -1.99733000
H -2.54871100 -1.05937100 -2.31631200
H -3.38049700 -2.07226800 -1.13928600

C 0.00003500 1.64237100 1.26831100
O 0.00003700 2.53345200 2.03014500
C -3.24369600 1.36116000 -1.03635300
C -3.37291500 2.60686600 -0.14755000
C -4.56163200 1.03630800 -1.75899000
H -2.49568200 1.58552200 -1.80627200
H -2.41105200 2.88911500 0.29091300
H -3.72905700 3.45634200 -0.74236600
H -4.08887400 2.45621800 0.66800300
H -4.49007000 0.13684000 -2.37850500
H -5.40090600 0.90674000 -1.07232400
H -4.81521100 1.86860500 -2.42746400
C -3.38225400 -0.49356300 1.39398700
C -2.91966700 -1.83258500 1.99032500
C -4.90652200 -0.50545300 1.20537800
H -3.12591500 0.29765600 2.11084300
H -1.83996200 -1.85822300 2.15368400
H -3.41306600 -1.99160000 2.95648600
H -3.19414600 -2.67472500 1.34442200
H -5.30921000 0.48607200 0.99038000
H -5.21502900 -1.18393500 0.40224600
H -5.38437800 -0.85706200 2.12821600
H 0.00001400 -1.12465100 -2.25154600
Ru 0.00000400 0.22046900 0.08870500

Ru-A3

H 0.00086100 1.38320500 -0.44936800
H -0.00474700 -1.98114000 0.00073900
C -1.23383800 -0.54315000 2.56629900
C -2.47539800 0.00338300 1.85959000
H -1.25377800 -0.26758600 3.63085700
H -1.19764400 -1.63322100 2.49989500
H -2.53676100 1.08560400 2.02063400
H -3.38225600 -0.43712300 2.28628800
P -2.35885300 -0.27348300 0.01180700
N -0.00011100 -0.02408900 1.92585900
C -3.26445000 1.21127900 -0.72444700
C -4.55204000 1.68996100 -0.03411300
C -3.46007900 1.03807800 -2.23832400
H -2.50576300 1.99070500 -0.58201800
H -4.42826100 1.81261900 1.04618100
H -4.83045500 2.67066200 -0.44006500
H -5.39750500 1.01942300 -0.20215100
H -2.52504700 0.76683100 -2.73779200

H -4.20490700 0.26898800 -2.46945400
 H -3.81143200 1.97791700 -2.68026100
 C -3.39135600 -1.81407300 -0.35494800
 C -4.91175700 -1.66344200 -0.19013700
 C -2.89881900 -3.02366000 0.45525500
 H -3.17215700 -2.00893500 -1.41323000
 H -5.34430700 -0.96015200 -0.90417300
 H -5.39401500 -2.63445200 -0.35792000
 H -5.18321900 -1.33834700 0.82061700
 H -1.82108100 -3.17162100 0.35753400
 H -3.13882000 -2.91652300 1.51970100
 H -3.40223100 -3.93035300 0.09943300
 P 2.35892300 -0.27425000 0.01141100
 C 1.23363100 -0.54336700 2.56603400
 C 2.47527300 0.00283200 1.85920800
 H 1.19711500 -1.63344100 2.49961700
 H 1.25381400 -0.26784100 3.63059900
 H 2.53684700 1.08505000 2.02018600
 H 3.38203100 -0.43779200 2.28600900
 C -0.00035900 -0.61588200 -2.13880500
 O -0.00022000 -0.83123000 -3.29132300
 C 3.26433200 1.21048300 -0.72517000
 C 3.46103100 1.03624700 -2.23877500
 C 4.55129300 1.69011000 -0.03434100
 H 2.50528000 1.98971600 -0.58383200
 H 2.52642200 0.76418600 -2.73861500
 H 3.81218500 1.97594600 -2.68117600
 H 4.20640500 0.26737700 -2.46891400
 H 4.42671800 1.81362000 1.04576300
 H 5.39709000 1.01970200 -0.20123000
 H 4.82965000 2.67056500 -0.44092100
 C 3.39202300 -1.81434200 -0.35515200
 C 2.89758500 -3.02472600 0.45262800
 C 4.91209900 -1.66388100 -0.18731600
 H 3.17487000 -2.00790500 -1.41409800
 H 1.82007600 -3.17260500 0.35231600
 H 3.40178100 -3.93110900 0.09712100
 H 3.13504500 -2.91870300 1.51776600
 H 5.34589200 -0.95997700 -0.89998900
 H 5.18168300 -1.33960600 0.82419900
 H 5.39474100 -2.63472600 -0.35501100
 H -0.00017400 0.99073900 2.03328800
 C 0.00148600 3.86164900 0.73942700
 O 0.00190000 3.36589400 1.80145200

O 0.00109900 4.41160800 -0.29077200
 Ru -0.00046300 -0.32682400 -0.31395800

RuATS3_4

H 0.00547500 1.51593400 -0.05182500
 H -0.03601200 -1.86414100 -0.43236500
 C -1.24348900 -1.06855100 2.43248000
 C -2.49403000 -0.38891900 1.86993700
 H -1.26036100 -1.03273100 3.53156000
 H -1.19886800 -2.11815600 2.13059500
 H -2.57295300 0.62301600 2.28235500
 H -3.39440100 -0.93081100 2.17640900
 P -2.37629400 -0.21797900 0.00942500
 N -0.01731400 -0.40835400 1.91842300
 C -3.26875500 1.40143900 -0.36718900
 C -4.55524300 1.72263200 0.41148600
 C -3.46058800 1.57955300 -1.88123600
 H -2.50821600 2.12401300 -0.04856300
 H -4.43637500 1.59166100 1.49125800
 H -4.81857700 2.77401700 0.24150900
 H -5.40847800 1.12090000 0.09106800
 H -2.52206600 1.44167800 -2.42688700
 H -4.19752400 0.87758000 -2.28604500
 H -3.82160400 2.59267200 -2.09410900
 C -3.41004200 -1.62189900 -0.71611700
 C -4.92766600 -1.52052600 -0.49850000
 C -2.90476200 -2.99228700 -0.23767000
 H -3.20649200 -1.54604300 -1.79254500
 H -5.36706600 -0.65670300 -1.00075000
 H -5.41353600 -2.41532200 -0.90679800
 H -5.18735400 -1.47004900 0.56516900
 H -1.83241100 -3.11568100 -0.40405500
 H -3.10919900 -3.14379000 0.82871900
 H -3.42821400 -3.78547100 -0.78439100
 P 2.34665300 -0.25024200 0.00220100
 C 1.22465800 -1.02249200 2.45158100
 C 2.45958300 -0.33201800 1.86776800
 H 1.20679000 -2.08208100 2.18411000
 H 1.23919800 -0.95227900 3.54892000
 H 2.50449500 0.69981500 2.23354700
 H 3.37295900 -0.83380100 2.20343800
 C -0.01087700 -0.04862300 -2.16156700
 O -0.00990300 0.02515200 -3.33048600
 C 3.26689300 1.32951300 -0.46551800

C 3.50829800 1.39534800 -1.98185600
 C 4.53298300 1.69302300 0.32805200
 H 2.50683600 2.08268500 -0.22939400
 H 2.58782000 1.22403200 -2.54818000
 H 3.88282300 2.38907300 -2.25426100
 H 4.25310100 0.66361100 -2.31199900
 H 4.37325600 1.66060900 1.41003300
 H 5.38304300 1.04840100 0.09299800
 H 4.82604000 2.71997700 0.07676700
 C 3.36428900 -1.70047000 -0.65222900
 C 2.80964400 -3.04838800 -0.16444000
 C 4.87502100 -1.63036600 -0.37993400
 H 3.20166200 -1.64436800 -1.73677900
 H 1.73933500 -3.14604300 -0.35913300
 H 3.32732100 -3.86403100 -0.68298300
 H 2.98084300 -3.18680300 0.90959000
 H 5.35590500 -0.79008400 -0.88393700
 H 5.09359400 -1.55972200 0.69169300
 H 5.35371700 -2.54641000 -0.74747100
 H -0.03609000 0.56709400 2.22492300
 C 0.13490600 3.09043600 0.95877900
 O 0.01967300 2.68181900 2.06968500
 O 0.27861800 3.87997300 0.09075600
 Ru -0.01328700 -0.20160100 -0.31950400

Ru-A4

H -0.07347000 1.80075600 0.13110700
 H -0.02376800 -1.73212700 -0.43810200
 C -1.25020900 -0.90175600 2.47120500
 C -2.49277400 -0.23331100 1.87575900
 H -1.25783500 -0.78787000 3.56474000
 H -1.23459500 -1.97229200 2.24835300
 H -2.53469500 0.80684200 2.21557200
 H -3.40376200 -0.73028400 2.22419500
 P -2.38281400 -0.18891800 0.01189500
 N -0.01720500 -0.29541300 1.90906700
 C -3.26952300 1.39136400 -0.50263700
 C -4.53463300 1.78345300 0.27820900
 C -3.50860800 1.41769000 -2.02057800
 H -2.50414500 2.14439600 -0.27942900
 H -4.37588100 1.78256800 1.36043000
 H -4.82263700 2.80346300 -0.00399300
 H -5.38529400 1.13375800 0.05896400
 H -2.59394500 1.20900100 -2.58385400

H -4.27026400 0.69302500 -2.32686400
 H -3.86099000 2.41110300 -2.32091800
 C -3.37282000 -1.65310300 -0.63411900
 C -4.88215200 -1.60084100 -0.35068500
 C -2.78736900 -2.98613600 -0.13944500
 H -3.21842700 -1.59958200 -1.71983700
 H -5.37464500 -0.76766100 -0.85561300
 H -5.35182000 -2.52392000 -0.71151400
 H -5.09371600 -1.52682100 0.72193300
 H -1.71885500 -3.07270800 -0.35195800
 H -2.93644400 -3.11494300 0.93859600
 H -3.30012600 -3.81558400 -0.64011000
 P 2.36140900 -0.22837000 0.00848700
 C 1.21728700 -0.88813400 2.48266300
 C 2.46368800 -0.23864500 1.87422200
 H 1.20029900 -1.96335500 2.28364100
 H 1.22526000 -0.75086200 3.57347900
 H 2.51390600 0.80756900 2.19376800
 H 3.37025700 -0.73437100 2.23595400
 C -0.00618300 -0.11880700 -2.16981000
 O -0.00606100 -0.16738700 -3.33645700
 C 3.26060900 1.33592000 -0.53257100
 C 3.51416300 1.32677700 -2.04853600
 C 4.52260400 1.73437400 0.25013300
 H 2.49860500 2.09997200 -0.33494900
 H 2.60246200 1.11565200 -2.61560600
 H 3.87796500 2.31067900 -2.36614200
 H 4.27170100 0.58892000 -2.33302300
 H 4.35322900 1.76612400 1.33028900
 H 5.36696700 1.06773900 0.05827300
 H 4.82669700 2.74236700 -0.05730700
 C 3.33530000 -1.71525500 -0.60759200
 C 2.72573800 -3.03261500 -0.10007200
 C 4.84241900 -1.67863400 -0.30999300
 H 3.19246000 -1.67502600 -1.69541300
 H 1.65879400 -3.10788400 -0.32468900
 H 3.23324600 -3.87654700 -0.58153500
 H 2.85899700 -3.14705100 0.98163400
 H 5.34928300 -0.85500100 -0.81645800
 H 5.04479400 -1.59828300 0.76395800
 H 5.30448800 -2.61003100 -0.65907100
 H -0.02954700 0.71967900 2.14645800
 C 0.08480200 2.75383200 0.81911000
 O -0.04545800 2.51872700 2.04270100

O 0.33821200 3.77609100 0.17971500
Ru -0.00933200 -0.15706100 -0.30871400

Ru-A4a

H 0.00002100 -3.99620300 0.68609200
H -0.00004400 1.72675400 -0.34021400
C 1.23159000 0.86149100 2.47932400
C 2.47476600 0.19763700 1.87906700
H 1.24585600 0.74945500 3.57370800
H 1.21466800 1.93270400 2.25632200
H 2.51838800 -0.84467100 2.21147400
H 3.38519500 0.69218100 2.23299700
P 2.36600100 0.16821100 0.01346700
N -0.00005300 0.25684700 1.92178500
C 3.23263600 -1.41683500 -0.51190400
C 4.47955300 -1.84845800 0.27650400
C 3.49097000 -1.42493300 -2.02728000
H 2.43960800 -2.14756900 -0.31396200
H 4.31134900 -1.85765200 1.35739200
H 4.75007400 -2.87099800 -0.01519900
H 5.34669700 -1.21454700 0.07497100
H 2.58942700 -1.18205300 -2.59810300
H 4.27569200 -0.71681600 -2.31401200
H 3.82012200 -2.42250400 -2.34119200
C 3.38336700 1.62409800 -0.61185100
C 4.88948700 1.54697500 -0.31688100
C 2.81459600 2.96183300 -0.11130100
H 3.23733700 1.58282900 -1.69936800
H 5.37384600 0.70882800 -0.82173800
H 5.37739100 2.46452800 -0.66791100
H 5.09038900 1.46343200 0.75708300
H 1.74746700 3.06110500 -0.32405200
H 2.96378500 3.08245600 0.96784900
H 3.33827900 3.78829600 -0.60590900
P -2.36606300 0.16818900 0.01341600
C -1.23171400 0.86147900 2.47929800
C -2.47486800 0.19761100 1.87901200
H -1.21479500 1.93269200 2.25629700
H -1.24600300 0.74944100 3.57368100
H -2.51848900 -0.84469800 2.21141800
H -3.38531200 0.69214600 2.23291800
C 0.00000000 0.16855800 -2.16443400
O 0.00010800 0.25455300 -3.33119300
C -3.23266000 -1.41687500 -0.51197100

C -3.49097500 -1.42499700 -2.02735100
C -4.47954700 -1.84857800 0.27644500
H -2.43960300 -2.14757900 -0.31403200
H -2.58943400 -1.18208100 -2.59816300
H -3.82007700 -2.42258500 -2.34126000
H -4.27572400 -0.71691900 -2.31410600
H -4.31133500 -1.85775000 1.35733200
H -5.34674000 -1.21473800 0.07491200
H -4.74999200 -2.87114200 -0.01524600
C -3.38339000 1.62410900 -0.61189900
C -2.81430900 2.96183500 -0.11168300
C -4.88945300 1.54727100 -0.31655800
H -3.23761100 1.58266100 -1.69944300
H -1.74721400 3.06091700 -0.32469500
H -3.33798100 3.78830000 -0.60629900
H -2.96323700 3.08264400 0.96748300
H -5.37408100 0.70914800 -0.82119000
H -5.09010500 1.46390400 0.75746700
H -5.37728600 2.46486300 -0.66758500
H -0.00005400 -0.75774200 2.14732000
C 0.00003700 -2.90001300 0.89346300
O 0.00010900 -2.54816200 2.09357400
O -0.00002000 -2.17638400 -0.15266200
Ru -0.00002900 0.13117500 -0.31196700

Ru-A4b

H -0.00032900 3.16263800 -0.51129800
H -0.00000300 -1.60238400 -0.83439700
C -1.23596100 -1.53405900 2.24717000
C -2.47493100 -0.74046600 1.82631400
H -1.24461200 -1.69133300 3.33519400
H -1.22007300 -2.51602300 1.76774900
H -2.52666100 0.18523600 2.40992700
H -3.38416500 -1.30995600 2.04353000
P -2.36804600 -0.24078800 0.02726400
N 0.00000000 -0.82155300 1.84359200
C -3.27420100 1.40494500 -0.07023100
C -4.55033500 1.56961800 0.77053200
C -3.49927100 1.82371200 -1.53210700
H -2.51445300 2.07356200 0.35137500
H -4.40402800 1.28279300 1.81595900
H -4.84577900 2.62616400 0.76535900
H -5.39206400 0.99557500 0.37619000
H -2.57586100 1.78020100 -2.11769600

H -4.24655000 1.19541200 -2.02826100
 H -3.86378100 2.85685000 -1.56805200
 C -3.34980100 -1.51929000 -0.94620200
 C -4.86714500 -1.51281600 -0.70563900
 C -2.78948900 -2.93530300 -0.73345500
 H -3.15989700 -1.23664500 -1.99005000
 H -5.33907300 -0.58453400 -1.03280900
 H -5.32862300 -2.33013500 -1.27318400
 H -5.11443400 -1.67076600 0.35008500
 H -1.71390800 -2.98673600 -0.92010900
 H -2.98158700 -3.29352200 0.28432900
 H -3.28567400 -3.62979100 -1.42126800
 P 2.36806500 -0.24074500 0.02728700
 C 1.23597700 -1.53401500 2.24719700
 C 2.47493200 -0.74039200 1.82634600
 H 1.22012100 -2.51598800 1.76779400
 H 1.24461800 -1.69127000 3.33522400
 H 2.52661700 0.18532200 2.40994300
 H 3.38417900 -1.30984800 2.04359500
 C 0.00001100 0.47191700 -2.03079400
 O 0.00000000 0.78395900 -3.15860200
 C 3.27416400 1.40501300 -0.07022900
 C 3.49919200 1.82377800 -1.53211000
 C 4.55031200 1.56971300 0.77050600
 H 2.51439900 2.07360200 0.35139000
 H 2.57576400 1.78026100 -2.11766900
 H 3.86369500 2.85691800 -1.56806700
 H 4.24646100 1.19548100 -2.02828500
 H 4.40402600 1.28291300 1.81594200
 H 5.39203500 0.99566200 0.37616100
 H 4.84575400 2.62626000 0.76530300
 C 3.34990500 -1.51920000 -0.94614800
 C 2.78973800 -2.93526100 -0.73333400
 C 4.86725500 -1.51255400 -0.70562300
 H 3.15995300 -1.23661400 -1.99000200
 H 1.71415700 -2.98680600 -0.91996100
 H 3.28597600 -3.62972700 -1.42113100
 H 2.98189200 -3.29342300 0.28446000
 H 5.33907200 -0.58423100 -1.03284000
 H 5.11459200 -1.67043700 0.35009900
 H 5.32880900 -2.32984300 -1.27315000
 H -0.00001900 0.10294700 2.28599600
 C -0.00020800 3.01512500 0.59833400
 O 0.00006300 1.78296700 0.97705600

O -0.00032400 4.00684100 1.33020300
 Ru 0.00000900 -0.09947400 -0.26893600

PNPRu

H 0.00000100 -0.91227000 1.32570100
 C 1.23443600 -2.35645100 -1.23918300
 C 2.47662000 -1.46831300 -1.33001600
 H 1.25801400 -3.11813300 -2.03221300
 H 1.19535800 -2.87239800 -0.27679800
 H 2.54873300 -1.04461100 -2.33839900
 H 3.38048100 -2.06474400 -1.16761600
 P 2.35455100 -0.02878200 -0.13923900
 N -0.00000200 -1.54122100 -1.34945400
 C 3.24371400 1.36799000 -1.04360400
 C 4.56165000 1.04755100 -1.76820900
 C 3.37292000 2.60823000 -0.14718900
 H 2.49571800 1.59707100 -1.81215000
 H 4.49006800 0.15189700 -2.39322300
 H 4.81524700 1.88392300 -2.43157200
 H 5.40092200 0.91376000 -1.08235000
 H 2.41104600 2.88779100 0.29296600
 H 4.08885500 2.45259500 0.66744800
 H 3.72908100 3.46132700 -0.73678700
 C 3.38221700 -0.50159500 1.37532000
 C 4.90649500 -0.51228500 1.18671000
 C 2.91965600 -1.84427000 1.96340900
 H 3.12582500 0.28519800 2.09701400
 H 5.30918000 0.48054900 0.97784600
 H 5.38431400 -0.86956900 2.10738600
 H 5.21504900 -1.18579700 0.37942200
 H 1.83994100 -1.87096100 2.12653900
 H 3.19422000 -2.68242000 1.31237300
 H 3.41299900 -2.00917700 2.92860900
 P -2.35455500 -0.02876400 -0.13922300
 C -1.23446400 -2.35641800 -1.23921600
 C -2.47662400 -1.46824700 -1.33005800
 H -1.19542400 -2.87237700 -0.27683600
 H -1.25805100 -3.11808900 -2.03225700
 H -2.54871100 -1.04451900 -2.33843100
 H -3.38049700 -2.06467000 -1.16768700
 C 0.00003500 1.63502100 1.26281800
 O 0.00003700 2.52137700 2.03014400
 C -3.24369600 1.36805600 -1.04354000
 C -3.37291500 2.60824600 -0.14705600

C -4.56163200 1.04767600 -1.76817000
 H -2.49568200 1.59717200 -1.81205700
 H -2.41105200 2.88778100 0.29314300
 H -3.72905700 3.46138200 -0.73661100
 H -4.08887400 2.45256200 0.66755100
 H -4.49007000 0.15205300 -2.39323100
 H -5.40090600 0.91386700 -1.08231800
 H -4.81521100 1.88408800 -2.43148800
 C -3.38225400 -0.50164900 1.37529300
 C -2.91966700 -1.84433000 1.96334600
 C -4.90652200 -0.51237300 1.18661400
 H -3.12591500 0.28512500 2.09702500
 H -1.83996200 -1.87097700 2.12654300
 H -3.41306600 -2.00931300 2.92850600
 H -3.19414600 -2.68246300 1.31225100
 H -5.30921000 0.48046100 0.97774700
 H -5.21502900 -1.18588000 0.37930500
 H -5.38437800 -0.86967800 2.10726200
 Ru 0.00000400 0.22043500 0.07444800

Ru-A5

H 0.59539500 5.05158400 0.20287800
 H -0.11069900 -1.59268000 -0.69169400
 C 1.20422900 0.73267200 -2.38782100
 C 2.45274800 0.84393100 -1.51127100
 H 1.23475300 1.50327000 -3.17159800
 H 1.16109300 -0.24168300 -2.88289400
 H 2.50532000 1.85199500 -1.08683100
 H 3.35749800 0.66889100 -2.10286300
 P 2.32092000 -0.29585000 -0.04691700
 N -0.03278100 0.89578200 -1.58224000
 C 3.30431500 0.55748800 1.30810800
 C 4.65016700 1.18629700 0.90946700
 C 3.43462500 -0.33563600 2.55052800
 H 2.62948900 1.38824400 1.54262100
 H 4.56497400 1.82089200 0.02271300
 H 4.99686800 1.82644600 1.73006000
 H 5.43114000 0.44516500 0.72412900
 H 2.46452200 -0.71939500 2.88269300
 H 4.09408700 -1.19218200 2.37179600
 H 3.86329400 0.24046900 3.37880600
 C 3.16713100 -1.92105600 -0.48511200
 C 4.69698000 -1.85429300 -0.61365200
 C 2.56239400 -2.55391100 -1.74925600

H 2.91784200 -2.56825400 0.36604900
 H 5.18638700 -1.60841800 0.33070900
 H 5.07736000 -2.83281200 -0.93121100
 H 5.01206100 -1.12324500 -1.36617200
 H 1.47508800 -2.64510000 -1.68907100
 H 2.81180200 -1.97507600 -2.64568500
 H 2.97737600 -3.55931800 -1.88584400
 P -2.42993800 -0.14599800 -0.03166500
 C -1.24126200 0.68746000 -2.41866900
 C -2.51350200 0.87467900 -1.59126300
 H -1.19600200 -0.32090100 -2.84034200
 H -1.24040600 1.40052500 -3.25572600
 H -2.58467800 1.92107500 -1.27717400
 H -3.40156100 0.64845000 -2.19002500
 C -0.08016100 -1.55137700 1.69328500
 O -0.09958200 -2.37226000 2.52068100
 C -3.31003100 0.89943500 1.26387600
 C -3.46867100 0.12504500 2.58124000
 C -4.61573800 1.59622400 0.84683200
 H -2.56307100 1.68689700 1.42759300
 H -2.52058400 -0.30711600 2.91738000
 H -3.82412400 0.79924300 3.36892300
 H -4.19866500 -0.68634500 2.48975400
 H -4.51396300 2.14131200 -0.09607600
 H -5.45279200 0.90155600 0.74842700
 H -4.88798500 2.32852500 1.61660400
 C -3.41249300 -1.72515400 -0.31516500
 C -2.88567900 -2.49428400 -1.53776200
 C -4.93574200 -1.55300900 -0.41285800
 H -3.18679500 -2.32079100 0.57938000
 H -1.80819800 -2.66912200 -1.48515200
 H -3.38372300 -3.46903200 -1.59490800
 H -3.10363300 -1.96200600 -2.47051400
 H -5.37206500 -1.17837500 0.51493500
 H -5.22034900 -0.87667900 -1.22636000
 H -5.39663600 -2.52606100 -0.62152500
 H -0.05954300 1.89638400 -1.25863300
 C 0.58712000 3.94797900 -0.00744600
 O -0.22419100 3.58279200 -0.90419900
 O 1.37790000 3.24839600 0.67052400
 H 0.30669800 1.45282100 1.12732400
 H -0.24521900 1.09346500 1.56109500
 Ru -0.05771000 -0.33594900 0.27469100

RuATS5_6

H 1.01650300 4.96520000 -0.30606200
H -0.11357100 -1.74931700 -0.49335900
C 1.18660900 0.26276700 -2.52830600
C 2.45739300 0.49206300 -1.70807900
H 1.22695700 0.86295100 -3.44889800
H 1.09378700 -0.78727800 -2.81871600
H 2.58077300 1.56510200 -1.52644900
H 3.33943600 0.15151700 -2.25980100
P 2.31402700 -0.32888300 -0.03460600
N -0.01829400 0.62756800 -1.74215600
C 3.27258400 0.79933200 1.12836000
C 4.62099700 1.35383300 0.63883800
C 3.38662600 0.17432600 2.52716600
H 2.58189400 1.64833100 1.19813300
H 4.56218000 1.76467700 -0.37368300
H 4.93024100 2.17183400 1.30112900
H 5.41645400 0.60562000 0.65436500
H 2.41115700 -0.14051900 2.91116300
H 4.05272200 -0.69555700 2.53474700
H 3.79838700 0.90809200 3.22992600
C 3.21360600 -1.98096500 -0.15490500
C 4.74402500 -1.90122800 -0.26269500
C 2.64889700 -2.83729300 -1.30046300
H 2.95827900 -2.47457400 0.79190600
H 5.20171700 -1.47223900 0.63053700
H 5.15217000 -2.91194900 -0.38548800
H 5.06495300 -1.31401600 -1.13045300
H 1.56138500 -2.93082500 -1.24916300
H 2.91301000 -2.41985100 -2.27887900
H 3.07875700 -3.84431800 -1.24932300
P -2.42101300 -0.14729000 -0.02623300
C -1.26480600 0.40459800 -2.51578900
C -2.49522500 0.73845700 -1.67011700
H -1.28203400 -0.64196700 -2.83232000
H -1.25907200 1.02762900 -3.42195300
H -2.50067200 1.81196600 -1.45057600
H -3.41367500 0.51564500 -2.22283700
C -0.09051000 -1.26333000 1.89094300
O -0.10899000 -1.89063400 2.87653200
C -3.29464100 1.00927700 1.17870000
C -3.49319100 0.33158200 2.54355700
C -4.57613600 1.70940200 0.69797200
H -2.52786000 1.78381100 1.30389200

H -2.56136100 -0.09708700 2.92525900
H -3.84373800 1.06798700 3.27594500
H -4.24211800 -0.46635000 2.49698900
H -4.45130000 2.18615700 -0.27858200
H -5.43196200 1.03340700 0.63771700
H -4.83642200 2.50037500 1.41205000
C -3.44724900 -1.71795500 -0.19411000
C -2.93521900 -2.60370300 -1.34201400
C -4.96394100 -1.51247400 -0.32792000
H -3.24893900 -2.24514300 0.74870000
H -1.86206800 -2.79612600 -1.26925900
H -3.45559600 -3.56804600 -1.31543800
H -3.13939200 -2.15110400 -2.31918600
H -5.40495700 -1.06303100 0.56359900
H -5.21828900 -0.88719900 -1.19082700
H -5.44924500 -2.48493500 -0.47606100
H 0.04639300 1.64545800 -1.54998100
C 0.68266400 3.90402500 -0.32408300
O 0.27183000 3.44299200 -1.40444000
O 0.77779100 3.31717000 0.80936900
H 0.26885500 2.04163500 0.88401400
H -0.12481300 1.26757200 1.14918100
Ru -0.05900100 -0.33560100 0.28163000

Ru-A6

H 0.62799000 5.15078000 -0.45072200
H -0.07329200 -1.88534100 -0.46540600
C 1.21125800 0.12503300 -2.55304600
C 2.46457200 0.42412000 -1.72878900
H 1.24678000 0.68210000 -3.50075700
H 1.14831500 -0.93969200 -2.79201700
H 2.56217600 1.50767000 -1.59706700
H 3.36073400 0.08112100 -2.25593200
P 2.32472400 -0.32486900 -0.02010200
N -0.01377600 0.48702800 -1.79737300
C 3.25327000 0.89581400 1.07711600
C 4.59840200 1.44709800 0.57426000
C 3.35635100 0.37775700 2.51938000
H 2.54188400 1.73041300 1.07964700
H 4.55417700 1.78077000 -0.46707500
H 4.87422500 2.31893600 1.18058900
H 5.41091900 0.72279400 0.66255400
H 2.38023600 0.07943300 2.91305300
H 4.03231200 -0.48086400 2.59755400

H 3.75166400 1.16538200 3.17167600
 C 3.29152800 -1.94734800 -0.06356100
 C 4.82197100 -1.82423400 -0.11583500
 C 2.80191500 -2.85522700 -1.20350400
 H 3.01425500 -2.42345100 0.88593200
 H 5.23463500 -1.36620700 0.78501700
 H 5.26343000 -2.82474000 -0.20347900
 H 5.15901100 -1.24465200 -0.98261300
 H 1.71702900 -2.98281300 -1.19155400
 H 3.09428500 -2.45950700 -2.18313800
 H 3.26166500 -3.84537200 -1.10295100
 P -2.39171900 -0.21115400 -0.03066900
 C -1.24766200 0.17539900 -2.56118300
 C -2.49381100 0.52643900 -1.74662500
 H -1.22695000 -0.89155800 -2.79772700
 H -1.25378800 0.73161100 -3.51005800
 H -2.55453400 1.61382500 -1.62556500
 H -3.39864400 0.21070300 -2.27608800
 C -0.07088200 -1.18541200 1.94879900
 O -0.09389900 -1.71768100 2.99172000
 C -3.25610200 1.06750400 1.05276400
 C -3.38284200 0.57365200 2.50157800
 C -4.57233300 1.68069600 0.54553600
 H -2.50022300 1.86246300 1.04384000
 H -2.42139300 0.23494600 2.89856700
 H -3.73882000 1.38817900 3.14343700
 H -4.09931300 -0.25020300 2.59184000
 H -4.51523800 1.99882100 -0.49988800
 H -5.42073700 1.00022200 0.64505200
 H -4.80206500 2.57264500 1.14169500
 C -3.43782700 -1.78370200 -0.05642800
 C -2.99067300 -2.72732200 -1.18447800
 C -4.96004300 -1.58508100 -0.11169500
 H -3.18462600 -2.26219100 0.89862600
 H -1.91354500 -2.90874100 -1.16573100
 H -3.49996500 -3.69202000 -1.07525100
 H -3.25880800 -2.32859600 -2.16982300
 H -5.35155600 -1.10528100 0.78751200
 H -5.26567800 -0.99105900 -0.98012000
 H -5.45056200 -2.56264500 -0.19771200
 H 0.01111300 1.50238100 -1.64970900
 C 0.42357300 4.06863200 -0.47765600
 O 0.24109300 3.46756700 -1.52557600
 O 0.40504600 3.56086400 0.73853000

H 0.22069300 2.55404300 0.72708800
 H -0.01047000 1.20849000 0.94442100
 Ru -0.03881500 -0.39160400 0.27837000

Mn-A2

P -2.26493700 -0.12919700 -0.04629800
 N -0.01729300 -1.66981700 -1.21965500
 C 1.00750100 -1.52932800 -2.28411800
 C -1.35519600 -2.12540000 -1.70754500
 C -2.38624800 -0.99741700 -1.69367600
 H -3.38366900 -1.39031500 -1.91780700
 H -2.14187300 -0.25924200 -2.46291800
 C 2.39086700 -1.36325400 -1.64514400
 H 3.09420100 -0.94787600 -2.37304200
 P 2.28030300 -0.25660200 -0.12487900
 C 0.09755700 1.19796000 1.48007600
 O 0.15834400 1.87740800 2.43355000
 Mn 0.01665100 0.08139800 0.11592500
 C 0.03963900 1.34413200 -1.13996500
 O 0.06041000 2.22840500 -1.91580200
 C -3.46150600 1.33263100 -0.16774000
 H -4.44162300 0.94683200 0.13671200
 C -3.06104700 2.45068900 0.80945300
 H -3.82655000 3.23659000 0.80766000
 H -2.95371200 2.09427600 1.83742700
 H -2.11132700 2.90811600 0.51540200
 C -3.60105900 1.89659200 -1.58998300
 H -4.02068100 1.16867600 -2.29023400
 H -4.27701400 2.76055300 -1.57455500
 H -2.64017500 2.24037600 -1.98541000
 C 3.36007600 1.19929800 -0.66527900
 H 2.95491000 1.40265200 -1.66589800
 C 3.14809900 2.46993200 0.17177800
 H 3.68914100 3.30752900 -0.28581700
 H 2.09287600 2.74588700 0.22937200
 H 3.52381600 2.36003000 1.19404500
 C 4.85339500 0.87413600 -0.81628700
 H 5.36742400 1.70744000 -1.31112800
 H 5.33696000 0.72722300 0.15525800
 H 5.02945600 -0.02229600 -1.42011200
 H 1.00311500 -2.40899500 -2.94427000
 H 0.74836700 -0.65675200 -2.89015200
 H 2.78264100 -2.34188400 -1.35121500
 H -1.68740800 -2.93492100 -1.05033900

H -1.26190000 -2.54840600 -2.71535400
 C 3.32170500 -1.19787700 1.13934400
 H 4.30304900 -1.35673900 0.67431900
 C 2.72222700 -2.57173900 1.47556900
 H 3.37365200 -3.09166700 2.18864700
 H 1.73426800 -2.46873400 1.93434200
 H 2.62384000 -3.22035000 0.59907100
 C 3.51087600 -0.38050400 2.42607200
 H 4.09509400 -0.95760300 3.15331900
 H 4.04175200 0.55909400 2.25200800
 H 2.54634100 -0.14472300 2.88869200
 C -3.13809600 -1.31847800 1.13469100
 H -2.47197900 -2.19060400 1.12340900
 C -4.54021400 -1.77730000 0.70936500
 H -4.91584400 -2.52523100 1.41880900
 H -5.26086300 -0.95192100 0.70441100
 H -4.55049800 -2.23765600 -0.28306800
 C -3.15225900 -0.76914200 2.56942800
 H -3.50289200 -1.54195200 3.26425900
 H -2.15602200 -0.45510200 2.89411300
 H -3.83095300 0.08570500 2.66714800
 H 0.31658900 -2.39387600 -0.58885400
 H -0.03614400 -1.01947500 1.30064500

Mn-A3

Mn -0.00000200 -0.37376600 -0.15996100
 P 2.27574300 -0.11545800 0.10299300
 P -2.27576500 -0.11556400 0.10304500
 O 0.00014500 -3.31310400 0.13547400
 O -0.00022400 -0.54566600 -3.09380600
 N -0.00000800 0.08880000 1.97474400
 C 1.23596100 -0.32847300 2.67228300
 H 1.26371200 -1.42245100 2.67838700
 H 1.22406400 0.01276300 3.71822700
 C -1.23585100 -0.32886100 2.67228300
 H -1.22399100 0.01220900 3.71828200
 H -1.26334900 -1.42284500 2.67820300
 C 3.12728600 1.40612200 -0.62855300
 H 2.48631000 2.20934900 -0.24258300
 C -3.50021800 -1.52296900 -0.21037400
 H -4.50060200 -1.07455500 -0.18077800
 C -2.44201400 0.24904100 1.93436800
 H -2.44550000 1.33963000 2.04823700
 H -3.37813300 -0.12048100 2.36143100

C -3.12717700 1.40625700 -0.62813100
 H -2.48609400 2.20931500 -0.24201500
 C 2.44194700 0.24957500 1.93421700
 H 3.37816400 -0.11956500 2.36140100
 H 2.44510600 1.34019800 2.04776500
 C 3.28285400 -2.14057700 -1.60225100
 H 2.31796900 -2.65453200 -1.66046200
 H 4.06601500 -2.88073100 -1.80818500
 H 3.31230600 -1.39786600 -2.40375200
 C 3.44681700 -2.61841000 0.86639900
 H 3.71422200 -2.24708400 1.85994000
 H 4.16240300 -3.41134100 0.61529400
 H 2.45790400 -3.08064500 0.92516700
 C 3.50005000 -1.52303400 -0.21023700
 H 4.50047100 -1.07468200 -0.18102900
 C 0.00014000 -2.13922100 0.05571900
 C -0.00004300 -0.48872700 -1.92238500
 C 3.06302800 1.46818500 -2.16071400
 H 3.72788200 0.73229000 -2.62522800
 H 3.38671500 2.45765600 -2.50643900
 H 2.05025100 1.29989100 -2.53520300
 C 4.55867400 1.65175400 -0.12857800
 H 4.63399400 1.62892700 0.96307900
 H 4.90278900 2.63975500 -0.45930100
 H 5.26465500 0.91701000 -0.53062500
 C -4.55853800 1.65191300 -0.12806100
 H -5.26455900 0.91727500 -0.53023500
 H -4.90257700 2.64000300 -0.45860400
 H -4.63384000 1.62888900 0.96359200
 C -3.44675300 -2.61872200 0.86587100
 H -2.45786700 -3.08107900 0.92407300
 H -4.16254200 -3.41145200 0.61472200
 H -3.71371800 -2.24776100 1.85966800
 C -3.28323400 -2.14016300 -1.60255900
 H -3.31289200 -1.39733200 -2.40394000
 H -4.06628600 -2.88041500 -1.80854200
 H -2.31826300 -2.65394700 -1.66099700
 C -3.06294400 1.46871000 -2.16029300
 H -2.05026600 1.30005700 -2.53491600
 H -3.38621500 2.45840800 -2.50574600
 H -3.72817200 0.73323700 -2.62493400
 H -0.00015400 1.10821800 1.95422700
 H 0.00004800 1.24210000 -0.35122000
 C 0.00005800 4.01038000 0.49324700

O -0.00032600 4.39547900 -0.60947100
O 0.00043600 3.67113700 1.61465100

MnATS3_4

Mn 0.00077800 -0.27001900 -0.14666400
P 2.28982800 -0.07526800 0.14237400
P -2.28863300 -0.07824800 0.14182700
O 0.00197100 -3.21488600 -0.30533400
O 0.00488700 -0.02318800 -3.07625500
N 0.00071000 -0.17627000 2.01623400
C 1.23398800 -0.71992700 2.63353100
H 1.24438300 -1.80029800 2.45887700
H 1.22365800 -0.55638300 3.72120500
C -1.23233300 -0.72045000 2.63353700
H -1.22232900 -0.55637400 3.72113400
H -1.24193600 -1.80092000 2.45941600
C 3.13985900 1.55405300 -0.29930000
H 2.55858000 2.26385400 0.30240100
C -3.49960500 -1.40854600 -0.43496700
H -4.50134400 -0.98568000 -0.29443800
C -2.45658100 -0.05346700 2.00743900
H -2.49501800 0.99802600 2.31489000
H -3.37905600 -0.52495700 2.35809500
C -3.14098600 1.54956100 -0.30102100
H -2.56034400 2.26071300 0.29957800
C 2.45786100 -0.05173600 2.00798100
H 3.38061100 -0.52300100 2.35820600
H 2.49572500 0.99952400 2.31627100
C 3.31022700 -1.71293400 -1.92886900
H 2.33110700 -2.16508400 -2.11657200
H 4.07434700 -2.42528700 -2.26356600
H 3.39272100 -0.82283300 -2.55827500
C 3.42294300 -2.69792500 0.39039700
H 3.61989300 -2.53222200 1.45352400
H 4.17900500 -3.40569400 0.02862400
H 2.44901100 -3.18395600 0.29180700
C 3.50233800 -1.40397100 -0.43509000
H 4.50363200 -0.98032400 -0.29374300
C 0.00175400 -2.04393500 -0.20998800
C 0.00262100 -0.12904400 -1.91033700
C 2.97709100 1.95987500 -1.77114200
H 3.58631700 1.33550000 -2.43303500
H 3.31093200 2.99574400 -1.90750800
H 1.93810400 1.89862400 -2.10318600

C 4.60784500 1.66122000 0.14168900
H 4.75650500 1.38594300 1.19092500
H 4.95277100 2.69575700 0.02375800
H 5.26423400 1.03319100 -0.46991700
C -4.60879900 1.65566200 0.14076500
H -5.26502700 1.02643600 -0.46976900
H -4.95474500 2.68977100 0.02202400
H -4.75649600 1.38135300 1.19039000
C -3.41953200 -2.70180900 0.39151000
H -2.44518300 -3.18718200 0.29369200
H -4.17492900 -3.41042900 0.03001300
H -3.61704900 -2.53537900 1.45442600
C -3.30629200 -1.71813800 -1.92846600
H -3.38922800 -0.82842800 -2.55837300
H -4.06949700 -2.43140100 -2.26331300
H -2.32658200 -2.16934400 -2.11532900
C -2.97935500 1.95416500 -1.77331500
H -1.94067600 1.89237000 -2.10614300
H -3.31305700 2.98999400 -1.91025800
H -3.58930500 1.32936200 -2.43414600
H 0.00056200 0.83332400 2.17581200
H -0.00214900 1.38310200 -0.07491300
C -0.00835300 3.10842400 0.58118300
O -0.01612500 3.72782900 -0.42558500
O -0.00181200 2.91439600 1.75519300

Mn-A4

Mn 0.00240500 -0.20965800 -0.13617000
P 2.32203800 -0.05357900 0.15335200
P -2.31665000 -0.05941800 0.15649700
O 0.00566000 -3.12743700 -0.42511200
O -0.00218600 0.07981300 -3.07163400
N 0.00904200 -0.20245000 1.99377700
C 1.23695400 -0.76641400 2.60923700
H 1.24787400 -1.84483800 2.42072200
H 1.21426300 -0.62000900 3.69853400
C -1.22369100 -0.74472700 2.61845900
H -1.19698800 -0.58536600 3.70584200
H -1.24522500 -1.82526000 2.44315900
C 3.16488900 1.58735200 -0.25189200
H 2.62471300 2.27838100 0.40667700
C -3.48715700 -1.40573100 -0.45274800
H -4.49517300 -0.99838100 -0.31462200
C -2.45609700 -0.06614700 2.01986800

H -2.48568300 0.98153300 2.33905000
 H -3.37463700 -0.54163200 2.37507000
 C -3.17160400 1.56958000 -0.26995100
 H -2.62357100 2.27811600 0.36209700
 C 2.47292600 -0.09021700 2.01544500
 H 3.38900300 -0.57998900 2.35684000
 H 2.51327000 0.95134100 2.35143600
 C 3.28209400 -1.64658500 -1.97934100
 H 2.29446100 -2.07744600 -2.17041500
 H 4.03128200 -2.36031500 -2.34243100
 H 3.37373200 -0.73860900 -2.58123700
 C 3.41365000 -2.69921400 0.31495700
 H 3.61935500 -2.56006200 1.37990200
 H 4.16453300 -3.39950300 -0.07040900
 H 2.43820800 -3.18114000 0.21217600
 C 3.49621200 -1.38613400 -0.47983700
 H 4.50314900 -0.97711100 -0.33894400
 C 0.00499300 -1.96422400 -0.29871100
 C -0.00014100 -0.02042100 -1.91038800
 C 2.93948900 2.05888500 -1.69511300
 H 3.44694400 1.41588800 -2.42137900
 H 3.34693400 3.06981500 -1.81606600
 H 1.87846800 2.10190600 -1.95053300
 C 4.65229500 1.64360500 0.12882700
 H 4.83897400 1.30264100 1.15247100
 H 5.00758000 2.67855300 0.05923700
 H 5.27058400 1.04426800 -0.54776600
 C -4.65298200 1.62866600 0.13336600
 H -5.27986800 1.01189400 -0.51922000
 H -5.01343400 2.66046100 0.04554800
 H -4.82238400 1.31109600 1.16745100
 C -3.39737500 -2.70660400 0.36097000
 H -2.42048400 -3.18650800 0.26209100
 H -4.14682000 -3.41530700 -0.01156500
 H -3.60046000 -2.55179200 1.42429100
 C -3.27656800 -1.68669700 -1.94925900
 H -3.37379500 -0.78801500 -2.56400800
 H -4.02399300 -2.40864500 -2.29951200
 H -2.28779000 -2.11596000 -2.13764300
 C -2.97004100 2.01448900 -1.72486600
 H -1.91337200 2.05460200 -1.99729100
 H -3.38017400 3.02296800 -1.85639400
 H -3.48923800 1.35891700 -2.43135800
 H 0.02296500 0.82329100 2.15631800

H -0.00378400 1.59423800 0.02219200
 C -0.01649700 2.67466800 0.55826200
 O -0.10698900 3.58416100 -0.26015700
 O 0.06329600 2.61405700 1.80016100

Mn-A4a

H -0.00059200 -3.84593600 -0.79911800
 C -1.23374700 0.92628700 -2.39973700
 C -2.44902000 0.15370200 -1.87480900
 H -1.20987800 0.88011300 -3.49897700
 H -1.28148500 1.98218700 -2.11615700
 H -2.41124400 -0.87051900 -2.25988500
 H -3.38329100 0.60408200 -2.22396100
 P -2.34882800 0.05350800 -0.01349200
 N -0.00002500 0.34037900 -1.83352800
 C -3.15178500 -1.58752200 0.44735700
 C -4.38323600 -2.03101300 -0.35890600
 C -3.39199100 -1.69418700 1.96289400
 H -2.33520000 -2.27662300 0.21036600
 H -4.21493300 -1.98094400 -1.43892200
 H -4.61042200 -3.07699700 -0.11687300
 H -5.27505500 -1.44392300 -0.12815500
 H -2.49944700 -1.43502300 2.53912900
 H -4.21053500 -1.05216100 2.30280400
 H -3.66076000 -2.72592400 2.21920800
 C -3.46962700 1.44618500 0.61016100
 C -4.98173900 1.18566700 0.51639300
 C -3.16001100 2.78363800 -0.08755100
 H -3.19749800 1.54192200 1.66943900
 H -5.30942500 0.34086700 1.12383900
 H -5.52142900 2.07159700 0.87337500
 H -5.29756000 1.00879200 -0.51757400
 H -2.10539600 3.05513500 -0.05944200
 H -3.48517900 2.76604000 -1.13336100
 H -3.71798900 3.58549400 0.41029700
 P 2.34870800 0.05372700 -0.01342500
 C 1.23356900 0.92684600 -2.39947700
 C 2.44903200 0.15442300 -1.87470600
 H 1.28097300 1.98267500 -2.11556700
 H 1.20979000 0.88101200 -3.49873300
 H 2.41147300 -0.86970100 -2.26003300
 H 3.38322200 0.60514400 -2.22363000
 C -0.00008100 -0.24220100 2.05324500
 O -0.00001400 -0.45570100 3.20134200

C	3.15184300	-1.58734800	0.44709100	H	-5.35906300	1.26859500	0.31931000
C	3.39198000	-1.69435300	1.96262200	H	-2.39749700	1.97636200	-2.01048400
C	4.38337500	-2.03056600	-0.35920400	H	-4.09039200	1.46379400	-2.01704400
H	2.33540600	-2.27654200	0.20993400	H	-3.66182200	3.08735600	-1.47382100
H	2.49939600	-1.43538100	2.53888600	C	-3.42625700	-1.40919600	-0.79209000
H	3.66079500	-2.72613700	2.21869600	C	-4.94461400	-1.17800400	-0.76073900
H	4.21046800	-1.05235500	2.30271900	C	-3.12792400	-2.83244800	-0.28516400
H	4.21515000	-1.98019200	-1.43921800	H	-3.09117000	-1.34172900	-1.83512900
H	5.27515200	-1.44351100	-0.12820800	H	-5.24134900	-0.24986500	-1.25220300
H	4.61057000	-3.07661100	-0.11744500	H	-5.44419600	-1.99989600	-1.28875700
C	3.46938200	1.44629100	0.61069400	H	-5.33338800	-1.16598700	0.26319300
C	3.15976800	2.78386500	-0.08677100	H	-2.06522400	-3.07503900	-0.27226500
C	4.98151800	1.18585900	0.51700200	H	-3.52799600	-2.98316500	0.72351600
H	3.19714400	1.54179400	1.66996500	H	-3.62107400	-3.55963100	-0.94081300
H	2.10513700	3.05530200	-0.05864200	P	2.35541200	-0.12377200	0.09203900
H	3.71769600	3.58565000	0.41124300	C	1.23233400	-1.37199000	2.31430800
H	3.48496900	2.76648300	-1.13257400	C	2.45595000	-0.54906900	1.90775300
H	5.30917600	0.34092900	1.12427400	H	1.26714800	-2.37510700	1.88005600
H	5.29744000	1.00926500	-0.51698000	H	1.20183100	-1.48472900	3.40781000
H	5.52113100	2.07172400	0.87426000	H	2.45117800	0.39765000	2.45967400
H	0.00030800	-0.66238200	-2.09824700	H	3.38077500	-1.07064500	2.17176300
C	0.00034000	-2.75838700	-1.03987100	C	-0.00001500	0.56158300	-1.88502500
O	0.00209700	-2.43546900	-2.24632300	O	-0.00012600	0.95121600	-2.98763600
O	-0.00053500	-2.00215900	-0.01371200	C	3.19877000	1.55695100	-0.01039800
Mn	-0.00007600	0.11974800	0.30993400	C	3.34139600	2.03883900	-1.46278700
C	-0.00019100	1.83094900	0.73116800	C	4.49978500	1.75508000	0.78540500
O	-0.00035900	2.94095000	1.10966800	H	2.43649900	2.18154200	0.46709200
Mn-A4b				H	2.39741700	1.97626100	-2.01066100
H	-0.00013800	3.02840200	-0.78022900	H	3.66181700	3.08725500	-1.47417900
C	-1.23225600	-1.37211600	2.31426700	H	4.09029000	1.46362700	-2.01727900
C	-2.45593100	-0.54926900	1.90774100	H	4.42166400	1.39172200	1.81437700
H	-1.20175700	-1.48491000	3.40776400	H	5.35909500	1.26867400	0.31908900
H	-1.26698800	-2.37521300	1.87996200	H	4.72272800	2.82811100	0.83831400
H	-2.45124800	0.39741000	2.45973100	C	3.42630900	-1.40921700	-0.79197400
H	-3.38071700	-1.07094000	2.17169700	C	3.12790900	-2.83243500	-0.28499000
P	-2.35538700	-0.12382500	0.09205800	C	4.94467300	-1.17807700	-0.76053200
N	0.00001300	-0.70986100	1.83018700	H	3.09129500	-1.34180600	-1.83504000
C	-3.19875100	1.55690100	-0.01020800	H	2.06520400	-3.07500300	-0.27215900
C	-4.49974200	1.75495600	0.78565400	H	3.62109600	-3.55966400	-0.94056000
C	-3.34144100	2.03892700	-1.46254400	H	3.52790400	-2.98310400	0.72372900
H	-2.43645500	2.18144100	0.46731100	H	5.24148900	-0.25001300	-1.25208200
H	-4.42159300	1.39149800	1.81458800	H	5.33336500	-1.16595700	0.26343000
H	-4.72268100	2.82798200	0.83867300	H	5.44426300	-2.00005400	-1.28841200
				H	-0.00003900	0.25085700	2.18676900

C -0.00005300 2.92229300 0.33035900
O 0.00001500 1.70439300 0.76070500
O -0.00010900 3.93518100 1.03059600
Mn 0.00000900 -0.11671300 -0.24347100
C 0.00002200 -1.71147800 -1.00299300
O -0.00002200 -2.71687000 -1.60603700

MnATS4_7

P 2.29978300 -0.36809100 -0.14301800
N 0.08637300 0.55731700 -1.72010400
C -1.11913400 0.61108200 -2.58034100
C 1.29853500 0.44211300 -2.57786300
C 2.36641600 -0.49043300 -1.98890400
H 3.35489600 -0.28676500 -2.41400500
H 2.10961200 -1.52647900 -2.22934900
C -2.35589700 0.99259800 -1.76857700
H -3.27121700 0.84344900 -2.34889000
P -2.35419900 0.01455900 -0.18792200
C -0.11160300 -0.55932600 1.84607100
O -0.18954000 -0.70115500 3.00277500
Mn -0.02784400 -0.32043600 0.07228900
C -0.10376500 -2.03510200 -0.26830800
O -0.13483600 -3.16303700 -0.58188200
C 3.38289500 -1.75115400 0.55204000
H 4.37978700 -1.31033500 0.66437900
C 2.90026200 -2.19181800 1.94383200
H 3.62672900 -2.88716500 2.38154000
H 2.78794900 -1.35155600 2.63458300
H 1.93829700 -2.71085600 1.88561200
C 3.51481500 -2.96265400 -0.38412100
H 3.97175000 -2.70136300 -1.34267500
H 4.15550300 -3.71556700 0.09052100
H 2.54763000 -3.43518800 -0.58125500
C -3.37583100 -1.50813000 -0.63588500
H -2.83815700 -1.87075000 -1.52255100
C -3.33633300 -2.62544200 0.42256300
H -3.62970000 -3.57623700 -0.03722600
H -2.34633400 -2.76136300 0.86197700
H -4.03815000 -2.43130100 1.23809500
C -4.82641100 -1.21074400 -1.04731700
H -5.30016900 -2.13152300 -1.40885000
H -5.41979800 -0.85196000 -0.19999800
H -4.89975900 -0.47194300 -1.85073000
H -0.98198700 1.34871800 -3.38668400

H -1.27179800 -0.36235300 -3.07198800
H -2.30939800 2.05259700 -1.50237900
H 1.73123300 1.44159200 -2.74209500
H 1.02182500 0.06521500 -3.57108300
C -3.42763000 1.05081700 0.96458700
H -4.32257000 1.29896200 0.37916600
C -2.72895700 2.36111100 1.35583600
H -3.41073200 2.97264700 1.95867100
H -1.83670300 2.17179600 1.96200200
H -2.43509600 2.96316700 0.49215200
C -3.86227500 0.28989500 2.22677400
H -4.40387400 0.97057100 2.89441700
H -4.52958600 -0.54479100 2.00253300
H -3.00244600 -0.09957900 2.78190800
C 3.24664700 1.21020900 0.26604000
H 2.68210900 1.98271500 -0.26925900
C 4.69233800 1.25016300 -0.25076400
H 5.11471600 2.24663800 -0.07458400
H 5.33495100 0.53130300 0.26826000
H 4.76023000 1.05242300 -1.32441500
C 3.18788700 1.52798000 1.76865300
H 3.61273500 2.52045500 1.95774700
H 2.16345300 1.52721000 2.15322300
H 3.76829800 0.80607700 2.35393500
H 0.18696000 1.97059900 -1.31514000
H 0.30694000 2.25566600 0.75060200
C 0.35501800 3.21404700 0.18260000
O 0.46931200 4.28126200 0.75907400
O 0.28228400 3.04876200 -1.11522700

Mn-A7

P 2.28480600 -0.43420600 -0.18524400
N 0.05784400 0.37868500 -1.73443900
C -1.13036800 0.62138700 -2.58130400
C 1.25291200 0.29389700 -2.60854100
C 2.33287000 -0.62392800 -2.02444200
H 3.31266700 -0.43503000 -2.47501100
H 2.06468600 -1.66526000 -2.22850400
C -2.34440500 1.01373900 -1.74336200
H -3.27116700 0.92187200 -2.31698600
P -2.35709000 -0.01840700 -0.19732300
C -0.06180900 -0.28769400 1.82747600
O -0.09200800 -0.21830400 2.99492200
Mn -0.03591200 -0.37719500 0.04149100

C -0.11127000 -2.12752200 0.05258000
O -0.13159300 -3.29599600 -0.04126300
C 3.37790400 -1.77946200 0.56095000
H 4.38410100 -1.34782100 0.60978100
C 2.93417400 -2.11695500 1.99477900
H 3.66419500 -2.79219400 2.45723600
H 2.85445100 -1.23016300 2.62934700
H 1.96345500 -2.62220400 2.00197200
C 3.46032700 -3.05130800 -0.29750800
H 3.89609100 -2.86032200 -1.28233500
H 4.09972800 -3.78573700 0.20701900
H 2.47937600 -3.51518400 -0.43848600
C -3.40962900 -1.50606200 -0.69470800
H -2.84717500 -1.87920800 -1.56180600
C -3.44912300 -2.63355400 0.35381100
H -3.74135700 -3.57271000 -0.13025700
H -2.48735400 -2.79877500 0.84182900
H -4.18863400 -2.43063300 1.13321100
C -4.83418000 -1.16270400 -1.15835000
H -5.32800800 -2.07021000 -1.52657600
H -5.44298600 -0.77416700 -0.33521000
H -4.85579200 -0.43040800 -1.97048200
H -0.92446500 1.42161200 -3.31010700
H -1.35253800 -0.28018000 -3.17520400
H -2.25636500 2.05973200 -1.43646000
H 1.66903900 1.29942600 -2.78558700
H 0.96533100 -0.08985900 -3.59782200
C -3.41174500 1.00998700 0.98200200
H -4.32002200 1.25756100 0.41724700
C -2.71195400 2.32394700 1.36356400
H -3.38336500 2.92679300 1.98649900
H -1.80420900 2.13833300 1.94656200
H -2.44616200 2.93449400 0.49658000
C -3.81756500 0.24572700 2.25224900
H -4.35022400 0.92278900 2.93079400
H -4.48378400 -0.59348900 2.04222000
H -2.94439700 -0.13758600 2.79024300
C 3.23796300 1.16420800 0.13675000
H 2.65190600 1.91432100 -0.40716700
C 4.66352700 1.18646000 -0.43440400
H 5.09801100 2.18351200 -0.29372700
H 5.32112100 0.47351200 0.07403800
H 4.68976200 0.96830600 -1.50572600
C 3.23813300 1.54639200 1.62481900

H 3.65444700 2.55255900 1.75137900
H 2.23316000 1.54739100 2.05568300
H 3.85651400 0.86119100 2.21491600
H 0.24255800 2.06383700 -1.15456800
H 0.34576900 2.53572200 0.92156400
C 0.39625800 3.40064900 0.23468900
O 0.49690600 4.54305500 0.62644400
O 0.33753100 3.07039800 -1.05261500

PNPMn

C 1.19497000 -1.78752400 -1.95322300
C 2.45332500 -0.93377100 -1.78209400
H 1.05057900 -1.99198100 -3.02657500
H 1.34103200 -2.77325200 -1.48042200
H 2.48271900 -0.17216600 -2.56956200
H 3.36836900 -1.52994500 -1.86164700
P 2.29813500 -0.01201500 -0.18499000
N 0.00003400 -1.12780900 -1.39853700
C 3.30013900 1.56553300 -0.41460600
C 4.61264300 1.45678600 -1.20631700
C 3.49838100 2.28852400 0.92734400
H 2.61150900 2.17171700 -1.01664100
H 4.47113300 0.96776500 -2.17474200
H 4.99905600 2.46439100 -1.40510100
H 5.38948900 0.91257900 -0.66383900
H 2.55910300 2.39062200 1.48097100
H 4.21277200 1.76140000 1.56896500
H 3.89372700 3.29655500 0.75589500
C 3.16571200 -1.04066000 1.13433100
C 4.67897300 -1.23428100 0.95945000
C 2.46907700 -2.40270400 1.29727700
H 2.99530100 -0.46836900 2.05563900
H 5.23107200 -0.29584600 1.04532800
H 5.05629500 -1.90604400 1.74074700
H 4.92533000 -1.68917900 -0.00657500
H 1.38536200 -2.30370600 1.40258300
H 2.66950900 -3.05704900 0.44200100
H 2.85091500 -2.90868500 2.19185900
P -2.29809600 -0.01202800 -0.18503400
C -1.19488900 -1.78753800 -1.95323500
C -2.45325000 -0.93378800 -1.78213900
H -1.34095300 -2.77326000 -1.48042100
H -1.05047800 -1.99201100 -3.02658100
H -2.48262600 -0.17218800 -2.56961100

H -3.36829100 -1.52996500 -1.86171000
 C 0.00001500 1.94058900 -0.09467100
 O 0.00000400 3.10753000 -0.21940600
 C -3.30010900 1.56551100 -0.41466000
 C -3.49822000 2.28857600 0.92726800
 C -4.61270100 1.45670100 -1.20621400
 H -2.61154000 2.17165900 -1.01680100
 H -2.55888700 2.39070800 1.48079700
 H -3.89358900 3.29659500 0.75580500
 H -4.21254500 1.76148100 1.56898700
 H -4.47129600 0.96763300 -2.17463100
 H -5.38947000 0.91250300 -0.66361400
 H -4.99915900 2.46428800 -1.40500100
 C -3.16572100 -1.04065400 1.13426600
 C -2.46933200 -2.40285000 1.29701200
 C -4.67903600 -1.23395500 0.95950200
 H -2.99512200 -0.46848200 2.05561400
 H -1.38558900 -2.30407400 1.40223200
 H -2.85119000 -2.90884600 2.19157600
 H -2.66996700 -3.05707000 0.44168800
 H -5.23092900 -0.29540400 1.04546300
 H -4.92556700 -1.68875600 -0.00652500
 H -5.05643800 -1.90567100 1.74080000
 C 0.00000300 0.20126800 1.74560300
 O -0.00009800 0.17846300 2.91819100
 Mn 0.00001700 0.17739400 -0.02625900

Mn-A5

P 2.29390500 -0.31545800 -0.09971800
 N 0.04197600 1.07676800 -1.48655300
 C -1.02902000 0.78865000 -2.47173000
 C 1.38260300 1.32677000 -2.09589500
 C 2.35612900 0.16771000 -1.89157900
 H 3.36039500 0.44376200 -2.22828700
 H 2.04075000 -0.70213400 -2.47548300
 C -2.38576400 0.89428400 -1.77046000
 H -3.18871100 0.53823200 -2.42240400
 P -2.34538000 -0.05902100 -0.16226300
 C -0.13635900 -1.21478500 1.70625600
 O -0.21873300 -1.77049300 2.72570500
 Mn -0.03254500 -0.29564700 0.17467200
 C -0.07522400 -1.78103200 -0.80645300
 O -0.09937900 -2.75996000 -1.43879400
 C 3.34482900 -1.87791100 0.07367600

H 4.33374700 -1.51434100 0.37724800
 C 2.82107000 -2.79704400 1.18839300
 H 3.52990700 -3.61827900 1.34894000
 H 2.69828100 -2.27383800 2.14031200
 H 1.85705400 -3.24071900 0.92038700
 C 3.52245900 -2.66303500 -1.23569200
 H 4.00286100 -2.06828100 -2.01758200
 H 4.16012300 -3.53505500 -1.04729800
 H 2.56943400 -3.03534700 -1.62403400
 C -3.30408500 -1.62086700 -0.61555400
 H -2.81659500 -1.90762800 -1.55688400
 C -3.11995700 -2.78749800 0.36857700
 H -3.57802700 -3.69141700 -0.05022400
 H -2.06815700 -3.01134600 0.55871700
 H -3.60077800 -2.59533700 1.33186900
 C -4.79227700 -1.38009400 -0.91412800
 H -5.22799300 -2.28622900 -1.35159500
 H -5.35865700 -1.15392500 -0.00546000
 H -4.95535600 -0.56460300 -1.62533500
 H -0.98782100 1.51327700 -3.29674600
 H -0.87801600 -0.20760300 -2.90008800
 H -2.58885800 1.94376000 -1.53835200
 H 1.77600700 2.22874100 -1.61769900
 H 1.27567800 1.54530700 -3.16533500
 C -3.46650200 0.93019300 0.98214000
 H -4.37908800 1.10747400 0.39861200
 C -2.85651200 2.29054400 1.35412000
 H -3.62162100 2.90235600 1.84715300
 H -2.03299000 2.16884900 2.06684600
 H -2.46992700 2.85290000 0.50069100
 C -3.83499800 0.15738200 2.25831200
 H -4.43510500 0.80037800 2.91304200
 H -4.42208800 -0.74121900 2.05702200
 H -2.94118000 -0.13708800 2.81976000
 C 3.27462700 1.00501000 0.80701300
 H 2.64491300 1.89746800 0.70533300
 C 4.65641200 1.30637600 0.21006800
 H 5.13550800 2.10487300 0.78951200
 H 5.32648600 0.43947400 0.23996400
 H 4.59709700 1.65181600 -0.82630200
 C 3.37591000 0.66800600 2.30400100
 H 3.81970900 1.51333700 2.84245500
 H 2.39589100 0.47119800 2.75140100
 H 4.01398400 -0.20479900 2.48413100

H -0.21435900 2.00939000 -1.08081500
H -0.02357500 5.15813700 0.53318600
C 0.18849300 4.10273800 0.21200000
O -0.55131100 3.67480900 -0.72328200
O 1.11265700 3.51282700 0.81443100
H -0.33850500 1.07734700 1.19419100
H 0.40462700 1.24224500 0.97507700

MnATSS_6

P 2.29015400 -0.29063900 -0.10085600
N 0.03601800 1.01311300 -1.56978600
C -1.02941800 0.66077500 -2.54265500
C 1.37528600 1.24324600 -2.19496700
C 2.36607300 0.11477400 -1.91547900
H 3.36754400 0.39162600 -2.26002300
H 2.07114100 -0.78829900 -2.45775700
C -2.39426700 0.76303700 -1.85563900
H -3.17542500 0.33278800 -2.48937100
P -2.33656600 -0.07846700 -0.18229100
C -0.13595900 -1.14690400 1.71943100
O -0.21918000 -1.65240300 2.76738900
Mn -0.03023500 -0.30480300 0.15378400
C -0.06468100 -1.81884000 -0.76429500
O -0.08926900 -2.83629400 -1.34235900
C 3.37139900 -1.82742800 0.13026400
H 4.35867600 -1.44104200 0.40988300
C 2.86496400 -2.70490300 1.28632400
H 3.59117600 -3.50158100 1.48865300
H 2.72517700 -2.13904100 2.21107700
H 1.91161600 -3.18150600 1.03689800
C 3.54882200 -2.66722700 -1.14454200
H 4.02388500 -2.10470000 -1.95324800
H 4.19137200 -3.52788500 -0.92238100
H 2.59577500 -3.05990100 -1.51221500
C -3.30815600 -1.66208800 -0.52639700
H -2.83171900 -2.01114800 -1.45210300
C -3.11089600 -2.76293000 0.52840600
H -3.57840000 -3.69116500 0.17843900
H -2.05616700 -2.97573300 0.71469600
H -3.57430800 -2.50581900 1.48522000
C -4.79964300 -1.44013800 -0.81978000
H -5.24648300 -2.37441100 -1.18046700
H -5.35088600 -1.14249500 0.07787900
H -4.97066400 -0.68024200 -1.58894000

H -0.99964400 1.34477500 -3.40259500
H -0.85001800 -0.35102900 -2.91929400
H -2.64657400 1.81670300 -1.70390200
H 1.75893700 2.18261200 -1.78508000
H 1.26426800 1.39018300 -3.27625000
C -3.46807000 0.98545900 0.88728500
H -4.40095100 1.08061300 0.31677900
C -2.89938100 2.39328600 1.12015800
H -3.65562800 3.00437700 1.62803100
H -2.01353900 2.36355500 1.76022300
H -2.62162700 2.91050500 0.19877400
C -3.77995300 0.32018800 2.23718200
H -4.38821600 0.99744800 2.84869900
H -4.33876500 -0.61246600 2.13058300
H -2.86316900 0.10661700 2.79785900
C 3.26930900 1.07230400 0.75110700
H 2.63431400 1.95632700 0.62868700
C 4.64575100 1.37052000 0.14043100
H 5.12191200 2.18967400 0.69320000
H 5.32245400 0.51020400 0.19364000
H 4.57974300 1.68272800 -0.90610000
C 3.37513100 0.79373300 2.25968500
H 3.79566700 1.66832300 2.76941500
H 2.39822100 0.58691600 2.70825600
H 4.03497700 -0.05525100 2.47139100
H -0.22562400 1.94425900 -1.20044400
H 0.42795800 5.07935500 0.47504000
C 0.24330100 4.00789500 0.23782600
O -0.32522000 3.74053800 -0.83794400
O 0.66147000 3.19838400 1.13477000
H -0.07608900 1.05211900 1.18620300
H 0.24894200 1.84651500 1.01084200

Mn-A6

P -2.26532100 -0.36070800 0.11675300
N -0.05052300 0.86338500 1.68200700
C 1.03199700 0.47819500 2.62078200
C -1.39076800 1.01976000 2.32704000
C -2.35750200 -0.10694600 1.96097200
H -3.36338300 0.12114900 2.32843900
H -2.04067300 -1.04183900 2.43132500
C 2.38784300 0.63766700 1.92761200
H 3.17763000 0.17176000 2.52486400
P 2.32347500 -0.08738100 0.19692600

C 0.14560100 -1.00695800 -1.78181000
O 0.22541500 -1.37025400 -2.89158600
Mn 0.03910000 -0.34907900 -0.14168400
C 0.11147400 -1.93012800 0.66868500
O 0.16352800 -2.99368400 1.16484800
C -3.34658300 -1.87037300 -0.25236200
H -4.35482300 -1.47692200 -0.42642900
C -2.88287200 -2.57777700 -1.53623800
H -3.59374900 -3.37083000 -1.79949300
H -2.81291900 -1.89724900 -2.38912000
H -1.90085800 -3.04095300 -1.39984500
C -3.43280400 -2.87037600 0.91111100
H -3.88822300 -2.43307400 1.80424500
H -4.05519100 -3.72286700 0.61229900
H -2.44973400 -3.26442000 1.18514900
C 3.35327900 -1.65819400 0.42224100
H 2.89281600 -2.08736500 1.32199500
C 3.18040000 -2.68632500 -0.70813500
H 3.66185100 -3.62989700 -0.42345100
H 2.12939000 -2.89935200 -0.91505300
H 3.64421300 -2.35355600 -1.64152100
C 4.84039100 -1.41788500 0.72278300
H 5.31448600 -2.36033100 1.02305800
H 5.37824400 -1.05095300 -0.15740100
H 4.99762900 -0.70251100 1.53643900
H 1.00215000 1.10698000 3.52266000
H 0.86799500 -0.55753300 2.93298100
H 2.63288800 1.70175900 1.85023900
H -1.79984000 1.97734900 1.99084500
H -1.27721400 1.08632100 3.41597900
C 3.44198900 1.07827000 -0.78157900
H 4.38337900 1.12671500 -0.21963200
C 2.86759700 2.49801700 -0.88066500
H 3.60790100 3.15668800 -1.35139500
H 1.96846100 2.51212600 -1.50158000
H 2.61550500 2.93313900 0.09019900
C 3.73630000 0.54137100 -2.19125300
H 4.33194500 1.27371900 -2.74975800
H 4.30065500 -0.39405300 -2.17745300
H 2.81115900 0.37213800 -2.75336000
C -3.26692600 1.07666900 -0.58414400
H -2.67187300 1.94979700 -0.29161000
C -4.68155500 1.25447300 -0.01266100
H -5.13844100 2.15791200 -0.43530900

H -5.33853500 0.41514300 -0.26542700
H -4.68496300 1.36946200 1.07536200
C -3.29490500 1.03050000 -2.11996100
H -3.71525400 1.96233000 -2.51639900
H -2.29395900 0.90831300 -2.54361900
H -3.92193300 0.20945100 -2.48536500
H 0.18369600 1.79605100 1.33433700
H -0.56007500 5.22676000 -0.41038900
C -0.36733600 4.16696300 -0.17976300
O -0.01179100 3.79360900 0.92716000
O -0.57717200 3.40671400 -1.23841100
H -0.02656100 1.09378900 -0.92187500
H -0.36351700 2.42684500 -1.03407200

Cis-2

Fe 0.00000000 0.22523800 -0.21711100
H 0.00000000 -1.24632000 -0.67725900
C -1.21162100 -1.36620300 2.06644700
C -2.49692400 -0.69741200 1.57445600
H -1.29809800 -1.62067400 3.13471600
H -1.05249000 -2.29477900 1.51507700
H -2.75950100 0.15442200 2.20934900
H -3.32918700 -1.40616700 1.64240900
P -2.22709000 -0.06446100 -0.16366000
N -0.00000800 -0.52008200 1.84892600
C -3.28440900 1.50019800 -0.23267400
C -4.68113700 1.48168300 0.41123000
C -3.32541400 2.07886700 -1.65671900
H -2.66942000 2.17730500 0.37305800
H -4.67084000 1.06283600 1.42238600
H -5.05081300 2.51178100 0.49323400
H -5.41243000 0.92330000 -0.17660900
H -2.32551300 2.15418400 -2.09495900
H -3.94100600 1.46820200 -2.32602100
H -3.76096600 3.08524800 -1.63983700
C -3.02913100 -1.34127900 -1.30792500
C -4.56547300 -1.37567500 -1.32076400
C -2.49009600 -2.75607200 -1.04105700
H -2.68011200 -1.03271000 -2.30191700
H -5.00489500 -0.45323500 -1.70448200
H -4.90488800 -2.19092100 -1.97203000
H -4.97901000 -1.56593200 -0.32370100
H -1.39894600 -2.78529400 -1.04618500
H -2.84327500 -3.14469000 -0.07839700

H	-2.85349500	-3.43868700	-1.81835000	H	-3.35100000	-0.78395400	1.95335800
C	0.00006500	0.59322400	2.82750800	P	-2.24931300	0.14074000	-0.09739800
H	0.00010000	0.21068200	3.85985700	N	0.00007600	-0.02653800	1.88737300
H	0.87952800	1.22054800	2.68249600	C	-2.99208900	1.84839300	-0.39899300
H	-0.87937500	1.22059600	2.68257100	C	-4.36868600	2.16960400	0.20716100
P	2.22708100	-0.06449500	-0.16366600	C	-2.92547800	2.22593900	-1.88697700
C	1.21154700	-1.36630500	2.06637500	H	-2.24959100	2.46510800	0.12288600
C	2.49689200	-0.69757600	1.57440700	H	-4.45926400	1.84711700	1.24937900
H	1.05233700	-2.29483600	1.51495200	H	-4.52245400	3.25601700	0.19174600
H	1.29802100	-1.62084100	3.13462900	H	-5.19000900	1.72062600	-0.35505200
H	2.75953600	0.15420000	2.20934800	H	-1.91875000	2.08222300	-2.28909200
H	3.32910700	-1.40639200	1.64230200	H	-3.62057200	1.63274500	-2.49092600
C	3.28441600	1.50016100	-0.23252100	H	-3.19540000	3.28071800	-2.01909100
C	3.32541600	2.07898200	-1.65650400	C	-3.33758100	-1.16178700	-0.94408100
C	4.68115400	1.48156800	0.41135700	C	-4.82968600	-0.83763400	-1.10543500
H	2.66943200	2.17720200	0.37329300	C	-3.19438800	-2.53592000	-0.26400100
H	2.32551700	2.15431000	-2.09474800	H	-2.89258500	-1.23433900	-1.94450400
H	3.76093200	3.08537600	-1.63951200	H	-5.00543300	0.04416100	-1.72468800
H	3.94103600	1.46840800	-2.32586400	H	-5.33223100	-1.68289300	-1.59275800
H	4.67087700	1.06260300	1.42246400	H	-5.32007000	-0.68337800	-0.13810800
H	5.41243500	0.92325200	-0.17656100	H	-2.15844700	-2.81579400	-0.06893100
H	5.05083400	2.51165400	0.49347400	H	-3.74393300	-2.56858300	0.68317800
C	3.02911000	-1.34122500	-1.30803300	H	-3.62470900	-3.30825600	-0.91242100
C	2.49014300	-2.75605000	-1.04119300	C	0.00020200	1.32453900	2.50207100
C	4.56545300	-1.37556100	-1.32096100	H	0.00023000	1.24825100	3.60063700
H	2.68002200	-1.03262300	-2.30199000	H	0.87537500	1.88763500	2.18468300
H	1.39899400	-2.78531500	-1.04626000	H	-0.87491500	1.88774700	2.18472500
H	2.85352400	-3.43861900	-1.81853400	P	2.24933500	0.14054900	-0.09745900
H	2.84339200	-3.14469200	-0.07856800	C	1.22245200	-0.75282000	2.33388200
H	5.00482100	-0.45307500	-1.70462800	C	2.49617400	-0.13543300	1.74327200
H	4.97905300	-1.56588400	-0.32393600	H	1.12190100	-1.78877200	2.00172400
H	4.90486100	-2.19074300	-1.97231100	H	1.27727600	-0.75499700	3.43458500
H	-0.00000400	0.52732800	-1.71420100	H	2.71673500	0.82452300	2.21751300
C	0.00000100	1.95607600	0.03924000	H	3.35090400	-0.78491700	1.95297500
O	0.00001800	3.12416500	0.13094000	C	2.99196200	1.84831400	-0.39885400
Cis'-2				C	2.92558800	2.22575700	-1.88688000
Fe	-0.00002800	-0.00489700	-0.30036700	C	4.36834700	2.16982600	0.20763000
H	0.00010600	1.54285400	-0.25353300	H	2.24926300	2.46495500	0.12281200
C	-1.22246000	-0.75253400	2.33392700	H	1.91898100	2.08175400	-2.28920000
C	-2.49606700	-0.13482500	1.74339800	H	3.19524800	3.28060400	-2.01899600
H	-1.27720400	-0.75469000	3.43463200	H	3.62097500	1.63272500	-2.49064700
H	-1.12220500	-1.78850900	2.00176700	H	4.45875100	1.84729300	1.24985300
H	-2.71621400	0.82532200	2.21744600	H	5.18994200	1.72111900	-0.35440100
				H	4.52181600	3.25628200	0.19232900

C 3.33784200 -1.16159200 -0.94436800
 C 3.19458100 -2.53601900 -0.26493100
 C 4.82997600 -0.83727800 -1.10525400
 H 2.89307100 -1.23382600 -1.94493100
 H 2.15856500 -2.81636700 -0.07099200
 H 3.62586100 -3.30790800 -0.91324900
 H 3.74325100 -2.56886400 0.68274800
 H 5.00580100 0.04461800 -1.72433100
 H 5.32010800 -0.68311800 -0.13778700
 H 5.33270900 -1.68241400 -1.59259400
 C -0.00031500 -1.66724400 -0.84367100
 O -0.00052800 -2.70022000 -1.40064300
 H -0.00003900 0.26697200 -1.79418800

TS3_4

C -0.06343800 3.16989100 0.31489900
 O 0.09227400 3.50006600 -0.81454200
 O -0.23541000 3.33588800 1.48025200
 Fe 0.00547500 -0.17961600 -0.19598500
 H -0.00453500 1.36907400 0.23395500
 H 0.01339500 -1.67492000 -0.54511000
 C -1.19993500 -1.69411600 2.12399100
 C -2.49520900 -1.01229100 1.68671500
 H -1.24880800 -1.96158300 3.19097600
 H -1.05813900 -2.61350100 1.55248300
 H -2.75429200 -0.19449300 2.36505300
 H -3.32289300 -1.72770400 1.72669100
 P -2.25379100 -0.30567100 -0.02456500
 N 0.00417400 -0.84236200 1.87897000
 C -3.19315700 1.33033500 0.02901300
 C -4.57294600 1.35976100 0.70849600
 C -3.23764900 1.98860000 -1.35902100
 H -2.51392300 1.92225700 0.65441200
 H -4.58449300 0.83653500 1.66948200
 H -4.85126700 2.40251500 0.90585400
 H -5.35807500 0.92903700 0.08351900
 H -2.24625800 2.04956100 -1.81559500
 H -3.89591300 1.44252100 -2.04358100
 H -3.62810900 3.01015500 -1.27677700
 C -3.16509700 -1.46141000 -1.20973400
 C -4.69923300 -1.42558600 -1.14868500
 C -2.67248000 -2.91059400 -1.06169100
 H -2.85008600 -1.10196300 -2.19844000
 H -5.10754200 -0.46031900 -1.45343300

H -5.10840500 -2.18074200 -1.83140800
 H -5.07554600 -1.65780000 -0.14591400
 H -1.58432400 -2.98105600 -1.12067400
 H -2.99637100 -3.34637500 -0.10921000
 H -3.10105000 -3.52519100 -1.86213600
 C -0.00283500 0.29829200 2.82789700
 H -0.02060500 -0.06330700 3.86746900
 H 0.87922400 0.91726400 2.67715200
 H -0.86795600 0.93291400 2.64925800
 P 2.26657600 -0.28676000 -0.01505500
 C 1.21384900 -1.68434800 2.12986600
 C 2.50563000 -0.99294500 1.69695100
 H 1.08154800 -2.60538200 1.55877800
 H 1.26090600 -1.95045700 3.19732000
 H 2.75708900 -0.17451200 2.37722500
 H 3.33800700 -1.70276000 1.73911300
 C 0.00732200 0.21857700 -1.87852200
 O 0.00964900 0.45294100 -3.02244400
 C 3.19131800 1.35852400 0.04006000
 C 3.25268200 2.00422000 -1.35305500
 C 4.55892200 1.40674000 0.74258700
 H 2.49524900 1.95093500 0.64710700
 H 2.26725900 2.05545600 -1.82283100
 H 3.63425800 3.02931500 -1.27362700
 H 3.92547800 1.45675100 -2.02218600
 H 4.55918700 0.89363600 1.70901400
 H 5.35784500 0.97620800 0.13509700
 H 4.82532300 2.45382100 0.93335400
 C 3.19843000 -1.43311000 -1.19281700
 C 2.71017800 -2.88505400 -1.05867200
 C 4.73118000 -1.39027900 -1.10556900
 H 2.89732400 -1.07056700 -2.18471800
 H 1.62352900 -2.96038900 -1.13638700
 H 3.15548300 -3.49442800 -1.85400600
 H 3.01991800 -3.32302200 -0.10248800
 H 5.14004700 -0.42223000 -1.40048300
 H 5.09091100 -1.62289500 -0.09682200
 H 5.15596300 -2.14173100 -1.78275200

Cis-TS3_4

C 0.01362400 3.23716900 -0.43666800
 O -0.01919500 3.46899700 -1.60374800
 O 0.04736300 3.56230200 0.71080900
 Fe 0.00044000 -0.13775900 -0.31989900

H 0.00621500 1.49670900 -0.36207000
 C 1.20281600 0.81858000 2.26123300
 C 2.51458500 0.24955100 1.71863000
 H 1.24483400 0.87197800 3.36072300
 H 1.05444600 1.82799600 1.87963100
 H 2.80877300 -0.64759500 2.26833400
 H 3.31336000 0.98263100 1.87199600
 P 2.33166900 -0.17656000 -0.09588600
 N 0.00395200 0.02676700 1.85011200
 C 3.07101000 -1.91868000 -0.24385900
 C 4.30297700 -2.28875600 0.59963800
 C 3.28275400 -2.28487100 -1.72250300
 H 2.25075900 -2.53811200 0.13212100
 H 4.18161800 -2.04687300 1.65948100
 H 4.45621700 -3.37342600 0.53680700
 H 5.22217600 -1.81443800 0.25127000
 H 2.40366400 -2.06266200 -2.33510800
 H 4.13636500 -1.74896800 -2.15060200
 H 3.48960800 -3.35751700 -1.81544500
 C 3.54201400 0.93549000 -1.02936400
 C 5.01615200 0.79340500 -0.61655900
 C 3.11925600 2.40835700 -0.98116200
 H 3.44167400 0.59925500 -2.06880100
 H 5.42920600 -0.18515100 -0.86391500
 H 5.61264700 1.54066500 -1.15388700
 H 5.16632200 0.97083800 0.45423900
 H 2.15762000 2.56182800 -1.46587800
 H 3.06608400 2.79064700 0.04472300
 H 3.85910000 3.01688600 -1.51484300
 C 0.02318000 -1.29082900 2.52899000
 H 0.01866000 -1.16910200 3.62299700
 H -0.84596400 -1.88054100 2.23709600
 H 0.91339800 -1.85102400 2.24237600
 P -2.33293600 -0.17902900 -0.09573700
 C -1.21112500 0.78834900 2.27031900
 C -2.50990800 0.18864900 1.73083600
 H -1.08962500 1.80304000 1.89170100
 H -1.24855300 0.83744000 3.37010500
 H -2.76157900 -0.73539200 2.25699000
 H -3.33334200 0.88635500 1.91574500
 C -3.07186700 -1.91512000 -0.28924000
 C -3.25900500 -2.25570700 -1.77716000
 C -4.31615900 -2.29982600 0.52978700
 H -2.25731300 -2.54023500 0.08993900

H -2.36767100 -2.02822200 -2.36957500
 H -3.47043000 -3.32540600 -1.89212400
 H -4.10107000 -1.70754400 -2.21236900
 H -4.21731500 -2.05931600 1.59246700
 H -5.23321000 -1.83425100 0.16530600
 H -4.45678300 -3.38587700 0.46132600
 C -3.54678700 0.96975300 -0.98086700
 C -3.17580400 2.44623200 -0.79434200
 C -5.02809500 0.75477000 -0.62765600
 H -3.40536400 0.72200300 -2.04042500
 H -2.20756600 2.67484300 -1.23292300
 H -3.92012900 3.07378200 -1.29877400
 H -3.16863200 2.73993500 0.26150900
 H -5.40766700 -0.20641800 -0.97605500
 H -5.21226400 0.82790700 0.45004600
 H -5.62896300 1.53344700 -1.11287500
 H -0.00361000 0.01391300 -1.82883000
 C 0.00133400 -1.84589200 -0.65322200
 O 0.00414100 -2.96749500 -0.98237300

Cis'-TS3_4

C 0.06885100 3.15689300 -0.16313200
 O -0.23606600 3.43472300 -1.28043000
 O 0.39650600 3.45130500 0.94748500
 Fe -0.00841300 -0.17967100 -0.27755900
 H 0.00635000 1.44039800 -0.10787400
 C -1.24368000 -1.18014400 2.29481600
 C -2.49928400 -0.47299200 1.77352100
 H -1.28439300 -1.26522500 3.39224400
 H -1.18743600 -2.19157900 1.88591800
 H -2.64842500 0.48089900 2.28685200
 H -3.38381100 -1.08068100 1.98693300
 P -2.29610400 -0.13567300 -0.05523400
 N 0.00463600 -0.47195200 1.89122500
 C -3.14524400 1.52344900 -0.33035800
 C -4.50403600 1.76636600 0.34680300
 C -3.17417500 1.88321000 -1.82386100
 H -2.42406300 2.19344000 0.15164300
 H -4.50945900 1.46457900 1.39887500
 H -4.72829700 2.84001100 0.31784900
 H -5.32406600 1.25172100 -0.15748600
 H -2.18460300 1.78704500 -2.27693500
 H -3.87228000 1.24967800 -2.38089700
 H -3.50180400 2.92179800 -1.95054800

C -3.31647600 -1.48579400 -0.91054200
 C -4.83351100 -1.25870900 -0.99624700
 C -3.05960900 -2.86978200 -0.28418100
 H -2.91277900 -1.49552200 -1.93049500
 H -5.09814900 -0.37454800 -1.57897200
 H -5.29820700 -2.12235900 -1.48824300
 H -5.28890200 -1.16772200 -0.00399300
 H -2.00189100 -3.09767900 -0.15026300
 H -3.55651500 -2.96292100 0.68775400
 H -3.47966100 -3.64392300 -0.93689700
 C 0.09420600 0.80311200 2.64215900
 H 0.14964900 0.60899400 3.72464000
 H 0.96539400 1.37255700 2.33017300
 H -0.77352100 1.42454400 2.43579400
 P 2.28206700 -0.19185100 -0.07254000
 C 1.18546700 -1.31793700 2.22853700
 C 2.49314600 -0.70490000 1.71826100
 H 1.02362700 -2.29438800 1.76512000
 H 1.23873200 -1.46571900 3.31904400
 H 2.76057000 0.17807700 2.30427700
 H 3.30967300 -1.42080100 1.84625300
 C 3.16283500 1.47116500 -0.15708400
 C 3.12307300 2.06167700 -1.57610300
 C 4.56631000 1.57795700 0.46374800
 H 2.49002400 2.07208400 0.46538500
 H 2.10912800 2.06894300 -1.98407900
 H 3.48546800 3.09661000 -1.55809700
 H 3.76302700 1.50392300 -2.26801600
 H 4.63844600 1.08036300 1.43588200
 H 5.34283800 1.16615200 -0.18373200
 H 4.80499900 2.63677700 0.62385800
 C 3.25061600 -1.47116000 -1.08411600
 C 3.05358400 -2.89301000 -0.52547400
 C 4.75192300 -1.22059300 -1.28528900
 H 2.76379500 -1.42111700 -2.06574100
 H 2.01476100 -3.12872800 -0.29122800
 H 3.39552400 -3.62421100 -1.26714700
 H 3.65113600 -3.04615500 0.37961800
 H 4.95844700 -0.28204600 -1.80312600
 H 5.29612600 -1.22034700 -0.33511800
 H 5.16965500 -2.02949200 -1.89789500
 H -0.01241100 0.18157800 -1.74788000
 C -0.03084500 -1.75184700 -1.02071800
 O -0.05153500 -2.69838000 -1.70996800

4

C -0.08877500 2.82873500 0.25817900
 O 0.59368900 3.40726100 -0.59098400
 O -0.84498500 3.20200600 1.16683500
 Fe 0.00874000 -0.09670400 -0.16687000
 H 0.00451800 1.62936200 0.19913700
 H 0.01922300 -1.55330500 -0.45487700
 C -1.19877200 -1.50821900 2.19116000
 C -2.50158300 -0.86726800 1.71832900
 H -1.24756600 -1.72325900 3.26911500
 H -1.03907100 -2.45250900 1.66675700
 H -2.76361800 -0.00881700 2.34307600
 H -3.32332700 -1.58532700 1.80507200
 P -2.27338600 -0.26866100 -0.03109000
 N -0.00354400 -0.65022900 1.91414400
 C -3.25682000 1.32983700 -0.12415100
 C -4.63980700 1.35794100 0.54850800
 C -3.31667400 1.86500100 -1.56457000
 H -2.60390100 2.00302700 0.44438200
 H -4.61930500 0.96526000 1.56976200
 H -4.97926300 2.39924700 0.61190800
 H -5.39707200 0.80401800 -0.01077100
 H -2.32297800 1.94299000 -2.01682200
 H -3.93862000 1.23766300 -2.21295600
 H -3.75397300 2.87024800 -1.56440000
 C -3.09269800 -1.54816900 -1.14865800
 C -4.62746000 -1.59094800 -1.08964900
 C -2.52247400 -2.95580300 -0.90755900
 H -2.79449400 -1.23172000 -2.15708000
 H -5.08551400 -0.67147100 -1.45828200
 H -4.99187300 -2.41167100 -1.71953700
 H -4.99285200 -1.77467300 -0.07294700
 H -1.43244800 -2.97673000 -0.97127100
 H -2.81810100 -3.34356400 0.07417600
 H -2.92133100 -3.64414400 -1.66166800
 C -0.04763600 0.55051000 2.78961300
 H -0.20072200 0.25557800 3.83790100
 H 0.89133900 1.09781100 2.71459200
 H -0.83426500 1.23275000 2.47175800
 P 2.28891300 -0.23159100 0.00469100
 C 1.21452200 -1.45685700 2.24084300
 C 2.50583700 -0.78903500 1.77055900
 H 1.09770900 -2.42217800 1.74439900

H 1.24993100 -1.63747300 3.32555000
 H 2.74269700 0.08352500 2.38466100
 H 3.34390800 -1.48528700 1.87824700
 C 0.02050100 0.13030400 -1.89016300
 O 0.02879400 0.19183200 -3.05239700
 C 3.24400300 1.38509000 -0.15367500
 C 3.43613300 1.76710400 -1.63062600
 C 4.54999800 1.51377500 0.64578100
 H 2.52651400 2.10517300 0.25444900
 H 2.49229000 1.74372200 -2.18094300
 H 3.82248200 2.79066600 -1.69438700
 H 4.15272600 1.11318600 -2.13866400
 H 4.41472500 1.28927500 1.70800200
 H 5.34641800 0.87051600 0.26422700
 H 4.90639200 2.54931100 0.57972200
 C 3.17408300 -1.52086400 -1.04991600
 C 2.58316900 -2.92503600 -0.84236600
 C 4.70089000 -1.56959600 -0.87762800
 H 2.94980300 -1.20952800 -2.07836100
 H 1.50192300 -2.94416800 -0.99448200
 H 3.04081000 -3.62099200 -1.55506400
 H 2.79568700 -3.30418300 0.16391900
 H 5.19125700 -0.65145400 -1.20515000
 H 4.98802500 -1.75960700 0.16264200
 H 5.10799800 -2.38938500 -1.48188100

Cis-3

C 0.00032300 2.89558600 -0.43900200
 O -0.00071700 3.31760800 -1.59559900
 O 0.00139500 3.41737700 0.68139600
 Fe -0.00002100 -0.10441700 -0.311105500
 H 0.00030500 1.67419900 -0.39197800
 C 1.20919800 0.84911800 2.25630400
 C 2.51815200 0.25922900 1.72688500
 H 1.24325100 0.90484700 3.35527900
 H 1.06817100 1.85965200 1.86923700
 H 2.79483000 -0.64406900 2.27585800
 H 3.32627200 0.98058600 1.88654100
 P 2.35340900 -0.15987000 -0.08899700
 N 0.00000300 0.06824800 1.84243400
 C 3.06053000 -1.91050200 -0.24690300
 C 4.29468100 -2.28957700 0.58916800
 C 3.25765900 -2.27663100 -1.72766500
 H 2.23811600 -2.52153700 0.13784000

H 4.18399600 -2.04038100 1.64838400
 H 4.43337600 -3.37616200 0.53021000
 H 5.21577500 -1.82774500 0.23025600
 H 2.37741400 -2.04548900 -2.33510400
 H 4.11321600 -1.74839000 -2.16054100
 H 3.45354400 -3.35101800 -1.82144300
 C 3.55845600 0.95467300 -1.02304700
 C 5.03590100 0.76526900 -0.64021400
 C 3.17506900 2.43680000 -0.92202300
 H 3.42849500 0.64680100 -2.06795200
 H 5.42274700 -0.21430000 -0.92337500
 H 5.63818000 1.51513800 -1.16681700
 H 5.20676900 0.90900500 0.43243000
 H 2.20905800 2.64626800 -1.37862900
 H 3.15772400 2.78805600 0.11574500
 H 3.92603500 3.03533000 -1.45147400
 C 0.00006000 -1.25207300 2.51680400
 H 0.00000900 -1.12960100 3.61005900
 H -0.88042600 -1.82661200 2.22784700
 H 0.88066000 -1.82647400 2.22791800
 P -2.35340400 -0.15981600 -0.08901000
 C -1.20925800 0.84901300 2.25631200
 C -2.51815600 0.25896100 1.72693000
 H -1.06833900 1.85956500 1.86927400
 H -1.24329400 0.90477500 3.35528900
 H -2.79461600 -0.64444700 2.27582900
 H -3.32640600 0.98015200 1.88666900
 C -3.06046200 -1.91042100 -0.24720200
 C -3.25722400 -2.27648000 -1.72803800
 C -4.29478200 -2.28954100 0.58859600
 H -2.23811300 -2.52145100 0.13770800
 H -2.37681200 -2.04535100 -2.33522700
 H -3.45312200 -3.35085800 -1.82190600
 H -4.11263000 -1.74819700 -2.16114800
 H -4.18432600 -2.04029100 1.64782800
 H -5.21582400 -1.82778700 0.22946900
 H -4.43338000 -3.37614200 0.52966300
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 C -3.17610400 2.43731000 -0.91934100
 C -5.03610600 0.76438800 -0.64090900
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 H -2.20985700 2.64802300 -1.37485500
 H -3.92698900 3.03603800 -1.44868700
 H -3.16001900 2.78720400 0.11891400

H -5.42231400 -0.21493700 -0.92580100
H -5.20768400 0.90637200 0.43185500
H -5.63842600 1.51476800 -1.16673400
H -0.00014800 -0.02478800 -1.82380300
C 0.00002200 -1.79357400 -0.64741000
O 0.00009900 -2.91331800 -0.97158300

Cis'-3

C 0.08101400 2.90635800 -0.11228600
O -0.63770500 3.40183400 -0.97878600
O 0.85663900 3.35487400 0.74180400
Fe -0.00609100 -0.08351400 -0.26107700
H 0.01086400 1.68730800 -0.08684400
C -1.22484900 -1.07357400 2.32476600
C -2.50752500 -0.43152400 1.78559000
H -1.26354500 -1.12939300 3.42347600
H -1.12806300 -2.09239500 1.94352100
H -2.70172700 0.52555400 2.27679500
H -3.36490200 -1.07382300 2.00796000
P -2.32303300 -0.12813500 -0.04781100
N -0.00188500 -0.32724200 1.90498800
C -3.23194600 1.47769400 -0.40010800
C -4.58326400 1.69572100 0.29913300
C -3.30797200 1.74277500 -1.91236700
H -2.52517600 2.21214000 -0.00015100
H -4.54470600 1.47351700 1.37012500
H -4.86623700 2.75079900 0.19894200
H -5.38689000 1.10118100 -0.14001800
H -2.31565700 1.70791300 -2.36748000
H -3.96003900 1.02972900 -2.42778100
H -3.71435600 2.74577800 -2.08611200
C -3.25581500 -1.55841400 -0.86337500
C -4.78589400 -1.42326000 -0.91198100
C -2.89868700 -2.91066800 -0.21705900
H -2.87664000 -1.56086400 -1.89250800
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H -5.21035100 -2.32735700 -1.36562800
H -5.21847100 -1.32898900 0.09008000
H -1.82646000 -3.07333500 -0.10036300
H -3.36821200 -3.01411900 0.76706700
H -3.28449600 -3.72100300 -0.84608400
C 0.02626900 0.97983400 2.61233600
H 0.14594000 0.82233600 3.69446200
H 0.82456300 1.61467900 2.23468900

H -0.90397600 1.51856100 2.43959500
P 2.31146300 -0.16385800 -0.07373200
C 1.20820200 -1.11056600 2.29311800
C 2.49920400 -0.48507200 1.75644200
H 1.08365000 -2.11739300 1.88827900
H 1.25670400 -1.19260000 3.38990300
H 2.70515700 0.46774500 2.25199500
H 3.34675700 -1.14178000 1.97401700
C 3.23802100 1.43795300 -0.38510000
C 3.22170000 1.81052300 -1.87612900
C 4.63731900 1.58163800 0.23513700
H 2.57939800 2.14664100 0.13051300
H 2.20775400 1.78547300 -2.28702400
H 3.60835600 2.82835400 -2.00495500
H 3.84873900 1.14385800 -2.47830600
H 4.66496900 1.26303400 1.28194700
H 5.40395300 1.02582900 -0.30846600
H 4.92507600 2.64012600 0.21310200
C 3.19640500 -1.59824200 -0.93516500
C 2.87242000 -2.94869100 -0.26856200
C 4.71926900 -1.46464300 -1.08383300
H 2.75616200 -1.60042700 -1.93956700
H 1.80615300 -3.10906100 -0.10014900
H 3.22562300 -3.76128700 -0.91362000
H 3.38901300 -3.04944600 0.69193100
H 5.00746600 -0.60611300 -1.69308400
H 5.22009000 -1.38418900 -0.11327700
H 5.10955300 -2.36201900 -1.57959000
H -0.00893900 0.30099100 -1.71898300
C -0.02094100 -1.59090400 -1.09386800
O -0.03055800 -2.50072200 -1.82688300

3

C -0.08473700 4.00562600 0.26920600
O 0.02416500 4.04477200 -0.89423400
O -0.19401700 4.02759900 1.43416700
Fe 0.00826100 -0.29625300 -0.20848700
H 0.00167000 1.14785900 0.41112700
H 0.01622100 -1.76374600 -0.72890000
C -1.19278000 -2.05431600 1.93503200
C -2.49028200 -1.32509100 1.58235400
H -1.24587500 -2.45238700 2.96072700
H -1.04683400 -2.89339100 1.25274200
H -2.75937900 -0.61171800 2.36625500

H -3.31235900 -2.04542900 1.51776600
P -2.24635100 -0.39734700 -0.02248400
N 0.00681100 -1.17402500 1.80139200
C -3.10933600 1.25770400 0.25915800
C -4.46681400 1.27878800 0.98031000
C -3.15162900 2.07617000 -1.04085900
H -2.37897700 1.73834200 0.92158600
H -4.46563400 0.69156300 1.90388700
H -4.70740000 2.31283600 1.25854900
H -5.28450100 0.91647200 0.35353300
H -2.17354700 2.11477900 -1.52806200
H -3.87281300 1.66506900 -1.75609500
H -3.45884700 3.10704400 -0.82683800
C -3.23884000 -1.34581200 -1.32176000
C -4.76713900 -1.29285700 -1.17718400
C -2.76973000 -2.80666300 -1.41546600
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H -5.22874700 -1.94356200 -1.93044000
H -5.09931500 -1.64845400 -0.19514600
H -1.68981700 -2.87799800 -1.56141100
H -3.03258500 -3.37123400 -0.51301900
H -3.26523100 -3.29786700 -2.26146700
C -0.01620000 -0.15944000 2.88432400
H -0.02367000 -0.64600100 3.87206000
H 0.85525500 0.48870400 2.81120200
H -0.89795600 0.47179000 2.78953500
P 2.26327500 -0.36198500 -0.01185400
C 1.22886000 -2.01956500 1.95324400
C 2.50906700 -1.25559900 1.61106300
H 1.11401000 -2.86626900 1.27440300
H 1.28146600 -2.41090800 2.98156600
H 2.73980400 -0.52039800 2.38679000
H 3.35545400 -1.94927700 1.57391800
C 0.00797600 0.29572400 -1.82955100
O 0.00769200 0.66315200 -2.94051600
C 3.09936500 1.31310800 0.23280500
C 3.16601900 2.08251200 -1.09583100
C 4.43648400 1.37414300 0.98864200
H 2.34483400 1.80877200 0.85596800
H 2.20025100 2.09108100 -1.60837500
H 3.45481900 3.12456000 -0.91320600
H 3.90963100 1.65367600 -1.77675600
H 4.41376700 0.82223500 1.93339100

H 5.27374200 0.99424900 0.39896800
H 4.66209600 2.41997900 1.23330600
C 3.28293100 -1.31919300 -1.28286500
C 2.82207300 -2.78278500 -1.37333700
C 4.80796800 -1.25941000 -1.10619500
H 3.02411600 -0.83086600 -2.23187600
H 1.74604800 -2.86100900 -1.54222100
H 3.33817500 -3.27962900 -2.20361800
H 3.06732700 -3.33835900 -0.46030900
H 5.20739400 -0.25483700 -1.25838000
H 5.11947100 -1.60593700 -0.11415300
H 5.28779000 -1.91488400 -1.84374100

TS4_4a

C -0.24496300 2.81750600 0.44725500
O -0.24955700 2.90948700 -0.80798200
O -1.07641700 3.22723200 1.29017700
Fe 0.05574200 -0.05202200 -0.14513800
H 0.64737800 2.26569200 0.87824300
H 0.09414700 -1.46660500 -0.54466600
C -1.14157000 -1.54596400 2.17230400
C -2.44071100 -0.87747400 1.72792500
H -1.18111300 -1.78390200 3.24562600
H -1.00269100 -2.48222800 1.62842200
H -2.66963000 -0.01040700 2.35425900
H -3.27457300 -1.57849700 1.83773700
P -2.23661800 -0.28879800 -0.02678600
N 0.06526700 -0.70075400 1.90265000
C -3.30218800 1.25297600 -0.17151900
C -4.66424300 1.23611200 0.54420400
C -3.42699800 1.70044200 -1.63694900
H -2.67756500 1.99666600 0.33838200
H -4.58506600 0.92393800 1.59032500
H -5.07055700 2.25522600 0.54509800
H -5.40118300 0.59400600 0.05613800
H -2.44454700 1.83116400 -2.09667200
H -4.01199900 0.99892300 -2.24201000
H -3.93757800 2.66995300 -1.67770200
C -2.98979700 -1.62919100 -1.12314000
C -4.52144400 -1.74093500 -1.06576500
C -2.36443700 -3.00880700 -0.85830900
H -2.70256100 -1.31806600 -2.13616500
H -5.02209300 -0.84679600 -1.44030600
H -4.84627000 -2.58223500 -1.69023100

H	-4.87935500	-1.93501700	-0.04831900	H	-0.00003600	-1.56151000	-0.54366900
H	-1.27398200	-2.98791200	-0.91477500	C	-1.20555000	-1.70554800	2.07767000
H	-2.65340200	-3.39557800	0.12563500	C	-2.50126000	-0.99932200	1.68463700
H	-2.72930200	-3.72255200	-1.60608800	H	-1.25368200	-2.03472900	3.12706500
C	0.05769600	0.46207200	2.83031400	H	-1.06733300	-2.59077500	1.45406500
H	-0.11286700	0.12683200	3.86321500	H	-2.74045500	-0.20399200	2.39536700
H	1.01703100	0.97781000	2.78851100	H	-3.33479200	-1.70851500	1.71446100
H	-0.70557500	1.18647900	2.54230000	P	-2.28869800	-0.23816200	-0.00489500
P	2.34381100	-0.18562000	0.00844300	N	-0.00001600	-0.84302100	1.88293500
C	1.27239200	-1.54828500	2.17037000	C	-3.19055300	1.41196100	0.08140800
C	2.57739700	-0.89135900	1.71824800	C	-4.50268800	1.48122000	0.87898300
H	1.12755700	-2.48318100	1.62468500	C	-3.35433600	2.01762200	-1.32202100
H	1.31664500	-1.78811800	3.24315300	H	-2.44596600	2.01341200	0.61552400
H	2.86054900	-0.07197200	2.38529700	H	-4.40337200	1.07681700	1.89062000
H	3.39011400	-1.62358900	1.75861700	H	-4.80235200	2.53169200	0.98151500
C	0.05973200	0.32444200	-1.85494200	H	-5.32486200	0.95598400	0.38712100
O	0.07242600	0.45700400	-3.00808900	H	-2.41839700	2.00627500	-1.88876600
C	3.29601000	1.43652400	0.04993400	H	-4.11122200	1.48500700	-1.90838300
C	3.20524200	2.16015000	-1.30321400	H	-3.67757700	3.06216000	-1.24198000
C	4.72525900	1.41874200	0.61680800	C	-3.23195400	-1.34232200	-1.20582000
H	2.68149500	2.00564100	0.75913700	C	-4.75072400	-1.40799600	-0.98309400
H	2.16210500	2.35326000	-1.57068500	C	-2.64402400	-2.76212000	-1.25262500
H	3.71761600	3.12773400	-1.23838900	H	-3.04714400	-0.87198600	-2.18056400
H	3.68602200	1.59199400	-2.10787500	H	-5.23854200	-0.44487000	-1.14460800
H	4.80311800	0.84723500	1.54717600	H	-5.19298500	-2.12004100	-1.69065900
H	5.45406100	1.01667500	-0.08945700	H	-5.00149100	-1.75509000	0.02569800
H	5.02706100	2.44849800	0.84387900	H	-1.57284300	-2.75659600	-1.46522700
C	3.17312300	-1.37409700	-1.19870200	H	-2.80216100	-3.29510700	-0.30755500
C	2.67321400	-2.81355500	-0.98745400	H	-3.14692200	-3.33830500	-2.03826600
C	4.70843700	-1.35175000	-1.22436000	C	-0.00000200	0.22947300	2.90863500
H	2.80875100	-1.03352600	-2.17635800	H	0.00000800	-0.20990300	3.91710800
H	1.58293600	-2.87909000	-0.99931300	H	0.87225400	0.86786400	2.78864900
H	3.05931400	-3.45283700	-1.78960000	H	-0.87225700	0.86786800	2.78866900
H	3.03390900	-3.22815000	-0.03920100	P	2.28866100	-0.23818000	-0.00491100
H	5.10452700	-0.39632400	-1.57319100	C	1.20550800	-1.70556700	2.07765400
H	5.14051700	-1.56760700	-0.24101100	C	2.50122400	-0.99935600	1.68461600
H	5.06849100	-2.12449100	-1.91454900	H	1.06727300	-2.59078700	1.45404300
4a				H	1.25364200	-2.03475400	3.12704700
C	-0.00000600	2.88788800	-0.17476800	H	2.74043500	-0.20403700	2.39535100
O	-0.00000800	1.81737700	0.54123400	H	3.33474400	-1.70856400	1.71443200
O	0.00002700	4.04814400	0.24374000	C	-0.00002500	0.16528100	-1.89104800
Fe	-0.00002200	-0.09022700	-0.17488000	O	-0.00002100	0.21842600	-3.05647700
H	-0.00003500	2.71467100	-1.27942600	C	3.19054600	1.41192100	0.08139100
				C	3.35411300	2.01768500	-1.32201900

C 4.50283100 1.48106000 0.87872700
H 2.44606500 2.01334600 0.61568300
H 2.41807900 2.00640800 -1.88860900
H 3.67740000 3.06220700 -1.24195300
H 4.11088500 1.48508800 -1.90854600
H 4.40368400 1.07659500 1.89035500
H 5.32488300 0.95580900 0.38667300
H 4.80257200 2.53150900 0.98127100
C 3.23194000 -1.34229900 -1.20585000
C 2.64430800 -2.76223000 -1.25239800
C 4.75076200 -1.40759900 -0.98336000
H 3.04688200 -0.87211400 -2.18062000
H 1.57310300 -2.75696400 -1.46487800
H 3.14724200 -3.33841200 -2.03801800
H 2.80266700 -3.29505300 -0.30727400
H 5.23832100 -0.44436500 -1.14502500
H 5.00178000 -1.75455200 0.02541700
H 5.19308200 -2.11959100 -1.69094200

5

C 0.27626900 4.07728000 -0.24319900
O 1.32712500 3.55390200 0.21396200
O -0.92009400 3.71756100 -0.11513000
H 0.43657900 5.01328700 -0.85889000
H 0.48225500 1.42174000 -0.31736100
H 2.19958900 1.09895400 -2.52103100
C 3.23979500 1.10813400 -2.18219300
C 3.35187800 1.01127400 -0.65310800
H 3.68597200 2.05136000 -2.51853600
H 3.77338000 0.29814100 -2.69022100
P 2.30850700 -0.35904400 0.09309800
C 4.82115900 1.00439400 -0.20521800
H 2.85513800 1.90053200 -0.24169200
Fe 0.04273300 -0.22510000 -0.14719200
C 2.49713000 -0.06731400 1.92109000
C 3.19366500 -1.98487000 -0.25033500
H 4.93146900 0.97310800 0.88343300
H 5.37513500 0.15873300 -0.62746800
H 5.31297100 1.91988700 -0.55517900
P -2.24391100 -0.31526500 0.02021900
C 0.02350100 -0.63660900 -1.84730300
C 1.21494100 -0.50828300 2.62165700
H 2.67967300 1.00093800 2.06824400
H 3.35624300 -0.60130800 2.33863400

C 2.94139100 -2.49477300 -1.67729000
C 2.83680400 -3.08014000 0.76560900
H 4.26114100 -1.75549400 -0.14244200
C -2.49928000 -0.25841000 1.86275400
C -3.14584200 1.18572900 -0.66699300
C -3.09101600 -1.87766600 -0.59793000
O -0.02361700 -0.96483200 -2.95966400
N -0.00995900 0.06585900 1.98152700
H 1.12276300 -1.59507400 2.57419700
H 1.23661900 -0.21904400 3.68238100
H 3.17861500 -1.75472700 -2.44533700
H 3.56573500 -3.37651100 -1.86429000
H 1.89760900 -2.79670300 -1.80628700
H 1.76744400 -3.31520300 0.73910700
H 3.38383800 -3.99695700 0.51581000
H 3.10663300 -2.81099000 1.79051300
C -1.19411500 -0.65105400 2.55162800
H -2.80073300 0.75421800 2.14037700
H -3.30670300 -0.92728600 2.17688200
C -4.52415400 1.52005200 -0.07334600
C -3.19188700 1.14317200 -2.20312500
H -2.45911400 1.99498600 -0.38290300
C -4.62345700 -1.87101800 -0.48888600
C -2.51514100 -3.13288400 0.07788500
H -2.82120500 -1.91557300 -1.66124900
C -0.09837500 1.51502400 2.31679300
H -1.25547000 -0.44655000 3.63059800
H -1.01315100 -1.71944100 2.41771300
H -4.52271700 1.52673800 1.02079500
H -4.81282200 2.52679500 -0.39942400
H -5.30707600 0.83439300 -0.40640300
H -3.57247200 2.09740000 -2.58492500
H -2.20135300 0.99004300 -2.64260900
H -3.85399600 0.35286700 -2.57385700
H -5.08220200 -1.11181600 -1.12479000
H -5.01291400 -2.84456400 -0.81001600
H -4.96150400 -1.70937000 0.54088100
H -1.42851500 -3.18807600 -0.01816800
H -2.76895400 -3.16839900 1.14366400
H -2.94635300 -4.02583300 -0.38930600
H -0.13958000 1.64593500 3.40753400
H 0.74443200 2.06171700 1.89413200
H -0.97867700 1.96105200 1.85725200
H 0.04473400 -1.69126600 0.13612200

H -0.30967000 1.42830500 -0.40362300

TS5_6

C -0.00996400 4.15952600 -0.15039800
O 0.91159400 3.29684700 -0.32246100
O -1.23737500 3.98412400 -0.04035600
H 0.36283600 5.21847400 -0.09228600
H 0.25572800 1.79289700 -0.53346600
H 2.07210600 1.11358700 -2.53194200
C 3.12821800 1.14574100 -2.24911600
C 3.31502500 1.10645800 -0.72459000
H 3.54586500 2.07958200 -2.64392500
H 3.64355900 0.32195700 -2.75403400
P 2.33430200 -0.26085100 0.11406900
C 4.80077200 1.15093000 -0.33910500
H 2.81626000 1.99773200 -0.32577700
Fe 0.06704900 -0.30243600 -0.15113900
C 2.48873300 0.17846300 1.91849100
C 3.34901900 -1.83688200 -0.06584500
H 4.95417200 1.13647800 0.74508000
H 5.36054400 0.31512500 -0.77247600
H 5.25226000 2.07489300 -0.72017900
P -2.21435600 -0.40495800 0.00910600
C 0.08985400 -0.95266500 -1.76928200
C 1.22299200 -0.27466600 2.64344400
H 2.62099100 1.26199700 1.98858900
H 3.36689500 -0.28128400 2.38238600
C 3.23532100 -2.44832600 -1.47093600
C 3.00083300 -2.89342300 0.99392900
H 4.38866100 -1.52630100 0.09724000
C -2.49434600 -0.26466900 1.84695600
C -3.10026800 1.07322300 -0.74714700
C -3.07157400 -1.98325000 -0.54778500
O 0.07349000 -1.44830200 -2.82082900
N -0.02422100 0.18875600 1.95957400
H 1.18727000 -1.36549300 2.67090300
H 1.22192600 0.08762400 3.68207600
H 3.47615300 -1.73888300 -2.26662500
H 3.92904400 -3.29283900 -1.56081300
H 2.22660600 -2.83099400 -1.65358200
H 1.95332900 -3.20374500 0.92060000
H 3.62232300 -3.78290400 0.83572700
H 3.18691800 -2.54527600 2.01411300
C -1.17703000 -0.54646600 2.56782100

H -2.85942300 0.74039700 2.07228700
H -3.26294600 -0.96460100 2.18972400
C -4.49267600 1.42788400 -0.20063700
C -3.10756900 0.97522400 -2.28096700
H -2.42356000 1.89539300 -0.47477000
C -4.60195600 -1.97956800 -0.41550100
C -2.47559600 -3.21238500 0.15812300
H -2.81747100 -2.05194500 -1.61364800
C -0.19073000 1.64680800 2.19879700
H -1.25788400 -0.27659600 3.63134400
H -0.94396300 -1.61121500 2.50451300
H -4.52461600 1.44758400 0.89284500
H -4.76272900 2.43274000 -0.54773800
H -5.27125300 0.74426300 -0.54815200
H -3.47793600 1.91424300 -2.70837900
H -2.10459600 0.80560800 -2.68565800
H -3.76066000 0.17133200 -2.63899100
H -5.07261800 -1.25232000 -1.07958100
H -4.99285000 -2.96816300 -0.68478600
H -4.92588800 -1.76916000 0.61002700
H -1.39140400 -3.26940200 0.03762800
H -2.70042000 -3.20803600 1.23123900
H -2.91619500 -4.12366700 -0.26288200
H -0.29933700 1.84509700 3.27525800
H 0.66756100 2.18988600 1.80972000
H -1.06016600 2.02918100 1.66746700
H 0.13342000 -1.72496000 0.31412700
H -0.22744600 1.20777200 -0.83656500

6

C -0.49676400 4.37097500 -0.02725600
O 0.47562800 3.59133200 -0.47556700
O -1.58573300 4.01636400 0.38317800
H -0.19060800 5.43003000 -0.07205100
H 0.21769600 2.60734300 -0.43134400
H 2.05696700 1.42233800 -2.34615600
C 3.11186200 1.46517000 -2.06173800
C 3.30961900 1.23703700 -0.55540000
H 3.49365800 2.45527900 -2.33882100
H 3.65677100 0.72950800 -2.66208200
P 2.35435100 -0.24502500 0.11373600
C 4.79799300 1.27741100 -0.17784900
H 2.80257100 2.06162000 -0.03760800
Fe 0.11159200 -0.33118700 -0.15803800

C 2.52447300 0.00346500 1.95816800
 C 3.44804300 -1.74463300 -0.22508500
 H 4.96425900 1.14552600 0.89643900
 H 5.37147800 0.50785700 -0.70546800
 H 5.22524800 2.24766800 -0.45910300
 P -2.14826700 -0.50119500 -0.01430300
 C 0.13108300 -0.69696200 -1.84616600
 C 1.26318200 -0.51837600 2.64505200
 H 2.66376200 1.07241900 2.14749500
 H 3.40477100 -0.50636800 2.36235800
 C 3.39603700 -2.17309900 -1.69937300
 C 3.10597200 -2.93697400 0.68070300
 H 4.47010900 -1.42356900 0.01171800
 C -2.44825200 -0.44220400 1.82816900
 C -3.12614100 0.95631800 -0.70323500
 C -2.97003400 -2.08660800 -0.62724700
 O 0.11820900 -0.96917100 -2.98250600
 N 0.01604800 -0.00012000 2.00667400
 H 1.23057300 -1.60688100 2.57090700
 H 1.26761600 -0.25274300 3.71360700
 H 3.67520200 -1.36900300 -2.38498400
 H 4.08915900 -3.00624600 -1.86853600
 H 2.39391100 -2.51664400 -1.97384600
 H 2.07804700 -3.27643000 0.51911000
 H 3.77650200 -3.77417900 0.45066700
 H 3.22783500 -2.70794900 1.74364400
 C -1.14249400 -0.76977500 2.55258700
 H -2.80054000 0.55816400 2.09237800
 H -3.23114300 -1.14284900 2.13620100
 C -4.52737500 1.23477000 -0.13292000
 C -3.14317400 0.92918100 -2.23987700
 H -2.48329200 1.79043200 -0.39776600
 C -4.50420800 -2.11656100 -0.55128500
 C -2.38493400 -3.32688100 0.06787900
 H -2.67718700 -2.13030100 -1.68460700
 C -0.14510100 1.43247900 2.36108200
 H -1.24268900 -0.56774400 3.63052100
 H -0.90700300 -1.82810700 2.42644700
 H -4.54861500 1.22267200 0.96113100
 H -4.84630900 2.23638100 -0.44792600
 H -5.27971300 0.52860000 -0.49149100
 H -3.55779200 1.86889100 -2.62400200
 H -2.13823300 0.81790700 -2.65773700
 H -3.76496700 0.11494500 -2.62868800

H -4.96869400 -1.38401200 -1.21388300
 H -4.86567800 -3.10608500 -0.85739600
 H -4.86874500 -1.93913300 0.46700500
 H -1.29606900 -3.35988600 -0.00608800
 H -2.65780200 -3.35844100 1.12955300
 H -2.79072000 -4.23249600 -0.39881600
 H -0.23816300 1.55177500 3.45130700
 H 0.71627300 2.00138800 2.01544100
 H -1.02426200 1.85030600 1.87534600
 H 0.21090200 -1.83206800 0.18492800
 H 0.01639100 1.22848700 -0.40511800

HCOOH

H -1.04586000 -1.06662500 0.00009300
 C 0.12972800 0.40168700 0.00000800
 H 0.09607100 1.50076600 0.00003700
 O 1.13896600 -0.26318100 -0.00000600
 O -1.11753800 -0.09235200 -0.00001600

3'

C 0.10378500 4.72733500 -0.11229000
 O 0.20260100 4.87166200 -1.26835100
 O 0.00582500 4.60459300 1.04699100
 Fe -0.01036500 -0.53879700 -0.18951700
 H -0.02295100 -2.11210000 -0.08542300
 H 0.00162900 1.01195000 -0.16533800
 C 1.20534200 0.38660400 2.41501800
 C 2.48959000 -0.21399700 1.84383400
 H 1.25517900 0.42180800 3.51469600
 H 1.08704300 1.40750000 2.04894700
 H 2.73234800 -1.16035400 2.33529200
 H 3.32963600 0.46283500 2.03233300
 P 2.24584600 -0.53180400 0.01867000
 N -0.01413300 -0.36706400 1.99386300
 C 3.10720300 -2.18453800 -0.28621800
 C 4.46168800 -2.45260700 0.39025900
 C 3.15890300 -2.50155500 -1.78833400
 H 2.37516700 -2.86569300 0.16485800
 H 4.46680100 -2.18353600 1.45095700
 H 4.68463000 -3.52530300 0.32962500
 H 5.28685000 -1.92528000 -0.09388700
 H 2.17475800 -2.40556900 -2.25627600
 H 3.85501200 -1.84262400 -2.31930100
 H 3.50195600 -3.53157900 -1.94351000

C 3.24709800 0.79546800 -0.87854800
 C 4.77053400 0.73166400 -0.69247300
 C 2.72820600 2.20333400 -0.54070600
 H 3.02026500 0.60748900 -1.93672900
 H 5.20778900 -0.16181400 -1.14220400
 H 5.23629800 1.59890400 -1.17697600
 H 5.05812000 0.75778400 0.36497200
 H 1.65224300 2.27900900 -0.70961400
 H 2.93363100 2.46885000 0.50340900
 H 3.23438100 2.94285500 -1.17256300
 C -0.03991700 -1.67559300 2.69471800
 H -0.04177300 -1.53238200 3.78633300
 H -0.92618700 -2.23942300 2.40754900
 H 0.82800300 -2.27045300 2.41435800
 P -2.26638700 -0.48454700 0.00980100
 C -1.21168600 0.42761300 2.40295200
 C -2.51063000 -0.13884500 1.83018800
 H -1.05985100 1.44086800 2.02844000
 H -1.26604000 0.47314000 3.50208200
 H -2.78657400 -1.07034600 2.33205700
 H -3.32963100 0.56686000 2.00472300
 C -0.00717300 -0.53876700 -1.91518400
 O -0.00480000 -0.49803600 -3.08484200
 C -3.15612700 -2.12549600 -0.27949900
 C -3.21132800 -2.45531900 -1.77867300
 C -4.51525000 -2.36463500 0.39795400
 H -2.43528600 -2.81388100 0.17839300
 H -2.22578000 -2.37593400 -2.24682100
 H -3.56765100 -3.48208400 -1.92513900
 H -3.89861500 -1.79199200 -2.31564600
 H -4.51737000 -2.08436100 1.45571400
 H -5.33134600 -1.82928900 -0.09275000
 H -4.75556600 -3.43414700 0.34830100
 C -3.24189500 0.84889500 -0.90709800
 C -2.69520000 2.25206500 -0.59439600
 C -4.76598600 0.81828400 -0.71572400
 H -3.02277000 0.63901600 -1.96271300
 H -1.62093300 2.31116400 -0.77969600
 H -3.19992300 2.99106200 -1.22817900
 H -2.88105200 2.53465600 0.44877800
 H -5.22242900 -0.07327400 -1.14976500
 H -5.04970600 0.86713400 0.34191200
 H -5.21573800 1.68676100 -1.21293100

TS3'_4'

C -0.00088800 3.33223200 0.00951200
 O 0.00023600 3.65431100 -1.13383600
 O -0.00227700 3.52299300 1.18470500
 Fe 0.00010500 -0.10275200 -0.23599700
 H 0.00015000 -1.63517800 -0.34989000
 H 0.00025400 1.52385500 -0.07626400
 C 1.21027300 0.52425300 2.42039400
 C 2.50690800 -0.03252100 1.82956800
 H 1.24260900 0.47788800 3.52035100
 H 1.08889000 1.56619300 2.12572900
 H 2.79700700 -0.96555600 2.31942200
 H 3.31896500 0.67962600 2.00744400
 P 2.26907600 -0.33093600 -0.00370100
 N 0.00007800 -0.20141400 1.92781600
 C 2.85365900 -2.10838200 -0.28089300
 C 4.13002500 -2.59541900 0.42451000
 C 2.89385500 -2.43366100 -1.78225900
 H 2.00966300 -2.65946200 0.14943700
 H 4.18155800 -2.29260000 1.47447500
 H 4.14980300 -3.69223100 0.40447200
 H 5.04176000 -2.25067900 -0.06870500
 H 1.95852400 -2.16476800 -2.28207500
 H 3.71379000 -1.91137500 -2.28817800
 H 3.05313300 -3.50860800 -1.92907200
 C 3.52103600 0.77826900 -0.87777900
 C 4.99364800 0.55318500 -0.49939400
 C 3.14711000 2.25800400 -0.71554200
 H 3.39518900 0.52073800 -1.93775200
 H 5.36318200 -0.42325100 -0.81570800
 H 5.61529700 1.31013500 -0.99317700
 H 5.16329100 0.64894100 0.57892100
 H 2.15940900 2.46927000 -1.12308500
 H 3.16489800 2.57041400 0.33528400
 H 3.87322400 2.88096000 -1.25165800
 C 0.00018800 -1.57817400 2.48053400
 H 0.00016400 -1.55221400 3.58079200
 H -0.87806900 -2.12367800 2.13882900
 H 0.87855300 -2.12352500 2.13886400
 P -2.26887200 -0.33122600 -0.00378400
 C -1.21025200 0.52405100 2.42036100
 C -2.50678100 -0.03292400 1.82949500
 H -1.08902700 1.56600500 2.12570500
 H -1.24261100 0.47766200 3.52031700

H -2.79674400 -0.96602100 2.31931100
H -3.31895400 0.67908900 2.00738300
C 0.00010600 0.07640300 -1.95895300
O 0.00009900 0.21464800 -3.11760300
C -2.85318000 -2.10875700 -0.28104400
C -2.89338100 -2.43398200 -1.78242200
C -4.12945700 -2.59602000 0.42437100
H -2.00908500 -2.65972300 0.14923800
H -1.95811500 -2.16493100 -2.28227500
H -3.05250800 -3.50894600 -1.92927000
H -3.71341600 -1.91179900 -2.28828600
H -4.18104500 -2.29320100 1.47433200
H -5.04125600 -2.25144900 -0.06884400
H -4.14903800 -3.69283500 0.40434100
C -3.52103400 0.77777400 -0.87785900
C -3.14737900 2.25758300 -0.71569300
C -4.99360300 0.55247300 -0.49943100
H -3.39517200 0.52022700 -1.93782700
H -2.15977300 2.46902100 -1.12339100
H -3.87366400 2.88038600 -1.25175400
H -3.16511200 2.57002600 0.33511700
H -5.36298000 -0.42404700 -0.81566200
H -5.16324200 0.64828800 0.57887800
H -5.61538600 1.30928100 -0.99326300

4'

C 0.00002000 2.92773300 -0.06705700
O 0.00002500 3.43512000 -1.19250300
O 0.00007700 3.37729400 1.08777000
Fe -0.00001400 -0.04148000 -0.21743500
H -0.00000800 -1.52437400 -0.33613500
H -0.00001900 1.72561700 -0.09848300
C 1.21218800 0.60939300 2.40953200
C 2.51167500 0.03858300 1.83620600
H 1.23557000 0.57615000 3.50945400
H 1.08471600 1.64942900 2.10257200
H 2.80143300 -0.88357000 2.34533000
H 3.32324300 0.75499300 1.99821400
P 2.28304700 -0.29065800 0.00926200
N -0.00002200 -0.12525400 1.92189500
C 2.80309400 -2.08745400 -0.26105600
C 4.02755400 -2.61917300 0.50033000
C 2.90440300 -2.39595100 -1.76384900
H 1.92384100 -2.61759600 0.12216900

H 3.98739400 -2.40816500 1.57281600
H 4.06390200 -3.70998000 0.38946500
H 4.97101600 -2.22488800 0.11658100
H 2.00964000 -2.08063800 -2.30957300
H 3.77163800 -1.90722600 -2.22075200
H 3.02086200 -3.47552600 -1.91445600
C 3.54256100 0.78186600 -0.89148200
C 5.01201700 0.49442600 -0.54439100
C 3.22582800 2.27378800 -0.71229400
H 3.38172100 0.53299300 -1.94860200
H 5.33596200 -0.49209000 -0.88084400
H 5.65227300 1.23298700 -1.04156900
H 5.20377200 0.57010900 0.53177100
H 2.24649700 2.54047800 -1.11138900
H 3.26620600 2.57748700 0.34015900
H 3.97558200 2.86823300 -1.24803400
C -0.00004500 -1.50100200 2.47729400
H -0.00005300 -1.46806700 3.57665000
H -0.87952000 -2.04796100 2.14028100
H 0.87941400 -2.04799100 2.14029200
P -2.28307300 -0.29066800 0.00924800
C -1.21222800 0.60941100 2.40950700
C -2.51171100 0.03858700 1.83619000
H -1.08474900 1.64944000 2.10252200
H -1.23561900 0.57618900 3.50943000
H -2.80146300 -0.88356200 2.34532400
H -3.32328300 0.75499600 1.99818600
C -0.00001000 0.04174100 -1.95769300
O -0.00000300 0.07180100 -3.11973200
C -2.80311300 -2.08746600 -0.26106300
C -2.90431100 -2.39600200 -1.76385600
C -4.02763200 -2.61915700 0.50024900
H -1.92389200 -2.61760300 0.12223900
H -2.00950200 -2.08071100 -2.30951800
H -3.02076900 -3.47558000 -1.91444300
H -3.77150600 -1.90728100 -2.22083800
H -3.98753800 -2.40814100 1.57273600
H -4.97106200 -2.22485900 0.11643300
H -4.06399400 -3.70996500 0.38939200
C -3.54258400 0.78185300 -0.89150800
C -3.22567600 2.27377300 -0.71260100
C -5.01202400 0.49461800 -0.54418900
H -3.38189900 0.53280300 -1.94861000
H -2.24639200 2.54029900 -1.11191900

H -3.97546300 2.86820400 -1.24831100
H -3.26583900 2.57764600 0.33980700
H -5.33610800 -0.49192100 -0.88044200
H -5.20363600 0.57049000 0.53198600
H -5.65226900 1.23316200 -1.04140500

TS4'_4a'

C 0.23226400 2.90726000 0.17298700
O -0.03485200 2.86080600 -1.06021000
O -0.27022600 3.59678300 1.08416800
Fe 0.01647800 -0.08542600 -0.15585000
H 0.02835100 -1.55257700 -0.32742600
H 1.04929800 2.19350700 0.49299100
C 1.14754100 0.38136600 2.58996100
C 2.43399500 -0.21111700 2.00851900
H 1.12181600 0.23868900 3.68016700
H 1.09912100 1.45480900 2.39727000
H 2.59865800 -1.22676100 2.37819600
H 3.29307300 0.38458900 2.33291500
P 2.30694600 -0.25278300 0.14326100
N -0.07865200 -0.23257300 1.98571400
C 3.00911700 -1.93644100 -0.32901700
C 4.33834100 -2.35404700 0.32087400
C 3.05052900 -2.12931200 -1.85275400
H 2.22577900 -2.59702700 0.06472100
H 4.35712800 -2.18036100 1.40094500
H 4.48950100 -3.42884900 0.16212200
H 5.19382500 -1.83776600 -0.11977500
H 2.08613200 -1.91198700 -2.32039900
H 3.80925300 -1.49388000 -2.32093600
H 3.30572200 -3.16975200 -2.08644700
C 3.45759500 1.13698400 -0.41057500
C 3.13527900 1.61789700 -1.83394700
C 4.96031100 0.88837800 -0.21835000
H 3.16874100 1.94208200 0.27719800
H 2.10453300 1.97589200 -1.90130800
H 3.80018900 2.45073300 -2.09488500
H 3.29192800 0.83097100 -2.57941500
H 5.20469300 0.52060900 0.78293400
H 5.35379400 0.17802400 -0.95144800
H 5.49973700 1.83284300 -0.36021700
C -0.19150500 -1.63192900 2.46910400
H -0.23189400 -1.65297800 3.56792400
H -1.08946200 -2.10420500 2.07734800

H 0.66157500 -2.21983500 2.13330000
P 2.29667800 -0.27066600 -0.01525300
C -1.27229000 0.55758300 2.43183600
C -2.57586800 0.04643800 1.80901900
H -1.09179900 1.59375400 2.13048800
H -1.33907000 0.52716800 3.52984900
H -2.92278200 -0.86581500 2.29970200
H -3.35959100 0.79687800 1.95124100
C 0.02737700 0.04270800 -1.90253700
O 0.00002600 0.06460900 -3.06230600
C -2.84077000 -2.05067900 -0.34011800
C -2.89794300 -2.32689700 -1.85194300
C -4.10097400 -2.56614800 0.37241900
H -1.98718300 -2.61268100 0.05561300
H -1.97376100 -2.03226300 -2.35806700
H -3.04289900 -3.39951900 -2.02570800
H -3.73080200 -1.80279200 -2.33218300
H -4.08327800 -2.38521500 1.45108000
H -5.02031600 -2.13177600 -0.02569100
H -4.16665200 -3.65186900 0.22991900
C -3.48488300 0.85737200 -0.94295600
C -3.20517800 2.33433100 -0.62591900
C -4.97487400 0.53687400 -0.74777100
H -3.22555400 0.68727600 -1.99627500
H -2.16838500 2.61744300 -0.82688400
H -3.85815000 2.95884200 -1.24856400
H -3.43718000 2.57263500 0.41852300
H -5.25821700 -0.42975600 -1.16876000
H -5.25987600 0.54896500 0.31044700
H -5.57585400 1.30147000 -1.25472200

4a'

C 0.28576000 2.86956300 -0.22137300
O 0.16680500 1.81691900 0.51340600
O 0.65209000 3.98464400 0.15544500
Fe -0.02409900 -0.12018300 -0.15328300
H -0.06553000 -1.60867800 -0.47953300
H 0.01184700 2.72689100 -1.29518300
C 1.12243100 -0.04272000 2.61924500
C 2.40910100 -0.53539000 1.95781000
H 1.11770600 -0.30151300 3.68913600
H 1.05286000 1.04063300 2.51960500
H 2.59480600 -1.58959600 2.18202100
H 3.25774400 0.02528000 2.35989800

P 2.26549700 -0.32856400 0.10493600
 N -0.09677400 -0.60440000 1.96405700
 C 3.06900100 -1.89185000 -0.56651500
 C 4.46882800 -2.23561900 -0.03493700
 C 3.02696100 -1.96504400 -2.10032000
 H 2.36840400 -2.64797600 -0.18645500
 H 4.54122500 -2.15859200 1.05406700
 H 4.71623200 -3.26979000 -0.30522900
 H 5.23939000 -1.59464200 -0.47125200
 H 2.02979000 -1.74991800 -2.49350400
 H 3.73342300 -1.26662200 -2.55986700
 H 3.30484800 -2.97317000 -2.43045900
 C 3.30837600 1.19993300 -0.24822800
 C 3.21075500 1.65383100 -1.71276100
 C 4.77434800 1.17519500 0.21178300
 H 2.77622300 1.94156000 0.36003800
 H 2.17782400 1.70294000 -2.06337500
 H 3.64398900 2.65547500 -1.81838800
 H 3.76360800 0.98646700 -2.38162400
 H 4.89858200 0.81090200 1.23568600
 H 5.39824500 0.56110900 -0.44428800
 H 5.17804100 2.19475300 0.18040800
 C -0.16586800 -2.06291900 2.22399700
 H -0.22745500 -2.26063800 3.30484100
 H -1.03423400 -2.49776000 1.73186300
 H 0.71535500 -2.56021900 1.82195900
 P -2.33168000 -0.21247500 0.00484300
 C -1.29531800 0.06425000 2.55515200
 C -2.58942900 -0.34861400 1.85174200
 H -1.13620800 1.13719900 2.44066000
 H -1.35256000 -0.16777100 3.62960200
 H -2.86206300 -1.37726600 2.10075100
 H -3.41414300 0.28454200 2.19163500
 C -0.03079300 0.12130700 -1.87332600
 O -0.07011400 0.21286400 -3.03531500
 C -3.08486300 -1.79823900 -0.68588100
 C -3.06259600 -1.81213700 -2.22232500
 C -4.45354000 -2.23744500 -0.13980700
 H -2.34366100 -2.53181900 -0.34425700
 H -2.06265300 -1.61550100 -2.61700500
 H -3.37525800 -2.79717800 -2.58857100
 H -3.74870400 -1.07316600 -2.64985900
 H -4.50796600 -2.19334400 0.95208100
 H -5.27581700 -1.64264000 -0.54252000

H -4.63409100 -3.27984900 -0.43020700
 C -3.36655600 1.26189900 -0.56670400
 C -3.11670600 2.48198200 0.33763400
 C -4.87711000 1.03222400 -0.71750300
 H -2.95142100 1.48534500 -1.55828600
 H -2.05794500 2.64464700 0.53619600
 H -3.51927100 3.38162800 -0.14223600
 H -3.63206600 2.37099100 1.29861800
 H -5.11681200 0.29245800 -1.48377000
 H -5.33619200 0.71511600 0.22519600
 H -5.35630900 1.97418200 -1.01250700

TS4a_5

Fe -0.04139700 -0.42331300 -0.18221500
 H -0.07924100 -1.85041300 0.15874500
 C -1.23898700 -0.55834900 2.54792500
 C -2.53694800 -0.12858000 1.86472400
 H -1.24321200 -0.25213000 3.60420700
 H -1.14291200 -1.64548400 2.51250700
 H -2.76891600 0.91497500 2.09014500
 H -3.37251400 -0.72665500 2.24130400
 P -2.32865600 -0.31872800 0.02298800
 N -0.02188400 0.00400500 1.87961000
 C -3.08002100 1.21945100 -0.75741700
 C -4.37208000 1.76922300 -0.13165200
 C -3.22897200 1.03282800 -2.27642800
 H -2.29242200 1.96617200 -0.58803800
 H -4.28086100 1.93383400 0.94591000
 H -4.59705000 2.74158600 -0.58603900
 H -5.23413800 1.12001700 -0.30347300
 H -2.30287300 0.68488100 -2.74404200
 H -4.02358000 0.32007400 -2.52243600
 H -3.49096300 1.99077000 -2.73977600
 C -3.34498400 -1.81646700 -0.48376700
 C -4.86008900 -1.67372100 -0.27373500
 C -2.82495000 -3.09160200 0.20058800
 H -3.14935200 -1.90818900 -1.55972100
 H -5.29616300 -0.89594100 -0.90381400
 H -5.35410200 -2.61840100 -0.53112200
 H -5.10702600 -1.44931500 0.76980200
 H -1.76112900 -3.25548000 0.01288100
 H -2.98090700 -3.05979600 1.28521200
 H -3.37491400 -3.95939500 -0.18130400
 C 0.01332600 1.48078200 2.05249300

H	0.02257400	1.74083700	3.12123500	H	-0.45533800	0.40180700	-0.43646700
H	0.88627600	1.91547500	1.56511900	H	-0.36459200	1.85696800	-2.59603900
H	-0.85223400	1.94209800	1.57885000	C	-0.22765900	2.93147100	-2.44138600
P	2.25606900	-0.45068700	-0.00005000	C	-0.09436100	3.28436500	-0.95255800
C	1.17414500	-0.61490900	2.53609400	H	-1.11061500	3.43497400	-2.85298600
C	2.48401800	-0.25115600	1.83826400	H	0.63513500	3.25477700	-3.03282400
H	1.02501100	-1.69643800	2.50422300	P	1.24364400	2.31531000	-0.06048100
H	1.20448200	-0.30703200	3.59142700	C	-0.01283700	4.80357200	-0.74174600
H	2.76288400	0.78458600	2.04701100	H	-0.99592800	2.90916800	-0.44551600
H	3.29497100	-0.88086800	2.21765700	Fe	1.20267300	0.03444100	-0.17155800
C	-0.06366500	-0.99895700	-1.83034500	C	0.82205900	2.57939400	1.73127700
O	-0.08150100	-1.50073200	-2.87958400	C	2.86434000	3.22790600	-0.34325900
C	3.10229900	1.02949500	-0.78987100	H	0.07427700	5.07551500	0.31545000
C	3.19768100	0.85163900	-2.31374900	H	0.82897800	5.25209400	-1.28054200
C	4.44906000	1.47076400	-0.19421800	H	-0.92802100	5.27228800	-1.12275800
H	2.38684700	1.83773900	-0.57847600	P	1.43865000	-2.23120900	0.13058100
H	2.23918800	0.57115700	-2.76152500	C	1.68896000	-0.04787200	-1.85226800
H	3.51165200	1.79517300	-2.77476400	C	1.31400400	1.37826900	2.53454100
H	3.93602300	0.09024700	-2.58912000	H	-0.26649000	2.67517000	1.78644300
H	4.41086100	1.58451300	0.89304200	H	1.25843100	3.50081300	2.12980000
H	5.26611600	0.78556300	-0.43433500	C	3.42762900	2.98956600	-1.75204900
H	4.71041700	2.45167100	-0.60902400	C	3.92935900	2.90366600	0.71416800
C	3.16627700	-2.01918100	-0.49334300	H	2.60743800	4.28987300	-0.24590400
C	2.58595700	-3.24639000	0.22906600	C	1.38175500	-2.38467400	1.98318400
C	4.69151000	-1.96302000	-0.31691500	C	0.01548500	-3.28530700	-0.50786800
H	2.94313900	-2.12216500	-1.56329600	C	3.06501200	-2.99962300	-0.42577200
H	1.50925300	-3.34621700	0.07199500	O	2.07365800	-0.12593200	-2.94380300
H	3.07081400	-4.15379300	-0.14931600	N	0.85957100	0.07574000	1.95055700
H	2.77301700	-3.20441900	1.30842900	H	2.40544600	1.36136100	2.54656900
H	5.15974900	-1.23896700	-0.98653200	H	0.96917800	1.44500000	3.57618900
H	4.97531900	-1.71337700	0.71151400	H	2.71118000	3.22291000	-2.54373900
H	5.12102700	-2.94576800	-0.54567000	H	4.30656700	3.62691100	-1.90496400
H	-0.09983400	2.24788800	-1.54633300	H	3.74884700	1.95098200	-1.87818000
H	0.05746500	1.67791700	-2.01704600	H	4.18639800	1.83927200	0.71233200
C	0.35577500	4.29124200	0.17944200	H	4.84336300	3.46611000	0.48928200
O	1.49358500	3.77189200	0.28874500	H	3.61718500	3.18361700	1.72405300
O	-0.71713600	3.80263600	-0.26361000	C	1.65838200	-1.01405500	2.59832700
H	0.27988800	5.36348700	0.53289000	H	0.39608900	-2.75572300	2.27347300
7				H	2.11454700	-3.11144600	2.34761800
C	-3.44581700	2.49521900	1.24836100	C	-0.21346400	-4.65594300	0.15028500
O	-4.56673400	2.15883600	1.66772400	C	0.06582800	-3.39779100	-2.03965600
O	-2.59808700	1.81578600	0.58425400	H	-0.84803500	-2.65715500	-0.25167400
H	-3.11952800	3.55057500	1.47927700	C	3.16263700	-4.52141100	-0.23625600
				C	4.26384600	-2.30440400	0.24094300

H	3.10483300	-2.78070900	-1.50064900	C	-1.69899200	2.34923000	-2.46941700
C	-0.58378900	-0.11536000	2.27053200	C	-1.76040500	2.59288600	-0.95453700
H	1.44177800	-1.02907100	3.67633600	H	-2.71584600	2.29809900	-2.87674400
H	2.71141700	-0.75852400	2.46647000	H	-1.18472900	3.16048100	-2.99493700
H	-0.23264500	-4.60418200	1.24298200	P	-0.10011400	2.38761100	-0.09437700
H	-1.18914500	-5.03969700	-0.17089000	C	-2.48192800	3.91044800	-0.63203000
H	0.53789900	-5.39278100	-0.14079200	H	-2.33946300	1.78338400	-0.49472500
H	0.13785300	-2.41768900	-2.52130300	Fe	1.03777600	0.40030300	-0.21202400
H	0.91389400	-4.00448500	-2.37461300	C	-0.57475600	2.43687400	1.70325800
H	-0.84837700	-3.87899900	-2.40477500	C	0.84802200	3.99125700	-0.39079400
H	2.46107000	-5.06595800	-0.87089700	H	-2.54604800	4.09785000	0.44413700
H	4.17206500	-4.85447100	-0.50508300	H	-1.99533500	4.77207200	-1.10190400
H	2.98842200	-4.81729400	0.80436800	H	-3.50827900	3.86752100	-1.01584300
H	4.25232900	-1.22352200	0.08422400	P	2.36965400	-1.44048300	0.11747300
H	4.29072700	-2.49617900	1.31969000	C	1.51239200	0.57535400	-1.88068500
H	5.19317500	-2.70061700	-0.18391000	C	0.44098000	1.62157300	2.49959600
H	-0.72811800	-0.13084600	3.36006400	H	-1.58349400	2.01650900	1.78456100
H	-1.18516400	0.68148100	1.82990700	H	-0.61155100	3.46060800	2.08926300
H	-0.93684100	-1.05857100	1.85430100	C	1.49771800	4.04066000	-1.78216200
H	2.64872700	0.12771100	0.15252200	C	1.90581100	4.26830100	0.68794300
H	-0.43861900	-0.39216800	-0.47550700	H	0.09125300	4.78286600	-0.32904100
C	-5.76723800	-0.91146700	0.53367900	C	2.30255600	-1.64940400	1.96661400
C	-4.40165400	-1.57824500	0.70791700	C	1.70750800	-3.05593300	-0.59227300
C	-3.88194300	-0.99852400	-1.57669300	C	4.19156500	-1.28830300	-0.33949500
C	-5.26943900	-0.36282600	-1.70059100	O	1.88454400	0.69632500	-2.97591300
H	-4.06399400	-1.46288900	1.74468000	N	0.67149000	0.26273000	1.91379700
H	-5.69317400	0.14069400	0.84916000	H	1.40558500	2.13178700	2.50578800
H	-6.53561600	-1.41327500	1.13385200	H	0.11194900	1.51150600	3.54328400
H	-3.16767100	-0.45813000	-2.20976400	H	0.78841300	3.85989200	-2.59356800
H	-3.93646500	-2.03287300	-1.94586600	H	1.93793200	5.03174200	-1.94540700
H	-5.20742900	0.71399300	-1.47050000	H	2.30325300	3.30468700	-1.86519600
H	-5.66520200	-0.47216100	-2.71731400	H	2.66444400	3.47943000	0.71516000
H	-4.49603200	-2.65504000	0.50578800	H	2.41739200	5.21121700	0.45981900
O	-6.20419500	-0.99679300	-0.82891200	H	1.47441400	4.36912100	1.68780600
N	-3.38352100	-1.01694400	-0.19377400	C	1.86918600	-0.32457200	2.59181600
H	-3.18417200	-0.04891900	0.09740700	H	1.59028800	-2.44390900	2.20374400
TS7_8							
C	-4.06768000	0.24313900	2.37455300	H	3.26930200	-1.95941900	2.37503200
O	-4.17294200	-0.96023700	2.67869600	C	2.14076900	-4.36675100	0.08426000
O	-3.55070300	0.76311000	1.33528600	C	1.90491000	-3.10926700	-2.11565800
H	-4.48202000	0.99034900	3.11012100	H	0.63290200	-2.93386400	-0.40650400
H	-1.00128500	-0.77426200	-0.58157200	C	5.02477600	-2.56601500	-0.15785200
H	-1.19330200	1.41168200	-2.71761800	C	4.85547300	-0.11491100	0.40003800
				H	4.16800600	-1.03934700	-1.40807000
				C	-0.51940900	-0.58250700	2.19534200

H 1.64906800 -0.46166100 3.66080800
H 2.67571700 0.40603100 2.50456900
H 2.00866000 -4.34271300 1.17000700
H 1.51946100 -5.18547300 -0.29869300
H 3.18143400 -4.62380200 -0.12391200
H 1.51103000 -2.21675700 -2.61143200
H 2.96126400 -3.21025000 -2.38670600
H 1.37612300 -3.97670100 -2.52715000
H 4.70491000 -3.37055200 -0.82255900
H 6.07433100 -2.34932200 -0.39045000
H 4.99013500 -2.93553400 0.87314800
H 4.31652900 0.82343100 0.25104800
H 4.92503100 -0.30637800 1.47704700
H 5.87755100 0.01626300 0.02638800
H -0.66583300 -0.68381900 3.28029600
H -1.41223100 -0.13565700 1.76102700
H -0.38529700 -1.57399200 1.76520300
H 2.22755600 1.22609900 0.13677200
H -0.20808600 -0.69893000 -0.77648300
C -4.27960800 -3.11251600 -0.01921400
C -2.83042900 -2.63422800 0.07006800
C -3.26304500 -1.18465400 -1.82861500
C -4.69952800 -1.71026200 -1.85791600
H -2.52673400 -2.61573600 1.11964400
H -4.89509400 -2.49432800 0.65134000
H -4.36696000 -4.15983100 0.29047900
H -3.24101300 -0.14020800 -2.15565200
H -2.65337600 -1.76975100 -2.53139500
H -5.34853700 -1.04775900 -1.26051200
H -5.08561600 -1.73533100 -2.88289900
H -2.17914000 -3.32876700 -0.47903900
O -4.77049600 -3.04409800 -1.36044900
N -2.66350100 -1.28382700 -0.49032600
H -3.08442100 -0.58887300 0.15543300

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C -4.33457800 0.89950000 1.46328100
O -3.39284100 0.62255400 2.22982800
O -4.56784900 0.42257900 0.30098500
H -5.08612500 1.65107900 1.80775100
H -1.85794300 -0.96751600 -0.19905500
H -1.42110100 1.33692200 -2.60183900
C -1.99120000 2.21353000 -2.28065100
C -1.86141200 2.46722100 -0.77186500

H -3.04406200 2.03982500 -2.53440000
H -1.65522200 3.07286200 -2.87065600
P -0.09090500 2.38869700 -0.13774400
C -2.64597600 3.72075500 -0.35715200
H -2.30932100 1.61125300 -0.25664900
Fe 1.07176900 0.45107500 -0.20909400
C -0.34475500 2.61779800 1.69532500
C 0.70828400 3.99388100 -0.73163200
H -2.60406600 3.90356400 0.72090900
H -2.28406100 4.61941300 -0.86870400
H -3.70196300 3.59840100 -0.62642800
P 2.38705000 -1.37083900 0.13312900
C 1.25154500 0.39810900 -1.92751900
C 0.79077400 1.91801400 2.43824600
H -1.31398800 2.17710600 1.95173200
H -0.38471300 3.67308700 1.98313800
C 1.24756100 3.85561900 -2.16415200
C 1.82688400 4.49238900 0.19547400
H -0.09046800 4.74610700 -0.72887500
C 2.63474100 -1.37318100 1.98433400
C 1.60571100 -3.04981300 -0.24333700
C 4.11868200 -1.37248500 -0.62451700
O 1.39442700 0.33929700 -3.08665700
N 0.97243400 0.50594200 1.98530300
H 1.73193800 2.43753900 2.24933300
H 0.60830600 1.93449000 3.52378200
H 0.49117300 3.51231000 -2.87470500
H 1.61552500 4.82698400 -2.51712500
H 2.08402200 3.15067100 -2.19642200
H 2.63447900 3.75711400 0.27452400
H 2.25727100 5.41443400 -0.21468100
H 1.46927300 4.72305700 1.20334400
C 2.27256700 0.00924800 2.52725900
H 1.99758600 -2.14394600 2.42563300
H 3.66551000 -1.62392500 2.25505500
C 2.12811500 -4.28727500 0.50552000
C 1.53231000 -3.29442300 -1.75901400
H 0.58104500 -2.86753100 0.10452500
C 4.92844100 -2.66668400 -0.45325600
C 4.94542500 -0.17216600 -0.13459900
H 3.92301800 -1.22506600 -1.69476600
C -0.13241500 -0.31710500 2.54316800
H 2.22903100 -0.01309600 3.62755800
H 3.03651600 0.73056400 2.23263100

H 2.19048200 -4.13001200 1.58652000
H 1.43669700 -5.12349600 0.34154800
H 3.11148400 -4.60919800 0.15663100
H 1.06567400 -2.45539100 -2.28364100
H 2.52436300 -3.45662700 -2.19415500
H 0.93450300 -4.19014600 -1.96635700
H 4.47829100 -3.51496000 -0.97242700
H 5.93287600 -2.52654400 -0.87167500
H 5.05219300 -2.93539900 0.60199200
H 4.41740500 0.77362400 -0.27349500
H 5.20423000 -0.26997100 0.92645800
H 5.88664000 -0.12612500 -0.69536100
H -0.10553700 -0.29594500 3.64406100
H -1.10024100 0.05520500 2.20972500
H -0.03455300 -1.35016200 2.21144000
H 2.33437900 1.33814000 -0.05845500
H -0.25319800 -0.42512200 -0.24968700
C -4.26033700 -3.17246400 0.63819100
C -2.93973400 -2.43173100 0.81856100
C -2.99935500 -1.96785000 -1.61430000
C -4.31541000 -2.73602600 -1.66464700
H -2.91209300 -1.90758000 1.77628300
H -5.10105300 -2.48477000 0.81718000
H -4.32636700 -3.99230700 1.35830600
H -2.99766500 -1.14284600 -2.33093600
H -2.15724700 -2.63081300 -1.83369700
H -5.16221100 -2.04237600 -1.54600900
H -4.41409800 -3.23600000 -2.63179900
H -2.09608800 -3.12379800 0.74457800
O -4.36123500 -3.74762300 -0.66226700
N -2.80379400 -1.39777500 -0.24962800
H -3.54439200 -0.58972700 -0.03813500

Ammonium formate salt (Morpholine)

C -3.06238100 0.05029900 -0.26163000
O -2.52964600 -0.43631400 0.84013100
O -2.46898200 0.56140700 -1.19701200
H -4.16187300 -0.05852400 -0.25013300
H -1.48720400 -0.33846900 0.82412100
C 2.05088500 1.18196000 0.24140600
C 0.54296700 1.11243400 0.46699400
C 0.63236800 -1.25037300 -0.12574600
C 2.13804100 -1.10138400 -0.32407900
H 0.24325600 1.80244200 1.26228900

H 2.58219300 1.01783800 1.19478100
H 2.33880400 2.16562200 -0.14239400
H 0.38935300 -2.25366500 0.23832900
H 0.11466400 -1.09671000 -1.07884700
H 2.66646000 -1.36137400 0.60936700
H 2.49320500 -1.77096700 -1.11355800
H 0.00789900 1.39092100 -0.44629700
O 2.47806100 0.22412300 -0.72580400
N 0.10162300 -0.25340100 0.83122500
H 0.45512800 -0.47465300 1.76357500

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C 3.67505500 -2.41396000 0.93127000
O 4.80432600 -2.08026800 1.32997800
O 2.79245000 -1.71605500 0.33535900
H 3.37553800 -3.48676400 1.11431200
H 3.32255000 0.19557700 -0.00686700
N 3.51891800 1.17801700 -0.24529000
C 4.13270500 1.19356900 -1.58741100
C 4.59661200 1.63746000 0.64705000
H 0.60058100 -0.39727500 -0.50482900
C 5.65771500 0.90807700 -1.41247800
H 3.99084800 2.18354600 -2.04159100
H 3.63249700 0.46472700 -2.23311600
C 5.88314400 0.96882300 0.11998100
H 4.67477400 2.73335500 0.58913100
H 4.37022300 1.37361400 1.68522800
H 5.93207500 -0.07238700 -1.81461100
H 6.25800400 1.65491100 -1.94396700
H 5.92888600 -0.04339300 0.53306000
H 6.79556800 1.50891400 0.39690600
H 0.24965800 -1.93905900 -2.73601100
C 0.21113400 -3.01029000 -2.51680700
C 0.21741400 -3.29221400 -1.00681300
H 1.09585500 -3.46899500 -2.97424800
H -0.66715000 -3.42976300 -3.01877800
P -1.07432500 -2.32492500 -0.04755700
C 0.20758900 -4.80156100 -0.72205200
H 1.14379300 -2.86462200 -0.59426900
Fe -1.05223400 -0.04282100 -0.17321800
C -0.54627900 -2.56756200 1.71799500
C -2.70081000 -3.25247100 -0.22597000
H 0.21331200 -5.02686400 0.34938800
H -0.65809000 -5.30134100 -1.17054700

H 1.10551900 -5.25905400 -1.15428600
P -1.28498200 2.22206100 0.12676600
C -1.62216600 0.03515400 -1.82810700
C -1.01826500 -1.37151200 2.54028500
H 0.54545100 -2.63907500 1.71277900
H -0.93753600 -3.49504700 2.14762500
C -3.38381200 -2.97190000 -1.57337900
C -3.67696200 -2.98127400 0.92789700
H -2.42434900 -4.31340700 -0.18972100
C -1.16218100 2.38806100 1.97532500
C 0.11120000 3.27000600 -0.57440400
C -2.93180600 2.98241000 -0.37585300
O -2.06518200 0.11581800 -2.89714900
N -0.60991400 -0.06557200 1.93216500
H -2.10794000 -1.37039500 2.60294800
H -0.62485700 -1.43029300 3.56505200
H -2.72965000 -3.15567100 -2.42940700
H -4.25921900 -3.62309000 -1.68144000
H -3.73493500 -1.93672600 -1.62820600
H -3.95267600 -1.92262500 0.97993100
H -4.59739200 -3.55409700 0.76375000
H -3.27544000 -3.28548200 1.89885300
C -1.39546700 1.01680600 2.60784800
H -0.17257500 2.77650600 2.22816800
H -1.89344500 3.10524800 2.36081200
C 0.35456500 4.65380900 0.05023500
C 0.01265800 3.35077100 -2.10602800
H 0.98601700 2.65109100 -0.33378700
C -3.03088500 4.50373300 -0.18183700
C -4.10488600 2.27990900 0.32755800
H -3.00482200 2.76442700 -1.44911200
C 0.84267900 0.14932400 2.18730500
H -1.13488800 1.03996300 3.67593500
H -2.44976600 0.74730200 2.52097600
H 0.38423400 4.62601600 1.14357500
H 1.32892200 5.02534900 -0.28885700
H -0.39594700 5.38840100 -0.24900300
H -0.06021600 2.35997400 -2.56530300
H -0.85254300 3.93992600 -2.42889200
H 0.90953500 3.83500300 -2.50828500
H -2.35369900 5.05207100 -0.83921900
H -4.05037300 4.83179800 -0.41662700
H -2.82341000 4.80053900 0.85237700
H -4.09304100 1.19936200 0.16825200

H -4.09790000 2.46971900 1.40702500
H -5.04960800 2.67223500 -0.06579300
H 1.03572900 0.16697100 3.26932400
H 1.43621700 -0.63645200 1.71793500
H 1.16090200 1.09760500 1.75589100
H -2.48169200 -0.14513500 0.21809600
H 0.56468500 0.39507600 -0.55831200

P-TS7_8

C -4.03984100 -1.09569500 2.42694500
O -3.67793600 -2.26099400 2.68157200
O -3.81949900 -0.39360300 1.39128700
H -4.65135900 -0.57480900 3.21891100
H -2.98421500 -1.38810700 0.06225800
N -2.39193900 -1.88504900 -0.62273600
C -3.03064600 -1.91088300 -1.96305600
C -2.21349900 -3.28041300 -0.16609000
H -0.80208900 -0.97765000 -0.61570200
C -3.22344300 -3.40097200 -2.33038900
H -2.40825700 -1.39643500 -2.70667700
H -3.99325900 -1.38600500 -1.92669900
C -3.23238600 -4.10627700 -0.96587200
H -1.19191000 -3.62623900 -0.39115400
H -2.37812700 -3.31987300 0.91419000
H -4.13211200 -3.57090400 -2.91630200
H -2.37516200 -3.75571000 -2.92854600
H -4.22103100 -4.02076000 -0.49815200
H -2.97707400 -5.16963400 -1.02649700
H -1.55752900 1.07659900 -2.82731000
C -2.34416400 1.78196400 -2.54359800
C -2.51744300 1.87743300 -1.02067200
H -3.27983000 1.44059000 -3.00127700
H -2.10557100 2.75422600 -2.98738300
P -0.89781900 2.12961400 -0.10042400
C -3.62104300 2.88062900 -0.65159000
H -2.82505400 0.89484200 -0.64538000
Fe 0.75801600 0.54787700 -0.19707500
C -1.42090200 2.00515000 1.67831400
C -0.42875200 3.93767500 -0.36218400
H -3.78448300 2.94543500 0.42804400
H -3.40448800 3.88647100 -1.02769300
H -4.56773700 2.56209700 -1.10437200
P 2.54759600 -0.85187300 0.15650400
C 1.22484900 0.87745800 -1.84663500

C -0.23130100 1.51950900 2.50286300
 H -2.26005300 1.30072100 1.72568200
 H -1.77513200 2.96405300 2.07040600
 C 0.29292500 4.16117700 -1.69986500
 C 0.41307800 4.51266500 0.78657300
 H -1.38233900 4.47921600 -0.38320600
 C 2.55883000 -1.01753600 2.01163600
 C 2.31792400 -2.60586700 -0.49135900
 C 4.25212600 -0.24046100 -0.35252600
 O 1.59976400 1.11525000 -2.92106200
 N 0.41333200 0.29861100 1.92007800
 H 0.53487900 2.29577300 2.54500700
 H -0.54329500 1.30134500 3.53465000
 H -0.25721400 3.76159800 -2.55513400
 H 0.43095600 5.23588300 -1.86885500
 H 1.28448300 3.69863300 -1.68943900
 H 1.36465300 3.98049700 0.88856100
 H 0.64301700 5.56412300 0.57623000
 H -0.10777000 4.48116800 1.74759500
 C 1.72899200 0.11665600 2.61067900
 H 2.14224800 -1.99228400 2.27832600
 H 3.57634800 -0.98713500 2.41346200
 C 3.12350600 -3.73614300 0.16969100
 C 2.44661200 -2.64483600 -2.02210700
 H 1.26153800 -2.77333400 -0.24401500
 C 5.40885400 -1.20639300 -0.05538800
 C 4.54295300 1.14298400 0.25189600
 H 4.16996200 -0.12119500 -1.44080400
 C -0.46146900 -0.87371100 2.19122900
 H 1.55413100 -0.06470300 3.68137100
 H 2.27124100 1.05881000 2.50983800
 H 3.08635400 -3.70103100 1.26251700
 H 2.69884400 -4.69969800 -0.13695600
 H 4.17323700 -3.73550200 -0.13260400
 H 1.81634900 -1.89310500 -2.50720500
 H 3.48033200 -2.48239400 -2.34659500
 H 2.13724900 -3.62740700 -2.39652100
 H 5.34419300 -2.12629400 -0.63893500
 H 6.35942800 -0.72380500 -0.31212400
 H 5.45550500 -1.47465300 1.00595600
 H 3.76852800 1.87072400 -0.00004200
 H 4.62571300 1.09529000 1.34389700
 H 5.50070100 1.51379200 -0.13122600
 H -0.57671700 -1.02009100 3.27440000

H -1.44461500 -0.72108700 1.75058600
 H -0.02613600 -1.77418400 1.75960600
 H 1.64609600 1.68028500 0.19548200
 H -0.01142500 -0.89388500 -0.76416200

Ammonium formate salt (pyrrolidine)

C -2.47488300 -0.25885700 -0.16991600
 O -2.06362000 0.90566000 0.18903700
 O -1.81872200 -1.30434900 -0.26028200
 H -3.56165400 -0.28205600 -0.41830900
 H -0.73924600 0.91213500 0.40101800
 N 0.43754400 0.95305900 0.52364300
 H 0.67455200 1.78568800 1.06141100
 C 1.07244800 1.01872100 -0.84185300
 C 0.93388100 -0.29073700 1.21988700
 C 1.64670000 -0.38317600 -1.06421800
 H 1.85852900 1.77802000 -0.83109900
 H 0.31109400 1.30628300 -1.56990600
 C 2.08314300 -0.80404300 0.34693700
 H 1.21765300 -0.04949700 2.24538100
 H 0.10030800 -0.99661500 1.21935200
 H 0.85943200 -1.05150100 -1.42628200
 H 2.46280700 -0.37777000 -1.79112600
 H 2.21920400 -1.88369100 0.45044300
 H 3.02551200 -0.31434700 0.61855200

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H 2.30165500 -1.45975800 1.05507600
 N 1.40405100 -2.02872300 1.48803900
 C 1.54737700 -2.17787300 2.97980400
 C 1.32200800 -3.40125300 0.87408100
 H 0.56741700 -1.46904300 1.24963500
 C 1.35712500 -3.67446500 3.25858300
 H 0.82241200 -1.53823200 3.48501400
 H 2.55461100 -1.84663500 3.24791300
 C 1.85534900 -4.33465100 1.96402000
 H 0.27441100 -3.61999100 0.64758800
 H 1.91255800 -3.38690100 -0.04448000
 H 1.90432400 -3.99549300 4.14899300
 H 0.29585800 -3.89970600 3.41446500
 H 2.95136300 -4.35123300 1.94245400
 H 1.49908300 -5.36019200 1.83542300
 H -0.00897500 0.89498500 3.12367800
 C 0.73086200 1.69954200 3.15202800

C	1.21659200	2.07804300	1.74552500	H	-2.30813100	0.93272100	-3.00895800
H	1.57884800	1.35850800	3.75834300	H	-2.73606300	-3.86380700	-1.77639600
H	0.28518000	2.55240200	3.67487100	H	-2.94989600	-4.77610300	-0.28442100
P	-0.18596000	2.32744400	0.50719000	H	-4.33061100	-3.96443500	-1.01945600
C	2.23821600	3.22400200	1.80449600	H	-3.38432600	-1.84524200	2.03979100
H	1.72399000	1.20079100	1.32306400	H	-4.75132000	-2.66147700	1.26569100
Fe	-1.66250900	0.66012400	0.10228400	H	-3.41786900	-3.60925300	1.92745000
C	0.76527100	2.43475300	-1.09732900	H	-5.81866100	-2.51957600	-0.76613100
C	-0.79079000	4.09431000	0.78789600	H	-6.79953300	-1.30573900	-1.58385700
H	2.59910500	3.51654800	0.81298500	H	-5.42813500	-2.03196000	-2.42512100
H	1.82752500	4.11463000	2.29272000	H	-4.52888600	1.58125300	-1.40309400
H	3.11203100	2.90994300	2.38875700	H	-4.84715600	0.56073400	-2.81871500
P	-3.05257400	-0.92582200	-0.73979200	H	-6.17329300	1.00902600	-1.74408000
C	-2.53026500	0.81766200	1.58753500	H	0.98403200	-0.52466000	-2.79178200
C	-0.08229500	1.82736500	-2.21199600	H	1.20318500	-0.24040900	-1.04756300
H	1.70561600	1.89033600	-0.97319200	H	0.09361200	-1.48725000	-1.58928300
H	1.02759700	3.46663600	-1.35075700	H	-2.53879700	1.74281600	-0.57843000
C	-1.72710400	4.19508800	2.00200000	H	-0.71054000	-0.44783800	0.71924800
C	-1.47594100	4.69353200	-0.44946500	C	7.04971100	0.61954600	-0.93104100
H	0.11074200	4.68534900	0.99135100	C	6.74509600	0.21357800	-2.38337300
C	-2.41629600	-1.15374900	-2.47847200	C	5.65423300	-0.85679500	-2.22552200
C	-2.92768100	-2.64090600	0.04604000	C	5.66608900	0.58806300	-0.26129400
C	-4.89170600	-0.52873900	-0.91920700	H	7.70515400	-0.12628100	-0.46528700
O	-3.13579000	0.91115500	2.58370300	H	7.53867200	1.59461600	-0.84554500
N	-0.63379800	0.49168500	-1.83476300	H	7.62127600	-0.15706900	-2.92342700
H	-0.93387800	2.47797400	-2.41962800	H	6.34923500	1.07365900	-2.93696400
H	0.50757800	1.73263000	-3.13694200	H	4.97502900	-0.90323600	-3.08330000
H	-1.28135100	3.79528400	2.91661800	H	5.16604900	1.56584200	-0.34388700
H	-1.97828800	5.24627000	2.19024700	H	5.70829600	0.33629700	0.80217100
H	-2.66336800	3.65824600	1.82120000	N	4.94814900	-0.44302000	-1.01324400
H	-2.37102500	4.12575200	-0.72260200	C	3.85638300	-1.14293000	-0.52952000
H	-1.78604600	5.72284600	-0.23062000	O	3.41485500	-2.10785300	-1.19529900
H	-0.81577000	4.73342600	-1.32103200	O	3.38189200	-0.70775200	0.59939500
C	-1.62533400	0.09123200	-2.87804400	H	6.09204300	-1.85966400	-2.10776000
H	-1.78032500	-2.04251600	-2.50540500				
H	-3.22886900	-1.32698300	-3.19188900				
C	-3.26169100	-3.86853100	-0.81691000	TS9_10			
C	-3.66386600	-2.68296400	1.39436100	H	1.92629700	-1.52496300	0.98141900
H	-1.85267000	-2.67543800	0.26142700	N	1.17562600	-2.10368400	1.39189800
C	-5.77333200	-1.66988600	-1.44985500	C	1.35077900	-2.21830300	2.86037200
C	-5.11209200	0.73371700	-1.76893100	C	1.25953100	-3.46065100	0.81187700
H	-5.20265400	-0.29683300	0.10817300	H	-0.32443300	-0.99335100	1.02731200
C	0.47751400	-0.49450300	-1.81591100	C	1.60206600	-3.71626300	3.16593400
H	-1.10586200	-0.07721800	-3.83429800	H	0.46328300	-1.85193300	3.39469400
				H	2.19732200	-1.59965600	3.18163800

C	2.07677800	-4.28437400	1.81941200	H	-3.50191900	-1.09879000	-3.14636100
H	0.25334600	-3.89537600	0.70349800	C	-3.71800000	-3.73839100	-0.75948700
H	1.73317300	-3.39387700	-0.17087900	C	-3.85008700	-2.53512200	1.47388300
H	2.32177700	-3.86091700	3.97779400	H	-2.12063400	-2.71604200	0.22502100
H	0.66663100	-4.20317700	3.46737100	C	-5.99936100	-1.26334100	-1.33809300
H	3.14472600	-4.08176400	1.67302700	C	-5.09784100	1.08638400	-1.52756100
H	1.92102500	-5.36477700	1.72724800	H	-5.25131600	-0.05827700	0.28039600
H	-0.13748500	0.80183700	3.15827300	C	0.26818400	-0.89957400	-1.71279200
C	0.60445700	1.60290100	3.22303600	H	-1.19359300	-0.18122900	-3.77538800
C	1.25143300	1.90147200	1.86209600	H	-2.24349000	0.97383500	-2.93182900
H	1.37544300	1.28637600	3.93569500	H	-3.29345400	-3.75818900	-1.76736900
H	0.11379200	2.48388200	3.64981400	H	-3.43280500	-4.67791000	-0.27087100
P	-0.00130300	2.17744100	0.48602400	H	-4.80635200	-3.73845800	-0.85216600
C	2.31604500	3.00299400	1.97759500	H	-3.42686700	-1.75265000	2.11164600
H	1.75703600	0.99333700	1.51304000	H	-4.93145200	-2.37353500	1.41025500
Fe	-1.63116600	0.60884100	0.11854100	H	-3.69178400	-3.49505000	1.97880100
C	1.02840300	2.00047800	-1.05151700	H	-6.11457100	-2.13771800	-0.69484300
C	-0.45773300	4.00424900	0.54372800	H	-6.98506400	-0.79089300	-1.42594200
H	2.79915800	3.21587200	1.01867300	H	-5.71229700	-1.60725600	-2.33817200
H	1.90195100	3.93893400	2.36846700	H	-4.43863500	1.84907800	-1.10672900
H	3.10093100	2.67981300	2.67193200	H	-4.85072300	0.96621100	-2.58878100
P	-3.21313500	-0.84505300	-0.69343800	H	-6.12802700	1.45687300	-1.47303500
C	-2.58660100	1.04258100	1.51273700	H	0.68345300	-1.10088800	-2.71046700
C	0.13858600	1.47552900	-2.17610700	H	1.09097100	-0.70989600	-1.02421600
H	1.83965500	1.30051400	-0.81863700	H	-0.27022600	-1.78321900	-1.37215900
H	1.48204700	2.95065900	-1.35305100	H	-2.36116800	1.69547400	-0.58711400
C	-1.37646500	4.34885200	1.72513100	H	-1.05554200	-0.69905300	1.15129600
C	-1.07374000	4.50681900	-0.77025900	C	7.03549100	0.71399000	-0.66407200
H	0.49829800	4.52346300	0.68327700	C	7.14488900	-0.03445000	-2.00324100
C	-2.65467300	-1.08930900	-2.45344100	C	5.98340800	-1.03772300	-1.93327500
C	-3.19770800	-2.56265300	0.08294200	C	5.51629300	0.83503700	-0.45728100
C	-4.99563800	-0.24811900	-0.77022900	H	7.47350300	0.10652200	0.13743300
O	-3.26956800	1.36205700	2.39778400	H	7.54428600	1.68326600	-0.66362000
N	-0.65155100	0.26954900	-1.76745600	H	8.11350400	-0.52184900	-2.15193400
H	-0.58013300	2.24108700	-2.47399700	H	6.99082400	0.66311900	-2.83582700
H	0.74417600	1.22350800	-3.05883200	H	5.60298100	-1.31224600	-2.92384700
H	-0.96113100	4.04645100	2.68983300	H	5.13818400	1.77300100	-0.89640800
H	-1.53611000	5.43320800	1.76129600	H	5.22057200	0.83462300	0.59551400
H	-2.35748600	3.87665000	1.61578600	N	4.96954500	-0.33731000	-1.14470400
H	-2.01125600	3.98963900	-0.99949600	C	3.81095500	-1.00135000	-0.70553300
H	-1.29780300	5.57654200	-0.67889700	O	3.58103100	-2.13557900	-1.19411800
H	-0.39780200	4.39042800	-1.62220500	O	3.09228200	-0.36037600	0.14328600
C	-1.69116300	0.03861100	-2.81940900	H	6.29311700	-1.97395500	-1.44338700
H	-2.16603900	-2.06333400	-2.53732500				

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H	1.71965300	-2.03437000	0.56122300	H	0.17471600	1.45491800	-3.31819600
N	1.27279800	-2.89166300	0.91566700	H	-1.05124300	4.14093000	2.60823300
C	1.65882200	-3.04309600	2.32742900	H	-1.97424800	5.39752700	1.77977300
C	1.92457900	-4.03029100	0.24622400	H	-2.56304100	3.73244700	1.78000400
H	-0.19638700	-0.17763800	0.73182400	H	-2.64650200	3.83190300	-0.87878700
C	3.12278300	-3.55783400	2.33663600	H	-2.14123400	5.51394300	-0.66442000
H	0.99957600	-3.78316800	2.80301200	H	-1.22320600	4.45816300	-1.73617200
H	1.53176700	-2.09707900	2.86403500	C	-2.06055300	-0.00583700	-2.74675400
C	3.29347700	-4.23647700	0.94876100	H	-2.23794300	-2.14766800	-2.41549100
H	1.29768600	-4.92568000	0.36496000	H	-3.75340100	-1.34975100	-2.80923000
H	2.03605300	-3.81199600	-0.81747400	C	-3.36970900	-3.97547900	-0.43934400
H	3.81731000	-2.71789500	2.44162000	C	-3.17078100	-2.79200000	1.80213800
H	3.31300000	-4.24277800	3.17017800	H	-1.71050100	-2.81328800	0.24152800
H	4.07451700	-3.73723400	0.36848700	C	-5.93421000	-1.76563800	-0.49312100
H	3.56062800	-5.29589900	1.03018300	C	-5.32269800	0.61752900	-1.04343500
H	0.25510900	0.90008800	2.91011000	H	-5.02468000	-0.35041200	0.84725400
C	0.81626500	1.83949900	2.91699600	C	0.13873800	-0.70499400	-1.95091000
C	1.22862200	2.27227700	1.50103800	H	-1.69046900	-0.17351500	-3.76857100
H	1.71637800	1.67882400	3.52243600	H	-2.73035200	0.85627700	-2.76348500
H	0.20953600	2.59301100	3.42969800	H	-3.16128000	-3.94637300	-1.51291700
P	-0.20767700	2.36597800	0.29588200	H	-2.89617700	-4.88170800	-0.04319800
C	2.10015200	3.53720500	1.53256700	H	-4.44791100	-4.08711700	-0.30645200
H	1.82087200	1.45476400	1.06589300	H	-2.69580800	-1.97952900	2.36065100
Fe	-1.62154700	0.57542500	0.15455700	H	-4.25277800	-2.72658400	1.95852200
C	0.62688200	2.28038900	-1.36253100	H	-2.83097100	-3.73637200	2.24200600
C	-0.90015800	4.11028700	0.41143000	H	-5.83101700	-2.58611400	0.21939700
H	2.41886100	3.85017800	0.53265200	H	-6.95950100	-1.38624900	-0.40727200
H	1.58592400	4.38127200	2.00550600	H	-5.82038400	-2.16966000	-1.50516900
H	3.00634600	3.34091500	2.11763300	H	-4.65612100	1.46030400	-0.84694400
P	-3.12836600	-1.05389200	-0.42593800	H	-5.30127400	0.40228300	-2.11786100
C	-2.38176700	0.85648600	1.70599300	H	-6.34438100	0.92496100	-0.79312200
C	-0.33408900	1.63945100	-2.36142900	H	0.46894600	-0.81442500	-2.99290600
H	1.52940800	1.67477400	-1.23197000	H	0.99299900	-0.46107600	-1.31819100
H	0.93412400	3.26837700	-1.72087900	H	-0.26075900	-1.65873200	-1.60764400
C	-1.65997800	4.34855300	1.72433100	H	-2.60975700	1.54255600	-0.39365600
C	-1.77458200	4.48839500	-0.79204500	H	-0.70918600	-0.78236300	0.67503200
H	-0.01477000	4.75778700	0.39959100	C	6.65908800	1.01010400	-0.00004900
C	-2.81857400	-1.23662100	-2.25184700	C	6.92707400	0.61054900	-1.46074100
C	-2.80509700	-2.75701000	0.30977800	C	5.82574200	-0.42245000	-1.73955300
C	-4.94818300	-0.62138200	-0.21354400	C	5.12254100	1.02399100	0.08089100
O	-2.94787000	1.06698300	2.69682000	H	7.06085700	0.24315200	0.67333300
N	-0.90981700	0.35150400	-1.85785200	H	7.10859100	1.96806100	0.27989600
H	-1.17272500	2.31089600	-2.55398700	H	7.93258100	0.21115500	-1.62600200
				H	6.80036900	1.48084300	-2.11654600

H 5.55454800 -0.47716100 -2.79981700
H 4.73036900 2.02882600 -0.14596900
H 4.74213400 0.74909100 1.06931400
N 4.70455700 0.04538000 -0.92540100
C 3.52863300 -0.71777100 -0.80645400
O 3.41248900 -1.70892100 -1.57092000
O 2.67803600 -0.30906200 0.06296000
H 6.14389800 -1.43429000 -1.44181100

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Fe 1.14075900 -0.00815800 -0.20453100
H 2.62358900 -0.02809100 -0.09416100
C 1.84957800 -1.23092200 2.44559000
C 1.31309100 -2.51806500 1.82257100
H 1.76185700 -1.27207800 3.54127300
H 2.90598800 -1.11498900 2.19549600
H 0.31142700 -2.74726800 2.19471400
H 1.95482300 -3.36212200 2.09459100
P 1.21231400 -2.29332400 -0.02078900
N 1.14433800 -0.01045600 1.94175300
C -0.35027000 -3.18324600 -0.56292700
C -0.64957600 -4.55132400 0.07325000
C -0.43940000 -3.24414000 -2.09659100
H -1.12589500 -2.48743800 -0.21356400
H -0.55314800 -4.54023500 1.16326100
H -1.68797300 -4.82275300 -0.15323100
H -0.01405100 -5.35129500 -0.31467100
H -0.31642400 -2.25768000 -2.55545000
H 0.31085300 -3.91575100 -2.52903400
H -1.42572600 -3.62026700 -2.39202600
C 2.69945900 -3.17475600 -0.76604600
C 2.68657500 -4.70459000 -0.62478200
C 4.02235600 -2.60530700 -0.22943900
H 2.63425600 -2.92523800 -1.83327600
H 1.86123400 -5.16692900 -1.16902700
H 3.61809100 -5.11452100 -1.03364400
H 2.62618800 -5.01829500 0.42347700
H 4.08395100 -1.52246900 -0.35794000
H 4.15660200 -2.83501400 0.83391400
H 4.85983600 -3.06230300 -0.76917200
C -0.24346000 0.01637500 2.48301400
H -0.21719300 0.01657700 3.58252600
H -0.78368600 0.88770000 2.11560800
H -0.81837600 -0.83225900 2.11473800

P 1.26794500 2.27461800 -0.00977400
C 1.89684300 1.18164300 2.44581100
C 1.40120900 2.48970400 1.83259700
H 2.94678300 1.02948000 2.18714900
H 1.81845100 1.22105900 3.54229300
H 0.41456900 2.75631900 2.21966300
H 2.07880000 3.30799300 2.09613000
C 1.41460300 -0.00678000 -1.92938800
O 1.69933200 -0.00596400 -3.05592200
C -0.28576300 3.19674200 -0.52429500
C -0.39949300 3.25971200 -2.05630400
C -0.54759300 4.57087300 0.11536700
H -1.06975500 2.51617000 -0.16288800
H -0.29972500 2.27176100 -2.51758800
H -1.38435900 3.65206100 -2.33502300
H 0.35422600 3.91968700 -2.50062600
H -0.42579700 4.56136500 1.20283200
H 0.09232300 5.35879100 -0.28969100
H -1.58611700 4.85912000 -0.08824400
C 2.76009100 3.13105800 -0.77230600
C 4.07820000 2.51832300 -0.27295500
C 2.78782500 4.65803200 -0.60507600
H 2.66608500 2.90193300 -1.84186400
H 4.10905500 1.43706600 -0.42365800
H 4.91680100 2.96503700 -0.81951600
H 4.23792800 2.72273100 0.79207800
H 1.96600100 5.14971100 -1.12846100
H 2.75079900 4.95552100 0.44899600
H 3.72291900 5.05160900 -1.02166900
H -0.54058600 -0.37929500 -0.21330500
H -0.51771700 0.41382200 -0.23870800
C -6.72313500 -0.65795500 0.15569600
C -6.69572400 0.74697000 -0.46896300
C -5.28252100 1.24684500 -0.12891900
C -5.30230800 -1.18013900 -0.11364500
H -6.89359500 -0.58022600 1.23680400
H -7.50265800 -1.30485600 -0.25944700
H -7.47925700 1.40998400 -0.08834100
H -6.81905600 0.67519600 -1.55686400
H -4.91003600 1.97718800 -0.85678200
H -5.26069300 1.74216700 0.85427300
H -5.26091500 -1.70708500 -1.08123700
H -4.94309200 -1.87997500 0.64601300
N -4.47317000 0.02736400 -0.12456100

C -3.15538200 0.03168200 0.38241000
O -2.64390700 1.17443800 0.58195200
O -2.62050500 -1.10368500 0.57161800

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Fe -1.32517400 0.00694700 -0.22246900
H -2.83356000 -0.01882600 0.11116800
C -1.69252100 1.17009700 2.54552100
C -1.27061200 2.47916000 1.87751000
H -1.48241900 1.20677200 3.62594000
H -2.76600600 1.02093000 2.41559900
H -0.24503800 2.74222700 2.14929700
H -1.90757200 3.29831200 2.22651300
P -1.36135800 2.26510500 0.02481700
N -1.01334100 -0.01816300 1.94524900
C 0.14029100 3.20149800 -0.63077600
C 0.49317400 4.56233200 -0.00670700
C 0.10857500 3.27947200 -2.16546000
H 0.94148000 2.50412400 -0.35880900
H 0.48287700 4.54261800 1.08758800
H 1.50946000 4.84175800 -0.31259900
H -0.17257300 5.36369300 -0.33476900
H -0.05162600 2.29708400 -2.61951500
H -0.67825500 3.95252700 -2.52350800
H 1.06421800 3.66479000 -2.54053900
C -2.90725300 3.20640900 -0.51897000
C -2.83396800 4.73776700 -0.42399600
C -4.15491100 2.69880700 0.22255600
H -3.01205300 2.92996300 -1.57659800
H -2.10032900 5.16485700 -1.11033300
H -3.80969600 5.16666600 -0.68419500
H -2.59216700 5.07323000 0.59084700
H -4.24645700 1.61175800 0.17406400
H -4.14057100 2.99641200 1.27790400
H -5.05268200 3.14067300 -0.22609100
C 0.42217700 0.00013400 2.32501700
H 0.53187200 -0.02995500 3.42022000
H 0.94957100 -0.84323300 1.88354300
H 0.89762600 0.90410800 1.94709000
P -1.29050900 -2.25723400 -0.04598500
C -1.65070900 -1.24698300 2.50769200
C -1.18497600 -2.51950700 1.80036600
H -2.72853500 -1.12998300 2.38185300
H -1.43891600 -1.30924700 3.58653000

H -0.14821300 -2.75127300 2.05815000
H -1.78973600 -3.37035300 2.13031200
C -1.73150400 0.02635600 -1.90020800
O -2.05454400 0.03968900 -3.02395200
C 0.23853400 -3.12153200 -0.72510400
C 0.23109300 -3.13074200 -2.26180300
C 0.61248500 -4.50058100 -0.15591800
H 1.01982600 -2.42261100 -0.40290600
H 0.05713200 -2.13189400 -2.67342900
H 1.20157800 -3.47727900 -2.63727100
H -0.53370800 -3.80322900 -2.66671100
H 0.56455600 -4.53386400 0.93691600
H -0.01359700 -5.30653500 -0.54554500
H 1.64820700 -4.73025200 -0.43651700
C -2.81315700 -3.21842700 -0.62345000
C -4.07031700 -2.79824600 0.15575200
C -2.69033200 -4.74944000 -0.62549800
H -2.93837300 -2.88240100 -1.66146200
H -4.20407200 -1.71420700 0.16268100
H -4.95599000 -3.24922300 -0.30772600
H -4.03373500 -3.14974400 1.19374400
H -1.94138500 -5.10732400 -1.33431600
H -2.43991200 -5.14333500 0.36610400
H -3.65112600 -5.19187000 -0.91716700
H 1.68978800 0.17953200 -0.48283300
H 0.23349900 0.01608500 -0.48178600
C 6.73343100 1.19946200 -0.07444800
C 7.08393900 -0.29308500 0.05201200
C 5.79490000 -0.91511500 0.60786700
C 5.27168000 1.18252500 -0.54601500
H 6.80375900 1.68724900 0.90482000
H 7.38463200 1.73931000 -0.76707700
H 7.94697500 -0.48103800 0.69614900
H 7.30287100 -0.71170200 -0.93690600
H 5.64099200 -1.95071100 0.29305800
H 5.77872800 -0.89522700 1.70610900
H 5.20408300 1.13389700 -1.64094700
H 4.70407500 2.05617400 -0.21484100
N 4.74324900 -0.04832200 0.06107400
C 3.44169500 -0.42500100 0.06882400
O 3.03894800 -1.47308700 0.58138800
O 2.64601800 0.47278400 -0.54530300

TS12_13

Fe	-1.37002700	0.02063600	-0.16423200	C	-0.27721100	-3.18197000	-2.44664500
H	-2.74958700	0.02379300	0.33944000	C	0.63346600	-4.41539500	-0.42514800
C	-1.26804300	1.20189600	2.57010600	H	0.88766500	-2.34359500	-0.83625100
C	-0.93814700	2.51522500	1.86087700	H	-0.63374200	-2.23139500	-2.85461300
H	-0.87110400	1.21149300	3.59598600	H	0.61235100	-3.46956800	-3.01886500
H	-2.35148200	1.07368000	2.62749700	H	-1.04660100	-3.93980900	-2.63375400
H	0.11355700	2.77894200	1.99341000	H	0.88531400	-4.37390100	0.63857700
H	-1.52552200	3.32917500	2.29675900	H	-0.05139300	-5.25327100	-0.57926100
P	-1.28645100	2.31498700	0.04041900	H	1.56077100	-4.64752700	-0.96255700
N	-0.72952000	0.00719900	1.84744800	C	-2.90677800	-3.23541800	-0.28713000
C	0.16788600	3.08688100	-0.87011100	C	-4.04789900	-2.69457700	0.59056800
C	0.76988700	4.37358500	-0.28145600	C	-2.78600800	-4.75854300	-0.12721500
C	-0.15823800	3.25592100	-2.36382800	H	-3.15222300	-3.01422900	-1.33382100
H	0.93174900	2.30206900	-0.78194000	H	-4.18837400	-1.61778800	0.46834100
H	1.03332300	4.27032400	0.77529600	H	-4.98509600	-3.19335000	0.31727100
H	1.69612500	4.60719500	-0.82018600	H	-3.86831600	-2.89934600	1.65235700
H	0.10744200	5.23714900	-0.38229200	H	-2.12701900	-5.20427900	-0.87465900
H	-0.54215900	2.33444800	-2.81223400	H	-2.41568700	-5.03587400	0.86614000
H	-0.89353000	4.04987800	-2.53579800	H	-3.77491300	-5.21767600	-0.24649200
H	0.75279200	3.52891000	-2.90850600	H	1.09655100	0.13273100	-1.83592100
C	-2.83224100	3.32022400	-0.32405600	H	0.47525500	-0.05080900	-2.22896800
C	-2.69044100	4.83144300	-0.08818700	C	6.78635100	0.89658200	0.30829000
C	-4.04299500	2.76470900	0.44367200	C	6.93196600	-0.61190800	0.04572700
H	-3.00625100	3.15199900	-1.39434400	C	5.54161700	-1.16302800	0.40615600
H	-1.96203700	5.29059400	-0.75945100	C	5.35524700	1.18995800	-0.16705500
H	-3.65550800	5.32037400	-0.26834000	H	6.87460900	1.09979000	1.38293200
H	-2.39868700	5.05859300	0.94311100	H	7.53620800	1.50382700	-0.20851000
H	-4.21277100	1.70574300	0.23409400	H	7.73811400	-1.07865800	0.62074700
H	-3.92298800	2.88451000	1.52658000	H	7.13760100	-0.78440600	-1.01786300
H	-4.94366200	3.31760200	0.15259900	H	5.25715300	-2.04031900	-0.18272900
C	0.75746900	0.02835600	1.86628600	H	5.50538600	-1.46520900	1.46594300
H	1.12511500	0.04604000	2.90297100	H	5.33429800	1.41772600	-1.24487700
H	1.17144400	-0.83563600	1.34540400	H	4.90803100	2.05018200	0.34428000
H	1.13405300	0.89978200	1.33289400	N	4.63541900	-0.04589100	0.13469600
P	-1.31555700	-2.28011400	0.01132600	C	3.30002100	-0.24609800	-0.27064400
C	-1.22756600	-1.21243500	2.55747000	O	2.83943300	-1.41726300	-0.12977000
C	-0.89444600	-2.50433400	1.81223300	O	2.70066600	0.78282900	-0.71505000
H	-2.31091600	-1.10523600	2.64771500				
H	-0.80335600	-1.23530900	3.57199800	13			
H	0.16860200	-2.74250300	1.89419400	Fe	0.26037000	-0.66856900	-0.19558100
H	-1.44302300	-3.34120900	2.25538900	H	0.83623200	-2.05141300	-0.26750300
C	-2.12966200	0.03778600	-1.73795700	C	-0.29828100	-2.26409700	2.30488900
O	-2.74594200	0.05000000	-2.72432100	C	-1.73137000	-2.33323500	1.77803700
C	0.08054700	-3.08202100	-0.95490400	H	-0.28857400	-2.42110100	3.39499800

H 0.30041500 -3.05195400 1.84396200
 H -2.39071300 -1.68523700 2.36083100
 H -2.11770600 -3.35183500 1.88562700
 P -1.74970000 -1.77636900 -0.00417200
 N 0.36487400 -0.96401300 1.98267700
 C -3.29047100 -0.71604300 -0.19710400
 C -4.55647000 -1.11468300 0.57683100
 C -3.59141000 -0.46300500 -1.68339900
 H -2.91639200 0.22749500 0.21579800
 H -4.36287000 -1.29148300 1.63905300
 H -5.28694000 -0.29777900 0.51613700
 H -5.03720500 -2.00875200 0.17189800
 H -2.70866400 -0.10390500 -2.22053700
 H -3.95604700 -1.36391200 -2.18920500
 H -4.37119100 0.30152800 -1.78184500
 C -2.01268900 -3.34024800 -1.02431000
 C -3.36685500 -4.03646600 -0.81409500
 C -0.86958300 -4.35022600 -0.83206200
 H -1.96739500 -2.98118500 -2.06075900
 H -4.20963500 -3.41556900 -1.12368000
 H -3.40268700 -4.95602200 -1.41122800
 H -3.52055900 -4.32396700 0.23233100
 H 0.10710000 -3.91213100 -1.04746600
 H -0.84925900 -4.74638800 0.19016800
 H -1.01976700 -5.20136400 -1.50689300
 C -0.30333500 0.12321400 2.73948200
 H -0.32214700 -0.11788700 3.81329400
 H 0.22265200 1.06107800 2.57145700
 H -1.32360600 0.25644500 2.38271400
 P 2.46753000 -0.02482800 -0.04719500
 C 1.79072000 -1.05058600 2.42646700
 C 2.68069800 0.02451500 1.79746100
 H 2.15436300 -2.04095800 2.14849300
 H 1.83408800 -0.98325800 3.52427900
 H 2.36210700 1.02264100 2.10818900
 H 3.71850800 -0.12014300 2.11691300
 C 0.26066500 -0.70834700 -1.92894000
 O 0.28837700 -0.82049800 -3.08962700
 C 2.98479700 1.66712100 -0.68939700
 C 3.13908300 1.66921400 -2.21866600
 C 4.16674100 2.35756600 0.01123600
 H 2.09526300 2.24625500 -0.42716200
 H 2.27533800 1.22265200 -2.71976700
 H 3.22634800 2.70168200 -2.57844100

H 4.03465000 1.13403600 -2.55238200
 H 4.04273900 2.38106800 1.09795200
 H 5.13198300 1.89522100 -0.20835200
 H 4.22100700 3.40022300 -0.32774300
 C 3.75235800 -1.25468000 -0.70503100
 C 3.64240400 -2.65118700 -0.07087300
 C 5.21626000 -0.78955700 -0.62315700
 H 3.47871700 -1.35047800 -1.76456600
 H 2.62041200 -3.03503900 -0.08375900
 H 4.27507500 -3.35283000 -0.62788800
 H 4.00106800 -2.64826200 0.96471200
 H 5.41871100 0.08923700 -1.23676100
 H 5.51435000 -0.56377600 0.40704300
 H 5.87310100 -1.59239800 -0.98092700
 H -0.12675100 2.54359600 -2.48324000
 H 0.02927900 2.95920900 -3.08010000
 C -3.27559600 4.56717300 -0.29810800
 C -2.09222600 5.53567200 -0.13746400
 C -1.08132100 4.71750600 0.67972400
 C -2.59172500 3.20235200 -0.48645300
 H -3.87872200 4.55989300 0.61791100
 H -3.93702200 4.82235000 -1.13150900
 H -2.36515500 6.47675700 0.34932000
 H -1.66981400 5.77621200 -1.12044600
 H -0.04149900 4.98629400 0.47391400
 H -1.24263300 4.85638400 1.76025100
 H -2.39328700 3.00031300 -1.54899300
 H -3.20555300 2.37824400 -0.10989100
 N -1.34888400 3.33630000 0.27363400
 C -0.41117700 2.32508500 0.44926500
 O 0.63664900 2.60837900 1.08545200
 O -0.73477900 1.18244800 -0.05342300

TS14_15

C 0.27551000 1.59665600 0.39041300
 H -0.63116700 2.05340900 0.80384300
 O 0.51325700 2.09792200 -0.85419900
 H 1.41259600 1.83037100 -1.10981000
 O 1.19912000 1.19699000 1.12998300
 O 3.20104900 -0.24595100 0.40159500
 H 2.37704400 0.30806900 0.65100600
 C 2.88957500 -1.28748300 -0.33835800
 H 3.78441000 -1.88208100 -0.58445000
 O 1.77628200 -1.60245500 -0.73365000

C -3.12298700 -0.06372600 -0.45885900
C -2.83637800 -1.05405800 0.68062800
C -1.41668900 -0.66326300 1.11988600
C -1.76912700 0.02645900 -1.17538200
H -3.92536900 -0.38828600 -1.12708400
H -3.40281000 0.91446800 -0.04978500
H -2.84439300 -2.08076700 0.29633000
H -3.55895400 -0.99544200 1.49982100
H -1.44831400 0.11737900 1.89204600
H -0.83927800 -1.49967200 1.52133300
H -1.61521500 0.97192400 -1.70474900
H -1.65904600 -0.78803700 -1.90206200
N -0.76041800 -0.11114000 -0.09499200
H 0.03634300 -0.68291100 -0.38128900

15

C -0.30056300 -1.43799400 0.08526200
H 0.40656800 -2.27195500 0.12923400
O -1.05247300 -1.52632700 -1.06218200
H -1.80540900 -0.89635800 -0.93084700
O -1.02970600 -1.38845300 1.25051900
O -2.82229500 0.25142300 -0.00902800
H -1.78851400 -0.78321500 1.06065100
C -2.40844100 1.44800100 -0.10443000
H -3.19235400 2.23477100 -0.13693700
O -1.21753800 1.84470500 -0.16499700
C 2.86665000 0.23021900 -0.68282400
C 2.59802900 0.88195500 0.68232100
C 1.42220400 0.06982000 1.21691100
C 1.46657200 -0.10883500 -1.21812500
H 3.41156200 0.88178200 -1.36976500
H 3.45222400 -0.68565200 -0.55262400
H 2.30703300 1.93125300 0.56151600
H 3.45726800 0.84247700 1.35614500
H 1.74693300 -0.90548000 1.59085500
H 0.82856500 0.56546800 1.98410300
H 1.41696900 -1.06609700 -1.73741500
H 1.07173900 0.66247900 -1.88103800
N 0.56244500 -0.15854600 0.00085400
H -0.14030400 0.65056600 -0.06904100

16

C 0.03647200 1.74286600 0.08101700
H 0.89566800 2.41419300 0.15003000

O -0.72126500 1.85635000 1.22585600
H -1.48301500 1.24777300 1.09922400
O -0.63943300 1.99202300 -1.09452200
O -2.03330200 -0.10972500 -0.07642600
H -1.41066800 1.38469900 -1.09336400
C -2.59401600 -1.27414700 -0.08944000
H -3.70886000 -1.24036400 -0.09257500
O -2.02393300 -2.36519400 -0.09762000
C 2.11663600 -1.35540000 0.70516700
C 2.57804800 -0.89210500 -0.68787300
C 1.43421600 0.00461500 -1.20150200
C 1.33916500 -0.15174200 1.22718200
H 1.44754600 -2.21880800 0.62509500
H 2.94510000 -1.62341000 1.36492200
H 2.76820300 -1.72568600 -1.36752600
H 3.50074700 -0.30997700 -0.60563100
H 1.78562900 0.94814300 -1.62042200
H 0.79918900 -0.48739600 -1.93854900
H 2.00385600 0.66143600 1.53385100
H 0.63694900 -0.36767000 2.03113300
N 0.57671700 0.30289600 0.01362900
H -0.33702300 -0.23536300 -0.04719400

TS16_17

C 0.55103000 1.75350100 0.08634400
H 1.57178800 2.14191900 0.16186800
O -0.12405800 2.14888200 1.23812200
H -1.02957700 1.79577100 1.18478900
O 0.00588700 2.25907800 -1.09127800
O -1.90784000 0.22164000 -0.16014300
H -0.89361000 1.89783800 -1.18077800
C -2.63885200 -0.86846800 -0.13250900
H -3.71933900 -0.64900200 -0.23445700
O -2.22809100 -2.01239200 -0.00937800
C 1.40618600 -1.82264600 0.70725100
C 2.01611200 -1.55361400 -0.67949500
C 1.29030700 -0.28746800 -1.18233500
C 1.11273000 -0.41708600 1.22439200
H 0.46521500 -2.37448700 0.61257600
H 2.07283700 -2.37876000 1.37112500
H 1.89063300 -2.39336500 -1.36722300
H 3.08908600 -1.35731000 -0.58824600
H 1.98477300 0.46137600 -1.57264300
H 0.55629300 -0.50424800 -1.96161000

H 2.02756400 0.09213100 1.55420000
H 0.38152700 -0.38099300 2.03311400
N 0.56356100 0.26398900 0.01488600
H -0.73436400 0.03823700 -0.07739800

17

C 1.40042300 1.23843800 0.08552000
H 2.48167900 1.07325200 0.17673400
O 1.01894700 1.94692600 1.22814900
H 0.05785500 2.08455000 1.18981800
O 1.21599500 1.95154400 -1.10344000
O -1.65498200 1.13545100 -0.16305500
H 0.26120800 2.06866700 -1.23966700
C -2.82590300 0.50984700 -0.12221900
H -3.65870400 1.22841000 -0.20275100
O -2.99006000 -0.68843500 -0.01116700
C 0.30035200 -2.24535500 0.72395900
C 0.90397200 -2.34354900 -0.69023400
C 1.04068100 -0.87721900 -1.16443700
C 0.81147800 -0.89515000 1.22063000
H -0.79283200 -2.21976100 0.67177000
H 0.59725800 -3.07062700 1.37656100
H 0.28426300 -2.93636200 -1.36786000
H 1.89052900 -2.81549500 -0.65096300
H 2.06605500 -0.65166500 -1.48021900
H 0.37871300 -0.63894700 -2.00043900
H 1.86704300 -0.95616500 1.52725800
H 0.23657100 -0.48267200 2.05175200
N 0.66657000 -0.03547500 0.01679300
H -0.84085400 0.47918000 -0.09275500

18

C 1.42690700 0.00001700 0.30807600
H 1.49607300 0.00010000 1.40787200
O 2.08215500 1.17116600 -0.10610400
H 1.88243800 1.27843700 -1.05104800
O 2.08222100 -1.17114100 -0.10597900
H 1.88187500 -1.27892600 -1.05073100
C -2.17278000 0.77702400 -0.15380800
C -2.17257600 -0.77711000 -0.15444200
C -0.73468300 -1.16655100 0.23101200
C -0.73460600 1.16667100 0.23063100
H -2.42100800 1.16089800 -1.14764700
H -2.89690800 1.19840900 0.54868100

H -2.41957800 -1.16019800 -1.14888900
H -2.89729400 -1.19934000 0.54692500
H -0.65757100 -1.32644800 1.32166600
H -0.38639600 -2.07700200 -0.26049700
H -0.65691100 1.32725600 1.32112500
H -0.38652600 2.07679100 -0.26162700
N 0.06760400 -0.00006900 -0.18542500

19

C 0.11193900 0.15129000 -0.41486300
H 0.46636800 -0.33147200 -1.33477100
O 0.63919900 -0.77227200 0.62695100
H 0.45436700 -0.34859400 1.48229500
O 0.64455500 1.40657300 -0.20514500
H 1.62010000 1.31797500 -0.27365600
C 3.87950700 -0.14892900 -0.03922200
H 4.96235800 -0.32834600 -0.09959800
O 3.24728300 -1.18845300 0.46168900
H 2.25287400 -1.01683000 0.51545000
O 3.37585800 0.90407800 -0.40708400
C -3.39805900 -0.87977200 -0.10636600
C -3.45641000 0.58122100 0.37619900
C -1.99010000 0.89497200 0.67853800
C -2.02216600 -1.00542500 -0.80226000
H -3.44425600 -1.55749800 0.75255800
H -4.22477600 -1.14071000 -0.77252400
H -4.10550000 0.72044000 1.24515400
H -3.81336900 1.23782200 -0.42493400
H -1.76349600 1.96358600 0.68739000
H -1.71172300 0.48045800 1.66462100
H -2.11324000 -1.06851300 -1.89384000
H -1.49228400 -1.90402500 -0.46106900
N -1.29869300 0.23088000 -0.43578800

TS19_20

C 0.12191400 0.21606400 -0.42494800
H 0.54256500 -0.29983900 -1.29039500
O 0.75514500 -0.98921800 0.70991200
H 0.60626200 -0.59247700 1.58365500
O 0.69171700 1.36037000 -0.04534800
H 1.69098800 1.26453100 -0.17100500
C 3.73611500 -0.11660400 -0.10339700
H 4.82144400 -0.24861700 -0.25844800
O 3.15028300 -1.15592900 0.37005800

H 1.97590500 -1.05052100 0.54182700
O 3.22596200 0.98087300 -0.39500500
C -3.29875600 -0.91134900 -0.05779000
C -3.43929800 0.57275800 0.31932100
C -1.99367000 0.99350200 0.60493100
C -1.99154200 -0.95905500 -0.86790500
H -3.19593300 -1.51695600 0.84936200
H -4.15023900 -1.29662600 -0.62454400
H -4.09604900 0.74012200 1.17684100
H -3.83288900 1.14596800 -0.52780900
H -1.81536800 2.06250000 0.46650800
H -1.70435500 0.72955400 1.63318300
H -2.17977200 -0.86212900 -1.94456100
H -1.43153800 -1.88367200 -0.69840700
N -1.23206400 0.20964200 -0.38205800

20

C -0.00161000 -0.34099800 -0.01915800
H -0.57022200 0.59676700 -0.07020800
O -1.44333900 2.79975100 0.08412100
H -1.46415000 2.85664300 1.04948200
O -0.55953500 -1.45249800 0.11790900
H -2.09764800 -1.46236200 0.15739000
C -3.75798500 -0.47030000 -0.05833100
H -4.84908400 -0.62199600 -0.05168400
O -3.25909300 0.62503000 -0.27374200
H -2.12561500 2.13384800 -0.11066200
O -3.11845000 -1.58852900 0.18535200
C 3.40325600 0.80299000 0.30271300
C 3.63965000 -0.64690200 -0.15685000
C 2.26548300 -1.31696400 0.01067600
C 2.00269500 1.10750100 -0.23771600
H 3.40235800 0.86121100 1.39693800
H 4.15269500 1.50201900 -0.07635100
H 4.41606100 -1.15885200 0.41660800
H 3.93640800 -0.66048000 -1.21121300
H 2.05597800 -2.07385100 -0.75000900
H 2.15029000 -1.78766600 0.99335700
H 2.04589100 1.39960000 -1.29430800
H 1.46335700 1.88218600 0.31093400
N 1.31686900 -0.19272200 -0.10248500

H₂O

O 0.00000000 0.12023200 0.00000000

H 0.75782100 -0.48086400 0.00000000
H -0.75782100 -0.48099500 0.00000000

21

C -0.23493600 -0.04923200 -0.01530100
H -0.76396100 0.91275500 -0.06009300
O -0.86117700 -1.12763200 0.06022200
H -2.43091600 -0.96495600 0.05951500
C -3.85383800 0.33720300 -0.00926500
H -4.95497700 0.39530400 -0.02685500
O -3.45034500 -0.91722800 0.04947100
O -3.14346700 1.32776200 -0.03843500
C 3.26006000 0.86959900 0.31268500
C 3.37308400 -0.57460700 -0.20701000
C 1.97004800 -1.15538700 0.02413000
C 1.85510600 1.29006000 -0.13428400
H 3.32443500 0.88617600 1.40631800
H 4.03269200 1.53254600 -0.08423900
H 4.14589000 -1.15531300 0.30224700
H 3.60464500 -0.57062600 -1.27782600
H 1.67298500 -1.89493700 -0.72389900
H 1.87452800 -1.61929300 1.01265700
H 1.86359700 1.65350900 -1.16914000
H 1.40307100 2.05690100 0.49919000
N 1.09296900 0.02841600 -0.04766700

22

C 1.71846100 0.48114000 0.00912100
H 1.94702600 1.56335100 0.05732300
O 2.59588300 -0.37361900 -0.10773100
C -1.89584600 0.49466500 -0.32820700
C -1.65684500 -0.94318800 0.16579100
C -0.14165600 -1.14200400 -0.00689000
C -0.65805200 1.24258800 0.18335800
H -1.91865200 0.52012300 -1.42361300
H -2.82735400 0.93001900 0.04260500
H -2.23505700 -1.68955200 -0.38471000
H -1.92699300 -1.02395500 1.22461200
H 0.29839300 -1.78702000 0.75955700
H 0.10971800 -1.57066800 -0.98457700
H -0.79743600 1.56073100 1.22545300
H -0.40240500 2.12352200 -0.41195300
N 0.39847500 0.22331400 0.08830200

aTS14_15

C -0.30092500 1.65593900 0.57926400
H -1.18265600 1.67886200 1.23570500
O -0.47534000 2.56854700 -0.43269800
H 0.40594100 2.73556900 -0.80805100
O 0.84613900 1.44199800 1.05398200
O 2.45679700 0.24920800 -0.52522900
H 1.88831100 0.78895600 0.12657300
C 3.00914200 -0.78625400 0.09570300
H 2.79444400 -0.82562100 1.18107300
O 3.69455100 -1.61723800 -0.46155700
C -2.89377800 -1.21560400 -0.54719800
C -2.25483600 -1.57787700 0.80226000
C -0.79689200 -1.12763800 0.62993200
C -2.23103000 0.12648900 -0.87890600
H -2.63378600 -1.96454400 -1.30413400
H -3.98389100 -1.14021000 -0.50460600
H -2.32764800 -2.64091600 1.04615200
H -2.73441100 -1.01480600 1.61103800
H -0.31728700 -0.81468300 1.56133000
H -0.18737000 -1.91814800 0.18183900
H -2.75556600 0.95203300 -0.38313600
H -2.17862400 0.35164300 -1.94526700
N -0.85631900 0.04047000 -0.30311000
H -0.16048200 -0.06188500 -1.03905500

bTS14_15

C 1.35856400 0.04283300 -0.67213300
O 2.30922200 -0.78206100 0.81253200
O 1.67736900 1.18991200 -0.92265700
H 1.53267100 -0.82385600 -1.32348200
H 2.75348900 -0.02296600 1.22169500
N 0.13343000 -0.24828100 0.24380700
H 0.95341000 -0.64693500 0.96219700
C -0.85103400 -1.24433000 -0.28583900
C -0.61086400 0.97480800 0.68349700
C -2.09536400 -0.41545900 -0.61309400
H -1.05698100 -1.97567800 0.50143500
H -0.42159900 -1.77147400 -1.14153500
C -2.09845000 0.63226800 0.50958000
H -0.33805700 1.22048400 1.71213300
H -0.29265400 1.79776000 0.03839300
H -1.97883600 0.06863100 -1.58957600
H -3.00219600 -1.02532300 -0.64098900

H -2.69214200 1.51895600 0.27199900
H -2.50095800 0.19485400 1.43001000

aTS19_20

C -0.17310800 -0.15082000 -0.35674700
H -0.75216500 0.70033500 -0.71086400
O -0.82814700 0.07026300 1.31757500
H -0.47098500 -0.67239100 1.83241900
O -0.61073800 -1.38473500 -0.68560600
H -1.57647500 -1.40288200 -0.53306800
C -3.62442900 0.24649400 -0.18729700
H -4.66193000 -0.05282000 -0.44056400
O -3.03116900 -0.62108200 0.59429100
H -1.96718300 -0.21008700 1.03581900
O -3.14469200 1.28364600 -0.63136300
C 3.16358700 0.99079100 0.39052900
C 3.46176700 -0.41946200 -0.14405800
C 2.09528700 -1.11267400 -0.08473000
C 1.78433200 1.31711100 -0.20326400
H 3.10342500 0.97116100 1.48435800
H 3.91794900 1.72868800 0.10673400
H 4.21732700 -0.95142800 0.43940100
H 3.80802100 -0.36758700 -1.18241500
H 1.98425700 -1.91746300 -0.81490600
H 1.90424800 -1.52682500 0.91508200
H 1.87136500 1.81980500 -1.17399300
H 1.17706600 1.94174300 0.45746500
N 1.15977500 -0.01051800 -0.38017900

TS14_15 (Piperidine)

C -3.42579600 -0.95787400 -0.01350800
H -4.42080100 -1.43199200 -0.03932900
O -3.50603700 0.30987600 0.30529100
H -2.57393000 0.76879800 0.33985400
O -2.40966700 -1.59490000 -0.26611700
O 0.60297000 2.19095900 -0.62443500
H 0.67645400 2.64289400 0.23394000
C -0.46462700 1.34710800 -0.51232600
H -0.77804700 1.02341100 -1.51373200
O -1.28449500 1.52721400 0.42709500
C 0.80355400 -0.56468700 1.23614400
C 1.23161600 -0.96760800 -1.17994800
C 2.64506100 -0.39797700 -1.04170500
C 2.21790300 -0.00412400 1.40814500

H 0.08664700 -0.03770200 1.87428000
H 0.80534600 -0.72725600 -2.16083400
H 2.62750900 0.67177500 -1.27556200
H 2.19941300 1.08614500 1.29637000
N 0.31419600 -0.43024700 -0.15230100
H 3.29221500 -0.88465500 -1.78013000
H 1.26415900 -2.06450300 -1.09869500
H 0.78800900 -1.62609900 1.52415200
H 2.55350500 -0.21275000 2.43024800
H -0.58454000 -0.92189300 -0.21651900
C 3.18555600 -0.60560900 0.38004300
H 4.17906100 -0.15396400 0.48140100
H 3.30385700 -1.68104300 0.57492600

15 (Piperidine)

C -3.21968800 -0.96877500 0.02003500
H -4.15260300 -1.57037600 -0.02885900
O -3.37961600 0.28033200 0.10813500
H -2.13756900 1.08542200 0.29157900
O -2.13963200 -1.61775300 -0.01932700
O 0.70161300 2.06249600 -0.64624800
H 0.72314900 2.58000500 0.17522100
C -0.35602500 1.17832700 -0.51976500
H -0.77728000 0.99963600 -1.51947900
O -1.24810800 1.61244300 0.39837500
C 0.72594000 -0.32927400 1.28238900
C 0.98392500 -0.93252400 -1.13693000
C 2.45897400 -0.53840000 -1.08675200
C 2.20598600 0.04845000 1.35079100
H 0.10514200 0.30227100 1.91957400
H 0.53689700 -0.71697500 -2.11090400
H 2.57512100 0.50253100 -1.40232100
H 2.32956000 1.12408100 1.19067100
N 0.14055700 -0.24295300 -0.10102700
H 2.99307200 -1.16154700 -1.81241600
H 0.87187200 -2.00501100 -0.94861500
H 0.58606700 -1.36796600 1.59767800
H 2.55234900 -0.16298200 2.36834300
H -0.78818800 -0.79178000 -0.05824900
C 3.03630900 -0.72823000 0.32149200
H 4.08005200 -0.39789200 0.35109400
H 3.03188600 -1.79634800 0.57883600

16 (Piperidine)

C -2.23881100 0.52320100 1.25572900
C -1.15239200 -0.55139900 1.24546200
C -1.15719500 -0.56793800 -1.23895400
C -2.24371200 0.50635700 -1.25939500
H -0.47379300 -0.45154400 2.09184300
H -1.76563300 1.51024300 1.32759800
H -2.83756900 0.38972600 2.16289000
H -0.48173700 -0.47930000 -2.08915600
H -1.59332500 -1.57302900 -1.24358600
H -1.77098000 1.49236400 -1.34637100
H -2.84594600 0.36072800 -2.16236400
H -1.58853000 -1.55630800 1.26519100
N -0.31676000 -0.45973000 0.00103200
H 0.17661600 0.49321600 -0.00542000
C 0.84059800 -1.50703300 0.00527000
H 0.34824700 -2.48415400 0.00956200
O 1.56813200 -1.34635900 1.16002700
H 2.16773000 -0.57623500 0.98840100
O 1.56717500 -1.35583500 -1.15138400
O 2.91840600 0.70997100 -0.00371700
H 2.16637000 -0.58387500 -0.98675200
C 2.24219100 1.78610800 -0.00585700
H 2.82941600 2.72950900 -0.00485400
O 0.99226500 1.90487400 -0.00906800
C -3.11561200 0.45268900 0.00026700
H -3.83857600 1.27511200 -0.00383000
H -3.69319600 -0.48145800 0.00763000

TS16_17 (Piperidine)

C -1.94802500 -0.18143300 1.24645000
C -0.65275100 -0.99467000 1.23425100
C -0.64927700 -1.05464700 -1.20751400
C -1.94447000 -0.24278400 -1.26303600
H -0.03440500 -0.75108100 2.09906700
H -1.69864800 0.88570600 1.29110000
H -2.50561700 -0.42472600 2.15823500
H -0.02895700 -0.85405800 -2.08180100
H -0.87893600 -2.13346000 -1.20427700
H -1.69583100 0.82135000 -1.35955200
H -2.49965700 -0.52965400 -2.16344800
H -0.88125500 -2.07264000 1.28325900
N 0.13932300 -0.71619300 0.00669400
H 0.67132500 0.82522100 -0.03228800
C 1.44488400 -1.42630100 0.02610300

H 1.30199900 -2.51388700 0.05477100
O 2.15499500 -1.09461800 1.18293800
H 2.28432000 -0.13136300 1.18972800
O 2.15653000 -1.15714400 -1.14611500
O -0.38273500 3.03827900 0.02262700
H 2.28368100 -0.19546400 -1.20659100
C 0.80776700 2.80689200 -0.03232700
H 1.57659400 3.59651700 -0.06327100
O 1.36699800 1.60085600 -0.06137500
C -2.79216000 -0.45747100 -0.00344200
H -3.67679800 0.18885600 -0.02048100
H -3.15519800 -1.49447800 0.02118500

17 (Piperidine)

C -1.94802500 -0.18143300 1.24645000
C -0.65275100 -0.99467000 1.23425100
C -0.64927700 -1.05464700 -1.20751400
C -1.94447000 -0.24278400 -1.26303600
H -0.03440500 -0.75108100 2.09906700
H -1.69864800 0.88570600 1.29110000
H -2.50561700 -0.42472600 2.15823500
H -0.02895700 -0.85405800 -2.08180100
H -0.87893600 -2.13346000 -1.20427700
H -1.69583100 0.82135000 -1.35955200
H -2.49965700 -0.52965400 -2.16344800
H -0.88125500 -2.07264000 1.28325900
N 0.13932300 -0.71619300 0.00669400
H 0.67132500 0.82522100 -0.03228800
C 1.44488400 -1.42630100 0.02610300
H 1.30199900 -2.51388700 0.05477100
O 2.15499500 -1.09461800 1.18293800
H 2.28432000 -0.13136300 1.18972800
O 2.15653000 -1.15714400 -1.14611500
O -0.38273500 3.03827900 0.02262700
H 2.28368100 -0.19546400 -1.20659100
C 0.80776700 2.80689200 -0.03232700
H 1.57659400 3.59651700 -0.06327100
O 1.36699800 1.60085600 -0.06137500
C -2.79216000 -0.45747100 -0.00344200
H -3.67679800 0.18885600 -0.02048100
H -3.15519800 -1.49447800 0.02118500

19 (Piperidine)

C 2.47937200 -1.39183400 0.45006500

C 1.82226100 -0.39576900 1.41906000
C 1.79587700 1.35966800 -0.29617700
C 2.47498300 0.42497000 -1.31272400
H 1.16933500 -0.91355700 2.12924500
H 1.69917400 -1.98271800 -0.04413800
H 3.10856800 -2.08894700 1.01727200
H 1.12101400 2.06157100 -0.78942800
H 2.57204600 1.95538900 0.20509700
H 1.71566600 -0.06100700 -1.94026700
H 3.10197000 1.02212700 -1.98647300
H 2.60964000 0.09862000 2.00693300
N 1.04554500 0.65251300 0.75045900
C -0.33126700 0.39809400 0.55928700
H -0.74261200 -0.03752900 1.47860800
O -0.64341100 -0.68093800 -0.43015200
H -0.42627200 -0.31870900 -1.30595400
O -0.97465600 1.55074200 0.15662600
H -1.93356900 1.34212200 0.10971300
C -3.97501400 -0.40289900 -0.13249500
H -5.03146700 -0.70636800 -0.12858500
O -3.18282000 -1.41589000 -0.40932500
H -2.21381200 -1.12496300 -0.41589900
O -3.63175700 0.74896200 0.09946600
C 3.31520700 -0.64648200 -0.60149500
H 3.73552500 -1.35009800 -1.32976700
H 4.16860800 -0.16102200 -0.10561200

19 (Piperidine)

C 2.47937200 -1.39183400 0.45006500
C 1.82226100 -0.39576900 1.41906000
C 1.79587700 1.35966800 -0.29617700
C 2.47498300 0.42497000 -1.31272400
H 1.16933500 -0.91355700 2.12924500
H 1.69917400 -1.98271800 -0.04413800
H 3.10856800 -2.08894700 1.01727200
H 1.12101400 2.06157100 -0.78942800
H 2.57204600 1.95538900 0.20509700
H 1.71566600 -0.06100700 -1.94026700
H 3.10197000 1.02212700 -1.98647300
H 2.60964000 0.09862000 2.00693300
N 1.04554500 0.65251300 0.75045900
C -0.33126700 0.39809400 0.55928700
H -0.74261200 -0.03752900 1.47860800
O -0.64341100 -0.68093800 -0.43015200

H -0.42627200 -0.31870900 -1.30595400
O -0.97465600 1.55074200 0.15662600
H -1.93356900 1.34212200 0.10971300
C -3.97501400 -0.40289900 -0.13249500
H -5.03146700 -0.70636800 -0.12858500
O -3.18282000 -1.41589000 -0.40932500
H -2.21381200 -1.12496300 -0.41589900
O -3.63175700 0.74896200 0.09946600
C 3.31520700 -0.64648200 -0.60149500
H 3.73552500 -1.35009800 -1.32976700
H 4.16860800 -0.16102200 -0.10561200

TS19_20 (Piperidine)

C 2.48466700 -1.37186600 0.42350100
C 1.76262200 -0.44363000 1.41040100
C 1.75219800 1.39502600 -0.24115500
C 2.48979200 0.51751200 -1.26394600
H 1.09164300 -1.00586700 2.06569700
H 1.73441500 -1.95647800 -0.12138200
H 3.11139900 -2.07581700 0.98376000
H 1.07289700 2.09664400 -0.72595800
H 2.48316000 1.98207400 0.33081100
H 1.75839900 0.03861300 -1.92812900
H 3.12031900 1.15702500 -1.89310600
H 2.50004100 0.06204200 2.04879000
N 0.98517900 0.59168700 0.72082700
C -0.35962700 0.43356200 0.60037500
H -0.81030800 -0.08994100 1.44538800
O -0.73358000 -0.89597400 -0.52432600
H -0.54731400 -0.52289600 -1.40151300
O -1.01998000 1.47555400 0.09491500
H -2.00755700 1.25430000 0.10787100
C -3.86472100 -0.35970100 -0.11211700
H -4.94114200 -0.60390900 -0.08594200
O -3.11431400 -1.35331100 -0.42519100
H -1.95355500 -1.11051800 -0.47480500
O -3.51516700 0.80460100 0.15545300
C 3.33519300 -0.55802100 -0.56379000
H 3.79808000 -1.21965400 -1.30491300
H 4.15685800 -0.07166700 -0.01876900

20 (Piperidine)

C -2.54500600 1.12454100 0.85104600
C -1.76308600 -0.00263000 1.53606000
C -1.81040700 -1.35769200 -0.54646100

C -2.62064000 -0.26880800 -1.26255600
H -1.05951800 0.38904500 2.27503200
H -1.82316000 1.83536700 0.43109500
H -3.14219300 1.65590300 1.60044000
H -1.12943000 -1.87154300 -1.22518700
H -2.48308400 -2.10164300 -0.10142100
H -1.93010800 0.38405800 -1.81050900
H -3.27441700 -0.74295300 -2.00307100
H -2.44800400 -0.68789900 2.05149700
N -1.01131100 -0.77012800 0.53658200
C 0.32115900 -0.73297500 0.49170200
H 0.77876100 -0.20613500 1.33989300
O 0.76068100 1.89726000 -0.96900400
H 0.63291000 1.14524700 -1.56205800
O 1.01858200 -1.25521000 -0.40419300
H 2.54852000 -1.07962000 -0.18509900
C 3.98130100 0.18186700 0.18334000
H 5.06551200 0.20331000 0.37546100
O 3.30855300 1.20301300 0.17372800
H 1.60976800 1.68412800 -0.53949900
O 3.55760500 -1.04593900 -0.01427400
C -3.43956200 0.56676800 -0.26632800
H -3.94641200 1.38516100 -0.78956700
H -4.22589000 -0.06094300 0.17603500

21 (Piperidine)

C -2.60759900 1.41029300 -0.36657400
C -1.49627500 1.22853400 0.67358000
C -1.64102600 -1.24710700 0.45364300
C -2.75423700 -1.10631100 -0.59108900
H -0.76269100 2.03702200 0.62091700
H -2.14978300 1.54541300 -1.35464100
H -3.16315700 2.32649000 -0.13675100
H -0.99642700 -2.10219400 0.24955700
H -2.07589800 -1.37422300 1.45410900
H -2.30447600 -1.11565700 -1.59204000
H -3.41540500 -1.97746400 -0.52458900
H -1.92525300 1.22965700 1.68484400
N -0.79915900 -0.04522300 0.46896000
C 0.52382600 -0.10383800 0.28203800
H 1.03192300 0.87024100 0.29229000
O 1.16597900 -1.15811200 0.10358100
H 2.72830500 -0.95677900 -0.04785400
C 4.11019000 0.37466600 -0.23412500

H 5.20392100 0.45633400 -0.34850500
O 3.37847700 1.34924500 -0.20345800
O 3.74060700 -0.88834300 -0.14047600
C -3.54596900 0.19448200 -0.38998100
H -4.29433900 0.30921300 -1.18193300
H -4.09656400 0.14185800 0.55974900

22 (Piperidine)

C -1.57750500 1.07829900 -0.39489600
C -0.30723400 1.34452600 0.42242200
C 0.17558500 -1.09099800 0.54353500
C -1.08781900 -1.40113000 -0.26852500
H 0.16845100 2.28264600 0.12207900
H -1.33307500 1.14234700 -1.46304300
H -2.31327500 1.86197500 -0.18084500
H 0.98760500 -1.78239300 0.31401300
H -0.04332700 -1.16446500 1.61866300
H -0.81893900 -1.47236800 -1.33029200
H -1.47680300 -2.38014100 0.03389800
H -0.56561500 1.42921600 1.48812300
N 0.65761400 0.25983700 0.25255700
C 1.92796400 0.47910200 -0.16626000
H 2.12237300 1.55143300 -0.35776900
O 2.79120200 -0.38006800 -0.32773200
C -2.15266200 -0.31066700 -0.07722700
H -3.02468300 -0.51464200 -0.70887700
H -2.50560200 -0.32670700 0.96370600

TS14_15 (N-methyl piperazine)

C 3.75160300 -1.01162200 -0.04851900
H 4.73708200 -1.50546900 -0.02496700
O 3.85263500 0.25048600 -0.37861300
H 2.92526800 0.72912500 -0.41697500
O 2.72579000 -1.62985400 0.21595800
O -0.16607700 2.22515300 0.62454600
H -0.27578000 2.65280900 -0.24226800
C 0.87422200 1.34948700 0.48189500
H 1.23389200 1.05513800 1.47768500
O 1.65746800 1.49543800 -0.49823600
C -0.50276300 -0.55810600 -1.14831800
C -0.84024100 -0.87229800 1.27480000
C -2.25216100 -0.31517600 1.11602800
C -1.93061700 -0.02577300 -1.24282200
H 0.15524800 -0.02382100 -1.84074500

H -0.41859800 -0.56914100 2.23933900
H -2.24722800 0.77272700 1.30388300
H -1.93031400 1.07803000 -1.16963400
N 0.05831500 -0.38673900 0.20737200
H -2.89552400 -0.77981600 1.87103700
H -0.87562700 -1.96954800 1.24942300
H -0.49147000 -1.62323600 -1.41327200
H -2.33037300 -0.28183500 -2.23000800
H 0.94455600 -0.90560100 0.24758900
N -2.77870500 -0.63078100 -0.21478300
C -4.16821800 -0.21548800 -0.35432900
H -4.78186100 -0.71299000 0.40410800
H -4.31124700 0.87628600 -0.24397500
H -4.54477400 -0.50595400 -1.34098000

15 (N-methyl piperazine)

C 3.51512100 -1.08719200 -0.07371500
H 4.41695500 -1.73562700 -0.06931800
O 3.72469000 0.14253100 -0.26313200
H 2.51233300 1.00433500 -0.39458500
O 2.41350500 -1.67142300 0.11671900
O -0.23991800 2.15474400 0.61862200
H -0.30991100 2.60046400 -0.24168600
C 0.77756400 1.22554300 0.49762400
H 1.22920400 1.08372600 1.48972000
O 1.64672500 1.57336200 -0.47677300
C -0.40200600 -0.34915400 -1.18506300
C -0.66127900 -0.78202500 1.24443800
C -2.11784600 -0.34842200 1.12570100
C -1.87202400 0.05456300 -1.22867700
H 0.20011000 0.24082400 -1.87722500
H -0.24219900 -0.49894700 2.21299400
H -2.21754400 0.72246900 1.36764600
H -1.97867800 1.14957700 -1.13133700
N 0.21315300 -0.19797700 0.17538300
H -2.69210700 -0.91145000 1.86916700
H -0.58788900 -1.86782100 1.14005200
H -0.30153100 -1.40582100 -1.44633900
H -2.25829100 -0.21796300 -2.21665800
H 1.11858700 -0.79340200 0.15534700
N -2.63647700 -0.66116200 -0.20773300
C -4.06304800 -0.38014400 -0.30979700
H -4.60850200 -0.96645800 0.43668500
H -4.31061600 0.68618100 -0.15285800

H -4.42555300 -0.66884700 -1.30171300

16 (N-methyl piperazine)

C -1.96600300 0.15431300 1.19757200
C -0.74279600 -0.75333500 1.23117300
C -0.74271300 -0.75325700 -1.23120500
C -1.96589800 0.15441400 -1.19761600
H -0.11256100 -0.53401100 2.09229800
H -1.64247400 1.21026700 1.26492500
H -2.57031100 -0.05822200 2.08541900
H -0.11240300 -0.53391200 -2.09226500
H -1.04200200 -1.80538600 -1.26117300
H -1.64228900 1.21035500 -1.26483200
H -2.57014200 -0.05798000 -2.08553700
H -1.04206400 -1.80547400 1.26109100
N 0.08768900 -0.55572100 0.00003000
H 0.46721200 0.45079900 0.00012400
C 1.36133300 -1.45791100 0.00003400
H 0.99085900 -2.48724000 0.00005700
O 2.06026100 -1.21248800 1.15665700
H 2.56581800 -0.37700600 0.98773500
O 2.06026600 -1.21255000 -1.15657200
O 3.16618500 0.98743600 -0.00031000
H 2.56572800 -0.37697400 -0.98769600
C 2.36559900 1.97428400 -0.00000400
H 2.83316500 2.98180900 -0.00005200
O 1.10996600 1.93992700 0.00037400
N -2.76722500 -0.09644300 -0.00007200
C -3.99516400 0.69075300 -0.00007600
H -4.58938700 0.44642400 0.88620700
H -3.81265100 1.78104300 -0.00002700
H -4.58931700 0.44648900 -0.88642100

TS16_17 (N-methyl piperazine)

C 1.92353900 0.11764100 -1.19228100
C 0.68364900 -0.77021700 -1.21794400
C 0.67065700 -0.76897800 1.21444900
C 1.91011500 0.11893000 1.20156700
H 0.07597600 -0.55010800 -2.09657600
H 1.62068200 1.17973200 -1.26781700
H 2.53022900 -0.10936700 -2.07574400
H 0.05405400 -0.54904600 2.08663700
H 0.97192100 -1.82529700 1.25974300
H 1.60546600 1.18094600 1.27242800

H 2.50697200 -0.10667600 2.09210100
H 0.98516300 -1.82657700 -1.25946400
N -0.15291700 -0.54653800 -0.00615700
H -0.61155400 0.79930400 -0.02385400
C -1.35945400 -1.45110500 -0.01159800
H -1.01374400 -2.49227800 -0.02316100
O -2.09508600 -1.23783000 -1.17190300
H -2.56798500 -0.39293200 -1.04431900
O -2.09277900 -1.25957500 1.15066500
O -3.06193600 1.16602100 0.06843200
H -2.54106400 -0.39542700 1.04980600
C -2.20212700 2.05795000 -0.00450300
H -2.50548100 3.11771700 -0.03293700
O -0.92153300 1.88822200 -0.05339300
N 2.71869800 -0.13316100 0.00933600
C 3.94779100 0.64941300 0.01626100
H 4.54779100 0.40510500 -0.86672700
H 3.76924900 1.74132800 0.01537900
H 4.53751100 0.40495400 0.90612800

17 (N-methyl piperazine)

C 1.92091000 0.11580100 -1.19191700
C 0.68864700 -0.78209200 -1.21515700
C 0.67537000 -0.78296100 1.21119500
C 1.90674500 0.11554300 1.20231900
H 0.08225300 -0.56889600 -2.09639300
H 1.60916300 1.17529200 -1.26945300
H 2.53024300 -0.10706200 -2.07457800
H 0.05979500 -0.57168200 2.08626100
H 0.98881100 -1.83679100 1.25629900
H 1.59241400 1.17469300 1.27587700
H 2.50593400 -0.10647700 2.09214600
H 1.00197500 -1.83599800 -1.25820300
N -0.14954400 -0.56201200 -0.00629600
H -0.63893400 0.88870700 -0.02739100
C -1.34397000 -1.46900400 -0.01275200
H -1.00194700 -2.51200100 -0.02479700
O -2.08488000 -1.26330600 -1.17446800
H -2.54936600 -0.41370000 -1.05714000
O -2.08364300 -1.28625900 1.15001800
O -3.06259400 1.17774100 0.07472300
H -2.51981100 -0.41606800 1.06247600
C -2.22209800 2.08004600 -0.00354000
H -2.52914000 3.13694000 -0.03327900

O -0.93200600 1.92735100 -0.05830000
N 2.71906600 -0.12479400 0.00999000
C 3.93674400 0.67498300 0.01767700
H 4.54028600 0.43983400 -0.86518700
H 3.74290100 1.76424600 0.01739500
H 4.52966300 0.43849400 0.90737800

19 (N-methyl piperazine)

C 2.25972800 -0.75463000 0.99000400
C 1.43873000 0.38924000 1.59718200
C 1.35613200 1.46727600 -0.58117000
C 2.19528700 0.32321000 -1.16539800
H 0.80657700 0.01035500 2.40569900
H 1.58350300 -1.57354600 0.68114800
H 2.94062200 -1.15497800 1.75034300
H 0.66252100 1.85591700 -1.32832300
H 2.03625900 2.28171100 -0.29887600
H 1.53449100 -0.44306500 -1.62215100
H 2.82642000 0.71613200 -1.97134000
H 2.13275900 1.12239700 2.02988800
N 0.60329200 1.08113000 0.61613400
C -0.73698300 0.64499000 0.48661200
H -1.16994600 0.52601300 1.48790700
O -0.89821700 -0.73501400 -0.05907000
H -0.60114300 -0.70310700 -0.98466500
O -1.43551500 1.52107700 -0.31783300
H -2.36812300 1.21275800 -0.34308700
C -4.25950400 -0.69492600 -0.16179200
H -5.28768800 -1.08335800 -0.15757600
O -3.37779100 -1.65735300 0.00242900
H -2.43611500 -1.29054900 -0.01409200
O -4.01771000 0.49676700 -0.30251100
N 3.05743500 -0.25936100 -0.13669700
C 3.92235000 -1.29568800 -0.68158600
H 4.59373100 -1.66804100 0.09963300
H 3.36465400 -2.16069200 -1.08914900
H 4.53581400 -0.88098900 -1.48864300

TS19_20 (N-methyl piperazine)

C 2.25498800 -0.85800900 0.89684800
C 1.34105200 0.13834700 1.61623900
C 1.30996600 1.52302100 -0.40834100
C 2.23574200 0.50812500 -1.08690800
H 0.68231200 -0.38310300 2.31528400

H 1.63761000 -1.64966700 0.43355200
H 2.91517000 -1.33366000 1.63095300
H 0.62783000 1.97251400 -1.12999100
H 1.91695300 2.32210800 0.03457600
H 1.63087300 -0.21886100 -1.66539700
H 2.87969400 1.03456900 -1.80054100
H 1.95733700 0.84443300 2.18683200
N 0.53058200 0.90158500 0.66663300
C -0.78976100 0.61031200 0.52170500
H -1.26147600 0.27411200 1.44662600
O -0.99450400 -0.97787000 -0.25127500
H -0.76283000 -0.82517300 -1.18232000
O -1.47660700 1.44178400 -0.25961900
H -2.44832800 1.15032600 -0.25481000
C -4.17367100 -0.59699200 -0.16349100
H -5.23267300 -0.90820500 -0.13277400
O -3.34355600 -1.57494200 -0.15757700
H -2.18868400 -1.26427500 -0.21312600
O -3.91742300 0.62144700 -0.19784800
N 3.07858000 -0.16125700 -0.09536700
C 4.04051400 -1.05809200 -0.72211700
H 4.69189900 -1.49512100 0.04222900
H 3.56644500 -1.88844700 -1.27923400
H 4.66746500 -0.49747400 -1.42377500

20 (N-methyl piperazine)

C -2.41058400 -0.41725100 1.25689700
C -1.57517900 -1.60749000 0.77919400
C -1.34289400 -0.51274500 -1.41479900
C -2.16629700 0.66264200 -0.88663700
H -0.98594300 -2.02181600 1.60041500
H -1.74600700 0.30324500 1.77136700
H -3.14713200 -0.77024100 1.98657700
H -0.58809600 -0.18384100 -2.12841900
H -1.99712200 -1.24461500 -1.90152500
H -1.47208200 1.42909000 -0.49497500
H -2.72677600 1.10730500 -1.71558700
H -2.23193700 -2.39173700 0.38642300
N -0.67315700 -1.17594000 -0.29143900
C 0.65172700 -1.20137600 -0.15832800
H 0.99816500 -1.68406600 0.76622200
O 1.24679900 2.14008300 -0.60743000
H 1.21042000 1.31182200 -1.10803800
O 1.46265300 -0.74465800 -0.99475500

H 2.96788700 -0.70966200 -0.44291900
C 4.23686900 0.22770200 0.68856400
H 5.25413700 0.10517300 1.09222100
O 3.54794600 1.20028600 0.94954500
H 1.95502200 1.94093100 0.02890400
O 3.90881700 -0.79608500 -0.07557800
N -3.11451700 0.19992100 0.13119900
C -3.99251200 1.27623500 0.57481200
H -4.72153900 0.88566100 1.29241100
H -3.45083600 2.11030900 1.05793100
H -4.54095000 1.68125800 -0.28179600

21 (N-methyl piperazine)

C -2.26624900 1.27506800 -0.17251500
C -1.07186700 1.21209600 0.78046400
C -1.18024000 -1.25235100 0.68096300
C -2.37798600 -1.12855400 -0.26163100
H -0.38743700 2.04370900 0.59783600
H -1.89594900 1.35569900 -1.21300600
H -2.84753900 2.17758900 0.04410800
H -0.56207800 -2.11203000 0.42188000
H -1.53058100 -1.36278200 1.71444300
H -2.02110900 -1.16657400 -1.30905800
H -3.04108000 -1.98609100 -0.10685500
H -1.42531500 1.26964400 1.81723700
N -0.35232200 -0.04802900 0.59472300
C 0.95409000 -0.09356600 0.30897800
H 1.44562100 0.88775200 0.25907700
O 1.59437000 -1.14463400 0.11362600
H 3.13231900 -0.93583900 -0.22874100
C 4.51915000 0.39309700 -0.37736000
H 5.59357600 0.47928300 -0.60967600
O 3.82930000 1.35657000 -0.09209000
O 4.12169200 -0.86295800 -0.45409900
N -3.12441500 0.10233500 0.00922500
C -4.32858700 0.18630100 -0.80857800
H -4.11751700 0.20595800 -1.89408900
H -4.97306800 -0.67538200 -0.60597000
H -4.88544800 1.09455000 -0.55625800

22 (N-methyl piperazine)

C -1.10249600 1.17208600 -0.24634500
C 0.24274700 1.40798000 0.44253500
C 0.52871300 -1.03262400 0.63188600

C -0.82430100 -1.21384000 -0.05713300
H 0.73371800 2.29379100 0.03062300
H -0.95138900 1.16304000 -1.34364100
H -1.77789200 2.00173400 -0.01090900
H 1.22785900 -1.81757800 0.34090000
H 0.39410200 -1.06361400 1.72110000
H -0.66281300 -1.34160600 -1.14520700
H -1.29826300 -2.12802700 0.31614500
H 0.07737700 1.57160700 1.51568800
N 1.11294300 0.25223400 0.25783300
C 2.35426600 0.34568600 -0.27926600
H 2.61828700 1.39036400 -0.53080100
O 3.12397200 -0.59077500 -0.47447600
N -1.70489600 -0.07686200 0.22632800
C -3.03491500 -0.27623800 -0.33499200
H -3.03502300 -0.36533200 -1.43770800
H -3.47704400 -1.18982600 0.07599200
H -3.68111100 0.56574200 -0.06561200

TS14_15 (morpholine)

C -3.38543900 -0.96237900 -0.03469100
H -4.37517400 -1.44670800 -0.06942500
O -3.47667000 0.30022100 0.29393000
H -2.54430200 0.76970300 0.34497700
O -2.36294800 -1.59127500 -0.28893700
O 0.62989500 2.19890600 -0.56040800
H 0.68842000 2.63196100 0.30863700
C -0.44284600 1.35035500 -0.48190600
H -0.76371100 1.08387300 -1.49912100
O -1.27121800 1.51750700 0.45880300
C 0.78753000 -0.58121600 1.19846100
C 1.25361100 -0.88142300 -1.20970000
C 2.66588900 -0.37529700 -0.93218700
O 3.08363700 -0.71815400 0.38751200
C 2.23012600 -0.10860900 1.35122400
H 0.12140100 -0.01637600 1.85892700
H 0.91113200 -0.53977200 -2.19314400
H 2.71503000 0.71299100 -1.07535100
H 2.28994800 0.98676500 1.26795700
N 0.30362400 -0.38966100 -0.18683400
H 3.36927700 -0.84953100 -1.62238800
H 1.25073000 -1.97917700 -1.21087600
H 0.71836000 -1.64383800 1.46317100
H 2.60670100 -0.39388200 2.33762000

H -0.58798200 -0.89461000 -0.27753900

15 (morpholine)

C -3.19584000 -0.97270300 0.00500100
H -4.12385500 -1.58026600 -0.04616400
O -3.36222500 0.27342100 0.11577000
H -2.12986000 1.08103100 0.31064500
O -2.11096500 -1.61353100 -0.05631200
O 0.70840400 2.07787700 -0.61532300
H 0.71799600 2.59676400 0.20576800
C -0.35253800 1.19543000 -0.50549800
H -0.77632500 1.03419400 -1.50678900
O -1.23915000 1.60808900 0.42540300
C 0.73668600 -0.34954700 1.26065900
C 1.01583800 -0.89688400 -1.14592700
C 2.48630200 -0.52722400 -0.98745200
O 2.94481800 -0.80563000 0.33314600
C 2.22759200 -0.02894200 1.28707900
H 0.16786600 0.31216200 1.91606900
H 0.64243300 -0.62157500 -2.13579500
H 2.65172000 0.52826100 -1.23804700
H 2.40515800 1.04163600 1.11843200
N 0.14683200 -0.23597600 -0.11575000
H 3.08085900 -1.14363600 -1.66715100
H 0.88700400 -1.97468800 -1.01501000
H 0.57323500 -1.38230700 1.57964100
H 2.62454400 -0.28832600 2.27231200
H -0.78389700 -0.79400700 -0.08830400

16 (morpholine)

C 2.27043100 0.52746600 -1.17082600
C 1.17111200 -0.52716500 -1.23011900
C 1.17108100 -0.52692400 1.23009700
C 2.27036500 0.52773400 1.17061300
H 0.52553800 -0.37610000 -2.09525800
H 1.82915500 1.53481900 -1.21790400
H 2.93490400 0.40449800 -2.02966100
H 0.52548600 -0.37571400 2.09519400
H 1.60049900 -1.53251700 1.27083600
H 1.82903900 1.53507800 1.21739800
H 2.93480000 0.40502700 2.02951300
H 1.60049100 -1.53278300 -1.27066100
O 3.06803700 0.38693600 -0.00007100
N 0.32115400 -0.44368900 -0.00002800

H -0.19063300 0.50705000 -0.00010400

C -0.81889800 -1.51172100 0.00004700
H -0.31001500 -2.48011000 0.00007300
O -1.54335300 -1.36348700 -1.15686500
H -2.15261000 -0.59997700 -0.99147600
O -1.54338100 -1.36341300 1.15690500
O -2.90948200 0.69064600 0.00002400
H -2.15267900 -0.59993500 0.99143800
C -2.24004200 1.76968200 0.00016900
H -2.82886400 2.71126600 0.00053900
O -0.98900600 1.89316600 0.00005500

TS16_17 (morpholine)

C 2.22631800 0.50108300 -1.16923000
C 1.11559400 -0.54271300 -1.21606100
C 1.11544800 -0.54263100 1.21625600
C 2.22617100 0.50116900 1.16948600
H 0.48659400 -0.39167300 -2.09475800
H 1.79714100 1.51419800 -1.22266300
H 2.89033300 0.36738100 -2.02764100
H 0.48634000 -0.39153500 2.09486600
H 1.55317600 -1.54924100 1.26991800
H 1.79698300 1.51428500 1.22278700
H 2.89007800 0.36753500 2.02799200
H 1.55332300 -1.54933000 -1.26960300
O 3.02656800 0.36500800 0.00018400
N 0.26195800 -0.44103500 0.00004300
H -0.37255100 0.80834800 -0.00002300
C -0.80658900 -1.50995000 0.00001300
H -0.31160900 -2.48891600 0.00008200
O -1.55915300 -1.41331000 -1.16168900
H -2.13951800 -0.63426100 -1.04778100
O -1.55930400 -1.41322100 1.16161100
O -2.85402100 0.83464200 -0.00026000
H -2.13965700 -0.63418500 1.04756200
C -2.12675900 1.84127000 -0.00024400
H -2.57702900 2.84772000 -0.00036600
O -0.83514200 1.85407500 -0.00009500

17 (morpholine)

C 2.21905100 0.52332900 -1.16945000
C 1.12795700 -0.54040900 -1.21244100
C 1.12781400 -0.54033600 1.21260700
C 2.21890100 0.52341100 1.16968000

H 0.50032500 -0.40309900 -2.09445200
H 1.77104500 1.52839000 -1.22446700
H 2.88614800 0.40140200 -2.02716000
H 0.50007200 -0.40298300 2.09453400
H 1.58824500 -1.53814600 1.26816800
H 1.77087800 1.52847100 1.22456600
H 2.88588900 0.40155200 2.02748500
H 1.58838300 -1.53822600 -1.26789400
O 3.02325600 0.40639700 0.00017100
N 0.27234600 -0.45041400 0.00003100
H -0.43962100 0.91698300 -0.00004000
C -0.76788000 -1.53295300 0.00001900
H -0.26510000 -2.50880600 0.00009700
O -1.52700200 -1.45709400 -1.16283600
H -2.10474300 -0.67627500 -1.06445700
O -1.52712800 -1.45696700 1.16277500
O -2.87147400 0.81640800 -0.00015700
H -2.10486900 -0.67616100 1.06422800
C -2.18361000 1.84209100 -0.00023500
H -2.65115900 2.83831300 -0.00040400
O -0.88331600 1.89509000 -0.00014100

19 (morpholine)

C 2.52226600 -1.34778400 0.35505000
C 1.83148600 -0.44375300 1.37801600
C 1.81385200 1.33139500 -0.29178600
C 2.52692300 0.37508800 -1.25223600
H 1.17974500 -1.03504900 2.02926700
H 1.77423400 -1.92948500 -0.20481200
H 3.20341500 -2.04403200 0.85470200
H 1.14522200 2.00077700 -0.83675700
H 2.57082200 1.94902900 0.20957900
H 1.79767000 -0.14783500 -1.89397900
H 3.21072100 0.92921900 -1.90356600
H 2.60178900 0.02211600 2.00752800
O 3.32048700 -0.57634900 -0.54528400
N 1.05243100 0.62360700 0.74517100
C -0.32860900 0.38119200 0.55148200
H -0.74205500 -0.05031300 1.47160000
O -0.64639200 -0.69179400 -0.43720100
H -0.44006000 -0.32617800 -1.31464000
O -0.95598300 1.54213400 0.15111900
H -1.91881900 1.34835600 0.11265700
C -3.97807700 -0.37474300 -0.11779000

H -5.03858600 -0.66298300 -0.10724400
O -3.20254400 -1.39837000 -0.40399900
H -2.23096500 -1.12185700 -0.41569400
O -3.61646700 0.77120600 0.11520800

TS19_20 (morpholine)

C 2.53279600 -1.32217700 0.33264700
C 1.76908500 -0.49178100 1.36546700
C 1.76829000 1.36485200 -0.24012500
C 2.55148500 0.46547700 -1.19982000
H 1.10372300 -1.12808800 1.95515600
H 1.82117500 -1.89204400 -0.28321700
H 3.20980500 -2.02276400 0.83062300
H 1.09878000 2.03166300 -0.78483300
H 2.47217400 1.97847900 0.33554500
H 1.86026900 -0.05281200 -1.88433900
H 3.24117800 1.06574400 -1.80125000
H 2.48423900 -0.01474600 2.04724400
O 3.34309300 -0.48451900 -0.49148500
N 0.98850700 0.55888600 0.70700100
C -0.35895800 0.41790400 0.59080100
H -0.81116200 -0.11104600 1.43118600
O -0.74695100 -0.90390600 -0.54725500
H -0.57731800 -0.52182200 -1.42424600
O -1.00715900 1.46874900 0.09524600
H -2.00058800 1.25840600 0.11055200
C -3.86415200 -0.33470800 -0.09234200
H -4.94320900 -0.56494400 -0.05199300
O -3.12859400 -1.33776400 -0.40564100
H -1.95738700 -1.10755300 -0.47763700
O -3.49945200 0.82893000 0.16269100

20 (morpholine)

C 2.67597400 -1.07160900 0.70042900
C 1.84240500 -0.04458400 1.46693000
C 1.80639400 1.32512500 -0.58489100
C 2.65973200 0.24381400 -1.25047800
H 1.18022900 -0.53971300 2.18138900
H 2.00404900 -1.81316100 0.24300600
H 3.36490200 -1.58351300 1.37785800
H 1.10911300 1.77122800 -1.29477100
H 2.45181600 2.11118800 -0.17556900
H 2.00723000 -0.47296100 -1.77356300
H 3.33648000 0.69564500 -1.98097500

H 2.50236700 0.63930100 2.01352600
O 3.47310600 -0.43629500 -0.29798100
N 1.04227900 0.72837600 0.51434200
C -0.29406700 0.71102700 0.52923500
H -0.72012300 0.17686700 1.38827900
O -0.76245700 -2.03255700 -0.56950100
H -0.52810100 -1.60601100 -1.40420000
O -1.01484800 1.26800100 -0.32214500
H -2.53982500 1.10251200 -0.07983600
C -4.05471500 -0.11196300 0.08305800
H -5.13834800 -0.09185000 0.27866900
O -3.45982300 -1.15908400 -0.12697200
H -1.66708500 -1.70690900 -0.40224600
O -3.54510200 1.09842000 0.11189400

21 (morpholine)

C -3.19584000 -0.97270300 0.00500100
H -4.12385500 -1.58026600 -0.04616400
O -3.36222500 0.27342100 0.11577000
H -2.12986000 1.08103100 0.31064500
O -2.11096500 -1.61353100 -0.05631200
O 0.70840400 2.07787700 -0.61532300
H 0.71799600 2.59676400 0.20576800
C -0.35253800 1.19543000 -0.50549800
H -0.77632500 1.03419400 -1.50678900
O -1.23915000 1.60808900 0.42540300
C 0.73668600 -0.34954700 1.26065900
C 1.01583800 -0.89688400 -1.14592700
C 2.48630200 -0.52722400 -0.98745200
O 2.94481800 -0.80563000 0.33314600
C 2.22759200 -0.02894200 1.28707900
H 0.16786600 0.31216200 1.91606900
H 0.64243300 -0.62157500 -2.13579500
H 2.65172000 0.52826100 -1.23804700
H 2.40515800 1.04163600 1.11843200
N 0.14683200 -0.23597600 -0.11575000
H 3.08085900 -1.14363600 -1.66715100
H 0.88700400 -1.97468800 -1.01501000
H 0.57323500 -1.38230700 1.57964100
H 2.62454400 -0.28832600 2.27231200
H -0.78389700 -0.79400700 -0.08830400

22 (morpholine)

C 1.60664300 -0.97657300 -0.38215500

C 0.34118900 -1.32899700 0.40034400
C -0.14948300 1.08702400 0.51887200
C 1.13910300 1.32650600 -0.26596600
H -0.08454900 -2.26952400 0.03875400
H 1.39298500 -0.99934100 -1.46279400
H 2.40027200 -1.69784900 -0.16716900
H -0.92626200 1.79820900 0.23278200
H 0.04820800 1.19133300 1.59413400
H 0.91569500 1.36874400 -1.34385700
H 1.59567800 2.27420200 0.03309900
H 0.59141200 -1.44688200 1.46344800
O 2.10241900 0.30605200 -0.00531200
N -0.64171500 -0.26116600 0.24372600
C -1.91943200 -0.48626700 -0.15211500
H -2.11482500 -1.56011100 -0.33128500
O -2.78176100 0.37385000 -0.30432300

23

C 1.28837900 -1.42795400 0.53199300
O 0.28860600 -0.74105400 0.95775300
O 2.04219700 -2.12223900 1.22371300
Fe -1.04993600 0.30887900 -0.16723900
H 1.46877100 -1.37541100 -0.56913800
H -2.12789800 1.12205200 -0.84977200
C -2.03491700 2.48860100 1.69308700
C -0.64294300 3.08020700 1.48087900
H -2.46011000 2.84601600 2.64361000
H -2.69737700 2.81058600 0.88719500
H -0.00802400 2.90269900 2.35288500
H -0.71473000 4.16608600 1.36031200
P 0.14461500 2.26568400 -0.00151100
N -2.02920100 0.99368100 1.68110100
C 1.95773200 2.04537700 0.44795900
C 2.64881400 3.14801300 1.26598000
C 2.78073100 1.66991400 -0.79561000
H 1.89365600 1.15497400 1.08379700
H 2.82935400 4.05659800 0.68568500
H 2.08365400 3.42736400 2.16030900
H 3.62513500 2.77962700 1.60457200
H 2.30180000 0.88001700 -1.38253100
H 2.93182300 2.53269700 -1.45405600
H 3.76844800 1.30089600 -0.49627200
C 0.05352400 3.52734900 -1.39894200
C 0.85760200 4.81528100 -1.16551700

C -1.40091000 3.86970500 -1.75960000
H 0.49450500 2.99585400 -2.25222100
H 1.93084800 4.62868600 -1.09886000
H 0.69652100 5.50463800 -2.00338100
H 0.54144500 5.33434500 -0.25358100
H -1.99697500 2.97652200 -1.95770900
H -1.89034700 4.43655500 -0.95880500
H -1.41704800 4.49836700 -2.65786800
C -1.37153400 0.50031900 2.91627100
H -1.90587800 0.86954600 3.80417700
H -1.35223900 -0.58688600 2.92655800
H -0.33604300 0.83144600 2.95111400
P -2.56377800 -1.41807400 -0.07582500
C -3.45224200 0.53534700 1.66716500
C -3.58214200 -0.96594400 1.41845000
H -3.95446700 1.08257900 0.86717000
H -3.93456000 0.80759100 2.61860700
H -3.21345600 -1.53644400 2.27489900
H -4.63618400 -1.23324100 1.29138400
C -0.51289100 -0.05310100 -1.77655300
O -0.23766000 -0.23232000 -2.89589600
C -1.82817300 -3.10293300 0.31928700
C -1.18378600 -3.72137700 -0.93138000
C -2.70648100 -4.11974900 1.06551300
H -1.01642600 -2.80699500 0.99338000
H -0.50696900 -3.02263700 -1.43257000
H -0.59668700 -4.60376400 -0.65114500
H -1.93547700 -4.04493300 -1.65960800
H -3.16179700 -3.70006400 1.96768600
H -3.50764400 -4.52603700 0.44320000
H -2.08247100 -4.96408000 1.38421700
C -3.78278300 -1.63433600 -1.49738600
C -4.57649900 -0.34466900 -1.76465500
C -4.74538900 -2.82531700 -1.36761400
H -3.13207200 -1.80926100 -2.36434500
H -3.92321600 0.52087000 -1.89439300
H -5.16917500 -0.46589100 -2.67902000
H -5.27764400 -0.12761000 -0.95019700
H -4.22514600 -3.78494500 -1.37888900
H -5.34441400 -2.76884100 -0.45140000
H -5.44510800 -2.82291000 -2.21233800
C 6.80299900 -2.56089500 -0.88071300
C 6.37397000 -2.74999000 0.60175400
C 5.58459200 -1.45549400 0.94335000

C 6.16074300 -1.21177300 -1.29104700
H 7.89391700 -2.50209200 -0.96234300
H 6.47437700 -3.38392400 -1.52336100
H 7.25134000 -2.85629500 1.24864300
H 5.75721500 -3.64290200 0.74520500
H 4.50665900 -1.63490000 0.85380800
H 5.77542400 -1.08783000 1.95623100
H 5.17288700 -1.38604500 -1.73642800
H 6.75571800 -0.64603400 -2.01448100
N 5.97713900 -0.43581500 -0.05142100
H 6.89079600 -0.07129800 0.21993600

TS23_24

C 1.24756500 -2.08696200 -0.25976200
O 1.03390900 -0.87598000 0.02695000
O 0.71376500 -3.14341600 0.07169400
Fe -0.55390900 0.50833800 -0.17413400
H 1.23512800 -2.05469700 -2.25336100
H -1.55678200 1.61503000 -0.21813300
C -0.24957600 2.08099900 2.41612800
C 1.08144200 2.49783300 1.78968100
H -0.18647600 2.12899000 3.51412500
H -1.03219300 2.77288800 2.09958500
H 1.90639300 1.90646800 2.19751200
H 1.29390300 3.54479900 2.03123600
P 1.00469600 2.19322600 -0.04701100
N -0.68467000 0.71062800 2.00298000
C 2.75920200 1.73850200 -0.54175400
C 3.92037000 2.49455500 0.12373300
C 2.90637900 1.69334200 -2.07106300
H 2.77993600 0.70234700 -0.18660500
H 4.03058300 3.51437300 -0.25206300
H 3.82043400 2.54687600 1.21223200
H 4.86039700 1.96940900 -0.08947100
H 2.14195800 1.06225300 -2.53309400
H 2.84716900 2.68976800 -2.52191800
H 3.88395000 1.27454000 -2.33927400
C 0.59479000 3.85534800 -0.83973000
C 1.70407700 4.91554200 -0.75634300
C -0.72310800 4.44072900 -0.30525900
H 0.43932100 3.59696000 -1.89548600
H 2.59892800 4.63182500 -1.31317800
H 1.34083700 5.85787800 -1.18463900
H 1.99472600 5.12083500 0.28025000

H -1.54876900 3.72933000 -0.37384700
H -0.62741500 4.76022700 0.73910000
H -0.99095800 5.32793000 -0.89111800
C 0.15190300 -0.29564300 2.70203000
H 0.01818000 -0.21095100 3.79076400
H -0.11484100 -1.29912700 2.37646300
H 1.20002000 -0.14726100 2.45273700
P -2.45338300 -0.79334400 0.02956600
C -2.10840100 0.54413700 2.43280200
C -2.75717900 -0.71801500 1.86715100
H -2.65217400 1.42271700 2.08112600
H -2.15714800 0.53822800 3.53274300
H -2.32279100 -1.61614400 2.31560000
H -3.82436200 -0.72605400 2.11283300
C -0.64306400 0.54683100 -1.91337900
O -0.79401500 0.67786900 -3.05972600
C -2.37238200 -2.62664700 -0.36098700
C -2.30892300 -2.86765500 -1.87780700
C -3.37545700 -3.56151900 0.33579000
H -1.37385300 -2.86300500 0.02423600
H -1.47199700 -2.32783400 -2.33110100
H -2.14571000 -3.93483400 -2.07121300
H -3.23354900 -2.58021000 -2.39098500
H -3.45756000 -3.36775700 1.41020900
H -4.37964500 -3.51103100 -0.09150100
H -3.02832100 -4.59660900 0.22331500
C -4.01232500 -0.09290200 -0.78561400
C -4.39693300 1.28993100 -0.23365700
C -5.24613300 -1.00858400 -0.75393000
H -3.70900600 0.03708800 -1.83278900
H -3.56582600 1.99717400 -0.26590300
H -5.21730500 1.70353400 -0.83225000
H -4.75420300 1.22237500 0.80053300
H -5.09359600 -1.93988900 -1.30108800
H -5.54592700 -1.25582700 0.27064700
H -6.09214600 -0.49070800 -1.22267300
C 4.06604000 -4.28186900 0.18243300
C 4.74329900 -3.09001600 0.87260200
C 3.64711300 -2.02299600 0.83870200
C 3.29064400 -3.62813900 -0.96547600
H 4.77266400 -5.03310800 -0.17986400
H 3.37125500 -4.77240000 0.87277800
H 5.61615900 -2.76035500 0.29736700
H 5.07149300 -3.30422600 1.89384500

H 2.94186200 -2.16264000 1.66101600
H 4.01313200 -0.99632600 0.85756600
H 2.37968500 -4.15229100 -1.24671500
H 3.91934500 -3.48805700 -1.84684400
N 2.89566300 -2.26867700 -0.45088600
H 3.11473900 -1.55977500 -1.14728500

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C -0.53294300 2.30002900 0.45130900
O -0.76255300 1.12912300 -0.03159500
O 0.41936800 2.64838500 1.19566900
Fe 0.31767700 -0.67349900 -0.19155000
H 0.24932000 4.22514400 -2.64641600
H 0.97445000 -2.01865700 -0.29135100
C -0.13822600 -2.33666200 2.28427300
C -1.57001400 -2.46843500 1.76716500
H -0.11262000 -2.50796400 3.37195300
H 0.49496000 -3.08864400 1.80964100
H -2.25676700 -1.86441100 2.36506900
H -1.90334000 -3.50677700 1.86107900
P -1.63179700 -1.88408800 -0.00537800
N 0.45874800 -1.00123100 1.97654100
C -3.21914300 -0.88830800 -0.16667100
C -4.45503900 -1.34639600 0.62251500
C -3.55391100 -0.64140100 -1.64684000
H -2.88063100 0.06914400 0.24595900
H -4.90831900 -2.25290600 0.21306000
H -4.23803200 -1.53040100 1.67896200
H -5.21711100 -0.55745600 0.58459900
H -2.69520600 -0.24600400 -2.19735700
H -3.89084300 -1.55412900 -2.15052200
H -4.36570600 0.09104400 -1.72837700
C -1.83750400 -3.44149900 -1.04754600
C -3.15141700 -4.20665500 -0.82357600
C -0.64099300 -4.39507500 -0.89434500
H -1.83019600 -3.06423400 -2.07841000
H -4.02992200 -3.62219600 -1.10369900
H -3.15583100 -5.11570600 -1.43771800
H -3.26918900 -4.52132700 0.21966200
H 0.30804900 -3.90159900 -1.11388300
H -0.58371100 -4.81124200 0.11851200
H -0.75762700 -5.23801000 -1.58582300
C -0.25519300 0.04056000 2.75484400
H -0.23921600 -0.20859600 3.82706900

H 0.20483200 1.01125600 2.57945100
H -1.28844500 0.11302800 2.41826900
P 2.47523500 0.11341300 -0.04535100
C 1.89173100 -1.02903000 2.40352200
C 2.72046700 0.10562300 1.79729000
H 2.30104100 -1.99097300 2.09094700
H 1.94413100 -0.99114600 3.50237600
H 2.36822600 1.07744600 2.15380000
H 3.76976600 -0.00316100 2.09275600
C 0.30639800 -0.67957800 -1.92572800
O 0.32880200 -0.76075900 -3.08891900
C 2.85126600 1.87158000 -0.59419400
C 2.87774400 1.99339500 -2.12553900
C 4.04680400 2.58212100 0.06295000
H 1.95241400 2.37259200 -0.22142400
H 1.97455200 1.57805400 -2.58245800
H 2.93319200 3.05041500 -2.41202900
H 3.74268700 1.49143300 -2.57302000
H 4.03350900 2.49064000 1.15344000
H 5.01501800 2.22324500 -0.29407200
H 3.99326500 3.65382200 -0.16810500
C 3.81488200 -1.00195400 -0.78629300
C 3.83755400 -2.40906300 -0.16559800
C 5.24109400 -0.42840400 -0.77468900
H 3.49227600 -1.10705800 -1.83103700
H 2.84779400 -2.86942800 -0.14285900
H 4.49840500 -3.05498200 -0.75628300
H 4.23600600 -2.38812700 0.85525900
H 5.34194000 0.46739300 -1.38923700
H 5.57267300 -0.18630000 0.24116600
H 5.93765500 -1.17624800 -1.17401600
C -2.89667200 5.11299700 0.49430800
C -3.31380000 4.40808700 -0.80709600
C -2.68494900 3.01501800 -0.65968900
C -1.46669500 4.59946800 0.73244600
H -2.94706800 6.20417300 0.43314100
H -3.55018700 4.79411400 1.31542300
H -2.88006100 4.92533000 -1.67111600
H -4.39769900 4.36599300 -0.95099200
H -3.35858300 2.34062700 -0.10852400
H -2.46614200 2.54153500 -1.62118600
H -1.20995100 4.51740200 1.79290200
H -0.72374400 5.26707900 0.27173500
N -1.45762100 3.27940700 0.09224100

H -0.06264600 3.95813100 -2.02468400

A3(HCOOH)

Fe -0.13896200 -0.45170300 0.19406600
H -0.30415000 -1.81813500 -0.53400300
C 1.14369600 0.00922600 -2.51381100
C 2.40705500 0.20263100 -1.67671500
H 1.21326400 0.58172900 -3.45046900
H 1.00404500 -1.04424900 -2.77040500
H 2.59067800 1.27354800 -1.53838100
H 3.28262000 -0.21629900 -2.18264000
P 2.12045300 -0.54049800 0.01171300
N -0.04420500 0.43548000 -1.73602700
C 3.07645500 0.59527700 1.17824400
C 4.45522500 1.10734900 0.73103300
C 3.12253100 0.01736600 2.60074400
H 2.39853500 1.45713000 1.19698800
H 4.44857400 1.49338500 -0.29263500
H 4.75906700 1.93480000 1.38486800
H 5.23240200 0.34282600 0.79743800
H 2.12619400 -0.25512700 2.96043800
H 3.75979700 -0.87200900 2.65972500
H 3.53526100 0.75967000 3.29470500
C 3.00069100 -2.21327800 0.00298400
C 4.53435600 -2.16764000 -0.07066800
C 2.44837800 -3.12207000 -1.10733800
H 2.71216800 -2.65336400 0.96684100
H 4.98159700 -1.71847200 0.81812700
H 4.92811100 -3.18855100 -0.15189600
H 4.88557700 -1.61385500 -0.94891200
H 1.35994500 -3.20227100 -1.06406000
H 2.72677200 -2.75351600 -2.10179900
H 2.87211500 -4.12808400 -1.00334800
P -2.36580300 -0.09960500 0.00476500
C -1.29395800 0.27597100 -2.51675100
C -2.49292600 0.70904400 -1.67423900
H -1.37412100 -0.77870300 -2.79284100
H -1.24489100 0.86610900 -3.44381300
H -2.45680700 1.79356200 -1.51994100
H -3.43391700 0.48506300 -2.18692000
C -0.20648200 -1.26872400 1.71500400
O -0.24952300 -1.86649100 2.72082300
C -3.10242500 1.18119200 1.18009500
C -3.24317200 0.61363000 2.60140400

C	-4.36935300	1.93263400	0.74062300	H	2.42960400	1.14879800	2.61714600
H	-2.28266900	1.90978800	1.20240800	H	4.04592500	0.43916900	2.49145900
H	-2.31243200	0.15561700	2.94933700	H	3.84383500	2.19075900	2.42179800
H	-3.50091100	1.41702000	3.30210600	C	3.08837200	-1.84302200	0.66278500
H	-4.03592700	-0.13965900	2.66429700	C	4.62186500	-1.86444900	0.56790900
H	-4.29057800	2.32826400	-0.27653100	C	2.51635700	-3.11117000	0.00759000
H	-5.26807800	1.31443200	0.79262300	H	2.80477100	-1.85895900	1.72373600
H	-4.52687500	2.78893500	1.40878300	H	5.09447400	-1.09392500	1.17967600
C	-3.53940400	-1.58285600	-0.03761000	H	4.99390100	-2.83395400	0.92204900
C	-3.21051800	-2.51265700	-1.21728800	H	4.96788100	-1.74364100	-0.46488600
C	-5.04278500	-1.26677200	-0.03037600	H	1.42585200	-3.14127700	0.05648800
H	-3.29279500	-2.12025800	0.88809500	H	2.81869200	-3.18874800	-1.04322400
H	-2.15161800	-2.77894500	-1.24555600	H	2.90709900	-3.99631400	0.52359000
H	-3.79285300	-3.43761900	-1.12896400	P	-2.28894000	-0.17866500	0.04037400
H	-3.47803600	-2.05133900	-2.17519800	C	-1.27937000	-0.70362300	-2.46931000
H	-5.36658200	-0.78351300	0.89346100	C	-2.48729100	-0.04224700	-1.80559700
H	-5.32933000	-0.62536800	-0.87142800	H	-1.30921600	-1.78946200	-2.34554800
H	-5.61203800	-2.19997600	-0.12538500	H	-1.27807900	-0.49107600	-3.54846500
H	0.01099800	0.99753900	0.80636700	H	-2.48792500	1.02515100	-2.05033200
H	0.06589400	1.43448400	-1.54749400	H	-3.42480000	-0.47245000	-2.17155300
C	0.84225600	3.80065800	-0.26680400	C	-0.00888700	-0.10074800	1.97192800
O	0.69984300	3.45181000	-1.41742700	O	0.00324600	-0.14071300	3.14096800
H	0.05072600	3.73965300	0.49562900	C	-3.22282500	1.29526400	0.76000100
O	2.00129400	4.31519800	0.16960800	C	-3.46350500	1.12828600	2.26994200
H	1.92234500	4.53320800	1.11446000	C	-4.49248000	1.75677600	0.02689600
ATS3_4(HCOOH)							
Fe	-0.02245800	-0.13321900	0.24200700	H	-2.47759600	2.09036200	0.64453300
H	-0.04101700	-1.64944500	0.29257300	H	-2.54859500	0.85679600	2.80505900
C	1.16230300	-0.85237300	-2.46130300	H	-3.82407600	2.07333800	2.69327800
C	2.44055300	-0.29867700	-1.83319600	H	-4.21901300	0.36589200	2.48536700
H	1.17039700	-0.68170600	-3.54796900	H	-4.32138400	1.90793800	-1.04293400
H	1.08002200	-1.92992200	-2.29451700	H	-5.32371200	1.05680200	0.14039700
H	2.58083400	0.74043900	-2.14965000	H	-4.81877300	2.71908500	0.44139300
H	3.31928500	-0.86254400	-2.16206300	C	-3.24855500	-1.72219000	0.55744900
P	2.24117000	-0.28219100	0.01886500	C	-2.69038500	-2.99404700	-0.10136900
N	-0.02526500	-0.20695400	-1.85182800	C	-4.76951600	-1.65722600	0.34162900
C	3.25667900	1.19893800	0.58406000	H	-3.05099300	-1.79207000	1.63539300
C	4.60243100	1.45610900	-0.11500100	H	-1.61044400	-3.08555300	0.03264500
C	3.39738800	1.23718200	2.11453700	H	-3.16694900	-3.87484100	0.34530200
H	2.58621000	2.01595100	0.29440000	H	-2.90840600	-3.01708100	-1.17509900
H	4.51214100	1.45826900	-1.20545100	H	-5.25211100	-0.88942600	0.94884000
H	4.97185200	2.44699000	0.17822500	H	-5.02327400	-1.47286600	-0.70843500
H	5.37109900	0.72984100	0.15861400	H	-5.21776300	-2.61903600	0.61997500
				H	-0.01682300	1.50817500	0.02399000
				H	0.02082100	0.80707900	-2.06442600

C -0.10153500 2.84171900 -0.81237100
O -0.13977800 2.56159100 -2.02576300
H -1.01122900 3.14893200 -0.26822600
O 1.01760400 3.52119100 -0.34648200
H 0.88664500 3.69618000 0.59962200

A4(HCOOH)

Fe -0.02359100 -0.09033400 0.23265200
H -0.04196100 -1.56694800 0.41033500
C 1.16750500 -0.85973100 -2.44901900
C 2.44367100 -0.29367800 -1.82749300
H 1.16732300 -0.67858500 -3.53400700
H 1.10613900 -1.94151300 -2.29700500
H 2.57258700 0.74576100 -2.14653300
H 3.32669100 -0.85194600 -2.15429500
P 2.24721300 -0.26551800 0.02183500
N -0.02684700 -0.23391300 -1.83191600
C 3.27323300 1.20489300 0.58704600
C 4.62257800 1.43692900 -0.11348200
C 3.41456400 1.24481600 2.11726700
H 2.61319400 2.02952500 0.29014100
H 4.53005300 1.44184600 -1.20362200
H 5.00974700 2.42067000 0.18025600
H 5.37765800 0.69595000 0.15917000
H 2.44693700 1.16789900 2.62212900
H 4.05554700 0.44172200 2.49634000
H 3.87030400 2.19500700 2.42093600
C 3.04934000 -1.83976800 0.68252700
C 4.58200000 -1.89390600 0.58985300
C 2.44833500 -3.09769500 0.03324200
H 2.76276100 -1.84035800 1.74264000
H 5.06894500 -1.13046900 1.19923400
H 4.93277900 -2.86953500 0.94839500
H 4.93138100 -1.78367800 -0.44281700
H 1.35689100 -3.10331500 0.07862800
H 2.75160500 -3.18939600 -1.01585600
H 2.81536700 -3.98846300 0.55663300
P -2.30099100 -0.16656800 0.03400200
C -1.26982700 -0.76140700 -2.44720300
C -2.49090600 -0.09451800 -1.81357400
H -1.29389500 -1.84577200 -2.30488200
H -1.26074500 -0.57016900 -3.53039000
H -2.49213300 0.96555700 -2.08742100
H -3.42247100 -0.54305500 -2.17218700

C -0.01597800 0.01252300 1.96471000
O -0.01159500 -0.00335300 3.13226800
C -3.23928000 1.32355500 0.70763300
C -3.48503800 1.20193300 2.22108400
C -4.51070800 1.74887900 -0.04458800
H -2.50048600 2.12140000 0.56604100
H -2.57125400 0.95600700 2.77013400
H -3.85499600 2.15745200 2.61109500
H -4.23560200 0.44071100 2.45704900
H -4.33228000 1.88360400 -1.11526400
H -5.33039400 1.03592400 0.07479900
H -4.85678600 2.71277500 0.34921200
C -3.21607400 -1.70741100 0.61965900
C -2.61958800 -2.99222200 0.02163500
C -4.73671500 -1.69356900 0.39524600
H -3.02200000 -1.72074200 1.70045100
H -1.53852600 -3.05032200 0.16678600
H -3.07636800 -3.86392900 0.50494300
H -2.82897900 -3.06827800 -1.05114900
H -5.24053700 -0.89154900 0.93752400
H -4.98946000 -1.60039700 -0.66709700
H -5.16293800 -2.64137600 0.74648300
H -0.01989300 1.65707600 -0.11094500
H -0.00785600 0.80673500 -2.06381100
C -0.09711400 2.67247300 -0.80959300
O -0.15478700 2.40330700 -2.06668100
H -0.98809200 3.16628000 -0.35477700
O 1.05744700 3.44795900 -0.42899400
H 0.93119500 3.70939300 0.49717700

A5(HCOOH)

Fe -0.04809700 0.12347800 -0.18263300
H -0.07793600 1.55694000 -0.70431700
C 1.15333100 1.55913500 2.23107600
C 2.40852800 0.80393800 1.79966000
H 1.14497200 1.69069600 3.32297400
H 1.12470900 2.55393400 1.77818800
H 2.49879000 -0.11828900 2.38350600
H 3.30604800 1.40052500 1.99156800
P 2.23758900 0.29992400 0.01265600
N -0.06261500 0.83807900 1.79077700
C 3.24102000 -1.28593400 -0.11874800
C 4.55979300 -1.36017500 0.67085400
C 3.44102000 -1.70328900 -1.58556600

H 2.55912000 -2.00932400 0.34283700
H 4.43192200 -1.08780900 1.72273100
H 4.92734700 -2.39424300 0.65131400
H 5.34698800 -0.72880800 0.25218000
H 2.50183700 -1.70410700 -2.14662300
H 4.14485600 -1.04821400 -2.11045000
H 3.84953800 -2.72025500 -1.62833300
C 3.12506400 1.62024400 -1.00563600
C 4.65408300 1.67038800 -0.85717400
C 2.53839800 3.02053100 -0.76033400
H 2.88643800 1.33455900 -2.03924100
H 5.14282800 0.76375000 -1.21802700
H 5.04968300 2.50824800 -1.44479000
H 4.95797300 1.83250500 0.18310300
H 1.45239200 3.03812400 -0.87681600
H 2.78536400 3.38628600 0.24307600
H 2.97011800 3.72810000 -1.47825500
P -2.33827700 0.19070300 0.02570800
C -1.29210500 1.55074000 2.20574600
C -2.52962800 0.75633800 1.79413400
H -1.28033200 2.53110800 1.72110800
H -1.29086600 1.71644900 3.29309200
H -2.60622100 -0.14340200 2.41391700
H -3.44065400 1.34133700 1.95566200
C -0.03655900 -0.35279100 -1.85078900
O -0.03098400 -0.58377300 -2.99605800
C -3.17414500 -1.49208100 0.00280700
C -3.29428700 -2.03864100 -1.42817000
C -4.48844500 -1.66397900 0.78120800
H -2.39845100 -2.06847100 0.51965400
H -2.34389500 -1.98825300 -1.96758000
H -3.60454200 -3.09016700 -1.40186600
H -4.04400000 -1.49282400 -2.01242200
H -4.43571100 -1.25432800 1.79417900
H -5.34192300 -1.20479800 0.27604800
H -4.70817000 -2.73482600 0.87844100
C -3.34611900 1.38339800 -1.02781000
C -2.86071600 2.83207500 -0.85021100
C -4.86856100 1.31099500 -0.83977700
H -3.10752400 1.07599500 -2.05498700
H -1.78308900 2.92626900 -1.00424600
H -3.36696100 3.47933900 -1.57626600
H -3.10145700 3.21353500 0.14872500
H -5.28011000 0.34676200 -1.14459900

H -5.15908000 1.49498900 0.20081000
H -5.35171100 2.08122800 -1.45377200
H 0.54194200 -2.83227600 -0.69712700
H -0.06160500 -0.09981100 2.20679800
C 0.13169700 -2.85411500 0.33646200
O -0.07694800 -1.63122100 0.85589200
H -0.79480600 -3.47971100 0.30051100
O 1.08260900 -3.57519800 1.17167800
H 1.18368300 -4.45628900 0.77837800

Fe-3(HCOOH)

Fe 0.00035100 -0.29816900 -0.17370400
H -0.00073200 1.16206100 0.43792500
H 0.00142200 -1.77173300 -0.61670200
C -1.20888100 -1.94698100 2.04687800
C -2.49857100 -1.22065600 1.66571900
H -1.25919800 -2.29311900 3.09084800
H -1.07584800 -2.82120600 1.40719200
H -2.74194800 -0.44985700 2.40168900
H -3.33542700 -1.92646300 1.66174000
P -2.26230000 -0.40958000 0.00124300
N 0.00044400 -1.08780700 1.86380400
C -3.16246800 1.24782600 0.12217300
C -4.47964700 1.30822800 0.91256000
C -3.31072100 1.88934000 -1.26707400
H -2.42181500 1.83778400 0.67606500
H -4.39322100 0.86688400 1.90998500
H -4.76636200 2.35841200 1.04967300
H -5.30506000 0.81262700 0.39674900
H -2.36771000 1.89653400 -1.82096600
H -4.05886000 1.37020100 -1.87577300
H -3.63893500 2.93038800 -1.16423400
C -3.22722500 -1.47060600 -1.22755400
C -4.75032200 -1.49905500 -1.02796000
C -2.68297500 -2.90730300 -1.28288600
H -3.01217600 -0.99496900 -2.19360200
H -5.21382100 -0.52333100 -1.18427000
H -5.20013700 -2.19175000 -1.74994500
H -5.02324700 -1.85295500 -0.02715600
H -1.60603200 -2.92979400 -1.46181900
H -2.88738200 -3.45077300 -0.35254000
H -3.17936600 -3.45405500 -2.09342600
C -0.00002500 -0.02849600 2.90499100
H 0.00021600 -0.47498200 3.91091100

H 0.87710600 0.60730300 2.79610300
 H -0.87779300 0.60644700 2.79618300
 P 2.26309200 -0.40799900 0.00126600
 C 1.21038700 -1.94606700 2.04698600
 C 2.49966300 -1.21892300 1.66584900
 H 1.07795900 -2.82041400 1.40734100
 H 1.26087000 -2.29212200 3.09097500
 H 2.74241500 -0.44789600 2.40181600
 H 3.33697300 -1.92418400 1.66200700
 C -0.00016000 0.14167200 -1.84819400
 O -0.00058500 0.37820500 -2.99235900
 C 3.16263900 1.24952100 0.12235800
 C 3.31004800 1.89136700 -1.26680400
 C 4.48009400 1.31039200 0.91231400
 H 2.42211100 1.83883800 0.67669400
 H 2.36675700 1.89836200 -1.82024200
 H 3.63809400 2.93246700 -1.16399700
 H 4.05799000 1.37245600 -1.87594300
 H 4.39456900 0.86780600 1.90926200
 H 5.30581300 0.81630000 0.39555000
 H 4.76567500 2.36073700 1.05052700
 C 3.22848600 -1.46854800 -1.22759400
 C 2.68518600 -2.90561200 -1.28268400
 C 4.75161800 -1.49597500 -1.02823800
 H 3.01294400 -0.99311000 -2.19363200
 H 1.60820000 -2.92882900 -1.46128700
 H 3.18169600 -3.45203800 -2.09337300
 H 2.89026100 -3.44893200 -0.35239700
 H 5.21446300 -0.51995800 -1.18469800
 H 5.02490800 -1.84958300 -0.02743100
 H 5.20179600 -2.18846000 -1.75019800
 H -0.00111000 2.37944200 -0.25528500
 C -0.00325300 4.14619500 0.49527600
 H -0.00253400 3.60589300 1.46154200
 O -0.00492300 5.35677600 0.42504300
 O -0.00210200 3.34656800 -0.56474900

Fe-TS3_4(HCOOH)

Fe 0.04348200 -0.10312900 -0.17814800
 H -0.07364600 1.49912900 0.27229300
 H 0.09044700 -1.58178100 -0.50154600
 C -1.14736400 -1.55831400 2.18910600
 C -2.44438400 -0.90499200 1.71763300
 H -1.19658900 -1.77239300 3.26772700

H -0.99938200 -2.50551000 1.66681800
 H -2.68557400 -0.03086200 2.32866200
 H -3.27670000 -1.60814500 1.82711000
 P -2.22439100 -0.34358800 -0.04585700
 N 0.05318000 -0.71257100 1.90799700
 C -3.25896300 1.21537800 -0.20137200
 C -4.61289800 1.25264000 0.52877700
 C -3.39921100 1.64856200 -1.67029500
 H -2.60686300 1.94703000 0.29594500
 H -4.53239200 0.95304300 1.57829400
 H -4.98979900 2.28331900 0.51984100
 H -5.37423100 0.62545800 0.05830000
 H -2.43197400 1.69854500 -2.17771700
 H -4.04997000 0.97868200 -2.24338800
 H -3.84133200 2.65096900 -1.71599900
 C -3.02736300 -1.67859200 -1.11664200
 C -4.56043000 -1.75304800 -1.03594900
 C -2.43042300 -3.06927800 -0.84747400
 H -2.74782600 -1.38460100 -2.13740200
 H -5.04616900 -0.85172900 -1.41331200
 H -4.91681300 -2.59375800 -1.64415500
 H -4.90722300 -1.92532100 -0.01064300
 H -1.34030100 -3.06770400 -0.91071500
 H -2.71902100 -3.44261300 0.14213700
 H -2.81518100 -3.78175200 -1.58679300
 C 0.04150300 0.46234300 2.81622700
 H -0.05983400 0.13823000 3.86290500
 H 0.97326300 1.01857800 2.71550200
 H -0.76412800 1.14647400 2.55415000
 P 2.31372800 -0.22556500 -0.01308800
 C 1.26601700 -1.54221900 2.18551700
 C 2.55578300 -0.86619600 1.72199000
 H 1.13373200 -2.48602100 1.65266500
 H 1.31819500 -1.76584100 3.26213500
 H 2.80874000 -0.02366600 2.37125200
 H 3.39042100 -1.57157400 1.78663500
 C 0.04876600 0.23431000 -1.87458900
 O 0.05921500 0.40314000 -3.03041000
 C 3.27297900 1.39881700 -0.05917700
 C 3.40015600 1.93502400 -1.49517400
 C 4.61615700 1.47288900 0.68614400
 H 2.57893300 2.06092900 0.47388100
 H 2.44433900 1.93068400 -2.02911000
 H 3.76468300 2.96879700 -1.47545100

H 4.11192700 1.34990600 -2.08695400
H 4.54820100 1.10297100 1.71330500
H 5.40926400 0.91770400 0.18093700
H 4.93662000 2.52078500 0.74123500
C 3.21508600 -1.44186900 -1.14319600
C 2.67685700 -2.87272100 -0.97785200
C 4.74665900 -1.45321400 -1.01955200
H 2.94922900 -1.09843500 -2.15175700
H 1.59227500 -2.92029200 -1.09184100
H 3.13091000 -3.52110400 -1.73638200
H 2.94023400 -3.28676800 0.00242000
H 5.20210900 -0.51006700 -1.32621700
H 5.07087200 -1.67634800 0.00324800
H 5.15742600 -2.23712300 -1.66765500
H 0.51843100 3.18295700 -1.18525600
C -0.19361400 2.88683200 0.59004400
H 0.84044900 2.97203000 0.99180700
O -1.16351900 3.09143800 1.35099000
O -0.26700500 3.46863500 -0.69331500

Fe-4(HCOOH)

Fe 0.04345500 -0.09372900 -0.17111700
H -0.07441300 1.54009900 0.29379400
H 0.08951300 -1.55946500 -0.51165000
C -1.14626200 -1.56794700 2.17829300
C -2.44483000 -0.91178900 1.71538500
H -1.19295900 -1.79175900 3.25489100
H -0.99744500 -2.51014100 1.64714800
H -2.68523600 -0.04297800 2.33424900
H -3.27636600 -1.61650100 1.82019800
P -2.22879800 -0.33475000 -0.04289100
N 0.05304300 -0.71754500 1.90378600
C -3.26166500 1.22400600 -0.18819500
C -4.61532200 1.25328500 0.54275700
C -3.40237400 1.66649700 -1.65422700
H -2.60836200 1.95269900 0.31529800
H -4.53353800 0.94736600 1.59037900
H -4.99401000 2.28333100 0.54076600
H -5.37614700 0.62769000 0.06903800
H -2.43462600 1.72447500 -2.15985000
H -4.05080800 0.99933900 -2.23329900
H -3.84736200 2.66796200 -1.69228700
C -3.02218700 -1.66458500 -1.12581000
C -4.55503700 -1.74497800 -1.04713200

C -2.41971000 -3.05484000 -0.86696500
H -2.74306400 -1.36117200 -2.14382900
H -5.04299600 -0.84146300 -1.41629300
H -4.90790200 -2.58094200 -1.66381300
H -4.90214100 -1.92813700 -0.02384000
H -1.32956000 -3.04918500 -0.93053700
H -2.70672600 -3.43640600 0.11985300
H -2.80176100 -3.76328800 -1.61147000
C 0.03613800 0.45382300 2.81785800
H -0.08818300 0.12497200 3.86033200
H 0.97678000 0.99880400 2.73886700
H -0.75596400 1.15027800 2.54358200
P 2.31614100 -0.21990000 -0.01065300
C 1.26712900 -1.54653500 2.18036700
C 2.55725300 -0.86803700 1.72107400
H 1.13676200 -2.48918000 1.64484700
H 1.31741600 -1.77322400 3.25622400
H 2.81056000 -0.02883000 2.37419400
H 3.39176100 -1.57387000 1.78217600
C 0.04589400 0.23968500 -1.87061200
O 0.05376300 0.39311400 -3.02759900
C 3.27028600 1.40641700 -0.06141300
C 3.41544000 1.92526300 -1.50230700
C 4.60196700 1.48968700 0.70255700
H 2.56861900 2.07494800 0.45313300
H 2.46729900 1.90910300 -2.04958600
H 3.77258500 2.96160000 -1.48888200
H 4.13949100 1.33835400 -2.07692700
H 4.51090900 1.15675800 1.74055300
H 5.39654600 0.90761500 0.23086600
H 4.93391000 2.53511100 0.72782700
C 3.21451900 -1.43311300 -1.14462200
C 2.66462200 -2.86111600 -0.99434900
C 4.74496900 -1.45522300 -1.00796000
H 2.95904000 -1.08004800 -2.15238700
H 1.58125000 -2.90103600 -1.12265300
H 3.12369300 -3.50786900 -1.75121100
H 2.91228500 -3.28321700 -0.01348600
H 5.20901200 -0.51134700 -1.29907800
H 5.05865700 -1.69244700 0.01490900
H 5.15638400 -2.23397100 -1.66176800
H 0.53613100 3.15658700 -1.19359900
C -0.18635400 2.82472400 0.58522500
H 0.84228700 2.96987400 0.99871000

O -1.16698200 3.05480000 1.34403800
O -0.25421300 3.43429700 -0.70509500

Fe-5(HCOOH)

Fe 0.03847400 -0.11014000 -0.19121100
H -0.52146700 2.72570100 -1.20318700
H 0.06749800 -1.59616800 -0.54582900
C -1.14044100 -1.68205300 2.12314600
C -2.43677000 -0.98675500 1.70945900
H -1.18761400 -1.97604200 3.18355100
H -1.00469300 -2.58943800 1.53109500
H -2.66022000 -0.15217500 2.37914700
H -3.27546500 -1.68643300 1.78972200
P -2.24301300 -0.31850900 -0.02173000
N 0.06132100 -0.82635300 1.89520500
C -3.21790900 1.28866200 -0.06390600
C -4.50422100 1.37451300 0.77355000
C -3.46300000 1.74314800 -1.51341900
H -2.49187300 1.98414000 0.37194900
H -4.33840800 1.10895700 1.82196400
H -4.86997700 2.40935900 0.76117000
H -5.30855300 0.74149400 0.38987700
H -2.55464600 1.69592700 -2.12231100
H -4.23286700 1.14303000 -2.01092200
H -3.80682900 2.78446500 -1.51941800
C -3.15078900 -1.54228800 -1.13682500
C -4.66729700 -1.64475500 -0.90697800
C -2.52115500 -2.94362000 -1.08414000
H -2.98217900 -1.14112200 -2.14499900
H -5.18978800 -0.71048400 -1.12037300
H -5.08667200 -2.41116400 -1.57064400
H -4.90571400 -1.94172900 0.12065800
H -1.45005300 -2.91948400 -1.29527500
H -2.66507500 -3.41406000 -0.10401600
H -3.00443000 -3.58936200 -1.82728400
C 0.07153800 0.26697100 2.89687300
H 0.11805200 -0.15216300 3.91344600
H 0.91815700 0.92683600 2.72668000
H -0.81895000 0.88097900 2.79076000
P 2.32513100 -0.21279700 -0.01874500
C 1.27368200 -1.67606000 2.08654500
C 2.55876600 -0.95701800 1.67774800
H 1.13953200 -2.56721100 1.47018500
H 1.33575700 -1.99763100 3.13821000

H 2.79365300 -0.15576400 2.38294500
H 3.40067900 -1.65631100 1.70646000
C 0.03769600 0.17396500 -1.89600700
O 0.04130900 0.28070500 -3.05935000
C 3.16872800 1.46645900 0.05109200
C 3.33317600 2.05016300 -1.36217100
C 4.46482900 1.60111000 0.86524200
H 2.38048400 2.03575400 0.55854700
H 2.40742700 1.99270300 -1.94302500
H 3.61877900 3.10706700 -1.30035400
H 4.11850200 1.53475900 -1.92666500
H 4.36993300 1.20262800 1.87963300
H 5.31630400 1.10610100 0.39078200
H 4.71969300 2.66429700 0.96121100
C 3.31318900 -1.29894400 -1.20109500
C 2.77520700 -2.73877900 -1.23451600
C 4.83194700 -1.30861700 -0.96939100
H 3.11699900 -0.84709700 -2.18244700
H 1.70292300 -2.77063200 -1.43970300
H 3.29217900 -3.30437000 -2.01897400
H 2.95696800 -3.25910200 -0.28639100
H 5.28622700 -0.32940400 -1.13323300
H 5.08713000 -1.63946000 0.04378700
H 5.30552200 -2.00903300 -1.66850300
H -1.04970500 4.60567100 -0.04237200
C -0.09828600 2.88908500 -0.18584000
H 0.86726300 3.43757100 -0.32824900
O 0.03052200 1.77034800 0.54360900
O -0.99047900 3.81082100 0.51053900

Ru-3(HCOOH)

H 0.04590400 1.35244600 -0.52636000
H -0.01255000 -1.99562200 0.04116400
C -1.21684900 -0.78790500 2.53996800
C -2.50858800 -0.31093000 1.87018000
H -1.27334100 -0.61561200 3.62576700
H -1.09111500 -1.85900500 2.37454400
H -2.72807700 0.72462600 2.14446500
H -3.34862200 -0.91295900 2.23245500
P -2.36306500 -0.40023300 0.00689600
N 0.00793600 -0.11823600 1.99870300
C -3.30896700 1.11008000 -0.61007800
C -4.65292500 1.46149300 0.05102300
C -3.41960300 1.09224100 -2.14234900

H -2.60568800 1.90703600 -0.34373400
H -4.60620300 1.43918800 1.14429100
H -4.93094600 2.48307600 -0.23669100
H -5.46623100 0.80499900 -0.26532900
H -2.44478900 0.94051300 -2.61606700
H -4.09690200 0.30618000 -2.49369000
H -3.81562500 2.05022300 -2.49900000
C -3.32489000 -1.94030900 -0.51491000
C -4.85133200 -1.85355500 -0.36096000
C -2.80111200 -3.19924700 0.19442100
H -3.08755900 -2.03321900 -1.58274100
H -5.29709400 -1.11691200 -1.03172800
H -5.29706400 -2.82580500 -0.60411600
H -5.14537500 -1.60835400 0.66567700
H -1.72021100 -3.31283000 0.08908600
H -3.04436600 -3.18741400 1.26351600
H -3.28161300 -4.08535700 -0.23674400
C 0.02706100 1.29798200 2.44531400
H 0.00154500 1.35535300 3.54371300
H 0.92711200 1.79412000 2.08524700
H -0.82636300 1.83672100 2.03742300
P 2.36225200 -0.43363100 0.00001900
C 1.21579400 -0.82186200 2.53544200
C 2.51918500 -0.37736200 1.86471200
H 1.06125600 -1.88874400 2.36581300
H 1.27965500 -0.65555300 3.62182500
H 2.77710500 0.64409800 2.15612900
H 3.34004900 -1.01400400 2.21132900
C -0.00479300 -0.71310700 -2.11053100
O -0.00853600 -0.96480900 -3.25408700
C 3.30578100 1.08519800 -0.60389100
C 3.41972300 1.07738000 -2.13612300
C 4.64752500 1.43692000 0.06023900
H 2.59235800 1.87437800 -0.33498900
H 2.44737000 0.92185800 -2.61346500
H 3.81132400 2.03953800 -2.48655400
H 4.10300700 0.29775300 -2.48998400
H 4.59887800 1.41668100 1.15342500
H 5.46052300 0.77823300 -0.25260900
H 4.92925300 2.45708900 -0.22928200
C 3.31739800 -1.96562900 -0.55252300
C 2.77806600 -3.23735300 0.12143800
C 4.84277600 -1.89142700 -0.38270600
H 3.08847300 -2.03125100 -1.62418300

H 1.69876000 -3.34490700 -0.00419100
H 3.26292000 -4.11562400 -0.32073900
H 3.00322000 -3.24935800 1.19448100
H 5.29830200 -1.13830300 -1.02816400
H 5.12881500 -1.67704300 0.65316900
H 5.28596400 -2.85855300 -0.64969000
H -0.37389300 2.68134400 -0.36793900
C 0.37316500 4.40571800 0.07281200
H 1.34559700 3.88133600 0.01258500
O 0.27912300 5.57922200 0.35865300
O -0.67482000 3.63381400 -0.20323200
Ru 0.00118700 -0.37092100 -0.29846100

Ru-TS3_4(HCOOH)

H -0.07620400 1.59567300 0.30140600
H 0.11568900 -1.69639500 -0.68909500
C -1.14455400 -1.66479100 2.14637100
C -2.44480000 -0.98221700 1.72023300
H -1.19247500 -1.92984600 3.21370700
H -1.00548500 -2.58614700 1.57754900
H -2.66219000 -0.12529700 2.36372100
H -3.27909000 -1.68214600 1.83768800
P -2.31494400 -0.36545600 -0.04007800
N 0.06374800 -0.81678600 1.90681900
C -3.32590300 1.21484500 -0.08568900
C -4.64772200 1.24327600 0.70153200
C -3.52070800 1.70103400 -1.53148600
H -2.64161700 1.91746800 0.41097300
H -4.53013000 0.90002100 1.73401400
H -5.00703000 2.27892600 0.74906300
H -5.43706200 0.64710700 0.23713600
H -2.57779800 1.72930600 -2.08488300
H -4.22469700 1.07312400 -2.08889200
H -3.92467000 2.72018300 -1.52443000
C -3.18734900 -1.65611400 -1.10815500
C -4.71432100 -1.72116200 -0.94528500
C -2.58510800 -3.05736500 -0.91785200
H -2.95933800 -1.32846300 -2.13109300
H -5.21065300 -0.80574000 -1.27201300
H -5.11047200 -2.54198700 -1.55571800
H -5.00634000 -1.91840700 0.09238300
H -1.50046800 -3.06162500 -1.04920600
H -2.81527200 -3.46038200 0.07522200
H -3.01938800 -3.74369700 -1.65428500

C 0.05504600 0.33232100 2.84931500
 H -0.06987100 -0.02244900 3.88319200
 H 0.99852300 0.87332500 2.77974300
 H -0.73435200 1.03952200 2.59521500
 P 2.41569500 -0.23749000 -0.00573700
 C 1.28289400 -1.65187900 2.13966700
 C 2.57760300 -0.95371700 1.71600200
 H 1.15288200 -2.56948700 1.56208900
 H 1.33832300 -1.92649600 3.20433700
 H 2.82102700 -0.13744100 2.40136600
 H 3.40766800 -1.66542100 1.77394800
 C 0.04443800 0.35670000 -2.06425400
 O 0.04456500 0.62701400 -3.20341800
 C 3.32218500 1.41220500 0.09022600
 C 3.41761000 2.06249300 -1.29848100
 C 4.66593000 1.47481900 0.83608700
 H 2.60118200 1.99791800 0.67621900
 H 2.44880000 2.07955300 -1.80808900
 H 3.76556700 3.09804200 -1.20603400
 H 4.12734900 1.53537000 -1.94544100
 H 4.64066100 0.96046100 1.80146400
 H 5.48790500 1.05404500 0.25318500
 H 4.91335100 2.52459600 1.03640200
 C 3.38824600 -1.38705300 -1.14402800
 C 2.89554000 -2.83830500 -1.02217000
 C 4.91551400 -1.33688400 -0.98878300
 H 3.12765200 -1.02760800 -2.14808100
 H 1.81348500 -2.91861200 -1.14908800
 H 3.37528600 -3.45022400 -1.79490700
 H 3.16374100 -3.27158100 -0.05167800
 H 5.33073600 -0.36852000 -1.27402100
 H 5.23106000 -1.55839700 0.03696100
 H 5.37239800 -2.09184500 -1.64015300
 H 0.36368800 3.32267900 -1.13155300
 C -0.23249900 2.94878900 0.67275000
 H 0.81857700 3.07424800 1.02058400
 O -1.16814800 3.08532600 1.49207400
 O -0.39985800 3.57008900 -0.58713200
 Ru 0.05060900 -0.11393300 -0.27926400

Ru-4(HCOOH)

H -0.08585600 1.64112100 0.31834200
 H 0.11311600 -1.67129000 -0.69081500
 C -1.14564400 -1.65554300 2.15113800

C -2.44577600 -0.97391300 1.72389600
 H -1.19246500 -1.91648800 3.21943300
 H -1.00771100 -2.57953100 1.58621800
 H -2.66167000 -0.11434000 2.36430700
 H -3.28029300 -1.67300000 1.84456000
 P -2.31743800 -0.36167500 -0.03757000
 N 0.06355300 -0.80956300 1.90774600
 C -3.32717000 1.21723300 -0.08800900
 C -4.65071500 1.24385700 0.69631500
 C -3.51982800 1.70105300 -1.53477500
 H -2.64337600 1.92087600 0.41129000
 H -4.53450800 0.90282700 1.72969600
 H -5.01195600 2.27893600 0.74141000
 H -5.43821300 0.64535700 0.23148600
 H -2.57564400 1.73303600 -2.08576100
 H -4.22033000 1.07051800 -2.09385300
 H -3.92718200 2.71885200 -1.52922800
 C -3.17906300 -1.65767400 -1.10616700
 C -4.70590200 -1.73011700 -0.94521700
 C -2.56820900 -3.05494500 -0.91392000
 H -2.95171100 -1.32895000 -2.12889400
 H -5.20551200 -0.81659200 -1.27238400
 H -5.09742100 -2.55255500 -1.55642000
 H -4.99858300 -1.92869200 0.09198600
 H -1.48361800 -3.05336200 -1.04660400
 H -2.79458100 -3.45762200 0.08012300
 H -2.99875500 -3.74532100 -1.64871600
 C 0.05725100 0.34432800 2.84508400
 H -0.07520800 -0.00523700 3.87967500
 H 1.00552500 0.87754500 2.77850200
 H -0.72520400 1.05801700 2.58388300
 P 2.41759400 -0.23582700 -0.00399200
 C 1.28120000 -1.64690700 2.14190800
 C 2.57796300 -0.95352000 1.71691800
 H 1.14869000 -2.56568000 1.56652400
 H 1.33580900 -1.91954700 3.20702700
 H 2.82528900 -0.13850900 2.40225900
 H 3.40527700 -1.66851200 1.77355200
 C 0.04183400 0.35485400 -2.06441600
 O 0.04093700 0.61061500 -3.20612400
 C 3.32406600 1.41343100 0.08881400
 C 3.42870100 2.05589800 -1.30298500
 C 4.66397300 1.47671100 0.84130700
 H 2.60078100 2.00388900 0.66754000

H 2.46343700 2.07112700 -1.81926300
H 3.77594900 3.09185000 -1.21326000
H 4.14281600 1.52533700 -1.94225600
H 4.63065000 0.97259200 1.81177800
H 5.48684100 1.04567800 0.26709700
H 4.91539900 2.52723300 1.03223400
C 3.38337700 -1.38649500 -1.14490600
C 2.87677300 -2.83385100 -1.03402200
C 4.91015000 -1.34964700 -0.98104400
H 3.13086200 -1.01868100 -2.14795800
H 1.79547200 -2.90483700 -1.17304700
H 3.35917600 -3.44663100 -1.80437300
H 3.13054600 -3.27391700 -0.06273700
H 5.33422800 -0.38247000 -1.25709700
H 5.21828300 -1.58069800 0.04485900
H 5.36464300 -2.10352900 -1.63525400
H 0.38515300 3.31004100 -1.13550800
C -0.23252400 2.90298700 0.66666500
H 0.80937400 3.07690800 1.03706000
O -1.18622400 3.06111500 1.47759500
O -0.38285200 3.55712800 -0.59719700
Ru 0.04971900 -0.10530900 -0.27481600

Ru-5(HCOOH)

H 1.10461100 3.19433000 0.12414300
H 0.04989200 -1.45498700 -0.94134900
C -1.16744500 -2.07758100 1.78267800
C -2.45428400 -1.28095600 1.56454000
H -1.21209300 -2.60241200 2.74968800
H -1.05919700 -2.83099600 1.00008500
H -2.61904100 -0.58832100 2.39365200
H -3.30952300 -1.96445200 1.55371700
P -2.34937000 -0.28296900 -0.01263600
N 0.05588200 -1.22096100 1.74297100
C -3.33866700 1.28435000 0.31102300
C -4.53844900 1.18358000 1.26570900
C -3.73096400 1.97676000 -1.00478000
H -2.56881400 1.90555600 0.78448000
H -4.26412100 0.76943900 2.24026300
H -4.93643000 2.19022200 1.44671800
H -5.35554500 0.57954300 0.86118800
H -2.89946500 2.03771400 -1.71388100
H -4.55653500 1.46437300 -1.50953900
H -4.05837700 3.00159100 -0.79768400

C -3.28671200 -1.28280900 -1.31106600
C -4.78625600 -1.47339400 -1.03026900
C -2.62959000 -2.64685800 -1.57462300
H -3.17632100 -0.67721200 -2.22041800
H -5.33390400 -0.52998100 -0.99708200
H -5.23188900 -2.08084400 -1.82751700
H -4.96019500 -2.00228200 -0.08645900
H -1.56927800 -2.55317400 -1.81904600
H -2.72339100 -3.31202900 -0.70829200
H -3.13286500 -3.13823100 -2.41584000
C 0.09446100 -0.36759400 2.95490800
H 0.04765500 -0.99163500 3.85974400
H 1.00461800 0.22675600 2.96568100
H -0.72925400 0.34146800 2.93746800
P 2.39473200 -0.22285000 -0.02984700
C 1.25723100 -2.10963000 1.71419600
C 2.55696800 -1.34335200 1.46160800
H 1.09564800 -2.83828100 0.91692100
H 1.32757700 -2.65972200 2.66568500
H 2.81333300 -0.72651900 2.32628000
H 3.38051400 -2.05315200 1.33362800
C 0.01875200 0.74799400 -1.90797100
O 0.02527700 1.16857200 -3.00349800
C 3.32975000 1.34887200 0.42625400
C 3.60589800 2.20069700 -0.82460300
C 4.58659800 1.22128700 1.30227800
H 2.56012800 1.86126000 1.01569100
H 2.71905000 2.30858500 -1.45719200
H 3.92128600 3.20753100 -0.52673000
H 4.40876200 1.77556700 -1.43642500
H 4.40830300 0.64533400 2.21482600
H 5.42526200 0.76098600 0.77364800
H 4.90820100 2.22330800 1.61317200
C 3.36233700 -1.06731800 -1.41207900
C 2.74352200 -2.42009200 -1.79662500
C 4.86690300 -1.23325700 -1.14673800
H 3.23308800 -0.38707600 -2.26404800
H 1.68462100 -2.33014400 -2.04762600
H 3.26985200 -2.82694100 -2.66822000
H 2.84082400 -3.15357400 -0.98747900
H 5.38194500 -0.27724700 -1.03907900
H 5.05929600 -1.82949600 -0.24758500
H 5.33049300 -1.76022400 -1.98957100
H -0.97325100 2.91980000 -0.90565700

C 0.14416700 3.05106200 0.66825000
H 0.14043100 3.77289900 1.51189800
O -0.04457500 1.78806000 1.10050600
O -0.89902200 3.57534800 -0.19782500
Ru 0.02326700 -0.00022100 -0.22943200

Mn-3(HCOOH)

H -0.00348500 1.27053800 0.37658900
H -0.19802500 -1.79038900 -0.65148700
C -1.36445100 -1.77648100 2.09313700
C -2.60704400 -0.96218400 1.72381900
H -1.42394500 -2.09471600 3.14611000
H -1.31902500 -2.67494000 1.47433600
H -2.74410900 -0.12612600 2.41488700
H -3.49856800 -1.59213500 1.81239800
P -2.40933300 -0.27961300 -0.00060800
N -0.09051500 -1.02981500 1.86756000
C -3.20756200 1.42705200 0.04251700
C -4.51173200 1.59078200 0.83915000
C -3.32963800 2.00766300 -1.37604500
H -2.43048000 1.99820300 0.56477000
H -4.43782600 1.18560800 1.85283300
H -4.73788600 2.66010300 0.93442400
H -5.36732400 1.12056800 0.34952100
H -2.38849700 1.93734800 -1.92964100
H -4.10469700 1.49806400 -1.95859400
H -3.60486800 3.06735100 -1.32144600
C -3.44620400 -1.39103600 -1.11853500
C -4.96725200 -1.27562200 -0.93422000
C -3.01339700 -2.86152600 -0.99910000
H -3.18797800 -1.04680400 -2.12828600
H -5.34871200 -0.29249700 -1.21668600
H -5.46777100 -2.01506900 -1.57130100
H -5.27060200 -1.47840300 0.09915900
H -1.93705300 -2.98576600 -1.13701600
H -3.28855900 -3.28035200 -0.02418600
H -3.52788200 -3.45457900 -1.76433700
C 0.03081100 0.04064300 2.88654300
H 0.03032300 -0.38385500 3.90256700
H 0.95267000 0.60091300 2.73626400
H -0.79467500 0.74493600 2.79425700
P 2.27372900 -0.58238200 -0.02301500
C 1.03844900 -1.99320400 2.03546500
C 2.39577800 -1.39933700 1.65214300

H 0.82123900 -2.84967600 1.39440700
H 1.06759600 -2.34841300 3.07783000
H 2.71430500 -0.65146100 2.38310400
H 3.15478900 -2.18871200 1.65891600
C -0.04019400 0.18537600 -1.95668500
O -0.02777500 0.42541700 -3.10627700
C 3.25922500 1.02016900 0.11523800
C 3.47106500 1.64085300 -1.27471500
C 4.56277100 0.99897900 0.92888900
H 2.54582900 1.65666300 0.65235000
H 2.53862300 1.70378300 -1.84211400
H 3.86405400 2.65884100 -1.17122000
H 4.19364800 1.06914100 -1.86669200
H 4.42794300 0.58228700 1.93144200
H 5.35817300 0.43613000 0.43516100
H 4.92139200 2.02823900 1.05324800
C 3.17731600 -1.71119500 -1.22951000
C 2.50510700 -3.09141000 -1.30517300
C 4.68576800 -1.86602200 -0.98213800
H 3.03152900 -1.21403500 -2.19725400
H 1.43828300 -3.01451300 -1.52680500
H 2.98059800 -3.68458200 -2.09510900
H 2.62174600 -3.64616300 -0.36673300
H 5.22984000 -0.93019600 -1.12418400
H 4.89964300 -2.23798900 0.02634300
H 5.09808200 -2.59409200 -1.69133400
H 0.22836600 2.50464300 -0.26963600
C 0.67177100 4.18861300 0.53750500
H 0.59780600 3.61981500 1.48478500
O 0.95700400 5.36674600 0.50467800
O 0.41709600 3.46214400 -0.54426900
Mn -0.06403900 -0.25184800 -0.25291900

Mn-TS3_4(HCOOH)

H -0.08639300 1.53427300 0.27242900
H 0.10372800 -1.63090600 -0.59256800
C -1.14310400 -1.58307900 2.16484400
C -2.44800000 -0.91954000 1.72404900
H -1.18424100 -1.81480000 3.24075300
H -1.01151600 -2.52385000 1.62664800
H -2.66296100 -0.03805400 2.33435900
H -3.28108600 -1.61558800 1.86952000
P -2.29475700 -0.37310400 -0.05154800
N 0.06434300 -0.74940500 1.88356000

C -3.29614800 1.20804400 -0.18287300
C -4.62484900 1.26861000 0.58996200
C -3.47619000 1.62473500 -1.65213500
H -2.61952400 1.93375600 0.28980400
H -4.51221900 0.98314600 1.64035700
H -4.99236500 2.30247000 0.57800800
H -5.40482700 0.64088400 0.15204800
H -2.52942200 1.62248200 -2.19951300
H -4.17774700 0.97243800 -2.18398600
H -3.87783300 2.64384500 -1.69711700
C -3.13814200 -1.70101900 -1.09317200
C -4.66649600 -1.77441400 -0.94740300
C -2.52388600 -3.08932100 -0.85314500
H -2.89981900 -1.39921000 -2.12154400
H -5.16565100 -0.87170400 -1.30389700
H -5.04787200 -2.61420700 -1.54129800
H -4.97021600 -1.94683600 0.09127300
H -1.43756400 -3.08306700 -0.96753700
H -2.76434200 -3.46464700 0.14833000
H -2.93989900 -3.80170800 -1.57525600
C 0.07958000 0.41632700 2.80065100
H 0.00710800 0.08837100 3.84917300
H 1.00830800 0.97355000 2.67574400
H -0.73271100 1.10346700 2.56617000
P 2.39732900 -0.25779200 -0.01951700
C 1.26485500 -1.60283200 2.13614100
C 2.57686600 -0.94214300 1.70712000
H 1.12053200 -2.52515800 1.56925300
H 1.31149100 -1.86677800 3.20451900
H 2.84037100 -0.12185900 2.37965400
H 3.39061400 -1.67165400 1.77218300
C 0.06332900 0.28958100 -1.97292100
O 0.08308300 0.49326100 -3.12970400
C 3.28502600 1.40334400 0.01686600
C 3.40668200 1.99147500 -1.39846600
C 4.61291200 1.49820300 0.78543900
H 2.55529700 2.01461400 0.56375700
H 2.45530600 1.96546500 -1.93943000
H 3.73129800 3.03699600 -1.34069000
H 4.14728300 1.45244600 -1.99903900
H 4.54206400 1.09268900 1.79903800
H 5.43179100 0.98806400 0.27380700
H 4.89409900 2.55436600 0.87986600
C 3.34659500 -1.42382100 -1.15561900

C 2.82825900 -2.86590400 -1.02955900
C 4.87404400 -1.39795700 -0.99629400
H 3.09362000 -1.06296000 -2.16061900
H 1.74642700 -2.92778100 -1.16664000
H 3.30651900 -3.49001700 -1.79340800
H 3.07883100 -3.29703300 -0.05349400
H 5.30521400 -0.43295700 -1.26936500
H 5.18273500 -1.63675100 0.02763800
H 5.32023000 -2.15270900 -1.65531300
H 0.43976400 3.22597700 -1.17957500
C -0.22748300 2.92963200 0.61071700
H 0.81252900 3.01665300 0.99614400
O -1.18829100 3.10251000 1.38766300
O -0.32958500 3.51573200 -0.66494100
Mn 0.04797200 -0.09272000 -0.25794000

Mn-4(HCOOH)

H -0.09721500 1.59652300 0.29689200
H 0.10384100 -1.59422100 -0.59970800
C -1.13894400 -1.58922700 2.15374200
C -2.44937700 -0.93313400 1.71885600
H -1.17935400 -1.83443700 3.22652400
H -0.99595500 -2.52184700 1.60407100
H -2.67293600 -0.06011800 2.33814800
H -3.27649600 -1.63795800 1.85537200
P -2.29794600 -0.36644100 -0.04973700
N 0.06067400 -0.73883000 1.88646600
C -3.29818900 1.21383600 -0.16912500
C -4.62971900 1.26275800 0.59970100
C -3.47443700 1.64458500 -1.63473300
H -2.62251000 1.93629900 0.31481800
H -4.52059900 0.96503700 1.64709200
H -4.99829500 2.29628000 0.59888800
H -5.40775900 0.63937700 0.15176900
H -2.52554200 1.65342400 -2.17829400
H -4.17145200 0.99569100 -2.17688900
H -3.87969100 2.66265100 -1.66957400
C -3.12552300 -1.68875500 -1.10889400
C -4.65395600 -1.77151100 -0.96940700
C -2.50333900 -3.07522200 -0.87924300
H -2.88523000 -1.37538800 -2.13324600
H -5.15579200 -0.86653300 -1.31636800
H -5.02921000 -2.60564000 -1.57500900
H -4.96037700 -1.95810800 0.06601600

H -1.41673600 -3.06179700 -0.99092600
H -2.74397800 -3.46056800 0.11828500
H -2.91284400 -3.78396500 -1.60853800
C 0.05236200 0.42372100 2.80913400
H -0.05589100 0.09057000 3.85268300
H 0.98969200 0.97349200 2.71911800
H -0.74596800 1.12036400 2.55148900
P 2.39875200 -0.24697000 -0.01424900
C 1.26947800 -1.57891000 2.14768800
C 2.57587100 -0.90576500 1.72093400
H 1.13759700 -2.50596800 1.58533300
H 1.31369900 -1.83704000 3.21731600
H 2.82073300 -0.07161500 2.38355900
H 3.40062100 -1.62093700 1.80338700
C 0.06180500 0.28310900 -1.96938000
O 0.08111100 0.44669900 -3.13124800
C 3.29012400 1.41151800 -0.01171300
C 3.42426300 1.96525700 -1.43997600
C 4.61298500 1.51605800 0.76380000
H 2.56009600 2.04052500 0.51468300
H 2.47657800 1.93177100 -1.98697100
H 3.75245800 3.01046300 -1.40300600
H 4.16691200 1.40990600 -2.02266100
H 4.53000000 1.14189000 1.78843700
H 5.43023700 0.98206400 0.27414100
H 4.90435800 2.57164800 0.82826600
C 3.33555600 -1.43534400 -1.13595300
C 2.80268700 -2.87067700 -0.99532100
C 4.86281700 -1.42400600 -0.97259100
H 3.08865400 -1.08257100 -2.14525900
H 1.72092900 -2.92431400 -1.13613700
H 3.27759100 -3.50776000 -1.75040800
H 3.04580800 -3.29317700 -0.01371200
H 5.30510800 -0.46480200 -1.24797600
H 5.16543900 -1.66281000 0.05313800
H 5.30276100 -2.18603700 -1.62735400
H 0.46726500 3.20353800 -1.18878900
C -0.22103500 2.86101700 0.60327100
H 0.80993600 3.01735300 1.01046100
O -1.19981700 3.06768100 1.37321400
O -0.30698200 3.48886300 -0.67906800
Mn 0.04766500 -0.07320300 -0.24649900

Mn-5(HCOOH)

H -0.48976000 2.88714100 -1.10470000
H 0.07984000 -1.54832300 -0.62799100
C -1.13157300 -1.68050700 2.10611000
C -2.43523700 -0.98654700 1.70691800
H -1.18647000 -2.00359300 3.15848600
H -0.99389000 -2.57371900 1.49336500
H -2.63955100 -0.13674000 2.36421300
H -3.27355900 -1.68230100 1.82278000
P -2.29215500 -0.34852900 -0.03963600
N 0.07157700 -0.82346700 1.90650900
C -3.28835100 1.24536000 -0.07214700
C -4.59680300 1.29129500 0.73430400
C -3.50148300 1.73006300 -1.51657600
H -2.58327000 1.94000300 0.39940900
H -4.46264300 0.96779700 1.77099700
H -4.95994200 2.32646100 0.76644500
H -5.39007700 0.68291400 0.29278400
H -2.57220700 1.72695000 -2.09409300
H -4.23346100 1.11712200 -2.05380500
H -3.88165100 2.75874600 -1.50782900
C -3.17460200 -1.61274600 -1.12649000
C -4.69925400 -1.68844200 -0.94788600
C -2.56290500 -3.01524400 -0.97534400
H -2.95979800 -1.26324700 -2.14469300
H -5.20299200 -0.76559200 -1.24152800
H -5.10057700 -2.49282100 -1.57684100
H -4.97761200 -1.91644600 0.08723100
H -1.47985400 -3.00817600 -1.11741200
H -2.77876300 -3.44207500 0.01098800
H -3.00238300 -3.68714500 -1.72214500
C 0.08905300 0.23755400 2.93772500
H 0.10826800 -0.20530400 3.94603800
H 0.95659900 0.88030100 2.80492100
H -0.78476200 0.87674800 2.83401700
P 2.38457500 -0.23986500 -0.03853900
C 1.27626500 -1.68701300 2.06368800
C 2.57393100 -0.98353300 1.66291900
H 1.12741400 -2.56136700 1.42663800
H 1.34795200 -2.03883600 3.10589400
H 2.81081300 -0.18061800 2.36607600
H 3.40618600 -1.69396000 1.70776900
C 0.00972500 0.36394500 -1.96553800
O -0.00922800 0.52807800 -3.13075600
C 3.24943800 1.42906000 0.05620100

C	3.40430500	2.03532600	-1.34789000
C	4.55401100	1.53306600	0.86136200
H	2.47806200	2.00369300	0.58277200
H	2.46972700	1.99527400	-1.91568600
H	3.70353000	3.08756400	-1.27144000
H	4.17634200	1.51921800	-1.92981200
H	4.46628400	1.10501400	1.86433100
H	5.39751400	1.04851900	0.36309500
H	4.81471500	2.59172800	0.98611600
C	3.36292900	-1.33712600	-1.21527800
C	2.79598800	-2.76532300	-1.25784400
C	4.87899500	-1.37425200	-0.97091200
H	3.17951800	-0.87633500	-2.19489600
H	1.72472700	-2.77213200	-1.47173700
H	3.30739400	-3.33771100	-2.04089600
H	2.96003800	-3.29262600	-0.31043700
H	5.35118600	-0.40358800	-1.13497300
H	5.12035200	-1.70586700	0.04542800
H	5.34507300	-2.08511700	-1.66441000
H	-1.18739300	4.57859800	0.19254700
C	-0.10680600	2.96091500	-0.06553400
H	0.85726100	3.51868800	-0.11093500
O	0.02867800	1.76288600	0.54880800
O	-1.03738600	3.76643800	0.70020800
Mn	0.04088800	0.00068100	-0.25127300

DBU

C	-2.12082300	1.15983900	-0.51291100
C	-2.96212500	0.01002900	0.06284300
C	-2.11231500	-1.18093600	0.53149200
C	-0.92401200	-1.48290200	-0.39976700
C	0.36890800	-0.72248300	-0.12278800
N	0.34323500	0.66516000	-0.04820200
C	-0.84635600	1.47283700	0.27768700
N	1.42808900	-1.46372200	-0.04738300
C	2.73220000	-0.84328700	0.17275200
C	2.79462700	0.60949400	-0.29209400
C	1.59798500	1.35633600	0.28012800
H	-2.73035900	2.07060500	-0.53902700
H	-1.83990100	0.95342300	-1.55190100
H	-3.67400200	-0.32191200	-0.70339100
H	-3.56409100	0.37765500	0.90331400
H	-2.74531600	-2.07287800	0.60011800
H	-1.73776300	-1.00250800	1.54693100

H	-1.22457500	-1.32136800	-1.44378700
H	-0.64132600	-2.53401100	-0.31954700
H	-1.05502500	1.43747500	1.35970500
H	-0.55798900	2.50532000	0.05895800
H	3.48852500	-1.44493200	-0.34762300
H	2.98364400	-0.90440400	1.24305000
H	2.76031200	0.65059700	-1.38755400
H	3.72399600	1.09344100	0.02686700
H	1.70450900	1.46049400	1.37205700
H	1.54155600	2.36937500	-0.13313900

LiOTf

S	0.77775700	0.28985500	0.00005400
O	0.88018800	1.74755900	0.00085700
C	-1.04338200	-0.10250000	0.00010900
F	-1.62512400	0.40494400	1.08968200
F	-1.21372600	-1.43285000	-0.00292100
F	-1.62640400	0.41014900	-1.08716700
O	1.29650200	-0.44377500	1.20802300
O	1.29720500	-0.44258900	-1.20849000
Li	2.07077000	-1.78414400	-0.00032400

Li-1

Li	-0.00039400	0.17487200	0.00585800
C	-2.72749800	0.77222400	0.92450400
C	-2.63952400	-0.75059900	-0.92611200
C	-4.12162600	0.63799700	0.32182900
C	-4.05413100	-0.73761900	-0.35788300
H	-2.58943300	-0.26976200	-1.90924900
H	-2.36947400	1.80314900	0.99034500
H	-4.29556800	1.42515100	-0.41915800
H	-2.65994400	0.30142900	1.91130400
H	-4.90146900	0.70278000	1.08425700
H	-4.80657600	-0.86857900	-1.13910300
H	-4.17781800	-1.53748000	0.37954500
H	-2.19468900	-1.74719200	-0.98769500
O	-1.84495200	0.04353600	0.01172800
C	2.73401200	0.94719000	-0.75071600
C	4.10886300	0.29209400	-0.67463100
C	2.63296200	-0.91834600	0.75317200
C	4.06645500	-0.40315200	0.69418200
H	2.72243600	1.93138500	-0.26988800
H	4.22730000	-0.44430600	-1.47614500
H	2.52592500	-1.89096900	0.26035900

H 2.22415600 -0.97886300 1.76518600
H 4.79357200 -1.21320400 0.78759200
H 4.24697500 0.31817500 1.49797600
H 4.91305900 1.02676800 -0.75882300
H 2.34047600 1.03626900 -1.76682200
O 1.84559800 0.06170000 0.00410700

Li-2

O -0.09369400 2.16698600 -1.17753100
Li -0.00276800 0.54058600 -0.02901900
C -0.07235800 2.77457500 -0.06956000
H -0.10368500 3.88723400 -0.09072200
O -0.01702100 2.21256400 1.06200500
C -2.66720800 -0.00554400 1.03643300
C -2.08386100 -1.42940400 -0.78022100
C -3.89526500 -0.17887800 0.15002500
C -3.59418600 -1.51285100 -0.55006200
H -1.84513200 -0.96408400 -1.74452900
H -2.41038500 1.03243500 1.26058000
H -3.95413300 0.63449500 -0.58163700
H -2.76806300 -0.55895600 1.97895400
H -4.82392700 -0.19286800 0.72661800
H -4.14452500 -1.64594100 -1.48497400
H -3.83465600 -2.35229700 0.11132700
H -1.57920200 -2.39827600 -0.72298900
O -1.56572600 -0.57750600 0.27901500
C 2.68211400 -0.06780800 -1.08020200
C 3.94838000 -0.72007300 -0.52802800
C 2.13799400 -1.22422400 0.92909100
C 3.61829800 -0.85575400 0.96579700
H 2.72379800 1.02542500 -1.01729300
H 4.09819300 -1.70802700 -0.97704400
H 1.99077300 -2.30329900 0.79721800
H 1.58014300 -0.89843800 1.81216700
H 4.21974000 -1.61187000 1.47703800
H 3.75875100 0.10269400 1.47756600
H 4.83874800 -0.11651500 -0.72180100
H 2.45480900 -0.35119200 -2.11172100
O 1.59689200 -0.53735700 -0.23115600

DBU-TS1_2

Fe 2.00936700 0.09447600 -0.18175300
H 0.40987800 -0.03444700 0.00708600
H 3.54111700 0.22819300 -0.28129400

B -1.46222800 -0.35977200 -0.11318100
H -1.40248000 -0.98142800 0.91013400
H -1.65793900 0.81971800 -0.08389100
H -1.31363000 -0.91301100 -1.16310800
C 3.15138100 -0.89249700 2.45233600
C 2.64987300 -2.24684800 1.95101300
H 3.20208700 -0.88679600 3.55244300
H 4.15739800 -0.70879800 2.07072100
H 1.70753800 -2.51499200 2.43724100
H 3.37271600 -3.02906500 2.20586800
P 2.35256700 -2.13485000 0.11310100
N 2.29550100 0.24013900 1.98701800
C 0.89819800 -3.29022000 -0.20363900
C 0.82340100 -4.60783400 0.58602800
C 0.68820800 -3.52060400 -1.70900800
H 0.07213400 -2.65988500 0.14046000
H 0.98195300 -4.46484200 1.65918700
H -0.17840700 -5.03966700 0.46506400
H 1.54008400 -5.35472400 0.23716900
H 0.66918000 -2.58032800 -2.26692100
H 1.46794300 -4.15740700 -2.14082100
H -0.27236400 -4.02176400 -1.87774000
C 3.87449000 -2.92965900 -0.68743400
C 4.01225100 -4.44852600 -0.49680400
C 5.17846300 -2.24016400 -0.25347600
H 3.73076900 -2.72613000 -1.75698400
H 3.21304700 -5.00850900 -0.98547100
H 4.95947800 -4.78684300 -0.93513700
H 4.02842100 -4.72696100 0.56311900
H 5.13447200 -1.15723800 -0.38640400
H 5.41195100 -2.45068300 0.79696000
H 6.01216400 -2.62563900 -0.85263600
C 1.01092600 0.21215000 2.72854400
H 1.18699200 0.31114300 3.81115100
H 0.36466600 1.02187700 2.39451500
H 0.48410300 -0.71979700 2.53451000
P 1.96551700 2.36182500 -0.11932600
C 3.01129000 1.51478100 2.29855500
C 2.33309700 2.73309700 1.67271900
H 4.02309100 1.41589900 1.90136800
H 3.08524700 1.63696000 3.39059600
H 1.38967100 2.95761900 2.17833700
H 2.97219300 3.61458000 1.78970000
C 1.86411700 -0.00625900 -1.89782900

O 1.78874400 -0.07342800 -3.06304100
C 0.30611100 3.20253600 -0.42232000
C -0.08843800 3.13397600 -1.90574600
C 0.06826400 4.60577100 0.16107200
H -0.35387000 2.51263900 0.11553400
H -0.01819300 2.11545000 -2.29717300
H -1.12604700 3.46555400 -2.03238300
H 0.53972200 3.78222000 -2.52701300
H 0.38646900 4.69038400 1.20480400
H 0.57012300 5.39210100 -0.40683000
H -1.00693300 4.82406700 0.13469500
C 3.27227800 3.29410800 -1.12284600
C 4.69650200 2.95025700 -0.65687600
C 3.11176700 4.82066600 -1.19366000
H 3.14354900 2.88574600 -2.13409800
H 4.86736900 1.87234000 -0.61851400
H 5.42380500 3.38707500 -1.35167300
H 4.90321300 3.36961000 0.33476900
H 2.19845700 5.12462900 -1.70825200
H 3.11371800 5.27864800 -0.19808400
H 3.95508000 5.24951200 -1.74933900
C -7.53027100 0.97989700 0.99223000
C -6.89723800 2.33657300 0.64679600
C -5.51630700 2.19528000 -0.00988800
C -4.65453600 1.08793600 0.62504400
C -4.81936000 -0.31277700 0.04936900
N -6.08808200 -0.86023200 -0.05207800
C -7.34833000 -0.09214900 -0.08719700
N -3.71720300 -0.93208400 -0.25194200
C -3.75887100 -2.29944700 -0.76410500
C -5.01178500 -3.05523800 -0.33670600
C -6.22917200 -2.19763000 -0.64642900
H -8.60660000 1.11455300 1.15050800
H -7.13139500 0.59148100 1.93630700
H -6.81203000 2.93106600 1.56506300
H -7.56238400 2.89620200 -0.02286300
H -4.97922700 3.14756100 0.06438800
H -5.62532600 1.99723900 -1.08314900
H -4.83723400 1.05299200 1.70739500
H -3.59858900 1.32132100 0.49809300
H -7.50299100 0.34698600 -1.08581100
H -8.13760900 -0.83845200 0.04193600
H -2.85899400 -2.81746200 -0.41485500
H -3.68843300 -2.27387600 -1.86162700

H -4.97347600 -3.26181500 0.73973300
H -5.08962800 -4.01668800 -0.85537200
H -6.37193600 -2.11825000 -1.73562400
H -7.13705300 -2.65241400 -0.23606000

DBU-BH₃

B 1.93220300 2.42347300 0.15577800
H 1.48688500 2.91958700 1.18052100
H 1.50719600 3.02354800 -0.82031000
H 3.14770100 2.46715900 0.16323700
C -2.32851600 -0.85594900 0.81992100
C -3.07431000 0.28962900 0.12689700
C -2.12289300 1.16308500 -0.69715900
C -0.81143500 1.48258600 0.03067700
C 0.28778800 0.43685000 -0.03369200
N 0.00634600 -0.87385800 -0.24343400
C -1.30119000 -1.55073400 -0.07253300
N 1.53041100 0.88178400 0.07120600
C 2.68714700 -0.03525200 0.14290700
C 2.30146600 -1.49875300 0.28949100
C 1.11354100 -1.76756100 -0.62061500
H -3.04244100 -1.62021400 1.14695500
H -1.82678700 -0.50164600 1.72782700
H -3.58117300 0.89952800 0.88447600
H -3.85786400 -0.11442200 -0.52549800
H -2.61405400 2.10886000 -0.94941500
H -1.89473100 0.67748300 -1.65344600
H -0.99695700 1.73063000 1.08380700
H -0.37343600 2.38273100 -0.40183900
H -1.73220200 -1.75894000 -1.06143700
H -1.06385000 -2.51998500 0.37540400
H 3.30576900 0.28798000 0.98424100
H 3.28589700 0.11568100 -0.76297200
H 2.02276700 -1.73017800 1.32352100
H 3.15045900 -2.13530600 0.02294400
H 1.38342500 -1.59101500 -1.66991800
H 0.76550400 -2.79772700 -0.53675900

Li-4

C -1.46960400 -0.01923500 -0.10592100
O -2.07984900 0.73250200 -0.91101500
O -2.00834800 -0.72916700 0.78613700
Fe 1.98784100 -0.03265200 -0.14778500
H -0.35143000 -0.06186600 -0.19220000

H	3.45017900	-0.08003800	-0.22263000	C	0.28555000	4.50494700	-0.82269000
C	2.84349500	-0.59094700	2.66426900	H	-0.23435500	2.43303000	-0.71879800
C	2.26945900	-1.98509200	2.41717400	H	0.54911000	1.74570700	-2.97014000
H	2.81207600	-0.34588100	3.73555200	H	-0.57040100	3.10738700	-3.04615700
H	3.88556800	-0.55772900	2.34064400	H	1.16015100	3.38196300	-3.27442200
H	1.29711900	-2.10167600	2.90408800	H	0.34720400	4.68426200	0.25487000
H	2.93258200	-2.74212400	2.84732200	H	0.97082900	5.19509400	-1.31992000
P	2.04398200	-2.21875600	0.58351400	H	-0.73127900	4.77148200	-1.13602000
N	2.12194600	0.47715600	1.89754100	C	3.57784900	2.87045300	-1.53697600
C	0.44536600	-3.18985900	0.39942900	C	4.91328600	2.37114400	-0.96096600
C	0.21096900	-4.35266100	1.37782800	C	3.62181100	4.39470100	-1.72547100
C	0.23168000	-3.62413200	-1.05929400	H	3.43585600	2.40239800	-2.51940400
H	-0.30540300	-2.42247600	0.62776500	H	4.94129100	1.28351600	-0.86127500
H	0.37180200	-4.06447000	2.42089300	H	5.72938900	2.67144500	-1.62799100
H	-0.83193100	-4.68149400	1.29200100	H	5.11663300	2.81399300	0.02062000
H	0.84317000	-5.21753800	1.16573200	H	2.77308500	4.76909700	-2.30015700
H	0.31709000	-2.78463700	-1.75655600	H	3.65144200	4.92519800	-0.76719500
H	0.94817100	-4.39301500	-1.36665600	H	4.53215600	4.66423500	-2.27413500
H	-0.77260900	-4.04816900	-1.17431400	Li	-3.72943900	0.03225400	0.01211400
C	3.48254100	-3.27439000	-0.01376600	C	-4.48568000	-1.28784000	-2.51598800
C	3.45206100	-4.74121100	0.44146300	C	-5.54149000	-2.22134200	-0.59557100
C	4.83303900	-2.63666900	0.35421900	C	-4.57796500	-2.79795400	-2.70644500
H	3.38314700	-3.24703500	-1.10630700	C	-5.75211100	-3.16148200	-1.78444400
H	2.60592000	-5.28954600	0.02377100	H	-4.90445600	-2.67464900	0.17378100
H	4.36605500	-5.24274100	0.10156400	H	-3.48723100	-0.87178500	-2.67054300
H	3.41799800	-4.83015300	1.53282300	H	-3.65606100	-3.28224200	-2.36561600
H	4.91098900	-1.60160200	0.01321200	H	-5.19731400	-0.75622000	-3.16043400
H	5.00649100	-2.65800800	1.43615800	H	-4.74709300	-3.07413700	-3.75048600
H	5.64099700	-3.20904800	-0.11537100	H	-5.75544400	-4.21143200	-1.48079600
C	0.74855300	0.63964600	2.44157500	H	-6.70493900	-2.94549900	-2.27967100
H	0.78372800	0.84689000	3.52017700	H	-6.47410500	-1.88878300	-0.13048800
H	0.24347200	1.46773400	1.94460500	O	-4.85104100	-1.05570200	-1.12840500
H	0.15742500	-0.25855400	2.26889800	C	-4.48002700	1.62450300	2.45086800
P	2.11964500	2.24002200	-0.52881400	C	-5.62498100	2.54585100	2.86367500
C	2.88832900	1.75295600	2.07786200	C	-5.91830600	1.93222400	0.57699000
C	2.36132600	2.88802000	1.20123900	C	-6.06569600	3.13080300	1.51360200
H	3.92481300	1.53400400	1.81435200	H	-3.53126900	2.17071800	2.37256100
H	2.86094300	2.04187400	3.13843500	H	-6.43742400	1.96565200	3.31463100
H	1.40675900	3.26605300	1.57551100	H	-6.82823700	1.32163800	0.54937500
H	3.06266000	3.72761100	1.22289300	H	-5.64770700	2.20806400	-0.44671700
C	2.07875600	-0.45157600	-1.84062800	H	-7.08681800	3.52035200	1.52194900
O	2.26322700	-0.72953500	-2.95456900	H	-5.39177000	3.93917900	1.20962300
C	0.54860200	3.03676900	-1.19335700	H	-5.30444400	3.30550500	3.58124100
C	0.42542900	2.80083700	-2.70756800	H	-4.34087700	0.76594500	3.11322300

O -4.84408000 1.12626000 1.13688500

Li-4a

C 0.79471700 0.31916400 -1.96198900
O 0.42500200 0.20011000 -0.74138400
O 1.98665600 0.51309600 -2.29414200
Fe -1.57171000 -0.21536600 -0.15564600
H 0.02411200 0.24672600 -2.74763000
H -2.94369600 -0.50047200 0.36503600
C -1.84849100 0.89063600 2.64515600
C -1.76668500 2.24646600 1.94711400
H -1.51607100 0.97704900 3.69028100
H -2.88388500 0.54516400 2.65015700
H -0.77177300 2.68608900 2.06050600
H -2.47381200 2.94360600 2.40813700
P -2.10285000 2.00935800 0.13024800
N -1.04128200 -0.16686300 1.95647000
C -0.97984800 3.23828000 -0.74514100
C -0.82027800 4.63892700 -0.13102200
C -1.32647900 3.31526700 -2.24068900
H -0.01284500 2.72939200 -0.65405400
H -0.57439500 4.60774800 0.93479300
H -0.00053800 5.16160800 -0.63935200
H -1.71563200 5.25228200 -0.25056400
H -1.41300600 2.32357000 -2.69535600
H -2.27021700 3.84440500 -2.40869900
H -0.54381300 3.86160800 -2.77976700
C -3.88658300 2.54427000 -0.15943300
C -4.16234500 4.04291300 0.03592800
C -4.86660900 1.71315000 0.68513700
H -4.06004900 2.29629900 -1.21486100
H -3.65161400 4.66037400 -0.70502000
H -5.23768200 4.22995400 -0.07029500
H -3.86955800 4.38812500 1.03388300
H -4.73261700 0.63979900 0.53421600
H -4.75736000 1.92806000 1.75434700
H -5.89437100 1.97187600 0.40562000
C 0.40041800 0.09937600 2.17870200
H 0.62617000 0.12692000 3.25475300
H 0.99959800 -0.68064200 1.71117700
H 0.68299900 1.04965100 1.72842500
P -1.20249400 -2.48094100 0.01480200
C -1.40172800 -1.47991200 2.58167300
C -0.82173300 -2.67509400 1.82777200

H -2.49102800 -1.54325700 2.57564000
H -1.06689600 -1.48704100 3.62950900
H 0.26284900 -2.73173900 1.95317100
H -1.23342800 -3.60466300 2.23377300
C -2.34214100 -0.33201600 -1.70987800
O -2.96702900 -0.43608100 -2.68795700
C 0.31459100 -3.14029000 -0.88090600
C 0.04778600 -3.25476400 -2.39040600
C 0.97917200 -4.41142900 -0.32649700
H 1.01889600 -2.31309400 -0.72938800
H -0.37589700 -2.33471100 -2.80470400
H 0.98462400 -3.45684300 -2.92245500
H -0.64183100 -4.07440400 -2.61821400
H 1.18196500 -4.34682500 0.74693100
H 0.38266900 -5.30935200 -0.50046900
H 1.94176600 -4.56156600 -0.83079700
C -2.65049200 -3.63002700 -0.35107500
C -3.87198700 -3.29122400 0.51984300
C -2.34380300 -5.13230600 -0.25716800
H -2.90541800 -3.39434800 -1.39247300
H -4.15640200 -2.23975800 0.44331700
H -4.72489200 -3.89945700 0.19723600
H -3.68898100 -3.52259800 1.57554100
H -1.62419200 -5.46042200 -1.00941900
H -1.96328300 -5.41230000 0.73153300
H -3.26753500 -5.70012900 -0.42152800
Li 2.55806600 0.44728500 -0.42300500
C 4.09072800 -1.52588000 1.35275100
C 4.55320200 -1.64650400 -0.98300400
C 4.95035200 -2.75887500 1.09319600
C 5.65340100 -2.38350900 -0.21983100
H 3.94027100 -2.32827600 -1.58244200
H 3.18120300 -1.73082400 1.92418500
H 4.31878500 -3.64284700 0.95228400
H 4.65937100 -0.73885500 1.86318600
H 5.64409100 -2.95819700 1.91379900
H 6.02515500 -3.24885900 -0.77402500
H 6.49784100 -1.71419000 -0.02231600
H 4.92867600 -0.85029100 -1.63164500
O 3.70045000 -1.04710000 0.03835700
C 2.98893900 3.34640900 -0.36095300
C 4.36040900 3.96458700 -0.59956100
C 4.57209300 2.15228300 0.95327500
C 5.11067900 3.55965600 0.67822400

H 2.36985800 3.98029300 0.28611700
H 4.82968900 3.51822300 -1.48338300
H 5.19653700 1.37773300 0.49625200
H 4.45923900 1.93513700 2.01953600
H 6.19719600 3.56432400 0.56121500
H 4.85296500 4.23618400 1.49983600
H 4.30790900 5.04655300 -0.74522500
H 2.43680500 3.11409700 -1.27425600
O 3.25581700 2.09312900 0.32655200

Li-4'

C 1.11201300 -0.55280700 0.43304800
O 1.80988600 -1.03104400 -0.49616700
O 1.55766900 -0.01088600 1.48251500
Fe-2.04511700 0.14550000 -0.16511100
H -0.00265400 -0.61780800 0.31978200
H -3.38086600 0.46958800 -0.67649000
C -3.26045700 1.77766900 2.02405200
C -2.24784800 2.84221400 1.60859600
H -3.52741400 1.89347600 3.08429100
H -4.17155500 1.88287000 1.43179400
H -1.41027500 2.88101000 2.31043900
H -2.71994000 3.82958500 1.62107700
P -1.58557800 2.40649200 -0.07641900
N -2.76261400 0.38241400 1.79700800
C 0.23340400 2.87811900 -0.02600200
C 0.60635000 4.21720300 0.63300200
C 0.87842600 2.73547600 -1.41457700
H 0.64249700 2.08401700 0.60995100
H 0.12949400 4.35954900 1.60745700
H 1.69021900 4.23367300 0.79979200
H 0.36057100 5.07807200 0.00731000
H 0.68859200 1.75456000 -1.86033800
H 0.51948800 3.50130000 -2.11099400
H 1.96477200 2.85148900 -1.32871200
C -2.47155600 3.50523800 -1.32019800
C -2.12036000 4.99786500 -1.23660800
C -3.99554700 3.31359600 -1.24679500
H -2.12973900 3.12068200 -2.28959700
H -1.07872800 5.19436000 -1.49657000
H -2.74550600 5.55697300 -1.94297500
H -2.30976300 5.40638800 -0.23790600
H -4.28481900 2.26479900 -1.34586900
H -4.40391800 3.69670600 -0.30454100
H -4.47052700 3.87510200 -2.05938100

C -1.62756800 0.09377800 2.71277600
H -1.90121700 0.32056200 3.75286900
H -1.35361300 -0.95882000 2.64700500
H -0.74874600 0.67615000 2.43577300
P -2.78653500 -2.02772300 0.02771500
C -3.90371700 -0.54706200 2.08277600
C -3.60563500 -1.99648800 1.69969300
H -4.75360200 -0.18109200 1.50345200
H -4.16582300 -0.47893700 3.14844100
H -2.93079200 -2.46498500 2.42093400
H -4.53201700 -2.57830400 1.71348400
C -1.62347500 -0.01278400 -1.85407700
O -1.46318800 -0.09135200 -3.00230300
C -1.45333400 -3.34762700 0.17314800
C -0.76178400 -3.58375000 -1.17896000
C -1.83492300 -4.67023400 0.85943100
H -0.72933800 -2.84423200 0.82732700
H -0.36777900 -2.65697500 -1.60427200
H 0.08500900 -4.26619000 -1.04421100
H -1.44059800 -4.04054600 -1.90694600
H -2.36890900 -4.51911800 1.80225000
H -2.44946600 -5.30995100 0.22266200
H -0.91758800 -5.22449000 1.09111300
C -4.08086100 -2.58386300 -1.21982800
C -5.33721900 -1.69981800 -1.14369400
C -4.47421500 -4.06695700 -1.14975700
H -3.59658800 -2.39964000 -2.18736600
H -5.10352900 -0.63629800 -1.23362500
H -6.01543200 -1.96664600 -1.96201200
H -5.88141400 -1.85747000 -0.20553400
H -3.64357100 -4.72916800 -1.40056200
H -4.85367800 -4.34613600 -0.16060800
H -5.27589900 -4.26084600 -1.87247500
S 5.77521800 -0.06673000 0.75072600
O 6.90860100 0.42060100 1.54243500
C 6.52165700 -0.78234900 -0.79425600
F 7.19824000 0.15874500 -1.46494500
F 5.55636700 -1.26557500 -1.59251600
F 7.35974900 -1.78094900 -0.48758500
O 4.81710700 0.95824300 0.22582000
O 4.99286500 -1.21350300 1.31436200
Li 3.31379100 -0.34600200 0.60935300

Li-4a'

C	0.21231600	-0.17045000	2.47258700	H	-2.26951200	-0.78164200	-2.84487000
O	0.17189900	-0.17228500	1.18809900	N	-0.59812200	-0.04061700	-1.82606500
O	1.28001800	-0.29155400	3.10912400	H	-0.32163600	-4.63032500	-0.37017100
H	-0.73801700	-0.05923300	3.01964700	H	-0.11153600	-5.06717200	1.32395800
Li	2.22531900	-0.36951200	1.40001100	H	-1.68872100	-5.26024100	0.55854700
O	3.96057500	-1.41063300	1.27875000	H	-2.03710900	-2.17723100	2.81297500
S	4.58215600	-0.22544000	0.60616900	H	-2.76169800	-3.74919900	2.44500500
O	5.89501100	0.20832100	1.09166400	H	-1.16391100	-3.66622300	3.19390700
C	4.88201100	-0.82025500	-1.13138600	H	-3.69874100	-4.68300100	0.54652700
O	3.53455400	0.83664400	0.44730600	H	-5.15889200	-4.32657400	-0.37501500
F	5.26616300	0.19633000	-1.91251500	H	-3.61660300	-4.50715500	-1.21594500
F	3.76048800	-1.35400800	-1.64468500	H	-4.55838500	-0.76294900	-1.12783700
F	5.83627000	-1.75771500	-1.13637800	H	-4.34818400	-2.13275300	-2.23458500
Fe	-1.60110300	0.19065800	0.09185500	H	-5.72619600	-2.09610800	-1.13220800
H	-2.80585100	0.43975600	-0.76164600	H	-1.82021300	1.29969300	-2.86735200
P	-2.06453700	-2.05863400	-0.11485700	H	-0.19454000	1.13679900	-3.55564100
P	-1.11303300	2.43205700	-0.15592800	H	-0.98897100	2.54036500	2.77395100
C	-2.72264700	0.44206100	1.39514000	H	0.39447300	3.58439000	3.12222600
C	-1.36918500	-2.43760000	-1.80107500	H	-1.06449700	4.26714000	2.39593600
C	-1.14369800	-3.18795400	1.07666800	H	1.48147300	4.13434300	-0.46113600
C	-3.86590800	-2.60550700	-0.15115600	H	0.48290500	5.24331500	0.48851200
C	-0.32508100	2.46375100	-1.84272200	H	1.87670100	4.45209700	1.22567000
C	0.19211500	3.12214300	1.01178900	H	-3.92480000	2.22811100	-1.16421500
C	-2.54767600	3.65156300	-0.21264900	H	-4.44519600	3.92108800	-1.21680600
O	-3.56581900	0.62958000	2.17781900	H	-3.16328300	3.36267200	-2.29470600
C	-1.26789100	-1.13669900	-2.59506500	H	-1.57634400	5.50356200	0.46474800
H	-0.38617400	-2.90028900	-1.67872200	H	-1.56645300	5.28885300	-1.29574600
H	-1.98931000	-3.15705200	-2.34547300	H	-3.05639900	5.73900400	-0.46341000
C	-0.80921000	-4.61379900	0.60894000	C	0.84618300	-0.35281000	-1.69494500
C	-1.82048200	-3.18947300	2.45703700	H	1.29860100	-0.49435700	-2.68638800
H	-0.19429500	-2.64869200	1.17544100	H	1.36698100	0.45446100	-1.18357600
C	-4.08420100	-4.11842800	-0.30435600	H	0.98064400	-1.26095100	-1.10954000
C	-4.66291800	-1.84576700	-1.22438600				
H	-4.24699700	-2.29777900	0.83131500				
C	-0.76099700	1.22057300	-2.61611200	Li-5			
H	0.76063300	2.48633800	-1.71733900	Fe	0.00000400	0.17845600	0.02640800
H	-0.59482900	3.36372100	-2.40481500	H	0.00010100	-0.36118700	1.38704300
C	-0.40817300	3.39023700	2.40143900	C	1.21097800	-2.52371600	-0.32929000
C	1.04397300	4.30682000	0.52660900	C	2.51278700	-1.76605200	-0.58928700
H	0.86406400	2.26092200	1.10138300	H	1.22280100	-3.49536200	-0.84297700
C	-3.57632500	3.25601500	-1.28485900	H	1.09442400	-2.70706700	0.74071700
C	-2.15060000	5.12598700	-0.38302500	H	2.77216600	-1.77990300	-1.65082500
H	-3.02397700	3.53409400	0.76968000	H	3.33608600	-2.25420600	-0.05924300
H	-0.72262700	-1.30487000	-3.53577500	P	2.29417700	0.00097700	-0.03752300
				N	-0.00003500	-1.75453600	-0.76426600

C 3.07336300 1.07421700 -1.37404300
 C 4.37167700 0.56504700 -2.01950600
 C 3.21920900 2.52758400 -0.89390300
 H 2.29227800 1.05852800 -2.14783300
 H 4.28759900 -0.46177900 -2.38629500
 H 4.61423300 1.19873800 -2.88095100
 H 5.21991600 0.61002100 -1.33275800
 H 2.28632600 2.92662100 -0.48420900
 H 3.99464600 2.62231200 -0.12712000
 H 3.50932300 3.16592200 -1.73593500
 C 3.26668900 0.19759400 1.55456000
 C 4.78650500 0.02815300 1.40872000
 C 2.72099800 -0.74199400 2.64302100
 H 3.05794600 1.22989800 1.86266500
 H 5.23439500 0.80445500 0.78486600
 H 5.25395400 0.09330100 2.39828400
 H 5.04986300 -0.94839800 0.98745000
 H 1.64878000 -0.60662400 2.80559100
 H 2.90301000 -1.79402000 2.39506700
 H 3.23642300 -0.53764600 3.58826700
 C -0.00020100 -1.61167800 -2.24339900
 H -0.00086000 -2.59524700 -2.73200800
 H -0.88155600 -1.05851400 -2.57085600
 H 0.88173400 -1.05957300 -2.57106800
 P -2.29422300 0.00099300 -0.03733400
 C -1.21092600 -2.52365400 -0.32881600
 C -2.51284500 -1.76614300 -0.58869700
 H -1.09412900 -2.70665500 0.74123400
 H -1.22282300 -3.49545000 -0.84221700
 H -2.77248000 -1.78022500 -1.65017200
 H -3.33598800 -2.25422100 -0.05834500
 C -0.00002100 1.72149200 0.84599200
 O -0.00014100 2.68036600 1.50345600
 C -3.07300700 1.07395500 -1.37427500
 C -3.21884700 2.52745200 -0.89449700
 C -4.37121100 0.56476300 -2.01990900
 H -2.29170700 1.05800700 -2.14784700
 H -2.28606100 2.92646800 -0.48456400
 H -3.50861400 3.16564600 -1.73675500
 H -3.99452700 2.62243800 -0.12799000
 H -4.28721600 -0.46223400 -2.38625000
 H -5.21962700 0.61016300 -1.33339500
 H -4.61341000 1.19816100 -2.88166800
 C -3.26694300 0.19800800 1.55452800

C -2.72128100 -0.74130000 2.64324200
 C -4.78672000 0.02838600 1.40839700
 H -3.05833300 1.23040300 1.86240100
 H -1.64905100 -0.60592100 2.80575400
 H -3.23668800 -0.53667600 3.58843700
 H -2.90332400 -1.79338700 2.39556700
 H -5.23448900 0.80438400 0.78407900
 H -5.04991100 -0.94836400 0.98747900
 H -5.25444300 0.09392500 2.39780400

Li-6

H 0.47895900 -0.16374500 -1.86810900
 H 2.03048800 -1.98364300 -2.18338900
 C 3.09854700 -1.80513800 -2.02730000
 C 3.37571700 -0.37743300 -1.53467200
 H 3.60577900 -1.96578900 -2.98563700
 H 3.47086300 -2.56217500 -1.33091000
 P 2.33272700 0.12816400 -0.05029700
 C 4.87872000 -0.11643900 -1.36224600
 H 2.99631100 0.31211100 -2.30178900
 Fe 0.06113900 -0.12101500 -0.20851700
 C 2.50542400 1.98086100 -0.05238000
 C 3.26076200 -0.42452200 1.48699800
 H 5.08875000 0.90537700 -1.02990800
 H 5.32943700 -0.80807600 -0.64353200
 H 5.38966500 -0.26206600 -2.32115700
 P -2.23045400 0.00789200 -0.04635100
 C 0.07992000 -1.85618100 0.04936100
 C 1.20118800 2.60207900 0.43777600
 H 2.74374900 2.29974600 -1.07121600
 H 3.33139500 2.30651900 0.58744400
 C 3.27394900 -1.94984500 1.66041600
 C 2.73795700 0.25792000 2.75945500
 H 4.28942900 -0.08263000 1.31907600
 C -2.50351200 1.84307000 0.06288400
 C -3.18600800 -0.54298200 -1.57424100
 C -3.00497600 -0.77503400 1.47919600
 O 0.07246500 -2.98955300 0.29054000
 N -0.00747100 2.02773200 -0.24050400
 H 1.08347300 2.40733900 1.50501700
 H 1.21271100 3.69104600 0.29125700
 H 3.68417300 -2.47177600 0.79230100
 H 3.89596400 -2.21054800 2.52446100
 H 2.26956100 -2.33993000 1.85065800

H 1.69870500 -0.01801700 2.96415600
 H 3.34340500 -0.06384700 3.61470800
 H 2.80107700 1.34909800 2.70947300
 C -1.20812100 2.50565300 0.52270600
 H -2.80755800 2.20484100 -0.92283000
 H -3.31476100 2.09065600 0.75460900
 C -4.59539300 0.03859600 -1.77934900
 C -3.18302200 -2.07413100 -1.70675900
 H -2.55402100 -0.13818300 -2.37627000
 C -4.54070700 -0.77230300 1.50938100
 C -2.44872300 -0.14683600 2.76719200
 H -2.65944500 -1.81544100 1.43387700
 C -0.07612500 2.54984000 -1.63330100
 H -1.28315000 3.59806300 0.42807500
 H -1.02794100 2.26729500 1.57224000
 H -4.62391200 1.12706400 -1.67317900
 H -4.92652300 -0.19642700 -2.79788400
 H -5.32898100 -0.38820500 -1.09276200
 H -3.61901100 -2.36177700 -2.66990000
 H -2.17281100 -2.49268600 -1.66348000
 H -3.78046400 -2.54793800 -0.92133300
 H -4.97432700 -1.39224900 0.72253400
 H -4.88090900 -1.17718500 2.46957400
 H -4.94923400 0.23989500 1.41827800
 H -1.35671500 -0.15329300 2.79183500
 H -2.79275000 0.88624900 2.88884300
 H -2.81166900 -0.71498400 3.63088200
 H -0.14295000 3.64593100 -1.62852400
 H 0.81049700 2.25346800 -2.19364700
 H -0.94715900 2.14279500 -2.14676300
 H 0.07312800 -0.00804000 1.26938700
 H -0.31793700 -0.20403300 -1.87680600

DBU-5

Fe -1.53785100 0.13349500 -0.09507900
 H -0.23617900 -0.61433400 0.71509200
 H -2.83104300 0.47404400 -0.72376700
 C -2.89421600 2.06845600 1.78497600
 C -1.77228500 3.00578800 1.34502900
 H -3.24098900 2.33213600 2.79400000
 H -3.74167500 2.16276800 1.10401300
 H -0.97097100 3.03615500 2.08936800
 H -2.15441600 4.02683200 1.24623500
 P -1.06116000 2.37659300 -0.25097400

N -2.48129000 0.62672100 1.76828100
 C 0.76242200 2.83558700 -0.21430200
 C 1.13196000 4.21315500 0.36050000
 C 1.41933600 2.60053700 -1.58367900
 H 1.16858300 2.07886000 0.46862500
 H 0.67940000 4.39666200 1.33948800
 H 2.21949000 4.25730900 0.49504300
 H 0.85281100 5.03601400 -0.30107100
 H 1.18724700 1.61122600 -1.98912000
 H 1.10716400 3.34972900 -2.31859200
 H 2.50799700 2.66773100 -1.48258400
 C -1.88935300 3.34112900 -1.63853500
 C -1.51235900 4.82926300 -1.70213200
 C -3.41863400 3.18913500 -1.60444400
 H -1.52103800 2.84838900 -2.54748800
 H -0.45892400 4.98382900 -1.94184700
 H -2.10131400 5.31562000 -2.48863700
 H -1.73366100 5.34718400 -0.76241000
 H -3.73039200 2.14248400 -1.57897300
 H -3.85259200 3.70184400 -0.73866800
 H -3.84601500 3.64851200 -2.50288300
 P -2.44225600 -1.95244300 0.22738100
 C -3.72596600 -0.19437300 1.92855400
 C -3.47338100 -1.68988400 1.75285100
 H -4.43012400 0.15260000 1.17031000
 H -4.16460000 0.00347400 2.91711400
 H -2.93878600 -2.10264900 2.61237800
 H -4.42786600 -2.22151800 1.68875100
 C -1.01694100 -0.22359900 -1.72854300
 O -0.76557600 -0.44161000 -2.83989600
 C -1.21684700 -3.30700400 0.68510100
 C -0.40979300 -3.75883000 -0.54253900
 C -1.75369100 -4.50847400 1.48108500
 H -0.53491500 -2.75800400 1.34851700
 H 0.05399400 -2.91680600 -1.06587900
 H 0.39258700 -4.43581300 -0.22867500
 H -1.03496200 -4.30107500 -1.25972700
 H -2.35705200 -4.20876400 2.34290200
 H -2.35357200 -5.18287000 0.86683600
 H -0.90365200 -5.08539500 1.86443800
 C -3.58852500 -2.58955400 -1.12013200
 C -4.76041200 -1.62130700 -1.34789600
 C -4.11037600 -4.01956700 -0.91509600
 H -2.95916600 -2.57594900 -2.01919000

H -4.41923900 -0.60167900 -1.54007400
 H -5.34129100 -1.95458100 -2.21522800
 H -5.43971800 -1.60349700 -0.48808400
 H -3.31084800 -4.76224700 -0.93762600
 H -4.65548800 -4.12581300 0.02938600
 H -4.80861100 -4.26522100 -1.72372800
 H 0.02623200 0.13110600 0.62216800
 C 5.84584300 -2.25594000 -1.30594300
 C 4.93394500 -1.95860900 -2.50638000
 C 3.86597100 -0.89966200 -2.19473500
 C 3.25239600 -1.05176200 -0.79086500
 C 3.97491300 -0.35901200 0.36167300
 N 5.33612700 -0.54946800 0.52870900
 C 6.27037700 -1.01390600 -0.51470200
 N 3.20661500 0.32200000 1.15720900
 C 3.78248500 0.99455000 2.32103000
 C 5.07848900 0.35258800 2.80762400
 C 6.01014800 0.17471100 1.61680800
 H 6.75553700 -2.75356900 -1.66095900
 H 5.36522000 -2.95865800 -0.61563800
 H 4.45001900 -2.89108800 -2.82270000
 H 5.53973300 -1.62179100 -3.35682800
 H 3.06418300 -0.96368400 -2.93932400
 H 4.29072600 0.10591600 -2.29968500
 H 3.14336400 -2.11907600 -0.55478100
 H 2.24649900 -0.62853400 -0.77714000
 H 6.51653600 -0.19171600 -1.20569300
 H 7.19616200 -1.25087300 0.01741300
 H 3.03196100 0.99628500 3.12184000
 H 3.96306800 2.05204600 2.07306000
 H 4.86502300 -0.62641300 3.25360700
 H 5.56488700 0.96523300 3.57419300
 H 6.36481900 1.15512900 1.26142500
 H 6.89603200 -0.40113900 1.90432800
 C -1.57089800 0.36985500 2.91708500
 H -1.26969200 -0.67749600 2.93104500
 H -0.66960100 0.97468300 2.82140700
 H -2.06872200 0.61181100 3.86537600

DBU-TS5_6

Fe 1.37553700 -0.08554200 -0.15933600
 H -0.03641600 0.29095200 0.71110100
 H 2.71679800 -0.28700600 -0.77006700
 C 3.07074400 -1.56735600 1.84359500

C 2.11825000 -2.72441200 1.55213400
 H 3.50921300 -1.67429200 2.84655900
 H 3.88602600 -1.56956400 1.11784900
 H 1.38181100 -2.83805100 2.35183700
 H 2.67686800 -3.66441700 1.50410300
 P 1.22125900 -2.37093000 -0.04187300
 N 2.39854600 -0.23265900 1.73706300
 C -0.51953500 -3.06540100 0.16170100
 C -0.68123100 -4.35630100 0.98041700
 C -1.22904600 -3.16604400 -1.19897500
 H -1.01012100 -2.25796200 0.71852800
 H -0.21017000 -4.28906200 1.96529400
 H -1.74947900 -4.54323800 1.14599600
 H -0.27368200 -5.23254600 0.47108400
 H -1.13697900 -2.24472700 -1.78164500
 H -0.83380600 -3.98774900 -1.80449700
 H -2.29702400 -3.35760600 -1.04461300
 C 2.09316700 -3.40023800 -1.35887900
 C 1.98487400 -4.92222400 -1.17243700
 C 3.56947500 -2.99718900 -1.50485200
 H 1.57680900 -3.12635500 -2.28807000
 H 0.95779100 -5.28397800 -1.24446400
 H 2.56239700 -5.42380600 -1.95813600
 H 2.39771900 -5.24609100 -0.21051600
 H 3.69001500 -1.92734600 -1.68754100
 H 4.14769900 -3.26074200 -0.61199000
 H 4.01085300 -3.53936900 -2.34899500
 P 1.89093100 2.14379200 -0.04087000
 C 3.46472500 0.81723900 1.80136100
 C 2.92588400 2.21526700 1.50643800
 H 4.21834400 0.54864000 1.05881700
 H 3.93976100 0.79166500 2.79298800
 H 2.30279300 2.57733500 2.32821800
 H 3.75696100 2.92119800 1.40922600
 C 0.81240400 0.00050100 -1.80253000
 O 0.54143700 0.04819400 -2.93402800
 C 0.43021300 3.29667200 0.26487100
 C -0.32518400 3.57968400 -1.04444000
 C 0.69629900 4.59151400 1.04949100
 H -0.21455100 2.66354900 0.88720300
 H -0.56786200 2.66310500 -1.59095400
 H -1.26781000 4.09399100 -0.82399400
 H 0.25206100 4.22805800 -1.71178000
 H 1.21763900 4.41193700 1.99414800

H 1.27749500 5.31799500 0.47765700
 H -0.26349700 5.06253200 1.29471200
 C 2.92824900 2.89858500 -1.41834700
 C 4.20707400 2.08417600 -1.67403500
 C 3.27818500 4.38329800 -1.23147000
 H 2.28583300 2.80248600 -2.30330100
 H 3.99390500 1.03124500 -1.87067800
 H 4.72799500 2.49528100 -2.54630800
 H 4.89850800 2.14200600 -0.82525000
 H 2.39718800 5.02768300 -1.24626600
 H 3.81898600 4.55932900 -0.29479900
 H 3.93207300 4.70684700 -2.05012200
 H -0.86049000 0.12319800 0.69592900
 C -5.86539800 1.14792200 -1.45760000
 C -5.19062200 0.42230400 -2.63135100
 C -3.92377100 -0.33955000 -2.21359100
 C -3.06543100 0.42704400 -1.19053400
 C -3.42348900 0.24836500 0.27882000
 N -4.71623000 0.39466200 0.70177600
 C -5.91609700 0.33366000 -0.16098900
 N -2.41119700 0.01762300 1.07328500
 C -2.60883100 -0.11858200 2.51483300
 C -3.83175800 0.65480000 2.99436800
 C -5.02503600 0.25848900 2.13673200
 H -6.89632900 1.39732600 -1.73289300
 H -5.36794300 2.10193800 -1.24927000
 H -4.94126500 1.15864300 -3.40502100
 H -5.89845400 -0.27976100 -3.08844100
 H -3.31218500 -0.53959400 -3.10003300
 H -4.18885600 -1.32198000 -1.80535800
 H -3.08525800 1.49899200 -1.42591600
 H -2.02447300 0.11400900 -1.27311600
 H -6.16802300 -0.71520600 -0.37675400
 H -6.72793200 0.72416300 0.45710900
 H -1.70031800 0.23520900 3.01586200
 H -2.71486900 -1.18263300 2.77233000
 H -3.65108000 1.73205900 2.90042500
 H -4.04654100 0.44397500 4.04658600
 H -5.32992300 -0.77492700 2.35677100
 H -5.88334700 0.90185500 2.35381100
 C 1.47928100 -0.06164500 2.89348300
 H 0.97596900 0.90254700 2.83485700
 H 0.71631000 -0.83906600 2.88432000
 H 2.03634000 -0.11790100 3.83941700

DBU-6

Fe -1.46783300 0.01216600 -0.20586700
 H -0.01782300 -0.02942700 0.46317700
 H -2.90436900 0.04447600 -0.74552700
 C -3.24125400 1.20197600 1.94353100
 C -2.46370100 2.48184800 1.63672400
 H -3.64725800 1.23753800 2.96631700
 H -4.07888200 1.10584900 1.25085500
 H -1.71690500 2.67755300 2.41102300
 H -3.14415900 3.33951100 1.63184800
 P -1.59311800 2.27210700 0.00086000
 N -2.40071000 -0.02352000 1.78226800
 C 0.05422200 3.17988500 0.18767200
 C 0.08253700 4.49151400 0.98856800
 C 0.73996500 3.33716700 -1.17919900
 H 0.62875300 2.43673300 0.75509000
 H -0.39626800 4.39489400 1.96766500
 H 1.12585500 4.78120700 1.16737000
 H -0.39604200 5.31907700 0.46080800
 H 0.76594800 2.39402600 -1.73348800
 H 0.23528200 4.08083000 -1.80495600
 H 1.77434800 3.67546100 -1.04435000
 C -2.62198500 3.24707600 -1.24775500
 C -2.64520500 4.76996200 -1.04499000
 C -4.06200900 2.71417300 -1.32670400
 H -2.13183600 3.02916700 -2.20602800
 H -1.66482600 5.22987000 -1.18136500
 H -3.32193900 5.22453200 -1.77891200
 H -3.01749600 5.04178100 -0.05063800
 H -4.08977300 1.63765000 -1.50674700
 H -4.61781700 2.92374600 -0.40511600
 H -4.59130600 3.21501400 -2.14589500
 P -1.66527200 -2.25187400 -0.11081000
 C -3.29570800 -1.21738600 1.87107100
 C -2.57358800 -2.51205400 1.49850700
 H -4.12246300 -1.04657200 1.17951300
 H -3.71159500 -1.29067400 2.88784500
 H -1.85249500 -2.79222900 2.27128800
 H -3.29485300 -3.33273100 1.43012000
 C -0.90339000 0.05361100 -1.83743500
 O -0.57592900 0.08906300 -2.96008700
 C -0.05341500 -3.22578800 0.06589600
 C 0.65324200 -3.35266000 -1.29349200

C -0.08663800 -4.57019600 0.81057200
H 0.53658300 -2.52949600 0.67492500
H 0.72941400 -2.38889800 -1.80595000
H 1.66974100 -3.73994900 -1.15397800
H 0.13191000 -4.04715800 -1.96056900
H -0.57065600 -4.49632200 1.78901100
H -0.59278000 -5.35494000 0.24445200
H 0.94237800 -4.90935400 0.98535300
C -2.69754400 -3.14035300 -1.42042800
C -4.11686600 -2.55653000 -1.51278200
C -2.77756000 -4.66836800 -1.27894700
H -2.17766700 -2.90331600 -2.35828300
H -4.10704800 -1.47520500 -1.66258400
H -4.64457400 -3.01699700 -2.35632900
H -4.69867200 -2.77355600 -0.60925100
H -1.81187500 -5.15747600 -1.41801200
H -3.17651300 -4.96680200 -0.30270000
H -3.45643300 -5.06948900 -2.04150000
H 1.64042900 -0.00494800 0.75392300
C 6.02160800 -0.63084100 -1.53109000
C 5.32198500 0.18498200 -2.62700800
C 4.04933800 0.87834700 -2.12258300
C 3.20964100 -0.01472300 -1.19351700
C 3.61180900 -0.01714700 0.26786800
N 4.87831500 -0.04645700 0.68984400
C 6.08531700 0.06888700 -0.17235000
N 2.60091900 -0.00719400 1.13208100
C 2.72780000 -0.05107000 2.59029600
C 4.06889200 -0.66656500 2.95628900
C 5.17117900 -0.00076100 2.14291000
H 7.05355600 -0.83862200 -1.83367200
H 5.54324300 -1.60848300 -1.40230800
H 5.07478200 -0.48201200 -3.46125800
H 6.00947500 0.94083900 -3.02416100
H 3.42403600 1.16692800 -2.97316100
H 4.30050200 1.80965400 -1.60164300
H 3.22381200 -1.05155500 -1.55042200
H 2.16515600 0.30048900 -1.22148300
H 6.33159700 1.13184100 -0.28868900
H 6.88872700 -0.38028300 0.41349300
H 1.89303600 -0.63937800 2.97849300
H 2.63869700 0.96511500 2.99201100
H 4.05687500 -1.74234400 2.75181300
H 4.27148600 -0.52974300 4.02146900

H 5.30485700 1.04596900 2.44265400
H 6.12074900 -0.51556200 2.29962400
C -1.41626700 -0.07739900 2.89119500
H -0.79615300 -0.96766900 2.79941100
H -0.75882200 0.78959000 2.85079500
H -1.92908300 -0.09579600 3.86484900

DBU-ATS1_2

Fe 1.52513100 0.02777400 -0.23625000
H -0.16011100 0.03044800 -0.10929700
H 3.03040900 0.05365700 -0.37080000
C 2.42291000 -1.10007300 2.37963700
C 1.78971800 -2.39799000 1.87018800
H 2.36965300 -1.09482600 3.48786300
H 3.51194400 -1.11563500 2.14429700
H 0.77933200 -2.49369900 2.28304400
H 2.35551100 -3.28836000 2.16567000
P 1.60483200 -2.22582300 0.03031100
N 1.75117300 0.05722000 1.81919200
C 0.00972400 -3.14906400 -0.38257500
C -0.27424800 -4.46502600 0.36076900
C -0.17246400 -3.31090200 -1.90004000
H -0.73642100 -2.42303000 -0.03794600
H -0.13946900 -4.37024300 1.44227700
H -1.31790200 -4.75858300 0.18856700
H 0.35264300 -5.29060000 0.01582900
H -0.03907100 -2.36350400 -2.43091300
H 0.53450500 -4.03456700 -2.32065300
H -1.18250700 -3.67732100 -2.12145700
C 3.01910400 -3.19219500 -0.76411000
C 2.98455600 -4.71681000 -0.57673300
C 4.38601300 -2.64432900 -0.32164100
H 2.90430700 -2.97293300 -1.83444500
H 2.12505000 -5.18044500 -1.06486000
H 3.88631000 -5.16103600 -1.01713900
H 2.97025800 -4.99841400 0.48243100
H 4.45879600 -1.56417300 -0.46558600
H 4.57991100 -2.86068200 0.73489500
H 5.18071000 -3.12470200 -0.90553000
P 1.52136700 2.28718400 -0.02141700
C 2.38559800 1.24847900 2.35085700
C 1.71044500 2.51325700 1.81281100
H 3.47299600 1.29458500 2.11263800
H 2.33446900 1.26705600 3.45905800

H 0.69950200 2.59168900 2.22844100
H 2.25257100 3.42624400 2.08222400
C 1.49356400 0.00298700 -1.97522700
O 1.58767800 -0.01373000 -3.14314000
C -0.11747600 3.12882200 -0.43215200
C -0.35758200 3.19286400 -1.94864200
C -0.42807500 4.47497900 0.24408000
H -0.82066100 2.39422600 -0.02058600
H -0.23664800 2.21418900 -2.42256500
H -1.37813500 3.53900000 -2.15440900
H 0.32681900 3.89263900 -2.44074200
H -0.24636400 4.45237300 1.32276200
H 0.14886100 5.30177300 -0.17630200
H -1.48939500 4.71487000 0.09920500
C 2.89591100 3.27928700 -0.85286600
C 4.27726800 2.84189900 -0.33807500
C 2.77575000 4.80917000 -0.78134300
H 2.82230900 2.97641300 -1.90595900
H 4.40407000 1.75745000 -0.37392600
H 5.06119500 3.29998800 -0.95342000
H 4.43945600 3.17033700 0.69472200
H 1.90463100 5.18743000 -1.32015100
H 2.72255300 5.16754200 0.25289900
H 3.66252100 5.26748000 -1.23757100
H -0.97113600 -0.10307500 0.29244600
C -6.05903400 0.61653400 -1.07552100
C -5.56291300 -0.17179800 -2.29719700
C -4.22956000 -0.88861900 -2.04089500
C -3.23183600 -0.03852500 -1.23356300
C -3.35012200 -0.11304100 0.28285400
N -4.55541500 0.01523300 0.90642800
C -5.87981800 -0.11390200 0.25935000
N -2.21596900 -0.25038500 0.92211200
C -2.15719900 -0.31071600 2.38126200
C -3.31302500 0.46093700 3.00500500
C -4.61654400 -0.02057900 2.38100100
H -7.12710700 0.83122600 -1.19408000
H -5.56030000 1.59024900 -1.00940300
H -5.45605400 0.51827800 -3.14304500
H -6.31791400 -0.91046900 -2.59290800
H -3.76655300 -1.15151500 -2.99800300
H -4.40389700 -1.83836700 -1.52148100
H -3.30849900 1.01243300 -1.53973500
H -2.21201900 -0.34838200 -1.46501200

H -6.13891200 -1.17734900 0.15269200
H -6.58748200 0.30485300 0.97872500
H -1.18431500 0.08319900 2.68848600
H -2.18912000 -1.36190500 2.70117700
H -3.18638400 1.53378000 2.81961200
H -3.34888100 0.31182500 4.08848900
H -4.84791700 -1.04179800 2.71551000
H -5.44846500 0.61933500 2.69065600

DBU-A2

Fe 1.60001000 0.04492000 -0.25672800
H 0.00972700 0.00752900 -0.40778200
H 3.14202200 0.07730800 -0.02784900
C 2.04827400 -1.14175800 2.45055700
C 1.53288600 -2.43393400 1.80713300
H 1.84766200 -1.18957100 3.54258300
H 3.15955800 -1.12387900 2.36322100
H 0.47508100 -2.57016700 2.05918800
H 2.07315500 -3.32091800 2.15684200
P 1.62757400 -2.20114000 -0.03697300
N 1.42909100 0.02088200 1.84871800
C 0.10706400 -3.11156600 -0.69972200
C -0.27227900 -4.46533200 -0.07623900
C 0.12196800 -3.18318000 -2.23468000
H -0.67558800 -2.39705400 -0.41625000
H -0.25023500 -4.44377200 1.01781500
H -1.29668500 -4.72719100 -0.37303000
H 0.37399100 -5.28097700 -0.40832100
H 0.31632900 -2.20447400 -2.68323000
H 0.88294800 -3.87977700 -2.60358300
H -0.84776800 -3.53492100 -2.60886600
C 3.13870100 -3.17642300 -0.63005200
C 3.03679500 -4.70797300 -0.56360300
C 4.41927800 -2.71543700 0.08503400
H 3.22477600 -2.88217200 -1.68502500
H 2.27399500 -5.10822800 -1.23438300
H 3.99466700 -5.15316500 -0.86211000
H 2.81953600 -5.05952200 0.45144800
H 4.53785200 -1.63052500 0.05357400
H 4.42399600 -3.02783700 1.13585800
H 5.29348400 -3.17253100 -0.39526300
P 1.48514200 2.28652100 0.01078000
C 1.98053700 1.20491500 2.47209000
C 1.37885100 2.47336100 1.85900900

H	3.09033000	1.25829500	2.37694900	H	-3.39661300	1.26760900	-1.38459200
H	1.78551100	1.21717600	3.56608700	H	-2.20329700	-0.00874000	-1.47625000
H	0.31473600	2.53181800	2.11548500	H	-6.11860400	-1.28352200	0.00442700
H	1.85953200	3.38661900	2.22719300	H	-6.60281600	0.08383800	0.99685500
C	1.87276100	0.06398600	-1.96670300	H	-1.20234700	-0.02527900	2.69920300
O	2.12154600	0.07686200	-3.11457400	H	-2.05815500	-1.55992400	2.52768200
C	-0.09269600	3.11458400	-0.62714600	H	-3.34148200	1.17896100	3.03641300
C	-0.08350300	3.23879200	-2.15859900	H	-3.39234100	-0.23077600	4.10354900
C	-0.55736300	4.41954500	0.04030700	H	-4.75083600	-1.49789500	2.51174500
H	-0.82499400	2.34053200	-0.36720800	H	-5.50319900	0.08572400	2.73342800
H	0.16570500	2.28871800	-2.64030400				
H	-1.07185400	3.54744600	-2.52207900	Li-A6			
H	0.63615000	3.99026400	-2.50201800	C	1.21433900	0.27386200	-0.71233000
H	-0.53250900	4.36312400	1.13279700	O	2.05580600	0.12992500	-1.63221300
H	0.03612700	5.28463000	-0.26334200	O	1.49234200	0.38445800	0.52055000
H	-1.59651200	4.62577300	-0.24878900	Fe-2.11073800	-0.14623400	-0.14331800	
C	2.92680700	3.37441600	-0.56094900	H	0.13642300	0.31202600	-1.00970500
C	4.24325700	2.96188300	0.11768200	H	-3.41945300	-0.39508900	0.46889100
C	2.73278600	4.89341500	-0.43098100	C	-1.61269500	0.94880800	2.61326800
H	3.01474400	3.12827400	-1.62782000	C	-1.57253000	2.29732000	1.89657600
H	4.42959500	1.88944100	0.02949200	H	-0.97714600	0.97466600	3.50880400
H	5.08045900	3.49721000	-0.34732900	H	-2.62961600	0.70457200	2.93106900
H	4.24182100	3.22043600	1.18292600	H	-0.53200600	2.59466700	1.73110800
H	1.94200500	5.27208400	-1.08168900	H	-2.04408200	3.07988700	2.49856300
H	2.49946400	5.18908600	0.59830800	P	-2.37089200	2.10764200	0.22504000
H	3.65926000	5.40893700	-0.71500900	N	-1.15573000	-0.13324700	1.69807800
H	-1.34844800	-0.11674100	0.40045100	C	-1.38768200	3.22584400	-0.92800000
C	-6.09526100	0.64263300	-1.00911800	C	-0.95151400	4.59289800	-0.37458300
C	-5.56004200	0.03074000	-2.31134700	C	-2.08346900	3.35999500	-2.29186000
C	-4.17841900	-0.61688600	-2.14000600	H	-0.47503500	2.63412700	-1.07922100
C	-3.24549700	0.19361100	-1.22231500	H	-0.44482700	4.51140100	0.59145400
C	-3.38329900	-0.08324000	0.26173700	H	-0.24250900	5.04879200	-1.07617700
N	-4.56395200	-0.16298700	0.88916800	H	-1.78832900	5.28547400	-0.26125900
C	-5.89394200	-0.23280000	0.22943900	H	-2.30983400	2.38543000	-2.73515000
N	-2.24301700	-0.21917100	0.92476900	H	-3.01911400	3.92390600	-2.21851300
C	-2.13693700	-0.47826600	2.36281300	H	-1.42975000	3.89629600	-2.98888300
C	-3.36588300	0.08394900	3.05710100	C	-4.12424000	2.76853800	0.36095800
C	-4.61581200	-0.42133800	2.34838800	C	-4.23759400	4.28027500	0.60809500
H	-7.17226100	0.81809000	-1.10644300	C	-4.92594300	1.99602800	1.42236100
H	-5.64591300	1.62453500	-0.82350000	H	-4.55697700	2.53959700	-0.62141600
H	-5.50804000	0.81776900	-3.07316100	H	-3.84448100	4.87112100	-0.22140200
H	-6.26579400	-0.71985800	-2.68646000	H	-5.29422400	4.54767900	0.72816800
H	-3.69307300	-0.71624500	-3.11592300	H	-3.71926900	4.58340300	1.52471500
H	-4.27728400	-1.63634500	-1.74905800	H	-4.91368800	0.91792500	1.24563000
				H	-4.54355800	2.18499800	2.43175000

H -5.96905800 2.33134600 1.40128600
P -1.66218800 -2.39728900 -0.13988400
C -1.13260000 -1.44655300 2.39809700
C -0.69099100 -2.55336500 1.44233500
H -2.14068500 -1.63643800 2.77485700
H -0.45583700 -1.39710100 3.26185700
H 0.36639000 -2.42059400 1.18968700
H -0.79493800 -3.53903300 1.90628700
C -3.02876400 -0.17004400 -1.62488100
O -3.74453800 -0.20429600 -2.54161800
C -0.49705400 -2.96816900 -1.50626900
C -1.24371700 -3.16133900 -2.83622200
C 0.41258800 -4.16535200 -1.18694000
H 0.15232000 -2.09105700 -1.61999500
H -1.84402500 -2.28699700 -3.10486200
H -0.51981300 -3.32369600 -3.64274300
H -1.90626000 -4.03251500 -2.81026600
H 0.96836200 -4.02926700 -0.25488400
H -0.13947100 -5.10568400 -1.11779000
H 1.14928300 -4.27672900 -1.99169400
C -3.10877400 -3.59199700 -0.03077700
C -3.99855900 -3.27241100 1.18219500
C -2.73058600 -5.08071800 -0.03174600
H -3.68565100 -3.37471100 -0.93940300
H -4.30850100 -2.22464900 1.20302300
H -4.90199500 -3.89152400 1.14226300
H -3.48856000 -3.50171400 2.12456300
H -2.25044100 -5.39011400 -0.96189100
H -2.06541300 -5.33192300 0.80196000
H -3.63904500 -5.68366100 0.08424400
Li 3.42930700 0.23348500 -0.18800900
C 4.33308700 2.84506300 -1.30741800
C 5.38125400 2.32562800 0.76848800
C 4.85133200 4.13908200 -0.68549100
C 5.97257900 3.62839800 0.23207700
H 4.77404300 2.49629500 1.66651900
H 3.27410700 2.87269100 -1.57562600
H 4.06390100 4.62164100 -0.09600200
H 4.91316900 2.55776600 -2.19295600
H 5.19956500 4.84856900 -1.44042200
H 6.22722400 4.32527100 1.03461400
H 6.87928300 3.42589500 -0.34841600
H 6.13192400 1.56165700 0.98933700
O 4.51569800 1.82643900 -0.28597700

C 4.63871700 -1.90818200 1.59479800
C 5.90371000 -2.75653900 1.49139800
C 5.30790600 -2.00325100 -0.69089800
C 5.84898600 -3.23525300 0.03281600
H 3.75905100 -2.51940700 1.83249000
H 6.79248000 -2.13808000 1.65833000
H 6.11305200 -1.31925900 -0.98535300
H 4.70309000 -2.23836400 -1.57116300
H 6.82136300 -3.54650700 -0.35709100
H 5.15318400 -4.07524500 -0.06840400
H 5.91269000 -3.57462500 2.21608200
H 4.71000500 -1.09457800 2.32281500
O 4.45858800 -1.32612600 0.27727900
H -0.17963000 0.08593300 1.42630000

Li-A6b

C -0.77256400 -0.13350400 -2.00015700
O -0.40502400 -0.07795700 -0.77290300
O -1.97384300 -0.19249600 -2.34644900
Fe 1.60554900 0.05025100 -0.13322800
H 0.01569700 -0.12737600 -2.77194500
H 2.95756300 0.16375900 0.50409800
C 1.12574200 -1.06044800 2.65261600
C 0.95561400 -2.37562600 1.89620600
H 0.51026000 -1.05876100 3.56271200
H 2.16607700 -0.92086300 2.95531400
H -0.10893800 -2.57910800 1.73444500
H 1.35889000 -3.21017500 2.47793700
P 1.74716000 -2.21768800 0.21666600
N 0.76610700 0.09814100 1.79007200
C 0.68350800 -3.29236700 -0.90114500
C 0.23586800 -4.66089500 -0.36065400
C 1.29676100 -3.40935800 -2.30531100
H -0.21573200 -2.67002400 -0.98464500
H -0.19026700 -4.59648100 0.64517800
H -0.53981300 -5.06995400 -1.01956700
H 1.05088800 -5.38675000 -0.33447600
H 1.55644800 -2.43160900 -2.72227100
H 2.20231800 -4.02510200 -2.30383400
H 0.58035800 -3.88181300 -2.98732400
C 3.46453300 -2.98177200 0.33475300
C 3.51231400 -4.51353000 0.44074800
C 4.27630100 -2.35400500 1.48072200
H 3.93522000 -2.68435300 -0.61139700

H 3.12308900 -5.00827700 -0.45115800
H 4.55413800 -4.83411000 0.56155000
H 2.95642500 -4.88030800 1.31076300
H 4.28463000 -1.26268300 1.43354900
H 3.88567300 -2.65659900 2.45895400
H 5.31352400 -2.70369900 1.42351900
P 1.48498900 2.34414900 -0.01681000
C 0.96772700 1.37622900 2.52629500
C 0.65101300 2.57424900 1.63466700
H 2.01216300 1.39884100 2.84539400
H 0.34317500 1.39338900 3.43013300
H -0.42746200 2.62183600 1.44265900
H 0.93480800 3.50940000 2.12742700
C 2.51458900 0.02380800 -1.61657000
O 3.22510300 0.01454700 -2.54042600
C 0.31839100 3.17949900 -1.23430500
C 0.91219100 3.21172400 -2.65124700
C -0.27291600 4.54219400 -0.83541600
H -0.50859800 2.45980800 -1.24089500
H 1.26845500 2.22824500 -2.97172400
H 0.14880600 3.53775900 -3.36719200
H 1.75005700 3.91272800 -2.72600100
H -0.67680400 4.54356100 0.18160000
H 0.45388400 5.35388100 -0.90937800
H -1.09977600 4.78439000 -1.51451600
C 3.10758800 3.29925400 0.03529100
C 3.95934200 2.88798100 1.24795800
C 2.98707700 4.82932300 -0.02197100
H 3.62638600 2.95734500 -0.87001600
H 4.09028900 1.80549100 1.31370900
H 4.95195100 3.34510400 1.16370000
H 3.51633600 3.24298100 2.18537100
H 2.56137300 5.18048500 -0.96359000
H 2.37969400 5.22314400 0.80034600
H 3.98550500 5.27369500 0.06993200
Li -2.57380000 -0.14290100 -0.48605000
C -3.67417800 1.87476200 1.53612900
C -4.32329700 2.19911400 -0.73606400
C -4.46949600 3.17482000 1.43167800
C -5.30610800 2.94074700 0.16522100
H -3.68502400 2.88944900 -1.29932000
H -2.69018300 1.99869200 1.99800700
H -3.79478700 4.02652800 1.29275000
H -4.22904300 1.10369100 2.08379300

H -5.07492100 3.35827200 2.32277900
H -5.66464600 3.86580700 -0.29296800
H -6.17268300 2.30894700 0.38929500
H -4.80061100 1.50798600 -1.43615800
O -3.48133000 1.42425600 0.16772000
C -3.35270500 -2.95223000 -0.64604300
C -4.79515700 -3.43977100 -0.69923100
C -4.60039300 -1.76571500 0.99927100
C -5.29112700 -3.10163700 0.71445900
H -2.69624400 -3.69432600 -0.17624800
H -5.35962700 -2.87964600 -1.45299800
H -5.21621000 -0.91401200 0.69118500
H -4.31878900 -1.64057000 2.04892500
H -6.37877900 -3.02132200 0.78419800
H -4.95788700 -3.86442300 1.42614300
H -4.86285000 -4.50439000 -0.93717300
H -2.93802900 -2.66523300 -1.61504000
O -3.38593800 -1.76130800 0.19083700
H -0.22970800 0.02161000 1.57055900

Li-A6'

C 0.93308800 -0.86642500 -0.74333900
O 1.85352700 -0.73766600 -1.58674000
O 1.11886400 -1.09287300 0.49279100
Fe-2.16521600 0.32280900 -0.16697100
H -0.12031400 -0.78204100 -1.10847100
H -3.38716700 0.84960900 0.44910700
C -1.01408700 1.17282000 2.48921700
C -0.28197500 2.20788900 1.63719000
H -0.40611000 0.90293300 3.36305300
H -1.96568700 1.56861300 2.85347000
H 0.72621900 1.84631000 1.40772600
H -0.17657400 3.15548300 2.17398500
P -1.18339500 2.39300800 0.01794900
N -1.31143100 -0.04402700 1.68511100
C 0.15148400 2.77390200 -1.25617600
C 1.27582500 3.72700400 -0.81830800
C -0.46618200 3.19598100 -2.59916100
H 0.61056000 1.78777800 -1.40278900
H 1.73138000 3.42717200 0.12959900
H 2.06791900 3.71035200 -1.57648200
H 0.93698800 4.76085200 -0.72082400
H -1.20972300 2.47579400 -2.95395600
H -0.94704800 4.17756300 -2.53691500

H 0.31923500 3.26013500 -3.36067300
C -2.32231800 3.88080000 0.16869300
C -1.61640400 5.24234200 0.25627400
C -3.29880500 3.71811700 1.34625900
H -2.90671400 3.84656300 -0.76014600
H -1.05127200 5.48177900 -0.64635700
H -2.36749400 6.03028500 0.38978000
H -0.93550600 5.29346300 1.11299100
H -3.84046600 2.76971000 1.30870200
H -2.77799300 3.78166000 2.30808700
H -4.03488700 4.52971500 1.31959700
P -2.98995800 -1.82236800 0.03907400
C -2.02276600 -1.05934600 2.50916100
C -2.28928000 -2.32025600 1.68860900
H -2.95917800 -0.61097400 2.85079700
H -1.42451700 -1.30500500 3.39684000
H -1.34613000 -2.84403300 1.50101500
H -2.94431300 -3.00931800 2.23041700
C -3.00324000 0.67553200 -1.65576300
O -3.66042300 0.95281900 -2.57528400
C -2.31383700 -3.07707000 -1.19112300
C -2.99862900 -2.93560600 -2.55972100
C -2.25200900 -4.54315000 -0.73223200
H -1.27790800 -2.73224000 -1.30361100
H -2.97698800 -1.90442000 -2.92535100
H -2.48064200 -3.55847300 -3.29766500
H -4.04295700 -3.26274800 -2.52898700
H -1.74935200 -4.65874800 0.23225100
H -3.23990500 -5.00282800 -0.65722700
H -1.67744000 -5.11991100 -1.46693600
C -4.85700600 -2.02207300 0.14331000
C -5.44209800 -1.16734400 1.28035100
C -5.35419300 -3.47044900 0.26045700
H -5.21108100 -1.60511100 -0.80831100
H -5.14717800 -0.11784800 1.20382500
H -6.53646800 -1.21493800 1.24302100
H -5.13318800 -1.54187500 2.26258300
H -5.12485700 -4.06369700 -0.62664500
H -4.93144700 -3.97838800 1.13451300
H -6.44430300 -3.46962800 0.37995800
S 5.37427100 -0.80207400 0.88538100
O 6.20846400 -0.84742300 2.08916600
C 6.55133000 -0.55981800 -0.53276200
F 7.22141300 0.59043700 -0.39208200

F 5.86875800 -0.52023500 -1.68783300
F 7.43041600 -1.56761600 -0.58851100
O 4.43123500 0.35511500 0.74977900
O 4.64223500 -2.05649500 0.51296900
Li 3.05456400 -0.92469200 -0.01441100
H -0.40348800 -0.45892200 1.40607800

Li-A6b'

C 0.06688900 0.05687200 2.63248200
O 0.13313800 0.03939600 1.34791300
O 1.08548600 0.14361200 3.34983600
H -0.92992300 -0.01254000 3.09811700
Li 2.15304600 0.16890900 1.71288900
O 3.70698700 -0.96978100 1.10959900
S 4.37640900 0.26690300 0.58855300
O 5.79842000 0.43742400 0.89320600
C 4.30165700 0.06293900 -1.25973600
O 3.47371800 1.43498500 0.85382000
F 4.79368700 1.14551600 -1.86925300
F 3.02400400 -0.10289500 -1.65850600
F 5.00170100 -1.00974700 -1.63942200
Fe -1.51429100 -0.06061900 0.04718100
H -2.56400300 -0.12843900 -1.02257600
P -1.28190900 -2.34748700 -0.13126000
P -1.54385300 2.23361600 -0.18607900
C -2.87953900 -0.12516800 1.12450300
C 0.06523400 -2.46526000 -1.41004200
C -0.58980700 -3.21990500 1.38435500
C -2.73756800 -3.35678100 -0.77038200
C -0.25300700 2.47743200 -1.50888600
C -0.89034200 3.21264000 1.28063100
C -3.13421700 3.03497300 -0.79799600
O -3.86925000 -0.17232500 1.73870700
C 0.00555200 -1.23099500 -2.30713000
H 1.02198000 -2.48492100 -0.87583200
H 0.00701500 -3.38263800 -2.00411600
C 0.22997200 -4.50155500 1.16262000
C -1.68147500 -3.41845700 2.44845500
H 0.10627300 -2.46301700 1.76298600
C -2.50939900 -4.87514400 -0.83251900
C -3.22657600 -2.84391000 -2.13561400
H -3.52763300 -3.15394900 -0.03513400
C -0.16140400 1.21018900 -2.35541800
H 0.70261300 2.65005700 -1.00062200

H	-0.44711200	3.35154200	-2.13837100	C	2.47724100	-1.32951800	-1.43070400
C	-1.91277200	3.23996400	2.42766400	C	2.95110700	1.57618500	-0.89152600
C	-0.29796300	4.60532400	1.00851800	C	3.34332800	-0.49226200	1.33569200
H	-0.05698900	2.57394600	1.59632900	C	-2.47724500	-1.32991800	-1.43032900
C	-3.53715500	2.48546600	-2.17684200	C	-2.95156600	1.57577500	-0.89196800
C	-3.14501000	4.57066400	-0.81874900	C	-3.34295700	-0.49207800	1.33601500
H	-3.88180000	2.69250800	-0.07033800	O	0.00002500	1.73748500	2.45635700
H	0.88736700	-1.18975000	-2.96010500	C	1.22802800	-2.20652000	-1.43097600
H	-0.88264300	-1.25377300	-2.94342200	H	2.58174700	-0.83608700	-2.40273100
N	-0.07930300	0.00668300	-1.48459800	H	3.37738700	-1.93249300	-1.27897300
H	1.02255200	-4.36871100	0.42033300	C	4.19175100	1.45458400	-1.79064300
H	0.71705900	-4.77798500	2.10581600	C	3.14074500	2.65959900	0.18248900
H	-0.38453900	-5.34986000	0.85381100	H	2.11133600	1.88560600	-1.53145800
H	-2.23203200	-2.49451600	2.65155700	C	4.85068800	-0.54439600	1.04835800
H	-2.40663200	-4.18173500	2.14742400	C	2.85461900	-1.81933600	1.93903100
H	-1.22775400	-3.74908500	3.38976000	H	3.15057100	0.30295000	2.06733600
H	-2.36223300	-5.31792700	0.15448800	C	-1.22788400	-2.20671500	-1.43067600
H	-3.38972000	-5.35629300	-1.27586000	H	-2.58205500	-0.83675600	-2.40246000
H	-1.64804200	-5.13422800	-1.45833300	H	-3.37725200	-1.93301100	-1.27823400
H	-3.43948400	-1.77243900	-2.12272300	C	-3.14067200	2.65965800	0.18166500
H	-2.49198300	-3.04114100	-2.92474100	C	-4.19260200	1.45385200	-1.79049600
H	-4.14803900	-3.37020900	-2.41039800	H	-2.11209900	1.88491300	-1.53243600
H	-1.04955300	1.09403300	-2.98116200	C	-2.85426400	-1.81915100	1.93934700
H	0.71439900	1.25479200	-3.01687000	C	-4.85039500	-0.54413400	1.04905800
H	-2.28974800	2.24032700	2.66516900	H	-3.14995400	0.30318800	2.06753500
H	-1.44612200	3.64356200	3.33364600	H	1.22038800	-2.86749800	-2.30713700
H	-2.77318800	3.87517500	2.19152700	H	1.18758200	-2.83161100	-0.53550400
H	0.42915000	4.59764000	0.19117100	N	0.00000800	-1.35764600	-1.42451200
H	-1.06001900	5.35218300	0.77691000	H	4.05210000	0.73896000	-2.60575100
H	0.23105400	4.94627600	1.90690000	H	4.39679100	2.42975400	-2.24827100
H	-3.56669400	1.39344200	-2.19246500	H	5.08351000	1.16094100	-1.23166900
H	-4.53508100	2.85659500	-2.43753800	H	2.25027500	2.78770900	0.80534000
H	-2.84912200	2.82552300	-2.95916700	H	3.98509000	2.42879400	0.83972000
H	-3.04949900	5.00179100	0.17960900	H	3.35055900	3.62180300	-0.29773900
H	-2.34541100	4.97742400	-1.44757100	H	5.25512700	0.43187800	0.77327600
H	-4.09740900	4.92000200	-1.23573200	H	5.37974600	-0.87844400	1.94859700
H	0.79344800	0.07845100	-0.95795000	H	5.08771600	-1.25440800	0.24825400
Li-A7				H	1.79438400	-1.78408600	2.20275400
Fe	0.00001800	0.07369200	0.07676900	H	3.00988900	-2.65646100	1.24907300
H	-0.00015100	-0.98008500	1.09512500	H	3.42466400	-2.03692800	2.84920700
P	2.27971300	-0.01017300	-0.12915900	H	-1.18719900	-2.83169400	-0.53513800
P	-2.27969900	-0.01018600	-0.12919900	H	-1.22028300	-2.86779700	-2.30676000
C	0.00000700	1.13530600	1.46201700	H	-2.24979100	2.78817900	0.80384600
				H	-3.35098100	3.62161300	-0.29884300

H -3.98452700 2.42898900 0.83957500
H -4.05352900 0.73756900 -2.60512800
H -5.08423900 1.16094800 -1.23094500
H -4.39749700 2.42875200 -2.24876900
H -1.79395800 -1.78404800 2.20279200
H -3.42411600 -2.03657100 2.84968500
H -3.00984100 -2.65632400 1.24951300
H -5.25488400 0.43218000 0.77420200
H -5.08764700 -1.25404300 0.24892800
H -5.37923700 -0.87827500 1.94939000
H -0.00014400 -0.83068800 -2.30422900

DBU-A3

Fe 1.58496200 0.17703900 -0.34475400
H 0.19522500 0.14212300 0.79084500
H 2.87606400 0.45276600 -1.02187200
C 3.74109700 -0.70793300 1.55910300
C 3.19435000 -2.10373900 1.26854700
H 4.17500300 -0.67804200 2.56859400
H 4.52796700 -0.43889400 0.84832200
H 2.50725000 -2.39246600 2.07026700
H 3.99727500 -2.84687600 1.22903900
P 2.19845600 -2.02911700 -0.29937600
N 2.65335100 0.29602400 1.44873400
C 0.78801100 -3.24642300 -0.03848800
C 1.12725900 -4.58329700 0.64094100
C -0.02092100 -3.44812000 -1.32919300
H 0.15615500 -2.68149000 0.65800900
H 1.68720900 -4.44725900 1.57081800
H 0.19318800 -5.09766100 0.89776100
H 1.70070500 -5.25204400 -0.00500400
H -0.30684000 -2.49629900 -1.78592300
H 0.53589500 -4.03041900 -2.07179100
H -0.94513400 -3.99170700 -1.10596200
C 3.29222500 -2.65221400 -1.69842900
C 3.59646400 -4.15768000 -1.68225800
C 4.60241800 -1.85110600 -1.77528500
H 2.70599900 -2.42528100 -2.59868100
H 2.69991000 -4.76685900 -1.80980800
H 4.27626000 -4.39865000 -2.50865700
H 4.09197600 -4.46347000 -0.75413700
H 4.42348200 -0.77364600 -1.80055800
H 5.25685900 -2.07313400 -0.92474100
H 5.14663200 -2.12792400 -2.68572300

P 1.30476400 2.43869000 -0.09760700
C 3.17851100 1.64983800 1.75969600
C 2.09813400 2.71005200 1.55705400
H 4.03517300 1.83763300 1.10556800
H 3.54023100 1.67636200 2.79758600
H 1.30054400 2.56056100 2.29170900
H 2.50602300 3.71843500 1.67909400
C 0.95202200 0.12895500 -1.97295500
O 0.63956100 0.11798800 -3.09297100
C -0.47255400 3.01761200 0.11378200
C -1.21918000 3.04791600 -1.22816600
C -0.69486700 4.30884900 0.91876200
H -0.87575800 2.19817900 0.71869200
H -1.12559700 2.10353900 -1.77284100
H -2.28728600 3.22366500 -1.05346600
H -0.85914200 3.85093200 -1.88080400
H -0.15396400 4.30461100 1.86909600
H -0.40840800 5.20850100 0.36878300
H -1.76222500 4.39811900 1.15583300
C 2.15810600 3.56477600 -1.34250000
C 3.67072000 3.29576800 -1.40375200
C 1.90030600 5.06742700 -1.15229400
H 1.72300600 3.25854900 -2.30301500
H 3.89498500 2.23681600 -1.55125900
H 4.10715500 3.85634500 -2.23859000
H 4.17240100 3.63096000 -0.48913100
H 0.85347200 5.33422100 -1.30829300
H 2.19824700 5.41051000 -0.15532400
H 2.49259700 5.63286600 -1.88212300
H 0.06065400 -0.39805900 0.23125800
C -6.04277000 1.06703800 -1.14015800
C -6.02354200 0.30384900 -2.47358300
C -5.12515800 -0.94138100 -2.43435900
C -3.81711400 -0.71974700 -1.65237400
C -3.87240100 -0.98229400 -0.15048000
N -4.85607600 -0.36929600 0.61367900
C -6.12762800 0.16961800 0.09920900
N -2.92670300 -1.74275300 0.30665500
C -2.87467000 -2.05389600 1.73434700
C -3.54208300 -0.99495100 2.60706700
C -4.92448300 -0.69471800 2.04579700
H -6.90701500 1.74137100 -1.12474900
H -5.15761400 1.70622000 -1.04404100
H -5.68050500 0.98338200 -3.26402300

H -7.04463700 0.00665300 -2.74422400
H -4.88002800 -1.24404800 -3.45866700
H -5.66844200 -1.78713800 -1.99495500
H -3.44983900 0.29918500 -1.83224400
H -3.04443500 -1.39707100 -2.01945000
H -6.85051500 -0.64470000 -0.07513400
H -6.53700900 0.76624600 0.92026200
H -1.82241300 -2.17114800 2.02173100
H -3.34653200 -3.03522100 1.90244300
H -2.92698000 -0.08842400 2.60936900
H -3.63139700 -1.33489200 3.64508900
H -5.59761700 -1.55245300 2.20808800
H -5.37140500 0.16208800 2.56260400
H 1.96390700 0.05085500 2.20114200
C -0.09558900 0.11075500 3.57785600
O -0.52603000 0.97659400 2.77714400
O 0.99452200 -0.52558900 3.53810700
H -0.75643700 -0.13251400 4.45251900

DBU-ATS3_4

Fe-1.41283700 0.06837000 -0.44567800
H 0.07909600 -0.14500300 0.32403800
H -2.80507900 0.08622900 -0.98371300
C -3.06585200 1.09189200 1.87098100
C -2.24503300 2.36086900 1.65200600
H -3.35059000 1.00581800 2.92902200
H -3.98477900 1.11758400 1.27745300
H -1.38775700 2.35760100 2.33291900
H -2.83423900 3.25852400 1.86534200
P -1.57569900 2.32375300 -0.08216800
N -2.28766300 -0.10184200 1.46027900
C 0.05186700 3.27156500 -0.02960300
C 0.13636600 4.46627200 0.93416900
C 0.52729500 3.64492400 -1.44342700
H 0.73900200 2.50390200 0.34418600
H -0.13273700 4.19138400 1.95809000
H 1.16977000 4.83429400 0.96006500
H -0.49915300 5.30228300 0.63169100
H 0.50100400 2.78979400 -2.12617400
H -0.07550500 4.44585700 -1.88363900
H 1.56347600 4.00124000 -1.40266300
C -2.76073700 3.33350500 -1.14762700
C -2.85304100 4.82686500 -0.79408700
C -4.17004800 2.72034700 -1.18467600

H -2.33183100 3.24176400 -2.15443800
H -1.90977500 5.35579000 -0.94283800
H -3.59979800 5.30688200 -1.43850600
H -3.17221200 4.98233200 0.24254200
H -4.15111700 1.66214700 -1.45410600
H -4.67650700 2.81993400 -0.21790400
H -4.77816000 3.25159900 -1.92647400
P -1.52790200 -2.21873800 -0.44800600
C -3.11295800 -1.32653500 1.61018500
C -2.29085400 -2.54963300 1.20908500
H -4.00406300 -1.21478100 0.98464000
H -3.44380100 -1.42635600 2.65423300
H -1.47311400 -2.66370300 1.93393900
H -2.89815100 -3.46030100 1.22220900
C -0.91237700 0.20842400 -2.10390500
O -0.68557400 0.30280300 -3.24485100
C 0.13592100 -3.10743800 -0.43240800
C 0.71316500 -3.24298700 -1.85091200
C 0.20838900 -4.42909300 0.34858600
H 0.75628500 -2.38319900 0.10733600
H 0.69402300 -2.29430600 -2.39681800
H 1.75712800 -3.57383900 -1.79536300
H 0.17123100 -3.98545600 -2.44607400
H -0.08117600 -4.29570500 1.39370000
H -0.41184500 -5.21625600 -0.08722900
H 1.24497800 -4.78995700 0.34421000
C -2.59832000 -3.08242700 -1.73805000
C -4.02015400 -2.49889500 -1.78526800
C -2.66930900 -4.61237400 -1.60816900
H -2.10618800 -2.83712300 -2.68864700
H -4.01638400 -1.41688700 -1.93424800
H -4.57300200 -2.95632100 -2.61453900
H -4.57576500 -2.71539600 -0.86558500
H -1.70013200 -5.09514200 -1.74697100
H -3.06690500 -4.91950700 -0.63440800
H -3.34482100 -5.01227600 -2.37454200
H 0.85201700 0.20942100 0.36083900
C 5.86538500 -0.72233100 -1.54911300
C 5.28213200 0.01250500 -2.76581000
C 4.00956300 0.80661900 -2.43484200
C 3.07390400 0.06971100 -1.45838100
C 3.35225100 0.27737400 0.02400900
N 4.60815000 0.08090300 0.53110800
C 5.86054600 0.09521200 -0.25316300

N 2.31165700 0.59606800 0.74670700
 C 2.44300200 0.81243300 2.18747100
 C 3.55911800 -0.04242100 2.77685600
 C 4.83585100 0.20319800 1.98381300
 H 6.90410600 -0.99997900 -1.76155100
 H 5.33157400 -1.66205800 -1.36767000
 H 5.06458500 -0.72375600 -3.54922000
 H 6.03432000 0.69396300 -3.18216700
 H 3.45865100 1.01229400 -3.35909000
 H 4.27020400 1.78668400 -2.01736200
 H 3.08608900 -1.00544600 -1.67694700
 H 2.04715000 0.40496700 -1.60917600
 H 6.16255200 1.13395600 -0.45539100
 H 6.61859600 -0.32022700 0.41567300
 H 1.47898600 0.58637900 2.65413800
 H 2.65087500 1.87681300 2.37363200
 H 3.27652200 -1.10033200 2.72603400
 H 3.73165900 0.20144800 3.82995900
 H 5.23959500 1.20071400 2.21077800
 H 5.60553100 -0.52608700 2.25813600
 H -1.51967700 -0.19542200 2.16450000
 C 0.02889800 -1.28441700 4.04518500
 O 0.02702200 -2.42024800 3.52658200
 O -0.54881000 -0.22129600 3.66772300
 H 0.62706800 -1.17456300 4.99466900

DBU-A4

Fe-1.53174200 0.07599300 -0.49078000
 H -0.03545100 0.07744400 0.04918500
 H -3.02327200 0.05625900 -0.89028300
 C -2.93657200 1.11932200 2.00226400
 C -2.14878700 2.38423700 1.66468200
 H -3.09584700 1.05166900 3.08868300
 H -3.91982800 1.14402000 1.52348800
 H -1.22079300 2.40143800 2.24609300
 H -2.71669800 3.28327000 1.92568500
 P -1.67522900 2.31347600 -0.13483300
 N -2.22406800 -0.08387000 1.51630600
 C -0.05940900 3.28679900 -0.23698200
 C 0.08616400 4.54363700 0.63657300
 C 0.33355600 3.56198600 -1.69747300
 H 0.64431200 2.54175400 0.15141100
 H -0.17220100 4.35486900 1.68284300
 H 1.13210900 4.87665800 0.61761700

H -0.52318900 5.37865600 0.28409300
 H 0.29200200 2.65509100 -2.30812400
 H -0.31567700 4.31108900 -2.16302400
 H 1.35939900 3.94768300 -1.74400100
 C -2.97368100 3.32535700 -1.06669500
 C -2.97768300 4.83849800 -0.79855000
 C -4.38986800 2.76497100 -0.85476600
 H -2.70494100 3.15902800 -2.11893200
 H -2.06088900 5.32929800 -1.12974500
 H -3.80849200 5.30395600 -1.34365900
 H -3.12268200 5.06346100 0.26419300
 H -4.43723500 1.68959600 -1.04045000
 H -4.74615500 2.95546700 0.16426900
 H -5.08624500 3.26332700 -1.53992800
 P -1.57283600 -2.20050400 -0.41377200
 C -3.05218700 -1.29502800 1.72779400
 C -2.27616100 -2.52993200 1.27517400
 H -3.97954300 -1.17035100 1.15999500
 H -3.31433600 -1.39318200 2.79214100
 H -1.45114200 -2.67926200 1.98263500
 H -2.90731800 -3.42444100 1.29901000
 C -1.08707500 0.17591100 -2.15607500
 O -0.82766300 0.23579700 -3.29773400
 C 0.11029500 -3.06289900 -0.42390000
 C 0.64609900 -3.22609200 -1.85588500
 C 0.24961700 -4.35802300 0.39201600
 H 0.72611800 -2.30384900 0.07237300
 H 0.58518500 -2.29412000 -2.42703400
 H 1.69866200 -3.53387800 -1.82918600
 H 0.10248800 -3.99644000 -2.41282600
 H -0.00425500 -4.20269900 1.44387300
 H -0.36449800 -5.17571100 0.00654800
 H 1.29469300 -4.69371300 0.35908300
 C -2.65445700 -3.15634300 -1.63716100
 C -4.10067200 -2.63472600 -1.64848500
 C -2.66097600 -4.68412200 -1.46721800
 H -2.20829100 -2.91808800 -2.61213800
 H -4.14466700 -1.55576200 -1.80980200
 H -4.66178000 -3.12821900 -2.45164000
 H -4.61622400 -2.85896700 -0.70698300
 H -1.68054900 -5.13498600 -1.63210900
 H -3.00863200 -4.98021300 -0.47104700
 H -3.34991100 -5.13074500 -2.19537000
 H 1.54948100 0.33457700 0.50514800

C 5.92948200 -0.80379800 -1.56554600
 C 5.20754500 -0.33114700 -2.83560900
 C 3.91933500 0.44433900 -2.52779700
 C 3.10718400 -0.17515200 -1.37738000
 C 3.51365800 0.23955700 0.02294900
 N 4.78495200 0.32912500 0.42964300
 C 5.98089100 0.24048100 -0.44754700
 N 2.50967900 0.49053300 0.85314300
 C 2.65159700 0.88867000 2.25737300
 C 3.97331900 0.35271700 2.78375900
 C 5.09480100 0.72982700 1.82422400
 H 6.96452700 -1.06522200 -1.81121800
 H 5.47330700 -1.71862500 -1.16993000
 H 4.97523700 -1.20510000 -3.45571500
 H 5.87646300 0.30363500 -3.42871300
 H 3.28198400 0.46985700 -3.41740600
 H 4.14766000 1.49002300 -2.29189800
 H 3.14873800 -1.26915000 -1.43229400
 H 2.05420700 0.09314500 -1.47954900
 H 6.19673400 1.23756300 -0.85259400
 H 6.80198400 -0.01069800 0.22581900
 H 1.78616300 0.49434300 2.80052900
 H 2.62744600 1.98404400 2.31959200
 H 3.92065700 -0.73650100 2.88651900
 H 4.18858800 0.77095100 3.77048200
 H 5.28327600 1.81041300 1.84607500
 H 6.02282600 0.22579700 2.10376900
 H -1.38698700 -0.19718300 2.12115500
 C 0.13863400 -1.36194500 4.09591200
 O -0.25969700 -2.52059700 3.86138600
 O -0.11098300 -0.28032900 3.48268400
 H 0.82464500 -1.24377200 4.98441400

Ru-2

H 0.00013900 0.81683600 -1.63420500
 H -0.00006100 -0.33642400 1.55926500
 C 1.21562400 -2.56682500 -0.14451500
 C 2.50930600 -1.81724000 -0.47120200
 H 1.27495200 -3.59814800 -0.52625100
 H 1.08030600 -2.61475800 0.93720800
 H 2.73833500 -1.88800500 -1.53806500
 H 3.34418800 -2.28781000 0.05867900
 P 2.35552100 -0.00415500 -0.02908200
 N -0.00004400 -1.90055000 -0.70529900

C 3.30771300 0.87959000 -1.40012800
 C 4.64337900 0.27865300 -1.86879400
 C 3.43634400 2.38096100 -1.09868200
 H 2.59293000 0.77569000 -2.22593100
 H 4.57940700 -0.79760300 -2.05596300
 H 4.93457000 0.75360500 -2.81397800
 H 5.45602600 0.44756400 -1.15888500
 H 2.47074900 2.82409900 -0.83717300
 H 4.13488500 2.57457900 -0.27728600
 H 3.81614500 2.90807700 -1.98186100
 C 3.31892600 0.22184100 1.58200500
 C 4.84827700 0.12387900 1.47329100
 C 2.81669600 -0.73396100 2.67641400
 H 3.05536300 1.24415900 1.88422900
 H 5.27771200 0.92291900 0.86639600
 H 5.28985800 0.20375700 2.47437300
 H 5.16836800 -0.83694000 1.05425300
 H 1.73240700 -0.68654300 2.79777200
 H 3.09525400 -1.77206400 2.45919000
 H 3.28082800 -0.46724200 3.63333000
 C -0.00004600 -2.04750400 -2.18295900
 H -0.00002300 -3.11167900 -2.46404000
 H -0.87770600 -1.56420600 -2.60843100
 H 0.87758000 -1.56416500 -2.60845400
 P -2.35550000 -0.00414100 -0.02903300
 C -1.21570000 -2.56685800 -0.14450900
 C -2.50937700 -1.81723600 -0.47112600
 H -1.08037000 -2.61482400 0.93721000
 H -1.27504000 -3.59816400 -0.52628800
 H -2.73853000 -1.88807700 -1.53795200
 H -3.34421400 -2.28773000 0.05888600
 C 0.00007300 2.04068900 0.62711100
 O 0.00008200 3.13804000 1.04008900
 C -3.30774000 0.87969300 -1.39999500
 C -3.43617800 2.38107200 -1.09850900
 C -4.64355000 0.27894100 -1.86849500
 H -2.59304700 0.77572600 -2.22587000
 H -2.47053800 2.82406000 -0.83691400
 H -3.81584500 2.90827900 -1.98169000
 H -4.13474900 2.57475700 -0.27715500
 H -4.57975300 -0.79731300 -2.05573200
 H -5.45607500 0.44791700 -1.15845600
 H -4.93482000 0.75397800 -2.81361100
 C -3.31889400 0.22177100 1.58206200

C -2.81676200 -0.73422500 2.67634600
C -4.84824500 0.12391100 1.47325000
H -3.05528600 1.24403600 1.88442300
H -1.73246800 -0.68695000 2.79770900
H -3.28087300 -0.46758700 3.63329600
H -3.09543000 -1.77226600 2.45896700
H -5.27760400 0.92306900 0.86645600
H -5.16834300 -0.83682400 1.05402500
H -5.28989100 0.20363600 2.47431500
Ru 0.00002100 0.30703700 0.00211200

Ru-3

C -0.08881800 4.07771200 0.33742100
O 0.00868900 4.11805500 -0.82708200
O -0.18628600 4.10107200 1.50341500
H 0.00096400 1.28032300 0.50119400
H 0.01901500 -1.78307300 -0.96229900
C -1.20112600 -2.14909400 1.85288000
C -2.49756500 -1.38773300 1.56009900
H -1.25880800 -2.61008700 2.85162800
H -1.06507400 -2.94676000 1.12100900
H -2.73177700 -0.70149000 2.37851400
H -3.32821500 -2.09886600 1.50264000
P -2.34582100 -0.38766600 -0.01756800
N 0.01108100 -1.27697000 1.77927700
C -3.22242000 1.23400500 0.39456700
C -4.55552700 1.18194700 1.16031200
C -3.31951700 2.13757300 -0.84423600
H -2.47634800 1.67934100 1.06389000
H -4.53481900 0.48189900 2.00099600
H -4.76786100 2.17617600 1.57293600
H -5.39883400 0.91333500 0.52030600
H -2.35118800 2.25044800 -1.34037800
H -4.03566700 1.74845300 -1.57667500
H -3.66384300 3.13729400 -0.55306000
C -3.37777700 -1.29896600 -1.31229000
C -4.90042500 -1.25051000 -1.11488400
C -2.91226100 -2.75556100 -1.46580100
H -3.13098100 -0.77083400 -2.24273100
H -5.30093600 -0.23951500 -1.20989000
H -5.38656100 -1.86683100 -1.88126700
H -5.20108400 -1.65009900 -0.13974300
H -1.83780600 -2.82292100 -1.64943700
H -3.14770900 -3.34863000 -0.57420900

H -3.43400900 -3.21928700 -2.31125400
C 0.00191600 -0.33502700 2.92692900
H 0.00425600 -0.88816000 3.87862200
H 0.87468600 0.31412600 2.88939300
H -0.88027600 0.30100100 2.88623900
P 2.36227000 -0.35591400 -0.00885800
C 1.23518400 -2.13160900 1.85853600
C 2.52177500 -1.35177600 1.57084200
H 1.11355300 -2.93146700 1.12652400
H 1.29510000 -2.59117000 2.85780800
H 2.74236200 -0.66198900 2.39006000
H 3.36293700 -2.05077600 1.51712100
C 0.00432800 0.53496800 -1.96372700
O 0.00183700 0.99630700 -3.04133200
C 3.21495500 1.27950200 0.39897700
C 3.31342400 2.17249900 -0.84748600
C 4.54196400 1.24893600 1.17628600
H 2.45711700 1.72308300 1.05683200
H 2.34927400 2.26898600 -1.35478700
H 3.64179000 3.17921400 -0.56227000
H 4.04210300 1.78562200 -1.56863100
H 4.52064100 0.55945300 2.02564500
H 5.39276400 0.97948400 0.54658400
H 4.74240400 2.25009500 1.57795400
C 3.41143000 -1.25729800 -1.29649400
C 2.96108200 -2.71847600 -1.45162400
C 4.93230100 -1.19443500 -1.08911500
H 3.16535300 -0.73244000 -2.22896600
H 1.88807400 -2.79693100 -1.63937300
H 3.49099000 -3.17719900 -2.29472200
H 3.19869500 -3.30898900 -0.55890100
H 5.32435800 -0.18007700 -1.18370200
H 5.22988400 -1.58903400 -0.11099500
H 5.42921200 -1.80804900 -1.85073100
Ru 0.00796600 -0.22964900 -0.28903600

Ru-TS3_4

C -0.09490600 3.31867200 0.39279100
O 0.41448700 3.73428300 -0.59549900
O -0.62960900 3.39936800 1.45320600
H -0.00355800 1.53426400 0.17233900
C -1.20734400 -1.63585900 2.16358000
C -2.51007800 -0.96983300 1.71530400
H -1.26779800 -1.89369400 3.23232900

H -1.05263000 -2.55841000 1.60104100
 H -2.76265800 -0.13044800 2.36934200
 H -3.33151400 -1.68874900 1.80145700
 P -2.35426700 -0.31929500 -0.03388500
 N -0.00319200 -0.77944600 1.93036000
 C -3.29238100 1.31484500 0.00315700
 C -4.65332500 1.36619600 0.71840000
 C -3.36820200 1.93255800 -1.40163600
 H -2.59273000 1.92212800 0.58943200
 H -4.64236100 0.86209900 1.68965400
 H -4.91815600 2.41470800 0.90275200
 H -5.45809700 0.93023000 0.12269900
 H -2.38380500 1.97994000 -1.87659500
 H -4.03802200 1.36714900 -2.05928800
 H -3.75781800 2.95571900 -1.34008900
 C -3.29951200 -1.52872500 -1.13467600
 C -4.82970400 -1.49575700 -1.00608300
 C -2.78987500 -2.96746600 -0.95001900
 H -3.02924200 -1.20505100 -2.14852900
 H -5.25432100 -0.54585200 -1.33583100
 H -5.26439300 -2.28228600 -1.63512000
 H -5.15950900 -1.68262500 0.02206700
 H -1.70511700 -3.03730000 -1.05781700
 H -3.06706700 -3.36590900 0.03293900
 H -3.25035900 -3.61592700 -1.70452800
 C -0.03435000 0.37671700 2.86053500
 H -0.09470100 0.02887100 3.90277300
 H 0.86305000 0.97995900 2.73645800
 H -0.88418000 1.01802600 2.63892600
 P 2.36906200 -0.28441900 -0.00270100
 C 1.22157400 -1.59547000 2.19734400
 C 2.51092200 -0.89607700 1.76091700
 H 1.10551300 -2.53084800 1.64711000
 H 1.27117800 -1.83607300 3.27067800
 H 2.72376700 -0.03780200 2.40395200
 H 3.35399200 -1.58589700 1.87432200
 C 0.01596100 0.24075000 -2.09065000
 O 0.02100800 0.46274400 -3.24046100
 C 3.29836100 1.35805300 -0.01413000
 C 3.46681100 1.87974400 -1.44980900
 C 4.60913600 1.46237200 0.78330300
 H 2.56189400 2.00466700 0.47780400
 H 2.51933900 1.87934900 -1.99562000
 H 3.83516300 2.91201000 -1.42898900

H 4.19049000 1.28486600 -2.01731500
 H 4.51955000 1.06846900 1.80028900
 H 5.44096200 0.94895300 0.29626400
 H 4.88817000 2.51981100 0.87088300
 C 3.35062300 -1.51097600 -1.05159800
 C 2.82876900 -2.94600100 -0.87313800
 C 4.87403500 -1.48598800 -0.85466100
 H 3.12428600 -1.19728000 -2.07930600
 H 1.74938200 -3.01364900 -1.02575100
 H 3.31909300 -3.60411100 -1.60003700
 H 3.06239300 -3.33435800 0.12509000
 H 5.32203500 -0.54109900 -1.16697200
 H 5.15342300 -1.67215600 0.18868800
 H 5.33199800 -2.27841900 -1.45924300
 Ru 0.00771300 -0.15350900 -0.28974200
 H 0.01722000 -1.78474600 -0.60487400

Ru-4

C -0.03680700 3.00816300 0.26576400
 O 0.87963800 3.63613100 -0.27823600
 O -0.96885300 3.33198800 1.02049900
 H -0.02200200 1.84066700 0.00761300
 H 0.01078600 -1.68068700 -0.49670600
 C -1.22209300 -1.36979500 2.29000500
 C -2.51910400 -0.73112000 1.79002200
 H -1.27698000 -1.52590500 3.37799100
 H -1.08401100 -2.34427900 1.81724300
 H -2.74184600 0.18127900 2.34995200
 H -3.35299600 -1.41927700 1.96408600
 P -2.37370900 -0.27871200 -0.01785400
 N -0.00651700 -0.55521900 1.97283800
 C -3.33215300 1.32572800 -0.20834700
 C -4.66302400 1.45423000 0.55071100
 C -3.48445400 1.69454400 -1.69291900
 H -2.62695800 2.03978000 0.23858100
 H -4.57186600 1.18558500 1.60754200
 H -4.99133800 2.50038300 0.51357600
 H -5.46094100 0.84751900 0.11628100
 H -2.52668400 1.66052100 -2.22229500
 H -4.18451000 1.03224300 -2.21394900
 H -3.87165200 2.71617900 -1.78167400
 C -3.25764800 -1.62997100 -0.99005800
 C -4.78551700 -1.66554600 -0.82880200
 C -2.66442800 -3.01788400 -0.69775500

H	-3.02339600	-1.37616800	-2.03261700	O	-0.31525600	3.08207400	-0.69983600
H	-5.26730400	-0.76764100	-1.21982300	O	-1.19890500	3.21104900	1.39633800
H	-5.18887500	-2.52040400	-1.38509700	H	0.55100900	2.30661700	0.94558100
H	-5.08489600	-1.78845300	0.21806100	H	0.09814200	-1.53292100	-0.60849300
H	-1.58228900	-3.04549900	-0.84680400	C	-1.12490000	-1.56127600	2.17643200
H	-2.87978200	-3.33939400	0.32783300	C	-2.44680100	-0.93493700	1.72892900
H	-3.11660400	-3.75520600	-1.37110400	H	-1.17879700	-1.82560000	3.24330800
C	-0.02217000	0.69618300	2.77372600	H	-0.93790900	-2.47830100	1.61388500
H	-0.14297300	0.46484200	3.84198300	H	-2.70647500	-0.08244700	2.36320300
H	0.91429300	1.23514000	2.63531900	H	-3.25295300	-1.66742500	1.84237500
H	-0.82049900	1.35795700	2.44155300	P	-2.32075600	-0.32040300	-0.03111400
P	2.37875900	-0.27554600	0.01135400	N	0.05287200	-0.66395700	1.95556000
C	1.20760000	-1.36031100	2.31888700	C	-3.40818700	1.21032300	-0.10096500
C	2.51122000	-0.73079400	1.82098400	C	-4.76788000	1.14930300	0.61643000
H	1.07642800	-2.34373300	1.86281500	C	-3.54235100	1.71313200	-1.54706600
H	1.25084100	-1.49701100	3.40992200	H	-2.78641300	1.93615600	0.43855000
H	2.74623000	0.17485300	2.38603800	H	-4.68939700	0.76213500	1.63730700
H	3.33789900	-1.42785100	1.99413700	H	-5.16961000	2.16737300	0.69075000
C	0.01194400	0.09711700	-2.11411800	H	-5.50779100	0.54760300	0.08364800
O	0.01225000	0.17929600	-3.27876000	H	-2.56225500	1.88714800	-1.99833600
C	3.32313000	1.33905100	-0.19240700	H	-4.10645900	1.01830600	-2.17963000
C	3.54589300	1.64839300	-1.68183200	H	-4.07896900	2.66924500	-1.55305500
C	4.60900300	1.52060400	0.62877800	C	-3.09055400	-1.65881900	-1.11654100
H	2.58507700	2.06950600	0.16236000	C	-4.61646200	-1.80202400	-1.00473100
H	2.61928800	1.56122200	-2.25732200	C	-2.42190500	-3.02544100	-0.89430300
H	3.90283800	2.67844200	-1.79223600	H	-2.84734600	-1.32570400	-2.13394600
H	4.29461600	0.98951400	-2.13472800	H	-5.14524400	-0.91753600	-1.36406900
H	4.45623200	1.32756900	1.69490000	H	-4.94691900	-2.65030900	-1.61648700
H	5.42591000	0.88161300	0.28490400	H	-4.93611700	-1.99976000	0.02453900
H	4.94600300	2.56050000	0.53638500	H	-1.33595700	-2.98063400	-1.00664800
C	3.29856200	-1.62186300	-0.93302400	H	-2.65013700	-3.42659800	0.09971500
C	2.69447500	-3.01053500	-0.66821400	H	-2.80582100	-3.74249400	-1.62911500
C	4.81785800	-1.65723000	-0.70425200	C	-0.03301200	0.49350100	2.88709500
H	3.10855500	-1.36628100	-1.98387000	H	-0.23066700	0.14253200	3.91017100
H	1.62039900	-3.03993300	-0.86701700	H	0.90989700	1.04010700	2.88585900
H	3.17918700	-3.74727700	-1.31920500	H	-0.80577900	1.19737700	2.57519000
H	2.86197100	-3.33176800	0.36637800	P	2.42374100	-0.16613300	0.01159100
H	5.31585600	-0.75413700	-1.06099800	C	1.30084800	-1.44080400	2.24235900
H	5.06935500	-1.79297600	0.35365700	C	2.57667400	-0.72485700	1.78934600
H	5.24788400	-2.50466700	-1.25174100	H	1.21115000	-2.39591700	1.72089800
Ru	0.00546800	-0.11021500	-0.27398200	H	1.35440300	-1.65234800	3.32078900
Ru-TS4_4a				H	2.76966300	0.15689800	2.40617300
C	-0.34308200	2.88456200	0.54009000	H	3.43414000	-1.39292700	1.92460300
				C	0.06347800	0.35109900	-2.06580300

O	0.07323300	0.51433100	-3.22021100	H	-2.50801300	2.04549200	-1.76943100
C	3.36505400	1.46241400	-0.11079500	H	-4.20690500	1.54054600	-1.78830600
C	3.57440900	1.85897200	-1.58197000	H	-3.75011700	3.08649100	-1.06462500
C	4.65671400	1.60116300	0.70968700	C	-3.34122300	-1.33332500	-1.20857100
H	2.63008800	2.16109000	0.30829100	C	-4.85466100	-1.39759100	-0.95205600
H	2.64160400	1.81906600	-2.15251700	C	-2.75797600	-2.75243700	-1.30139600
H	3.94748900	2.88804700	-1.63483700	H	-3.17207400	-0.83706900	-2.17335700
H	4.30895000	1.21736200	-2.07971400	H	-5.34026000	-0.42791800	-1.07765000
H	4.51116400	1.35090400	1.76470100	H	-5.31671200	-2.08879600	-1.66742900
H	5.46918400	0.98135800	0.32373100	H	-5.08372800	-1.76954100	0.05311100
H	4.99347200	2.64435200	0.66969800	H	-1.69007200	-2.74332500	-1.53237600
C	3.34535900	-1.44609700	-1.01917900	H	-2.90358200	-3.30912000	-0.36818400
C	2.74896100	-2.85162000	-0.83702500	H	-3.27373900	-3.30684800	-2.09408600
C	4.86597100	-1.48867300	-0.80034600	C	0.00000300	0.08345000	2.92842400
H	3.14752000	-1.12911300	-2.05141300	H	0.00002200	-0.38427600	3.92381400
H	1.67683900	-2.87763200	-1.04643900	H	0.87220700	0.72486200	2.82388600
H	3.24293400	-3.54671900	-1.52557600	H	-0.87220800	0.72485800	2.82392100
H	2.91027800	-3.23056700	0.17861200	P	2.36762300	-0.26717300	0.00009700
H	5.35992200	-0.56734300	-1.11365000	C	1.21284800	-1.82286100	2.02513200
H	5.12312800	-1.67686800	0.24799900	C	2.51214100	-1.09767100	1.67004900
H	5.29514100	-2.30595700	-1.39233100	H	1.07690300	-2.68152600	1.36484700
Ru	0.05666900	-0.01686300	-0.25021800	H	1.26361100	-2.19584700	3.05955700
Ru-4a				H	2.74076400	-0.33130800	2.41532500
C	0.00018700	3.07225700	-0.00665300	H	3.34320500	-1.81034400	1.68981900
O	0.00006400	1.97332800	0.66414900	C	-0.00003600	0.39176000	-2.03767200
O	0.00035900	4.21562700	0.45694600	O	-0.00001200	0.62301700	-3.18489500
H	0.00012700	2.94442900	-1.11909800	C	3.25741700	1.37953800	0.18242800
H	-0.00005400	-1.61720600	-0.73570100	C	3.43761800	2.04343400	-1.19190000
C	-1.21289900	-1.82283400	2.02515000	C	4.55419500	1.42179900	1.00599900
C	-2.51217800	-1.09761200	1.67008500	H	2.49547400	1.95070900	0.72675900
H	-1.26365400	-2.19582100	3.05957600	H	2.50810200	2.04541000	-1.76948500
H	-1.07698400	-2.68150100	1.36486100	H	3.75027200	3.08632900	-1.06467600
H	-2.74076200	-0.33124100	2.41536500	H	4.20695600	1.54033400	-1.78831800
H	-3.34326200	-1.81026000	1.68987900	H	4.44477300	0.95505400	1.98953100
P	-2.36767200	-0.26711700	0.00012700	H	5.39302400	0.94085800	0.49710500
N	-0.00001700	-0.95974100	1.87296600	H	4.83329900	2.46880700	1.17746300
C	-3.25741600	1.37963300	0.18245600	C	3.34115800	-1.33338400	-1.20859800
C	-4.55420300	1.42197100	1.00601100	C	2.75785700	-2.75247100	-1.30148100
C	-3.43754000	2.04357400	-1.19186300	C	4.85458300	-1.39770100	-0.95201100
H	-2.49546500	1.95076200	0.72681800	H	3.17206200	-0.83708500	-2.17337100
H	-4.44482600	0.95522800	1.98954800	H	1.68995800	-2.74331000	-1.53248400
H	-4.83324800	2.46899700	1.17746700	H	3.27361300	-3.30687400	-2.09418000
H	-5.39305600	0.94108200	0.49711100	H	2.90342100	-3.30919500	-0.36828700
				H	5.34019700	-0.42801400	-1.07745900

H 5.08359100 -1.76977100 0.05312600
H 5.31666600 -2.08882700 -1.66744000
Ru -0.00002700 -0.08421900 -0.25586100

Ru-5

C 0.24001900 4.22557600 -0.27938400
O 1.29833900 3.59400500 -0.01029800
O -0.95906100 3.88688600 -0.13257800
H 0.40194800 5.25587400 -0.72138800
H 0.43534500 1.60914800 -0.60151000
H 2.46192100 0.84828400 -2.61391500
C 3.47152800 0.93564900 -2.20078800
C 3.46691500 0.99699900 -0.66568900
H 3.91355600 1.85555600 -2.60074800
H 4.06901400 0.09827500 -2.57600300
P 2.40467700 -0.33399100 0.12523600
C 4.89762200 1.07854200 -0.11090600
H 2.91970700 1.90408600 -0.37473000
C 2.49273300 0.10243500 1.93815700
C 3.32547000 -1.96553500 -0.05033800
H 4.92278600 1.16432800 0.97996500
H 5.50026200 0.20952000 -0.39746700
H 5.39625600 1.96654200 -0.51738600
P -2.34382700 -0.32587000 0.03235700
C 0.04168300 -0.83391200 -2.02327200
C 1.20995300 -0.31063500 2.66047500
H 2.64501300 1.18345900 2.00007900
H 3.35377800 -0.36735900 2.42360500
C 3.09909200 -2.59938900 -1.43212300
C 2.96620100 -2.97303400 1.05263500
H 4.38791300 -1.71127300 0.05305300
C -2.52268400 -0.12896400 1.88166000
C -3.25371000 1.14534400 -0.70900900
C -3.24182700 -1.91088000 -0.43499800
O 0.01339000 -1.22986500 -3.11820000
N -0.02429400 0.21477100 2.00044000
H 1.12817000 -1.39924500 2.67816500
H 1.23637500 0.04088400 3.70260800
H 3.34119700 -1.92503800 -2.25732400
H 3.73076500 -3.48961100 -1.53506900
H 2.05760800 -2.91570400 -1.54934200
H 1.90093900 -3.22739100 1.03046700
H 3.52875700 -3.90034100 0.89240200
H 3.21578300 -2.61161800 2.05432100

C -1.21353600 -0.46801700 2.59815100
H -2.81828700 0.90313800 2.08565200
H -3.32510100 -0.76700200 2.26626000
C -4.61537200 1.52509300 -0.10426100
C -3.33453600 1.01511800 -2.23833200
H -2.55409900 1.96125100 -0.47944800
C -4.76765400 -1.86797700 -0.25883900
C -2.65228400 -3.12186000 0.30587300
H -3.01645400 -2.02585000 -1.50331600
C -0.11931600 1.68329800 2.22124800
H -1.29006600 -0.19162500 3.66044500
H -1.02805600 -1.54265900 2.54219100
H -4.59145600 1.58364900 0.98800000
H -4.89847000 2.51852100 -0.47283800
H -5.41255900 0.83396400 -0.38816700
H -3.70582200 1.95165200 -2.66970700
H -2.35645400 0.81267100 -2.68635400
H -4.02083100 0.21749100 -2.54355100
H -5.24408900 -1.16724000 -0.94684900
H -5.18459900 -2.86126900 -0.46321600
H -5.05466000 -1.59729000 0.76326900
H -1.57250000 -3.20741700 0.16313600
H -2.85390800 -3.07188900 1.38225500
H -3.11912100 -4.03942300 -0.07008200
H -0.16248900 1.89883100 3.29915800
H 0.72358500 2.19818000 1.76081500
H -0.99913800 2.08971900 1.72607000
H 0.04434700 -1.80069900 0.19062500
H -0.34148100 1.53204700 -0.73702200
Ru 0.03929100 -0.26358900 -0.25266000

Ru-TS5_6

C -0.04780100 4.24176100 -0.16725700
O 0.86794100 3.38212900 -0.39876800
O -1.27023700 4.06399800 -0.03019200
H 0.33486800 5.29386200 -0.07977200
H 0.23530800 1.96287900 -0.65503100
H 2.33514000 1.00938300 -2.55525600
C 3.35752000 1.12485500 -2.18323900
C 3.42004200 1.12343600 -0.64814000
H 3.74122900 2.07898700 -2.56311600
H 3.97200000 0.33177600 -2.62147100
P 2.42553500 -0.26266800 0.14379800
C 4.86969800 1.23128700 -0.15103800

H 2.86047700 2.00301300 -0.30565900
C 2.49546500 0.19051900 1.95726800
C 3.45994500 -1.82881400 0.00544800
H 4.94089600 1.25682700 0.94116600
H 5.48698100 0.40112700 -0.51127600
H 5.32022800 2.15720400 -0.52831800
P -2.31331400 -0.39217100 0.01828900
C 0.10529700 -0.99130400 -1.96652700
C 1.21000800 -0.23161000 2.67041200
H 2.64287500 1.27250800 2.02055200
H 3.35392000 -0.27241400 2.45402600
C 3.37952900 -2.44602800 -1.39949300
C 3.08426000 -2.87916000 1.06181200
H 4.49359200 -1.51168000 0.19309400
C -2.51738000 -0.12413100 1.85778500
C -3.21595200 1.05196700 -0.78327800
C -3.22094100 -1.98829700 -0.39719200
O 0.10907500 -1.44442700 -3.04135200
N -0.02603800 0.26252000 1.98681600
H 1.14645200 -1.32109800 2.70078300
H 1.21735500 0.13397700 3.70824600
H 3.65432700 -1.74347800 -2.19029000
H 4.06289500 -3.30101200 -1.46583600
H 2.36974700 -2.81307400 -1.60968300
H 2.04153700 -3.19675700 0.95618000
H 3.71482900 -3.76641000 0.93019700
H 3.23453400 -2.52300200 2.08515800
C -1.21012300 -0.42197800 2.59500900
H -2.83049900 0.91053200 2.02190400
H -3.31255600 -0.75993900 2.26054200
C -4.60022300 1.42940900 -0.22959000
C -3.24802800 0.89087400 -2.31119200
H -2.53360200 1.88115000 -0.55114200
C -4.74263200 -1.95080300 -0.18610100
C -2.60884100 -3.18495200 0.34883200
H -3.02051500 -2.12185900 -1.46833500
C -0.14524300 1.72982400 2.19110300
H -1.29852300 -0.11882900 3.64915700
H -1.00805700 -1.49458400 2.56785800
H -4.63155800 1.44358900 0.86398700
H -4.85403000 2.43971400 -0.57258700
H -5.39005000 0.76076700 -0.58058900
H -3.63073600 1.80876000 -2.77217600
H -2.25124100 0.70585200 -2.72377300

H -3.90375000 0.06961300 -2.62224900
H -5.24152700 -1.26820700 -0.87597400
H -5.15822900 -2.95074100 -0.35899300
H -5.00834400 -1.66013000 0.83635400
H -1.53319600 -3.27055100 0.17853900
H -2.78097000 -3.11579200 1.42936000
H -3.08371200 -4.11025100 0.00273000
H -0.23305900 1.95639100 3.26397700
H 0.72384400 2.23759400 1.77941000
H -1.01032900 2.12516100 1.66182800
H 0.12095400 -1.83479400 0.31146500
H -0.22107200 1.33573100 -0.97088000
Ru 0.06428800 -0.32390000 -0.23632700

Ru-6

C -0.68776700 4.47206500 -0.02523800
O 0.30707300 3.76904000 -0.54633000
O -1.72929600 4.03666300 0.42786200
H -0.45060400 5.54917000 -0.05229900
H 0.10728900 2.77548100 -0.52215400
H 2.25703100 1.42184400 -2.35290800
C 3.29792000 1.47397100 -2.02133500
C 3.42360800 1.27593300 -0.50332900
H 3.68898700 2.46058600 -2.29782400
H 3.87370300 0.72985100 -2.58079900
P 2.45925200 -0.21124000 0.14250400
C 4.89074300 1.34234200 -0.05272300
H 2.87909200 2.10058200 -0.02422700
C 2.52857900 0.07811200 1.99298800
C 3.58013400 -1.70254500 -0.12578600
H 5.00663100 1.22428900 1.02975300
H 5.49993100 0.57653800 -0.54443100
H 5.31654000 2.31620600 -0.32316300
P -2.24348200 -0.51562500 -0.00857300
C 0.17599300 -0.72596600 -2.04506400
C 1.25658500 -0.43522800 2.67148300
H 2.65308300 1.15285900 2.15653300
H 3.39966100 -0.40889200 2.44296400
C 3.57325600 -2.16020200 -1.59228400
C 3.22614900 -2.88023700 0.79385300
H 4.58963100 -1.36083300 0.13422500
C -2.46921000 -0.34969800 1.84231200
C -3.25064700 0.90372400 -0.73123100
C -3.07851700 -2.13885800 -0.49442200

O 0.19180400 -0.98020700 -3.18805500
 N 0.00872300 0.08378200 2.03204500
 H 1.21996500 -1.52419300 2.60602000
 H 1.26119600 -0.15971500 3.73756600
 H 3.88212100 -1.37193000 -2.28353800
 H 4.26403500 -3.00213200 -1.72184500
 H 2.57623600 -2.49974000 -1.89185200
 H 2.21281000 -3.24509300 0.59854100
 H 3.92168600 -3.70780900 0.60851200
 H 3.30044300 -2.62625700 1.85545900
 C -1.16446600 -0.66562400 2.57850700
 H -2.79687900 0.67161700 2.05417500
 H -3.26009300 -1.01393700 2.20654000
 C -4.64321500 1.18765800 -0.14208400
 C -3.29700800 0.81412600 -2.26435200
 H -2.61026200 1.75429300 -0.46878100
 C -4.61171300 -2.16058700 -0.39511400
 C -2.48538600 -3.32544500 0.28180800
 H -2.79992100 -2.25742700 -1.54995600
 C -0.13978600 1.52591100 2.35516600
 H -1.27512900 -0.43491800 3.64957600
 H -0.93575600 -1.72844800 2.48371100
 H -4.64716700 1.19507600 0.95215300
 H -4.97062100 2.18193800 -0.47065700
 H -5.39758100 0.47210700 -0.47636100
 H -3.74255100 1.72677800 -2.67762000
 H -2.29663000 0.71074300 -2.69545000
 H -3.90495900 -0.03066500 -2.60697000
 H -5.08485600 -1.48031100 -1.10556500
 H -4.97532000 -3.17052900 -0.62086600
 H -4.96351400 -1.90703600 0.61127300
 H -1.39649300 -3.36064600 0.20600700
 H -2.75525800 -3.28456200 1.34386800
 H -2.88859200 -4.26263100 -0.11975300
 H -0.22762700 1.66692800 3.44294600
 H 0.72522300 2.07977900 1.99398100
 H -1.01800500 1.93896800 1.86370900
 H 0.23962700 -1.94951900 0.18068000
 H -0.01550300 1.35644300 -0.55123700
 Ru 0.12119600 -0.33497800 -0.24409000

Mn-2

H -0.00001100 -1.52424800 0.10814600
 C 1.21713100 1.31572400 2.19691000

C 2.50211600 0.59332700 1.78150100
 H 1.25150300 1.56293400 3.27025200
 H 1.12215000 2.25101500 1.64099400
 H 2.72839200 -0.22185200 2.47284100
 H 3.34626200 1.28695300 1.83852200
 P 2.29318700 -0.10104800 0.05098100
 N -0.00002100 0.50407800 1.90435500
 C 2.95432500 -1.86899100 0.19261900
 C 4.25006700 -2.12296200 0.98139200
 C 2.98958900 -2.55264300 -1.18324100
 H 2.13290000 -2.32702600 0.75637700
 H 4.27857300 -1.58731900 1.93511500
 H 4.32285200 -3.19353100 1.21116700
 H 5.14679100 -1.85325900 0.42005300
 H 2.03723300 -2.45184400 -1.71059300
 H 3.77645300 -2.14046100 -1.82424100
 H 3.19398000 -3.62377100 -1.06496300
 C 3.51357100 0.87167900 -1.02804100
 C 4.99934300 0.50768500 -0.88841700
 C 3.34969800 2.39080600 -0.84603100
 H 3.18985900 0.62237100 -2.04738800
 H 5.21478800 -0.51674500 -1.19671300
 H 5.59656500 1.17062600 -1.52731500
 H 5.35636200 0.64116700 0.13896200
 H 2.32447500 2.73136300 -0.98539900
 H 3.69061800 2.71653600 0.14355100
 H 3.97206500 2.91016100 -1.58475600
 C -0.00003000 -0.69120800 2.78353400
 H -0.00002800 -0.39454000 3.84399000
 H -0.87568200 -1.30587300 2.58600700
 H 0.87561200 -1.30588800 2.58600600
 P -2.29319600 -0.10104500 0.05097400
 C -1.21715600 1.31574500 2.19691100
 C -2.50215000 0.59338000 1.78147600
 H -1.12214900 2.25104000 1.64100500
 H -1.25153900 1.56294400 3.27025500
 H -2.72849100 -0.22176600 2.47283500
 H -3.34626600 1.28704600 1.83844300
 C 0.00001200 -0.55454900 -1.95025500
 O 0.00003600 -0.97233400 -3.04747900
 C -2.95430600 -1.86899800 0.19263900
 C -2.98958200 -2.55265400 -1.18322000
 C -4.25002200 -2.12299800 0.98144700
 H -2.13286100 -2.32701400 0.75638300

H -2.03722900 -2.45186200 -1.71057700
H -3.19398100 -3.62378000 -1.06493900
H -3.77644700 -2.14046900 -1.82421700
H -4.27853500 -1.58731100 1.93514500
H -5.14677000 -1.85337600 0.42011000
H -4.32274100 -3.19356000 1.21127500
C -3.51356400 0.87168500 -1.02807600
C -3.34975400 2.39080500 -0.84596800
C -4.99933100 0.50764700 -0.88855900
H -3.18978200 0.62244600 -2.04741600
H -2.32450300 2.73139600 -0.98506700
H -3.97195900 2.91018500 -1.58481200
H -3.69091000 2.71648200 0.14355100
H -5.21473600 -0.51677100 -1.19691700
H -5.35640500 0.64106900 0.13880900
H -5.59653300 1.17061000 -1.52745400
Mn 0.00000000 0.03574200 -0.29495800
C -0.00003200 1.72697000 -0.83739000
O 0.00007100 2.80765000 -1.30730600

Mn-3

C 0.06065500 4.17142700 -0.27238500
O -0.02762100 4.08070200 -1.43444700
O 0.15098300 4.30080600 0.88708900
H 0.00317300 1.10143900 0.25301600
C -1.22655900 -2.05323900 1.96445400
C -2.51861900 -1.29470900 1.64659700
H -1.26640200 -2.45083000 2.99133200
H -1.11620500 -2.90096200 1.28494600
H -2.79252500 -0.63785900 2.47550800
H -3.33945400 -2.01016000 1.53498900
P -2.29500600 -0.27899700 0.08352400
N -0.01214500 -1.20089600 1.80373800
C -2.90391000 1.45168100 0.56062000
C -4.12740400 1.60285100 1.47874800
C -3.03553100 2.33429800 -0.69030600
H -2.03247600 1.81064100 1.11907700
H -4.07070600 0.97483200 2.37310600
H -4.18281300 2.64315100 1.82418700
H -5.07063200 1.38212400 0.97493400
H -2.14677200 2.27375400 -1.32435200
H -3.90375400 2.05470800 -1.29718800
H -3.17014500 3.38325900 -0.39871400
C -3.58038400 -0.95762800 -1.13134300

C -5.05153900 -0.72668300 -0.75218500
C -3.35351700 -2.44907200 -1.42538800
H -3.36873500 -0.40020100 -2.05371200
H -5.32462700 0.32961400 -0.75198500
H -5.69931000 -1.22865000 -1.48174500
H -5.29003000 -1.14287600 0.23333800
H -2.35255300 -2.65984500 -1.79946600
H -3.52107000 -3.06638400 -0.53441400
H -4.07093100 -2.78213000 -2.18512100
C -0.01666800 -0.15567400 2.85529500
H -0.01836200 -0.61074800 3.85816900
H 0.85899500 0.48344500 2.75668800
H -0.89460800 0.47981300 2.75267800
P 2.28497600 -0.30074900 0.08321100
C 1.20126700 -2.05279100 1.97419100
C 2.49471800 -1.29451900 1.66225100
H 1.09521400 -2.90288500 1.29673400
H 1.23487000 -2.44723400 3.00252000
H 2.75404500 -0.62358400 2.48468800
H 3.31997900 -2.00818000 1.57340200
C 0.00035900 0.31086300 -1.91777500
O 0.00490100 0.77885500 -2.99325000
C 2.91540200 1.42775900 0.53764500
C 3.04789900 2.29877400 -0.72143800
C 4.14653600 1.57415200 1.44629900
H 2.05162600 1.80079200 1.09871100
H 2.15098000 2.24975600 -1.34517400
H 3.20700200 3.34683000 -0.43888900
H 3.90279300 1.99911800 -1.33743500
H 4.08863600 0.95408200 2.34606700
H 5.08410600 1.33962700 0.93833300
H 4.21444800 2.61662200 1.78282500
C 3.55875100 -1.01556900 -1.12364000
C 3.32664200 -2.51448600 -1.37226300
C 5.03490300 -0.77818300 -0.76879400
H 3.33795500 -0.48415700 -2.05912600
H 2.32019100 -2.73507500 -1.72517400
H 4.03219900 -2.86978100 -2.13306400
H 3.50735900 -3.10615500 -0.46679100
H 5.30938600 0.27744500 -0.79387400
H 5.28659800 -1.17489600 0.22144100
H 5.67201300 -1.29594700 -1.49669200
Mn -0.00559400 -0.41341000 -0.30988100
C -0.01639700 -2.05044600 -0.99974200

O -0.02373300 -3.09756800 -1.53926700

Mn-TS3_4

C -0.00739900 3.13115900 0.00999000
O 0.06890200 3.39774900 -1.14589000
O -0.08828500 3.39880500 1.16961900
H 0.00257200 1.37789500 0.04574800
C -1.21637000 -1.37222200 2.31127900
C -2.46023200 -0.59165300 1.88380600
H -1.22118300 -1.52770700 3.40163500
H -1.21361300 -2.35629700 1.83702300
H -2.54541400 0.33846500 2.45227600
H -3.35802900 -1.17542300 2.10686400
P -2.32189500 -0.15409600 0.07043400
N 0.04717300 -0.68618600 1.91197600
C -3.11485800 1.55914100 -0.00108400
C -4.45172600 1.76679000 0.73089000
C -3.16222000 2.11694700 -1.43282000
H -2.36180200 2.13435500 0.54944400
H -4.45588600 1.32746700 1.73303700
H -4.62873100 2.84323900 0.84918100
H -5.30094200 1.35914100 0.17935800
H -2.19152500 2.05375700 -1.92922100
H -3.89632800 1.59141500 -2.05223400
H -3.45412600 3.17374500 -1.40948400
C -3.44568800 -1.38521200 -0.84454300
C -4.93230900 -1.02190100 -0.97677500
C -3.33943800 -2.80380300 -0.25422100
H -3.00881600 -1.40384300 -1.85143500
H -5.09599100 -0.08453900 -1.51124600
H -5.44330700 -1.81189700 -1.54155800
H -5.42240700 -0.95379800 0.00000800
H -2.31318800 -3.14010300 -0.11055500
H -3.86473600 -2.87234500 0.70462900
H -3.82192600 -3.51340200 -0.93683500
C 0.21223200 0.53275100 2.74064100
H 0.22301400 0.27420200 3.81081300
H 1.14239000 1.03804600 2.48993500
H -0.59165200 1.23764000 2.54525200
P 2.33460100 -0.22734400 0.01954300
C 1.19142400 -1.60925200 2.16951700
C 2.53007800 -1.02864400 1.70508300
H 0.98069000 -2.53483800 1.62929900
H 1.23924900 -1.84977100 3.24344800

H 2.90456400 -0.29463400 2.42161000
H 3.27433000 -1.83045800 1.66608100
C -0.01488600 0.22509400 -1.98449000
O -0.01299400 0.53304500 -3.11287700
C 3.08060500 1.50783600 0.19871000
C 3.29276000 2.13840700 -1.18853200
C 4.31089200 1.71047600 1.09823800
H 2.25239600 2.03937000 0.67728200
H 2.41222800 2.03171500 -1.82722200
H 3.49444900 3.21092900 -1.08363300
H 4.14894200 1.69509300 -1.70806300
H 4.17382100 1.29956300 2.10284600
H 5.22349900 1.27935200 0.68168200
H 4.48651200 2.78715600 1.21690700
C 3.53276800 -1.17045200 -1.10412400
C 3.15710400 -2.65509400 -1.22824600
C 5.01976400 -1.04700100 -0.73379900
H 3.38190500 -0.70668200 -2.08765800
H 2.15309200 -2.80550800 -1.62144700
H 3.85881300 -3.14668000 -1.91263100
H 3.23006700 -3.17625100 -0.26607800
H 5.40294500 -0.03378800 -0.86165000
H 5.21268600 -1.35987700 0.29866300
H 5.61154100 -1.70089600 -1.38623700
Mn-0.00648500 -0.26399700 -0.28521000
C -0.08278600 -1.96993100 -0.76456500
O -0.16475600 -3.06579800 -1.18070000

Mn-4

C -0.13135400 2.86840500 0.16104200
O 0.18422900 3.39648100 -0.90651000
O -0.56380200 3.27620000 1.24634600
H 0.01622500 1.66033600 0.14849100
C -1.19585600 -1.42448500 2.27227300
C -2.48628700 -0.72797500 1.83813700
H -1.21300300 -1.60713800 3.35755900
H -1.10849300 -2.39309900 1.77485600
H -2.66807500 0.16402000 2.44359000
H -3.33581600 -1.39685900 2.00060000
P -2.33723100 -0.19010500 0.05438800
N 0.02501600 -0.63600400 1.92427000
C -3.22181300 1.47142000 0.03698500
C -4.62124100 1.53234300 0.67420300
C -3.19933800 2.12826800 -1.35354200

H -2.54821800 2.05591400 0.67504800
H -4.68080100 0.98903000 1.62264200
H -4.86716000 2.58002800 0.88652500
H -5.39925000 1.14480700 0.01340500
H -2.18222000 2.23191100 -1.73887600
H -3.79241900 1.57253700 -2.08742300
H -3.62578600 3.13634900 -1.28625700
C -3.30666600 -1.45795800 -0.97560000
C -4.79033200 -1.15988100 -1.23470300
C -3.18013400 -2.88075200 -0.40021700
H -2.78433100 -1.43313800 -1.93990000
H -4.95080000 -0.20240300 -1.73304500
H -5.19887700 -1.94074200 -1.88828200
H -5.37500900 -1.17247400 -0.30950200
H -2.15534000 -3.16632000 -0.16199100
H -3.78769400 -2.99449100 0.50396500
H -3.55638000 -3.60027400 -1.13659200
C 0.04743500 0.60192700 2.74461200
H -0.03363600 0.35494200 3.81347600
H 0.97504900 1.14548200 2.57919800
H -0.75365400 1.27728500 2.45447700
P 2.36493000 -0.16410300 0.06450800
C 1.22898200 -1.46069100 2.24986600
C 2.53305200 -0.78524100 1.82072800
H 1.11585900 -2.41522800 1.72989900
H 1.24875400 -1.66721200 3.33083500
H 2.76602100 0.06198200 2.47022500
H 3.36191100 -1.49059200 1.92584500
C 0.01992900 0.37480000 -1.93469200
O 0.02511800 0.66089900 -3.06325200
C 3.19334000 1.52862500 0.10025500
C 3.20527600 2.17956800 -1.29258100
C 4.55928600 1.64159400 0.79941500
H 2.47181400 2.08852700 0.70848200
H 2.19517700 2.27818200 -1.69454900
H 3.62304800 3.19088600 -1.21694200
H 3.82572500 1.62413200 -2.00341600
H 4.59700100 1.10539300 1.75266900
H 5.37802700 1.27780400 0.17552900
H 4.75980300 2.69837800 1.01401000
C 3.39771700 -1.34345800 -1.00439900
C 3.23111900 -2.81003100 -0.56397100
C 4.89759600 -1.03497600 -1.12429900
H 2.94596100 -1.23213600 -1.99815500

H 2.19411500 -3.11113800 -0.41967600
H 3.65630300 -3.46471000 -1.33357600
H 3.77849900 -3.00740700 0.36387900
H 5.09720200 -0.05185400 -1.55306400
H 5.40510200 -1.10092000 -0.15621800
H 5.36066700 -1.77870200 -1.78455700
Mn 0.01456300 -0.15906800 -0.23183100
C 0.00923400 -1.81188900 -0.83908800
O -0.00175100 -2.86444500 -1.35249200

Mn-TS4_4a

C -0.11077000 3.09568100 0.25395500
O -0.05731400 3.30841100 -0.98067200
O -1.03549000 3.32040400 1.07651500
H 0.81870600 2.62866400 0.70028800
C -1.17996100 -1.26525300 2.38183400
C -2.45126400 -0.57425300 1.88797800
H -1.20707100 -1.36760500 3.47705800
H -1.10626400 -2.26934100 1.95850500
H -2.59967500 0.37716900 2.40662300
H -3.32198200 -1.19576900 2.11603100
P -2.29179800 -0.20519000 0.06524700
N 0.06201900 -0.53058800 1.99142100
C -3.25597700 1.39254800 -0.15233900
C -4.65939000 1.44020100 0.47656200
C -3.25392200 1.88094400 -1.61062900
H -2.61584000 2.09095500 0.40358200
H -4.68129100 1.03573200 1.49362400
H -4.97737000 2.48831400 0.54044700
H -5.40935500 0.91034800 -0.11446100
H -2.23802000 2.09661700 -1.94799100
H -3.72008700 1.17156400 -2.30295500
H -3.82030500 2.81799500 -1.67475400
C -3.16351900 -1.62520500 -0.84841900
C -4.66195600 -1.44441100 -1.13536500
C -2.95711000 -2.98054700 -0.14737900
H -2.63862400 -1.65755000 -1.81099700
H -4.87912500 -0.55372400 -1.72734800
H -5.01812700 -2.31096800 -1.70619400
H -5.24939400 -1.40004100 -0.21296800
H -1.91528300 -3.19867000 0.08747900
H -3.53941000 -3.03942000 0.77832500
H -3.31484500 -3.78080500 -0.80563600
C 0.10560300 0.76696900 2.72383800

H -0.08280800 0.60373800 3.79459300
 H 1.08778500 1.22471400 2.61534400
 H -0.61933700 1.47863800 2.32248800
 P 2.44403600 -0.14470900 0.15843100
 C 1.24171100 -1.36725700 2.37430100
 C 2.57335300 -0.76335200 1.92238300
 H 1.10051200 -2.34747300 1.91096900
 H 1.24677300 -1.51232100 3.46502500
 H 2.85666500 0.08112500 2.55617700
 H 3.36325500 -1.50977000 2.03605600
 C 0.07703300 0.45261000 -1.86511500
 O 0.05692600 0.72633200 -2.99262100
 C 3.40539000 1.47866500 0.24706400
 C 3.27069800 2.32417400 -1.02850300
 C 4.87403800 1.32436400 0.67138400
 H 2.87673700 2.00874600 1.04954100
 H 2.22458000 2.53793500 -1.27068200
 H 3.77800100 3.28548400 -0.87825300
 H 3.74881100 1.84231500 -1.88821100
 H 5.29118700 2.31302200 0.89641300
 H 4.99567100 0.70641200 1.56711800
 H 5.48679100 0.89186100 -0.12634300
 C 3.54561600 -1.28294900 -0.87639400
 C 3.23317900 -1.14971800 -2.37649300
 C 3.51725700 -2.75939900 -0.44910200
 H 4.56370600 -0.91644400 -0.70700400
 H 3.21903500 -0.11072500 -2.71527200
 H 3.99987500 -1.67643500 -2.95715600
 H 2.26747100 -1.59899200 -2.62471900
 H 3.86947700 -2.90827600 0.57514300
 H 2.52197400 -3.20126300 -0.54028800
 H 4.18645800 -3.33028300 -1.10408400
 Mn 0.08342900 -0.12192100 -0.15641600
 C 0.12979800 -1.75877100 -0.77063900
 O 0.15693700 -2.83078400 -1.23994300

Mn-4a

C 0.00283300 2.91199300 -0.26844000
 O 0.00227900 1.80142100 0.38599700
 O 0.00781000 4.04197600 0.22445600
 H -0.00183300 2.81034900 -1.37911700
 C -1.20485600 -1.54428300 2.16882100
 C -2.51590500 -0.86385800 1.76673700
 H -1.24068500 -1.82691800 3.23281100

H -1.06633900 -2.45979200 1.58810200
 H -2.75452100 -0.04991800 2.45497500
 H -3.33780200 -1.58164200 1.84414800
 P -2.36988600 -0.16926800 0.03378300
 N -0.01547700 -0.67715300 1.92052100
 C -3.13765500 1.54699800 0.14618900
 C -4.43169800 1.72193900 0.95799900
 C -3.25535100 2.19126600 -1.24528700
 H -2.34014600 2.07239200 0.68233400
 H -4.38334400 1.24201800 1.93996000
 H -4.59968200 2.79215700 1.13214800
 H -5.31173300 1.33612700 0.43935600
 H -2.33440700 2.09205100 -1.82650500
 H -4.06849900 1.75010800 -1.83114900
 H -3.46872200 3.26179100 -1.14362700
 C -3.49470600 -1.25382400 -1.03831100
 C -5.00121800 -0.96824300 -0.93753300
 C -3.25993100 -2.75465400 -0.78900100
 H -3.16442700 -1.02488000 -2.06018100
 H -5.26922400 0.03456200 -1.27403700
 H -5.54461700 -1.67989600 -1.57151700
 H -5.36898900 -1.09924100 0.08598600
 H -2.21379000 -3.04870100 -0.85922700
 H -3.63936100 -3.06005000 0.19244600
 H -3.81333100 -3.33172100 -1.53930500
 C -0.07424700 0.48923900 2.83578800
 H -0.08362500 0.14659500 3.88130200
 H 0.77604400 1.14438700 2.66892000
 H -0.96139300 1.08438800 2.63794800
 P 2.36562000 -0.14158400 0.05094900
 C 1.21997700 -1.45831000 2.22375700
 C 2.49451200 -0.70819000 1.82835200
 H 1.15659200 -2.39875800 1.67149500
 H 1.24576100 -1.70409600 3.29701900
 H 2.63441700 0.17220000 2.46048200
 H 3.36459400 -1.35095300 1.99201700
 C 0.00545500 0.30329600 -1.99842300
 O 0.00587500 0.52395200 -3.14602800
 C 3.15882200 1.56561500 0.06463400
 C 3.24747500 2.16163300 -1.34979500
 C 4.47612400 1.74547100 0.83728200
 H 2.38473400 2.12273900 0.60365500
 H 2.30153300 2.08046800 -1.89230300
 H 3.50384300 3.22589400 -1.28925900

H 4.02031200 1.67358100 -1.95268200
H 4.44896100 1.28655900 1.83013700
H 5.33696800 1.33930100 0.30217700
H 4.65974500 2.81734300 0.98295300
C 3.46236000 -1.32964100 -0.94048400
C 3.27899500 -2.79180400 -0.49257300
C 4.96514900 -1.01108500 -0.97287800
H 3.06839600 -1.23543700 -1.96089100
H 2.23712400 -3.10506100 -0.43971800
H 3.78122900 -3.45122900 -1.21022000
H 3.74278400 -2.96754600 0.48412200
H 5.18548200 -0.04100400 -1.42175400
H 5.40624200 -1.03619200 0.02929000
H 5.47914300 -1.77196900 -1.57338200
Mn 0.00215600 -0.13959200 -0.28015400
C 0.02675900 -1.81788400 -0.82843300
O 0.05574300 -2.89002100 -1.30568900

Mn-5

C 0.11780100 4.21697100 -0.23578700
O 1.19396100 3.61629600 0.02681800
O -1.06837200 3.84847700 -0.06225000
H 0.24487300 5.24366300 -0.69357800
H 0.40966600 1.40347800 -0.38292000
H 2.28524600 1.10513700 -2.60357600
C 3.28846600 1.23732800 -2.18754900
C 3.28538000 1.25939300 -0.65154900
H 3.67413800 2.19258800 -2.56275800
H 3.93186100 0.44712600 -2.58949400
P 2.36615100 -0.19382100 0.10485200
C 4.70557800 1.46137800 -0.10067100
H 2.66282900 2.10721600 -0.33812200
C 2.48338700 0.15184600 1.93429500
C 3.46913600 -1.69419500 -0.22240300
H 4.73266000 1.49693300 0.99281800
H 5.39666900 0.67831300 -0.43219800
H 5.10225300 2.41639700 -0.46571900
P -2.33087200 -0.22124400 0.03575900
C 0.03542100 -0.57615500 -1.94728000
C 1.21756200 -0.34896300 2.62996000
H 2.59382000 1.23210600 2.05933800
H 3.36379100 -0.30814100 2.39040500
C 3.13419200 -2.35310800 -1.57109800
C 3.46688400 -2.73984500 0.90450500

H 4.48347900 -1.28341500 -0.28755400
C -2.51960400 -0.14556500 1.89715700
C -3.13305300 1.37010500 -0.55992900
C -3.51434600 -1.55374100 -0.63355000
O 0.02468000 -0.74671200 -3.09846700
N -0.02533100 0.16312300 1.97554900
H 1.18076300 -1.44085200 2.59887300
H 1.22076200 -0.04716700 3.68785500
H 3.13022600 -1.64044400 -2.39966000
H 3.88195900 -3.12188200 -1.79956800
H 2.15659200 -2.84305900 -1.54419200
H 2.47998000 -3.18489300 1.05517600
H 4.15047200 -3.55469100 0.63698500
H 3.81189900 -2.33382800 1.85906400
C -1.20598700 -0.52147300 2.58439600
H -2.82107100 0.87089500 2.16358700
H -3.31097000 -0.80873200 2.25230400
C -4.59351800 1.55325800 -0.12150300
C -2.99002400 1.53291900 -2.08150400
H -2.51739900 2.15368500 -0.10060300
C -4.58310300 -2.01252100 0.36963800
C -2.81489400 -2.76743000 -1.25868300
H -4.02650200 -1.02395100 -1.44536400
C -0.13024100 1.62675500 2.23422600
H -1.25996900 -0.27209600 3.65457400
H -1.03884400 -1.59883000 2.50514400
H -4.72301800 1.46993800 0.96225600
H -4.93646400 2.55355900 -0.41269500
H -5.26188800 0.83012300 -0.60145000
H -3.38019300 2.51239900 -2.38009000
H -1.94629900 1.48616300 -2.40464400
H -3.55243900 0.77415000 -2.63871100
H -5.13685700 -1.18033600 0.81174800
H -5.30769700 -2.65509900 -0.14452400
H -4.14644700 -2.60370600 1.18246400
H -2.05427500 -2.47888900 -1.98838500
H -2.34062500 -3.39821600 -0.50271000
H -3.55753900 -3.38273200 -1.78077600
H -0.15221700 1.81347100 3.31771500
H 0.69546800 2.16486100 1.77142600
H -1.02479300 2.03844800 1.77236600
H -0.37824000 1.36402600 -0.45098200
Mn 0.02394100 -0.31281400 -0.17954700
C 0.04662500 -2.07161000 0.11406100

O 0.06722700 -3.22322300 0.28970800

Mn-TS5_6

C -0.12050500 4.22368700 -0.18776300
O 0.79550600 3.36565500 -0.40088300
O -1.31960500 4.03967200 0.09490200
H 0.22590000 5.28984900 -0.26863000
H 0.16770200 1.79864700 -0.46758700
H 2.25829700 1.13962300 -2.61153600
C 3.26016200 1.30463100 -2.20522500
C 3.26784800 1.33632800 -0.66938100
H 3.61705600 2.26641300 -2.59223700
H 3.92231800 0.52874100 -2.60454100
P 2.35407800 -0.11969000 0.09683400
C 4.69066800 1.55021700 -0.13010300
H 2.64373000 2.18292300 -0.36298400
C 2.49478000 0.23472000 1.92605400
C 3.47994000 -1.60583800 -0.22698800
H 4.72611900 1.59077600 0.96297800
H 5.38252700 0.76846800 -0.46254200
H 5.08149700 2.50471100 -0.50328800
P -2.32656800 -0.26585600 0.09168300
C 0.03897400 -0.62701100 -1.92123700
C 1.23042200 -0.24234700 2.64194900
H 2.62611100 1.31327800 2.04621100
H 3.37283100 -0.23640400 2.37540100
C 3.15858700 -2.26844700 -1.57719800
C 3.48108800 -2.65545800 0.89596400
H 4.49122200 -1.18678900 -0.28627600
C -2.50541500 -0.01894700 1.93714400
C -3.21792300 1.23513500 -0.61189800
C -3.41806900 -1.74420400 -0.34997300
O 0.05732000 -0.81601700 -3.07029300
N -0.01500900 0.26379600 1.98906500
H 1.18452100 -1.33404200 2.63123500
H 1.24642700 0.07938600 3.69426200
H 3.15757000 -1.55768200 -2.40714000
H 3.91110200 -3.03465000 -1.79926900
H 2.18249700 -2.76158900 -1.55648800
H 2.49705100 -3.10950700 1.03825500
H 4.17331200 -3.46349500 0.62956000
H 3.81667600 -2.25092200 1.85457400
C -1.19529600 -0.38893100 2.63365900
H -2.75514200 1.02959200 2.11799700

H -3.32426000 -0.61104800 2.35336500
C -4.65546100 1.41928800 -0.10168300
C -3.17173000 1.29649000 -2.14637500
H -2.60319800 2.06612600 -0.23902200
C -3.40297100 -2.87406200 0.69230200
C -3.06215200 -2.29976700 -1.73880600
H -4.43805300 -1.34348000 -0.38970100
C -0.10528900 1.73223600 2.20962200
H -1.23750300 -0.10117800 3.69499600
H -1.03767100 -1.46970700 2.58944800
H -4.72335900 1.40552300 0.99046500
H -5.03788200 2.39090700 -0.43711800
H -5.33442200 0.65332100 -0.49293300
H -3.51664100 2.28197800 -2.48070400
H -2.16004100 1.15443600 -2.53722600
H -3.82604400 0.54976700 -2.60879500
H -3.75124400 -2.54888800 1.67627900
H -4.07714400 -3.67292200 0.36088200
H -2.40939000 -3.31555100 0.80579800
H -3.07404300 -1.53334600 -2.51702800
H -2.07109500 -2.76370800 -1.73832300
H -3.78825600 -3.07099000 -2.02260900
H -0.14952200 1.94907600 3.28714400
H 0.75156100 2.23696800 1.77084600
H -0.98046300 2.14913800 1.71620500
H -0.40341000 1.26828500 -0.69169200
Mn 0.01223500 -0.30736900 -0.16604600
C 0.06081500 -2.04973900 0.16259700
O 0.06658300 -3.20919300 0.31199300

Mn-6

C -0.64183400 4.36557900 -0.05428700
O 0.04129800 3.54620400 -0.84228900
O -1.28157500 4.06099500 0.93366700
H -0.55489300 5.40350800 -0.41791000
H -0.02313600 2.58731300 -0.52359700
H 2.11109200 1.84047400 -2.11967500
C 3.08001600 2.03387900 -1.65270900
C 3.10369700 1.63393000 -0.16990600
H 3.28997800 3.10535000 -1.75230200
H 3.84761300 1.50027400 -2.22323000
P 2.38217900 -0.08328400 0.13737000
C 4.49360800 1.88310000 0.43588300
H 2.37999900 2.27018300 0.35518800

C 2.52595700 -0.22097000 2.00224000
C 3.70393000 -1.25626200 -0.54632000
H 4.54734500 1.62372300 1.49770400
H 5.27461500 1.32251200 -0.08901200
H 4.74853200 2.94640600 0.34719300
P -2.20831000 -0.44180300 0.01146200
C 0.10116200 -0.26879400 -1.97572200
C 1.29640300 -0.94104700 2.55954300
H 2.60296300 0.78943200 2.41318800
H 3.43255500 -0.74919000 2.30912700
C 3.46729400 -1.54084000 -2.03978500
C 3.82455600 -2.58125200 0.22448400
H 4.65798400 -0.72544600 -0.44221900
C -2.44421700 -0.78260800 1.84091800
C -3.03963800 1.23534700 -0.24625000
C -3.24911700 -1.73953700 -0.89537800
O 0.05651100 -0.16036100 -3.14164900
N 0.02531500 -0.37171000 2.02453100
H 1.32288300 -1.99639400 2.27806700
H 1.29194500 -0.88933700 3.65988900
H 3.37626700 -0.63019600 -2.63693100
H 4.30748100 -2.11884600 -2.44409100
H 2.55777300 -2.13110500 -2.18819500
H 2.90038700 -3.16312800 0.18057200
H 4.61549500 -3.19056700 -0.23014800
H 4.09417200 -2.43871600 1.27464100
C -1.11587700 -1.23127300 2.45783900
H -2.80620100 0.12656200 2.32722800
H -3.20502500 -1.55013000 2.01278700
C -4.40363100 1.50691500 0.41086800
C -3.05309100 1.62600200 -1.73255800
H -2.31433200 1.88801800 0.25140700
C -4.77013000 -1.52280900 -0.89060000
C -2.93879600 -3.16373100 -0.40475800
H -2.89265500 -1.65769300 -1.93076800
C -0.16180100 0.98859500 2.58811700
H -1.18994800 -1.22092700 3.55684200
H -0.88521500 -2.25401100 2.15041900
H -4.44269400 1.19089400 1.45782300
H -4.59098600 2.58805400 0.39732000
H -5.23206800 1.02897200 -0.11569900
H -3.32302300 2.68403100 -1.83656100
H -2.07654800 1.48595300 -2.20286500
H -3.78683600 1.04477200 -2.30164300

H -5.06765600 -0.61378900 -1.41604600
H -5.25734600 -2.36459900 -1.39865400
H -5.17379200 -1.47998100 0.12724500
H -1.87707400 -3.40504000 -0.43415900
H -3.29967000 -3.32243000 0.61789700
H -3.45927700 -3.88695200 -1.04387300
H -0.22866500 0.94514600 3.68640500
H 0.67054200 1.63071200 2.30858700
H -1.06382300 1.44717100 2.19156000
H 0.00315600 1.20886100 -0.14247800
Mn 0.11485700 -0.41545500 -0.21716400
C 0.32000900 -2.17777300 -0.31551300
O 0.49256900 -3.33232900 -0.45757400

'Bu-2

Fe 0.00000500 -0.10599100 -0.13800900
H -0.00003800 -1.60968700 -0.47940300
H 0.00000700 1.38574700 0.34069000
C 1.20865900 -0.10824300 2.65308900
C 2.49793600 -0.44232600 1.90321700
H 1.27116200 -0.47271400 3.69110100
H 1.07018700 0.97264900 2.68747000
H 2.72150500 -1.50937400 1.98023500
H 3.33931100 0.08768500 2.36053400
P 2.29594600 -0.01978000 0.09211300
N 0.00003700 -0.68329600 1.99443600
C 3.42972900 -1.32648100 -0.77934400
C 4.79735100 -1.53916700 -0.09483200
C 3.64269300 -0.93625500 -2.25509900
H 4.69408800 -1.83300600 0.95438900
H 5.32155400 -2.35744100 -0.60546900
H 5.44664400 -0.66595600 -0.13872200
H 2.69302800 -0.78211300 -2.77645900
H 4.24766700 -0.03338800 -2.36837300
H 4.17107200 -1.74862700 -2.77069900
C 3.11326500 1.73287600 -0.07864900
C 4.65107700 1.74441500 -0.01002700
C 2.59982700 2.62695600 1.07003600
H 5.11816500 1.25872100 -0.86911500
H 4.99419000 2.78721600 -0.00532200
H 5.03028600 1.27636100 0.90374300
H 1.50877100 2.65757300 1.09907900
H 2.97265000 2.30461600 2.04768700
H 2.96411000 3.64935600 0.90776000

C	0.00015600	-2.15267400	2.19864200	H	2.49957400	-3.03585000	0.26169900
H	0.00017400	-2.39433000	3.27304900	H	1.75048100	-2.65174400	-1.29179400
H	-0.87553000	-2.59868800	1.73173900	H	3.34350600	-3.43548200	-1.23589000
H	0.87594500	-2.59851800	1.73176000				
P	-2.29592300	-0.01981900	0.09214400	'Bu-3			
C	-1.20861100	-0.10834300	2.65313900	C	0.06679400	4.80747900	-0.24466500
C	-2.49788800	-0.44239600	1.90325200	O	-0.01478700	4.75712500	-1.40998700
H	-1.07016700	0.97255000	2.68758400	O	0.14804300	4.88314000	0.91980800
H	-1.27110200	-0.47287300	3.69113200	Fe	-0.00499500	-0.28617100	-0.09009100
H	-2.72143300	-1.50945000	1.98021300	H	0.00292600	1.25772600	-0.08203200
H	-3.33927000	0.08757800	2.36060200	H	-0.01317400	-1.83924700	0.04047600
C	-0.00001800	0.18197800	-1.83938900	C	-1.21282600	-0.96522900	2.62174300
O	-0.00008700	0.30469600	-3.00407500	C	-2.50559800	-0.46612600	1.97760500
C	-3.42970300	-1.32648100	-0.77934800	H	-1.27348000	-0.86442800	3.71731900
C	-3.64271600	-0.93618000	-2.25508000	H	-1.07189800	-2.02157700	2.39087700
C	-4.79730200	-1.53920200	-0.09478500	H	-2.74259800	0.54313800	2.32198400
H	-2.69305700	-0.78195300	-2.77642900	H	-3.34044100	-1.10414900	2.28399900
H	-4.17103500	-1.74856700	-2.77071900	P	-2.30221300	-0.41189200	0.11965200
H	-4.24775000	-0.03335300	-2.36832800	N	-0.00436300	-0.24567400	2.12157900
H	-4.69399300	-1.83333500	0.95434600	C	-3.42728400	1.08702800	-0.37589900
H	-5.44649700	-0.66589900	-0.13839000	C	-4.81654200	1.09993600	0.29717200
H	-5.32163500	-2.35727500	-0.60560600	C	-3.58817500	1.12721100	-1.90770500
C	-3.11334100	1.73279100	-0.07859800	H	-4.75062900	1.02630100	1.38727200
C	-2.59990200	2.62688800	1.07007400	H	-5.30668900	2.05612600	0.07150300
C	-4.65115500	1.74424500	-0.00987900	H	-5.47875300	0.31090300	-0.05659000
H	-1.50884800	2.65762100	1.09902200	H	-2.61965600	1.14429600	-2.41703200
H	-2.96430200	3.64925900	0.90786700	H	-4.16313700	0.28039400	-2.29035500
H	-2.97260100	2.30447700	2.04775000	H	-4.12557500	2.04084700	-2.19345800
H	-5.11828900	1.25856600	-0.86894600	C	-3.12460000	-2.05333900	-0.50524300
H	-5.03028100	1.27612200	0.90389200	C	-4.66354100	-2.07008000	-0.46401100
H	-4.99431100	2.78702900	-0.00510000	C	-2.63440200	-3.21999200	0.37889800
C	-2.65497000	2.36429000	-1.40828200	H	-5.11224300	-1.37943900	-1.18099700
H	-3.08268200	3.37151000	-1.49758000	H	-5.01050100	-3.07722000	-0.72961100
H	-1.56702500	2.45661000	-1.44370700	H	-5.05818900	-1.84597200	0.53210600
H	-2.98074800	1.79374300	-2.28213300	H	-1.54418500	-3.26961100	0.41685800
C	-2.70021500	-2.68627600	-0.75659300	H	-3.02274000	-3.15946800	1.40053200
H	-1.75042600	-2.65159700	-1.29201000	H	-3.00148900	-4.16152600	-0.04928900
H	-2.49942900	-3.03593800	0.26146900	C	-0.00074900	1.12916900	2.67873400
H	-3.34340100	-3.43542700	-1.23613800	H	-0.01042400	1.10002100	3.77973600
C	2.65480400	2.36435800	-1.40830500	H	0.88144100	1.67014600	2.34369900
H	1.56686100	2.45672000	-1.44366100	H	-0.86867400	1.68215100	2.32683100
H	3.08254300	3.37156100	-1.49767000	P	2.28900200	-0.43480400	0.11713700
H	2.98050700	1.79376600	-2.28215600	C	1.20017900	-0.97097400	2.62284500
C	2.70029600	-2.68630500	-0.75641800	C	2.49473900	-0.48166700	1.97474200

H	1.05257600	-2.02740300	2.39652400	O	-0.00045000	3.89181100	0.86466300
H	1.26309600	-0.86640500	3.71792300	Fe	0.00002600	0.07467400	-0.07375100
H	2.73680300	0.52828000	2.31341500	H	0.00010300	1.71759500	-0.01177800
H	3.32716100	-1.12208500	2.28291600	H	-0.00000200	-1.43767400	-0.09489600
C	-0.00331800	-0.20752300	-1.81431900	C	-1.20159100	-0.74737400	2.62956300
O	-0.00126100	-0.09281300	-2.97957800	C	-2.49994600	-0.29581700	1.96625800
C	3.43008100	1.04827900	-0.39065500	H	-1.27425100	-0.62528400	3.72163500
C	3.60697600	1.06468200	-1.92129200	H	-1.03594600	-1.80544200	2.42843300
C	4.81214100	1.05939000	0.29713700	H	-2.75524800	0.72057700	2.27662900
H	2.64352700	1.08088500	-2.44032300	H	-3.32232500	-0.94214000	2.28948100
H	4.15296100	1.97077300	-2.21458800	P	-2.30109600	-0.28330100	0.11043900
H	4.18008200	0.20902400	-2.28638200	N	-0.00004000	-0.01501200	2.12997900
H	4.73246000	1.02312200	1.38819500	C	-3.62763600	1.01462700	-0.43317900
H	5.46438600	0.24753100	-0.02192600	C	-4.96212000	0.92140500	0.33751700
H	5.32163400	1.99893700	0.04571000	C	-3.88405100	0.91849400	-1.95041200
C	3.09518100	-2.08789600	-0.49880300	H	-4.82659200	1.07545000	1.41246100
C	2.58741500	-3.24599400	0.38670100	H	-5.62509600	1.72100700	-0.01738500
C	4.63368900	-2.12175500	-0.44859300	H	-5.48928700	-0.02044000	0.19479100
H	1.49652000	-3.28408100	0.41734500	H	-2.95149900	0.97162900	-2.52107700
H	2.94792600	-4.19286500	-0.03521800	H	-4.41254300	0.00713400	-2.23947700
H	2.96918700	-3.18523600	1.41080100	H	-4.50580100	1.76727700	-2.26315200
H	5.09474800	-1.43757700	-1.16387500	C	-2.90689600	-2.04124000	-0.45372700
H	5.02390800	-1.89964900	0.54973500	C	-4.43089300	-2.25264600	-0.37543200
H	4.97132900	-3.13326600	-0.70951000	C	-2.26837400	-3.11785800	0.44873600
C	2.71460500	2.35385300	0.01420700	H	-4.98755300	-1.63801200	-1.08491800
H	1.72435100	2.42151100	-0.43799600	H	-4.64923800	-3.30022200	-0.62010300
H	2.59931900	2.44497100	1.09936300	H	-4.82346000	-2.07034000	0.62987900
H	3.32005300	3.20586600	-0.32084100	H	-1.18053400	-3.03412800	0.48034100
C	-2.70545800	2.38001400	0.05718900	H	-2.65938100	-3.08685400	1.47061000
H	-2.61205300	2.45885100	1.14562200	H	-2.51679200	-4.10543300	0.03990500
H	-1.70506000	2.44215300	-0.37320100	C	-0.00059800	1.35398600	2.69735700
H	-3.29399200	3.24237300	-0.28138200	H	-0.00127300	1.31298800	3.79806200
C	-2.65400500	-2.32293800	-1.94808600	H	0.87328100	1.90212100	2.35418800
H	-2.96151500	-1.54044800	-2.64685400	H	-0.87414500	1.90190300	2.35301700
H	-1.56702800	-2.41639900	-1.99493900	P	2.30114900	-0.28311500	0.11046200
H	-3.09055400	-3.26676300	-2.30018200	C	1.20191200	-0.74650400	2.62989100
C	2.62792500	-2.35740100	-1.94272500	C	2.50001800	-0.29468500	1.96627200
H	3.04914800	-3.31100300	-2.28708200	H	1.03678000	-1.80476700	2.42939400
H	1.53969400	-2.43155900	-1.99491200	H	1.27457000	-0.62378500	3.72189000
H	2.95269700	-1.58472700	-2.64451100	H	2.75482500	0.72201500	2.27604600
'Bu-TS3_4							
C	-0.00013000	3.47577800	-0.25077700	H	3.32272900	-0.94042000	2.28982200
O	0.00007300	3.59828800	-1.43571100	C	0.00000800	0.23473400	-1.79899700
				O	0.00001000	0.37984400	-2.95630400
				C	3.62757500	1.01471300	-0.43369600

C	3.88402800	0.91802800	-1.95089000	H	-1.04045200	-1.74952500	2.45771100
C	4.96204000	0.92187300	0.33708500	H	-2.76418200	0.77387200	2.27744100
H	2.95148300	0.97079000	-2.52160100	H	-3.32485300	-0.89110000	2.31230900
H	4.50563700	1.76679800	-2.26394400	P	-2.32434500	-0.25152800	0.12177800
H	4.41268300	0.00665000	-2.23959800	N	-0.00001200	0.03203900	2.11488100
H	4.82651500	1.07705000	1.41186700	C	-3.65718700	1.02485800	-0.44739600
H	5.48892700	-0.02027100	0.19532400	C	-4.98596400	0.92680000	0.33225400
H	5.62525200	1.72092000	-0.01862700	C	-3.91852600	0.89608900	-1.96125900
C	2.90709100	-2.04124300	-0.45298400	H	-4.84722800	1.10284100	1.40331100
C	2.26860700	-3.11754500	0.44988300	H	-5.65962700	1.71144600	-0.03487600
C	4.43109600	-2.25257100	-0.37460300	H	-5.50109900	-0.02454000	0.20844800
H	1.18077800	-3.03371700	0.48162800	H	-2.99006200	0.95185600	-2.53818400
H	2.51688100	-4.10526500	0.04131300	H	-4.43950700	-0.02498400	-2.23199600
H	2.65977200	-3.08625500	1.47169000	H	-4.55041800	1.73345500	-2.28325500
H	4.98775100	-1.63815400	-1.08428400	C	-2.89108300	-2.02432400	-0.42513400
H	4.82364900	-2.06994200	0.63065500	C	-4.41090000	-2.25895800	-0.32962500
H	4.64946900	-3.30021900	-0.61894200	C	-2.22676100	-3.08122300	0.48156100
C	3.04165400	2.41230300	-0.15720300	H	-4.98350900	-1.66364200	-1.04271400
H	2.19985500	2.62098500	-0.81471900	H	-4.61241800	-3.31325800	-0.55836800
H	2.71753600	2.54126600	0.87947000	H	-4.79722700	-2.06913600	0.67657400
H	3.81527500	3.16550000	-0.35489700	H	-1.14063500	-2.97953700	0.50907000
C	2.43024400	-2.29329300	-1.89733400	H	-2.61337100	-3.05043700	1.50483100
H	1.33957100	-2.28021200	-1.95988700	H	-2.45742400	-4.07591000	0.08031000
H	2.82437400	-1.56359400	-2.60911700	C	0.00002300	1.41951900	2.63998400
H	2.77188100	-3.28498600	-2.22165200	H	-0.00011000	1.40898500	3.74030400
C	-3.04179700	2.41214900	-0.15612700	H	0.86972800	1.96328700	2.27974200
H	-2.71742700	2.54063100	0.88052400	H	-0.86943900	1.96348600	2.27947400
H	-2.20017900	2.62121200	-0.81375500	P	2.32435900	-0.25154800	0.12176200
H	-3.81552600	3.16538000	-0.35325900	C	1.20290300	-0.68707100	2.63702500
C	-2.43001100	-2.29272100	-1.89816400	C	2.50715700	-0.24514600	1.97718200
H	-2.82430100	-1.56286500	-2.60970200	H	1.04041700	-1.74954300	2.45772800
H	-1.33934100	-2.27940500	-1.96072900	H	1.26448800	-0.54102800	3.72598200
H	-2.77146200	-3.28437400	-2.22280500	H	2.76421300	0.77381100	2.27743400
'Bu-4				H	3.32478400	-0.89118600	2.31233200
C	-0.00005000	3.11906200	-0.26923200	C	-0.00001900	0.19522100	-1.80210100
O	0.00014900	3.36022000	-1.48334900	O	0.00001300	0.22653800	-2.96229100
O	-0.00026200	3.81320700	0.75150000	C	3.65717500	1.02493500	-0.44733800
Fe	0.00001600	0.11334600	-0.05295400	C	3.91836200	0.89630400	-1.96123900
H	0.00003500	1.92915200	-0.02724000	C	4.98602700	0.92676600	0.33216800
H	0.00004700	-1.36344600	-0.10758200	H	2.98983900	0.95217500	-2.53805900
C	-1.20293200	-0.68706200	2.63703500	H	4.55027300	1.73365900	-2.28322900
C	-2.50718400	-0.24510000	1.97720100	H	4.43925500	-0.02478000	-2.23211800
H	-1.26448900	-0.54103900	3.72599600	H	4.84741200	1.10252400	1.40328600
				H	5.50120900	-0.02450500	0.20804700

H	5.65959600	1.71155500	-0.03483300	C	-3.78662900	1.38591800	-1.73981500
C	2.89114000	-2.02430200	-0.42516600	H	-4.74244200	1.17252400	1.61415500
C	2.22698200	-3.08114500	0.48170600	H	-5.43192400	2.12688400	0.30470500
C	4.41097600	-2.25888700	-0.32987500	H	-5.51195100	0.36794500	0.23926400
H	1.14085700	-2.97947600	0.50940000	H	-2.85364300	1.41634400	-2.31053000
H	2.45758500	-4.07587100	0.08051700	H	-4.41348300	0.58513500	-2.13908500
H	2.61374400	-3.05026300	1.50492000	H	-4.30980700	2.33200100	-1.92597000
H	4.98345300	-1.66358000	-1.04308000	C	-3.10773900	-1.84599000	-0.65319200
H	4.79745800	-2.06901100	0.67625300	C	-4.64234300	-1.94092400	-0.55722600
H	4.61247400	-3.31319100	-0.55861300	C	-2.52974600	-3.07973400	0.07209100
C	-3.08250400	2.43243500	-0.20114200	H	-5.15227900	-1.19739200	-1.17247900
H	-2.75187200	2.58514400	0.83017400	H	-4.95425400	-2.92825600	-0.92060100
H	-2.25016600	2.64919400	-0.86965800	H	-5.00046300	-1.84758400	0.47275400
H	-3.86913000	3.17112700	-0.40179400	H	-1.43729500	-3.07869100	0.08778500
C	3.08250900	2.43247500	-0.20089000	H	-2.90019000	-3.16670100	1.09790900
H	2.25009600	2.64929400	-0.86929500	H	-2.85378000	-3.98004100	-0.46460100
H	2.75198400	2.58510800	0.83047100	C	0.04980700	0.85839100	2.80453300
H	3.86910400	3.17119900	-0.40155900	H	0.04726300	0.71800000	3.89477600
C	2.42553300	-2.27877500	-1.87273800	H	0.97043700	1.36274600	2.51710000
H	2.76076000	-3.27571700	-2.18646500	H	-0.78682500	1.50082100	2.52966100
H	1.33613600	-2.25720400	-1.95074800	P	2.29442500	-0.44276200	0.16153100
H	2.83413400	-1.55802900	-2.58477700	C	1.07754500	-1.33644900	2.50869000
C	-2.42567600	-2.27870600	-1.87277700	C	2.42927800	-0.86149800	1.97983100
H	-2.83442800	-1.55796400	-2.58473100	H	0.85304400	-2.32950400	2.11619000
H	-1.33629200	-2.25705400	-1.95095200	H	1.10927500	-1.41072800	3.60608400
H	-2.76088000	-3.27565900	-2.18649600	H	2.75749100	0.02881200	2.51818300
'Bu-TS4_5							
C	0.41864700	3.67111500	-0.22179900	H	3.17816100	-1.63329400	2.17352200
O	0.10151200	3.39529300	-1.40935600	C	-0.02507400	0.22390400	-1.71992700
O	0.90221900	4.71037700	0.26660900	O	-0.01671200	0.30288000	-2.87669700
Fe	-0.04267200	-0.06342800	0.01618200	C	3.51835800	1.02669600	-0.11860000
H	0.22695900	2.82446700	0.52138000	C	3.18051300	1.68484900	-1.47451600
H	-0.12539400	-1.48426900	-0.28533500	C	5.01115700	0.64827300	-0.09168000
C	-1.32026900	-1.13193700	2.55834600	H	2.16054400	2.07785100	-1.50335800
C	-2.58494700	-0.49999100	1.98236500	H	3.86347200	2.52949300	-1.63142700
H	-1.35902800	-1.12462100	3.65751300	H	3.31339500	1.00250800	-2.31713200
H	-1.24720000	-2.17145400	2.24041400	H	5.29893700	0.14139800	0.83479000
H	-2.77201900	0.47616600	2.43790000	H	5.30690800	0.02549500	-0.93848000
H	-3.45020500	-1.12798000	2.21754200	H	5.60051400	1.57202000	-0.15289600
P	-2.38359100	-0.24438400	0.14473700	C	2.96281400	-2.01852600	-0.74886900
N	-0.06318600	-0.45208400	2.11187700	C	1.90964000	-3.14435700	-0.67714800
C	-3.53319200	1.25220900	-0.22540900	C	4.25596300	-2.58646900	-0.12441700
C	-4.87813300	1.20623100	0.52893800	H	1.00022700	-2.89552300	-1.22569400
				H	2.34045700	-4.04722000	-1.12863400
				H	1.63554900	-3.39612700	0.35166900

H 5.07528200 -1.87140300 -0.08198000
H 4.08951600 -2.97768100 0.88367200
H 4.59042900 -3.43113500 -0.73940300
C -2.76791600 2.50943300 0.22991300
H -2.49577800 2.47775600 1.29097300
H -1.86911200 2.67383000 -0.36862700
H -3.41850800 3.38339200 0.09557900
C 3.29796600 2.07785200 0.99035300
H 3.85124800 2.98419100 0.71781400
H 2.25477500 2.37532700 1.10244200
H 3.68349000 1.74935700 1.96021500
C -2.68078100 -1.92148600 -2.13301300
H -1.59518000 -1.98883000 -2.23497800
H -3.11234800 -2.82527400 -2.58137400
H -3.02743200 -1.06800900 -2.71982000
C 3.20897000 -1.70120000 -2.23767100
H 2.32751900 -1.26797100 -2.71922200
H 4.05262000 -1.02475100 -2.39174500
H 3.44281700 -2.63537700 -2.76361100

^tBu-5

C 0.01052300 2.91430800 -0.95601600
O -0.02044200 2.07242300 0.01958800
O -0.06625700 4.14139800 -0.85916000
Fe 0.00300100 0.02649600 -0.09243300
H 0.12086500 2.46727200 -1.97248600
H 0.00658700 -1.48116000 -0.07403500
C -1.19131900 -0.94364400 2.57263000
C -2.50954700 -0.44664100 1.98740700
H -1.23817800 -0.92389500 3.67262800
H -1.02636500 -1.97751100 2.27003100
H -2.78148400 0.51937100 2.41731900
H -3.31104700 -1.14370800 2.25325800
P -2.35778500 -0.24254500 0.13795700
N 0.00311300 -0.16506700 2.11983600
C -3.57282200 1.22040000 -0.20832100
C -5.03932500 0.99711300 0.21853500
C -3.52006600 1.55471600 -1.71135700
H -5.12279400 0.58990600 1.23141200
H -5.54538200 1.97117100 0.22110500
H -5.59622600 0.35160400 -0.45955900
H -2.50447000 1.78836500 -2.04465200
H -3.90383900 0.73714500 -2.32907500
H -4.14399400 2.43500600 -1.91148800

C -3.06041800 -1.90486100 -0.57184300
C -4.58779600 -2.06182800 -0.45147100
C -2.42195300 -3.08124600 0.19777500
H -5.12722000 -1.43189600 -1.16090900
H -4.85018900 -3.10168600 -0.68441900
H -4.95868000 -1.85187600 0.55605000
H -1.33121900 -3.02967500 0.19864900
H -2.77536800 -3.14195700 1.23177700
H -2.71373400 -4.01640200 -0.29639800
C 0.00141400 1.16016500 2.78507400
H -0.00025900 1.03677600 3.87852100
H 0.87742500 1.73244900 2.48796100
H -0.87368200 1.73157100 2.48405500
P 2.36172100 -0.23644500 0.13696500
C 1.19911200 -0.94149500 2.57205000
C 2.51584700 -0.44178100 1.98604400
H 1.03619400 -1.97556700 2.26885500
H 1.24645100 -0.92210600 3.67202300
H 2.78641300 0.52464700 2.41607200
H 3.31908500 -1.13715400 2.25088600
C -0.00057100 -0.04089000 -1.82999000
O -0.00633600 -0.11761900 -2.99200400
C 3.57325000 1.22921600 -0.20571900
C 3.53129000 1.55680300 -1.71046100
C 5.03733900 1.01667000 0.23497600
H 2.51571400 1.77412000 -2.05460300
H 4.14502100 2.44466200 -1.90867000
H 3.93259700 0.74159900 -2.32008000
H 5.11419400 0.61439300 1.25035500
H 5.60416200 0.37152600 -0.43517400
H 5.53756200 1.99377200 0.23783200
C 3.06897400 -1.89358900 -0.57845700
C 2.44137900 -3.07499500 0.19225700
C 4.59790100 -2.04057900 -0.46653900
H 1.35031100 -3.03044700 0.19728800
H 2.73723000 -4.00775400 -0.30404500
H 2.79882800 -3.13466700 1.22496100
H 5.12916700 -1.40239000 -1.17483400
H 4.97202000 -1.83395800 0.54046000
H 4.86652800 -3.07715000 -0.70685500
C 3.05239200 2.44740200 0.59533600
H 1.97137600 2.56354400 0.54048900
H 3.34304500 2.38679300 1.64924400
H 3.52124600 3.35404700 0.19257800

C -3.06765400 2.44028100 0.59983500
H -3.35176700 2.36743500 1.65484200
H -1.98909600 2.57781800 0.53741000
H -3.55613700 3.34049300 0.20590100
C -2.66628200 -2.03855200 -2.05540600
H -1.58490500 -2.11338200 -2.18107800
H -3.11067700 -2.95631200 -2.46153800
H -3.02532100 -1.20458500 -2.66478100
C 2.66765500 -2.02688300 -2.06026100
H 3.11775500 -2.93964900 -2.47129400
H 1.58625100 -2.11117700 -2.17961200
H 3.01548200 -1.18817100 -2.66966100

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C 0.10755100 4.50841100 -0.50919100
O 0.23087900 4.22957400 0.70872200
O -0.48613200 3.88835800 -1.42566900
H 0.61042000 5.47616400 -0.83552000
H 0.39524200 1.52541900 0.49307500
H 2.66160900 1.69067800 -1.98363500
C 3.64245100 1.48042500 -1.54605200
C 3.53141400 1.07924300 -0.06303200
H 4.23823300 2.39826800 -1.62464300
H 4.13827700 0.71727100 -2.15209300
P 2.31108700 -0.40111900 0.12186700
C 4.93527400 0.80291300 0.51808300
Fe 0.00402200 -0.06079300 0.03633200
C 2.51676200 -0.89220200 1.91044200
C 2.93063000 -1.92408100 -0.89572700
H 4.89561500 0.48167900 1.56368000
H 5.50318500 0.06408600 -0.04484500
H 5.50729600 1.73854900 0.49263100
P -2.30095000 -0.38350700 0.15407100
C -0.01578300 0.33912000 -1.67853600
C 1.20817400 -1.46409500 2.44668600
H 2.81253400 -0.00260200 2.47207900
H 3.31815800 -1.62546300 2.04186800
C 2.42994000 -1.81106500 -2.34884600
C 2.33210300 -3.20863000 -0.28449900
C -2.48725300 -0.77589400 1.96745800
C -3.50389200 1.09685200 -0.10439500
C -2.95960600 -1.94724400 -0.76595700
O -0.03154800 0.57733100 -2.81068100
N 0.02160800 -0.60378800 2.14041000

H 1.01822000 -2.43719900 1.99367500
H 1.27679000 -1.61045800 3.53473800
H 2.78049600 -0.90554400 -2.84993600
H 2.80568500 -2.66859400 -2.92074200
H 1.33973700 -1.83342000 -2.39715100
H 1.24168500 -3.16731600 -0.22817900
H 2.59907900 -4.05552000 -0.92858100
H 2.73264600 -3.42274200 0.71097300
C -1.19840100 -1.39368200 2.49967100
H -2.71613000 0.15613100 2.49075900
H -3.32487200 -1.45613900 2.15080900
C -4.84841200 0.92107600 0.63399700
C -3.76019500 1.33114700 -1.60639900
C -4.49025700 -2.11029800 -0.69305300
C -2.33725400 -3.20864300 -0.13055800
C 0.06938900 0.61176000 2.99735600
H -1.25049300 -1.49689300 3.59329000
H -1.06621700 -2.39065200 2.08157400
H -4.71702000 0.84347700 1.71748600
H -5.45903900 1.81361000 0.44950700
H -5.42455200 0.05971400 0.29787100
H -4.31055800 2.27256400 -1.72570300
H -2.82914700 1.42779200 -2.17200600
H -4.36399400 0.54236500 -2.06216600
H -5.02544900 -1.34226100 -1.25481200
H -4.75736600 -3.07797300 -1.13576900
H -4.85980100 -2.11282600 0.33708400
H -1.24591200 -3.16208400 -0.10375700
H -2.71174900 -3.39193000 0.88106800
H -2.61775300 -4.07689600 -0.73963600
H 0.09196500 0.32977700 4.05891100
H 0.95357400 1.20379300 2.76680700
H -0.80502200 1.23464600 2.81349500
H 0.00441500 -1.50622100 -0.30146100
H -0.39661400 1.53862100 0.46267600
C -2.81640900 2.35756000 0.46128100
H -2.49487700 2.22852800 1.50071300
H -1.96402700 2.69326600 -0.13911200
H -3.55004300 3.17441500 0.45922300
C 2.94839000 2.27522700 0.71675500
H 1.99191600 2.63535600 0.33534200
H 2.83241900 2.06228100 1.78481300
H 3.65479800 3.11104000 0.63787600
C -2.52018700 -1.89403600 -2.24253100

H -1.43185400 -1.90890300 -2.33471400
H -2.90900400 -2.77905600 -2.76164300
H -2.89900600 -1.01446200 -2.76763700
C 4.46181900 -2.08922400 -0.90583600
H 4.96269300 -1.29983400 -1.46973300
H 4.88863100 -2.12843200 0.10092800
H 4.70423900 -3.03949100 -1.39774900

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C 0.12608000 4.45855500 -0.16195400
O 0.08308200 3.63756200 0.81224500
O 0.39752200 4.25016300 -1.35649900
H -0.12016200 5.52000700 0.12975200
H 0.08822600 2.05581700 0.12822100
H 2.00228600 1.92388800 -1.78897700
C 3.01415000 1.50991000 -1.78732700
C 3.43628800 1.05753700 -0.37196000
H 3.69070200 2.30840400 -2.11755800
H 3.07065900 0.70943800 -2.52923600
P 2.30519900 -0.42246800 0.14821200
C 4.94665700 0.75701800 -0.35017000
Fe -0.01259100 -0.13830700 -0.05743600
C 2.46492900 -0.56081900 2.00553100
C 3.05352000 -2.08012600 -0.52073500
H 5.28293000 0.39697600 0.62741800
H 5.25374400 0.03881100 -1.11303900
H 5.48745000 1.69015900 -0.55327000
P -2.33931700 -0.30136700 0.10939300
C 0.00024000 -0.30516200 -1.79380200
C 1.12217300 -0.96608000 2.61041600
H 2.78891100 0.40368900 2.39963600
H 3.22569000 -1.28730100 2.30121700
C 3.25619300 -1.99487200 -2.04665300
C 2.05872400 -3.22671200 -0.24343500
C -2.53399000 -0.20869800 1.96047900
C -3.49102900 1.10066500 -0.54313200
C -3.08186100 -2.02170300 -0.36828400
O 0.00945300 -0.43361400 -2.94922400
N -0.01979300 -0.13321600 2.12067000
H 0.89620000 -2.00097100 2.34836200
H 1.17234900 -0.90142700 3.70799900
H 4.04550300 -1.29523300 -2.32955400
H 3.55068100 -2.98370200 -2.42007500
H 2.33922500 -1.70972100 -2.56914000

H 1.12024700 -3.09419600 -0.78303200
H 2.51517700 -4.16777500 -0.57557500
H 1.82975900 -3.33388300 0.82137600
C -1.27864900 -0.75399800 2.63770500
H -2.69255100 0.83972900 2.22610300
H -3.41288400 -0.76038100 2.30962200
C -4.82580400 1.20890600 0.22425600
C -3.76394400 0.92508600 -2.05001500
C -4.61626400 -2.09028000 -0.24328600
C -2.50547900 -3.10726400 0.56549100
C 0.09737700 1.23279700 2.69259200
H -1.33743300 -0.59548000 3.72465100
H -1.20095000 -1.82683000 2.46569300
H -4.67440800 1.41877800 1.28746300
H -5.39483600 2.05107700 -0.18947800
H -5.45261000 0.32165400 0.13691100
H -4.27052000 1.82373100 -2.42387600
H -2.83706200 0.81368200 -2.62142800
H -4.41185200 0.07348900 -2.27079400
H -5.12937000 -1.46328200 -0.97437600
H -4.93430900 -3.12451800 -0.42599300
H -4.96424300 -1.81828000 0.75814500
H -1.41310700 -3.11185000 0.56949200
H -2.86529000 -3.00402900 1.59359500
H -2.84205600 -4.08711200 0.20458400
H 0.10071500 1.18326100 3.79152600
H 1.01012500 1.71342000 2.35225100
H -0.72789000 1.85725600 2.35995800
H -0.09378600 -1.61065800 0.04990600
H 0.13016700 1.50733200 -0.45318100
C 3.19623600 2.24252200 0.58694300
H 2.14586800 2.52561100 0.67848600
H 3.61182100 2.06186100 1.58349700
H 3.72300000 3.11523300 0.18034200
C -2.73285900 2.42947300 -0.36035100
H -2.38759100 2.59306300 0.66323500
H -1.86464300 2.50215400 -1.01617800
H -3.41074900 3.25527400 -0.61212700
C -2.67164800 -2.37827600 -1.81088800
H -1.58771200 -2.46850400 -1.90643400
H -3.10968000 -3.34926700 -2.07420000
H -3.02154600 -1.65124400 -2.54686800
C 4.38678800 -2.47562200 0.15018300
H 4.73625900 -3.41044100 -0.30586900

H 5.17863700 -1.73916300 0.02345400
H 4.27119700 -2.67258200 1.22011200

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C -0.59703300 4.75559900 -0.15555000
O -0.13453500 3.84394000 -1.00265800
O -1.00307800 4.56207600 0.97283700
H -0.56203500 5.75480400 -0.62120800
H -0.15307900 2.91544600 -0.61001800
H 2.85268300 0.67343100 -2.67959500
C 3.79329500 0.76460800 -2.12750200
C 3.55165200 1.03926100 -0.62994600
H 4.34735300 1.60661500 -2.56213300
H 4.38436300 -0.13693400 -2.30426000
P 2.34243900 -0.28162400 0.10463900
C 4.90401900 1.15389100 0.10578200
Fe 0.04081600 -0.11750200 -0.13779300
C 2.53333400 -0.03123100 1.94649900
C 3.08747700 -2.04234200 -0.21442200
H 4.78046800 1.38271200 1.16889700
H 5.52375900 0.26214100 0.02057500
H 5.47029300 1.98468000 -0.33512500
P -2.24344500 -0.47083800 0.09384000
C 0.03861700 -0.24923700 -1.86249800
C 1.23583000 -0.41203200 2.65818400
H 2.77345500 1.02048300 2.12259400
H 3.36283100 -0.61455400 2.35849600
C 2.64383600 -2.52909100 -1.60891500
C 2.52579900 -3.02954200 0.83041100
C -2.46742000 -0.10067800 1.90905800
C -3.55438700 0.67591500 -0.74617100
C -2.82990900 -2.30910400 -0.11058300
O 0.02705900 -0.27585300 -3.03110300
N 0.02984500 0.21851600 2.04366600
H 1.09226000 -1.49149400 2.60930600
H 1.29361500 -0.13144800 3.72184700
H 2.99920700 -1.88217500 -2.41494500
H 3.05483500 -3.53122100 -1.78746700
H 1.55529600 -2.59610000 -1.67536100
H 1.43411100 -3.03674500 0.83693600
H 2.86763700 -4.04009600 0.57320000
H 2.88666700 -2.81684500 1.84146200
C -1.17490000 -0.41036800 2.66252900
H -2.72191600 0.95893800 2.00069500

H -3.29554300 -0.66532100 2.34998300
C -4.89378800 0.75896200 0.01606300
C -3.80551100 0.23418300 -2.20223700
C -4.35307100 -2.51929900 -0.00927500
C -2.19158200 -3.17653500 0.99502100
C 0.02864100 1.66600900 2.37270200
H -1.26165100 -0.07936900 3.70921200
H -1.00462600 -1.48632300 2.67380700
H -4.76720600 1.16487900 1.02436600
H -5.56126700 1.44465100 -0.52206800
H -5.41053100 -0.19663300 0.09811300
H -4.40976400 0.99844700 -2.70765300
H -2.87170400 0.13172500 -2.76342200
H -4.35348700 -0.70793400 -2.27324900
H -4.90775200 -2.05144500 -0.82438800
H -4.56098100 -3.59618500 -0.05641900
H -4.75887900 -2.15721500 0.94090400
H -1.10371200 -3.08258700 1.01226100
H -2.58650800 -2.93848600 1.98754400
H -2.43466700 -4.22802600 0.79566200
H 0.01707600 1.81053700 3.46455800
H 0.91533900 2.14451200 1.96186200
H -0.83366400 2.16027500 1.93303200
H 0.12594300 -1.62184000 0.13787900
H -0.04263700 1.45331800 -0.31884700
C 2.84973600 2.40639800 -0.52255300
H 1.93275600 2.43046300 -1.10902500
H 2.60122000 2.67545300 0.50952400
H 3.52371200 3.18212700 -0.90837600
C -2.96251800 2.09652200 -0.79409200
H -2.68564800 2.47453100 0.19390600
H -2.08030100 2.13918100 -1.43285900
H -3.71577200 2.77968900 -1.20787100
C -2.32557800 -2.83438000 -1.46968400
H -1.23721700 -2.75997300 -1.53585500
H -2.60010000 -3.89197100 -1.57396100
H -2.75763000 -2.29963300 -2.31905500
C 4.62332900 -2.11591100 -0.11640400
H 4.92941600 -3.16635700 -0.20471500
H 5.12658300 -1.56867300 -0.91557500
H 4.99759500 -1.75200300 0.84548700

Cy-2

Fe 0.00668500 -0.13724500 0.31926200

H	0.00863000	-1.70732100	0.18282100	C	-4.36610600	1.99355500	0.73792400
H	0.01647400	1.41901100	0.57048800	H	-2.41381100	1.28665700	-2.08642000
C	1.23334500	0.29043200	3.05616800	H	-2.59474200	3.63159300	-2.17769200
C	2.50297200	-0.21384400	2.37366100	H	-3.63058500	4.44245000	-0.22923300
H	1.28394800	0.11548900	4.14219400	H	-5.85840600	3.56979100	0.61056300
H	1.13281000	1.36600300	2.89387700	H	-4.98255600	1.12653300	0.99027500
H	2.70654100	-1.25571300	2.63528800	H	-4.13230500	1.03728900	-1.83171500
H	3.36239500	0.37070600	2.71715100	H	-4.10596800	3.12621000	-2.91617500
P	2.26781300	-0.09058200	0.52544600	H	-4.92792200	4.71732500	-1.37824400
N	0.00445500	-0.35118700	2.50185700	H	-5.89762000	2.45663400	-0.74529000
C	-0.03722100	-1.76711700	2.94850300	H	-4.07885500	2.45649300	1.68920100
H	-0.04568800	-1.82632400	4.04783600	C	3.11766600	1.53621500	0.11331600
H	-0.92375200	-2.26130300	2.55536400	C	2.75888200	2.05451300	-1.30748100
H	0.82719000	-2.30700700	2.56625700	C	3.71090700	3.18087100	-1.77953900
P	-2.25373500	-0.03770000	0.53020500	C	4.22511500	4.00834300	-0.59677100
C	-1.18415500	0.36486600	3.05338800	C	5.07986300	3.13391200	0.34955300
C	-2.48509000	-0.07458400	2.38504500	C	4.63555500	1.64801400	0.35113300
H	-1.02419200	1.43055400	2.87454900	H	2.78553000	1.24004500	-2.03741700
H	-1.23860800	0.20684100	4.14200200	H	4.57006100	2.74779500	-2.30913300
H	-2.75346200	-1.09552800	2.67222900	H	4.80783900	4.86847100	-0.94597500
H	-3.30253900	0.56993000	2.71784800	H	6.13510200	3.18581100	0.05462700
C	-0.00437300	0.01357900	-1.40232300	H	4.93161100	1.18737400	1.29887200
O	-0.01676900	0.09269700	-2.56946100	H	1.72735200	2.41860000	-1.28907700
C	-3.28265800	-1.50505700	-0.03450400	H	3.19391700	3.81785300	-2.50655800
C	-3.01356700	-1.88715000	-1.51710400	H	3.36570400	4.42106300	-0.05244900
C	-4.11429700	-2.81013300	-2.09209700	H	5.02427300	3.53581000	1.36857100
C	-4.69643000	-3.72430300	-1.00813000	H	5.16518900	1.10125000	-0.43783600
C	-5.40676100	-2.89340700	0.08733900	C	3.26587700	-1.53300300	-0.15334800
C	-4.79585300	-1.47838300	0.25203500	C	3.41415400	-1.49659900	-1.68779300
H	-2.93695500	-0.99504600	-2.14468900	C	3.85225900	-2.87700400	-2.23304700
H	-4.92516800	-2.20474800	-2.51890500	C	4.79842200	-3.62637400	-1.26349800
H	-5.39336800	-4.44995200	-1.44292300	C	5.58087300	-2.63808600	-0.39159800
H	-6.47245300	-2.79213600	-0.15236400	C	4.63321300	-1.83251000	0.52830500
H	-5.00373700	-1.11058400	1.26209200	H	2.47431100	-1.20088100	-2.16346300
H	-2.03961200	-2.38366000	-1.57060000	H	2.96480400	-3.49105700	-2.42673800
H	-3.70405200	-3.39880900	-2.92064400	H	4.21664400	-4.29011400	-0.61005000
H	-3.88131400	-4.31096300	-0.56435700	H	6.32791200	-3.15970600	0.21827700
H	-5.35511900	-3.42896400	1.04322200	H	5.13644500	-0.91358400	0.83761400
H	-5.28246900	-0.78045800	-0.43910100	H	4.15544900	-0.73614400	-1.96062700
C	-3.07303300	1.57067900	-0.01764800	H	4.34635000	-2.73239100	-3.20159000
C	-3.28286500	1.66790400	-1.54342100	H	5.48160300	-4.27370100	-1.82539400
C	-3.54860300	3.13179900	-1.97133500	H	6.14039200	-1.95313000	-1.04226200
C	-4.33073900	3.93079400	-0.90282900	H	4.44852800	-2.40596800	1.44410900
C	-5.21928900	2.99799000	-0.07258400	H	-2.84974400	-2.30027600	0.58873000

H -2.28379000 2.28994800 0.23329100
H 2.58668100 -2.36552100 0.07227900
H 2.62469400 2.20133500 0.83648400

Cy-3

Fe -0.06929600 0.12051800 0.33641300
H -0.00038200 -1.45369500 0.27402800
H -0.12653800 1.68642200 0.50552100
C 1.10098600 0.79879500 3.04835300
C 2.41098400 0.36711500 2.39425300
H 1.16377600 0.68998800 4.14257800
H 0.90900400 1.85093400 2.82532500
H 2.69984800 -0.63659000 2.71671100
H 3.21622400 1.04158800 2.70223600
P 2.17691500 0.35437500 0.54152000
N -0.06635400 0.02416600 2.53278400
C 0.01313200 -1.36528900 3.05078000
H 0.01725200 -1.36846300 4.15186700
H -0.83254500 -1.94981000 2.69338200
H 0.91584600 -1.85126800 2.68657500
P -2.33260200 0.13002900 0.54538900
C -1.31211300 0.66109200 3.05388400
C -2.56711400 0.09214900 2.39702900
H -1.23900900 1.72937600 2.83666800
H -1.35975600 0.54030600 4.14748200
H -2.73900600 -0.94523300 2.69943400
H -3.44239100 0.66234200 2.71936900
C -0.06700900 0.12629700 -1.39141600
O -0.05983900 0.08018100 -2.56013500
C -3.30243900 -1.37361800 -0.02579100
C -3.05148000 -1.70974400 -1.52275900
C -4.11259800 -2.68336300 -2.08847800
C -4.60582700 -3.65570500 -1.01076000
C -5.32939700 -2.89378100 0.12588800
C -4.80797800 -1.44404800 0.29378000
H -3.04449900 -0.80125300 -2.13192000
H -4.97050800 -2.11827800 -2.47663200
H -5.27203000 -4.41138200 -1.44259000
H -6.40763900 -2.85983800 -0.07321400
H -5.02114600 -1.09786300 1.31053500
H -2.05361400 -2.14892300 -1.61337600
H -3.69312600 -3.22705900 -2.94274700
H -3.74387600 -4.20280400 -0.60675400
H -5.20672400 -3.43978500 1.06937500

H -5.35291800 -0.77637200 -0.38349800
C -3.19914700 1.71997400 0.02331500
C -3.27499300 1.90710000 -1.50568600
C -3.57112900 3.38320100 -1.86431400
C -4.50215500 4.06851700 -0.83496300
C -5.40555000 3.03859600 -0.14826700
C -4.57310600 2.03371200 0.68275200
H -2.34246000 1.59677400 -1.98554700
H -2.62803900 3.93851100 -1.93277100
H -3.90293600 4.57785200 -0.06870800
H -6.13844800 3.53171400 0.50119900
H -5.16097000 1.12522100 0.83488300
H -4.06538900 1.26311500 -1.90915800
H -4.02540200 3.41918700 -2.86210500
H -5.09984600 4.84696600 -1.32279800
H -5.98469000 2.50381600 -0.91270600
H -4.39537800 2.45789900 1.67778100
C 2.87364900 2.02352300 0.02453000
C 2.49625200 2.40339800 -1.43498300
C 3.35086600 3.57530700 -1.97711800
C 3.75262800 4.53788900 -0.85445200
C 4.65590200 3.82506000 0.17995800
C 4.36795200 2.30493400 0.27374600
H 2.61012400 1.54512300 -2.10375500
H 4.26062100 3.18688800 -2.45413200
H 4.26412600 5.41857700 -1.25983900
H 5.71124600 3.96821400 -0.08295700
H 4.69021600 1.93897800 1.25346000
H 1.43592700 2.67235200 -1.45709400
H 2.79617500 4.10186500 -2.76254600
H 2.84334800 4.91030000 -0.36469800
H 4.51843700 4.28666500 1.16555800
H 4.96706800 1.76766200 -0.47069500
C 3.31833400 -1.02494300 -0.03610400
C 3.49905800 -1.06709300 -1.56665600
C 4.06355200 -2.43626100 -2.01882300
C 5.01585500 -3.06101500 -0.97176000
C 5.71069100 -1.96895500 -0.15055000
C 4.68961400 -1.15999300 0.68528500
H 2.54922000 -0.87794500 -2.07500600
H 3.23438100 -3.12502400 -2.21828600
H 4.44990000 -3.71189000 -0.29156700
H 6.46915900 -2.40047000 0.51303700
H 5.11650900 -0.18136100 0.91716000

H 4.18280600 -0.26544600 -1.86966500
H 4.59087900 -2.30402100 -2.97146500
H 5.75277400 -3.70422600 -1.46624800
H 6.24745500 -1.29792000 -0.83411500
H 4.53225200 -1.66332400 1.64602800
H -2.80868200 -2.15436700 0.56989800
H -2.47418400 2.45885700 0.38775200
H 2.71281500 -1.89994500 0.23092100
H 2.30313700 2.68512400 0.69123600
C 1.07359000 -4.39084500 -0.26322500
O 0.72547700 -4.31648700 -1.37676500
O 1.42274500 -4.49979500 0.84840600

Cy-TS3_4

Fe 0.00194800 0.00150100 0.32364200
H -0.00390200 -1.60963000 0.23117700
H 0.01806900 1.54645300 0.48377900
C 1.17870700 0.63788500 3.03931000
C 2.48354000 0.16789600 2.40222900
H 1.22382600 0.52607300 4.13387500
H 1.02167300 1.69546700 2.81475900
H 2.75199900 -0.83490300 2.74345500
H 3.29903200 0.83206100 2.70507900
P 2.26808900 0.13674600 0.54795200
N -0.00627700 -0.10004000 2.50924800
C 0.03413200 -1.49992400 3.00169900
H 0.01572100 -1.52159800 4.10224600
H -0.80851300 -2.06394600 2.60997400
H 0.93652800 -1.99606700 2.64958600
P -2.26922000 0.15364200 0.52097900
C -1.23502500 0.56320600 3.03943900
C -2.50421900 0.04690100 2.36745400
H -1.12951700 1.63377300 2.84659900
H -1.28854000 0.42075000 4.12972900
H -2.69639600 -0.99788200 2.62931500
H -3.36665000 0.62327500 2.71338600
C 0.01261400 0.07859900 -1.40799200
O 0.01946400 0.11840600 -2.57404400
C -3.34111700 -1.24703800 -0.12039700
C -3.17250100 -1.48311100 -1.64639300
C -4.27278800 -2.41395000 -2.21452500
C -4.75428000 -3.41808200 -1.16056900
C -5.41978000 -2.68709100 0.03011200
C -4.83520000 -1.26930500 0.25638200

H -3.19758800 -0.53470800 -2.19086100
H -5.12982500 -1.81668400 -2.55276200
H -5.45360900 -4.13831300 -1.60029500
H -6.50011900 -2.60119100 -0.13968900
H -4.99620600 -0.97070000 1.29733500
H -2.18499200 -1.91735000 -1.82657100
H -3.89240900 -2.93227700 -3.10207500
H -3.89448900 -4.00274300 -0.80823800
H -5.29618700 -3.28483900 0.94126100
H -5.37548000 -0.54485100 -0.36349400
C -3.00252700 1.83224700 0.08676800
C -3.01945000 2.13326800 -1.42558000
C -3.19106400 3.65020800 -1.67822500
C -4.11004200 4.32456700 -0.63040900
C -5.10424000 3.31366100 -0.04823900
C -4.37144400 2.19662800 0.73151800
H -2.10100000 1.78595200 -1.90700100
H -2.20742700 4.13518600 -1.67102600
H -3.50618900 4.73743900 0.18857100
H -5.82464400 3.80908500 0.61318800
H -5.02593600 1.32421200 0.80146800
H -3.84583100 1.58650300 -1.89460000
H -3.60114600 3.79520500 -2.68509400
H -4.63755600 5.17416200 -1.07883300
H -5.69043500 2.87535500 -0.86656200
H -4.19605800 2.53559500 1.75902200
C 3.03401000 1.77109000 0.02068600
C 2.68528800 2.15678800 -1.44484900
C 3.59657800 3.28390200 -1.98868700
C 4.02703900 4.23900400 -0.87057400
C 4.88921600 3.49769300 0.17851400
C 4.53694500 1.99173300 0.28183700
H 2.76294900 1.28974700 -2.10720300
H 4.49347900 2.85124100 -2.45154600
H 4.57915400 5.09373300 -1.27789700
H 5.95205700 3.59354100 -0.07514900
H 4.83588800 1.62167800 1.26737200
H 1.63980500 2.47711700 -1.47701300
H 3.07337000 3.82558400 -2.78527100
H 3.12911000 4.65347700 -0.39363200
H 4.76223900 3.97290000 1.15908000
H 5.11853300 1.42267300 -0.45268600
C 3.35680200 -1.29480200 -0.00413000
C 3.55863100 -1.34861900 -1.53178600

C 4.09134700 -2.73418200 -1.96964400
 C 5.03919000 -3.36529300 -0.92120300
 C 5.73503200 -2.28039600 -0.09177100
 C 4.71299400 -1.47048900 0.74010700
 H 2.62222800 -1.13507300 -2.05541100
 H 3.24599000 -3.40720200 -2.15221300
 H 4.46959200 -4.01652200 -0.24478300
 H 6.48535800 -2.71900100 0.57646300
 H 5.15415000 -0.50560500 1.00136800
 H 4.26787400 -0.56703600 -1.82794800
 H 4.61327500 -2.62338100 -2.92794700
 H 5.77593600 -4.00882900 -1.41538400
 H 6.28131100 -1.60908100 -0.76740600
 H 4.52790100 -1.99088900 1.68678500
 H -2.86757600 -2.09385800 0.39491300
 H -2.23971900 2.49062800 0.52132700
 H 2.71813400 -2.14916100 0.25580600
 H 2.48611500 2.46043300 0.67818600
 C -0.21829800 -3.32548600 -0.24445800
 O 0.18033900 -3.34472800 -1.36297000
 O -0.67651000 -3.79562800 0.74830800

Cy-4

Fe -0.01250100 -0.07232500 0.33393100
 H -0.06168200 -1.86954500 0.20687200
 H -0.01243200 1.42175400 0.44381000
 C 1.21471000 0.50939200 3.03142400
 C 2.48890700 -0.01080800 2.37551000
 H 1.25191000 0.36229600 4.12094500
 H 1.11318600 1.58097600 2.84192500
 H 2.66934700 -1.05737300 2.63590200
 H 3.35122200 0.56135200 2.73132600
 P 2.27813300 0.10621600 0.53126100
 N -0.01203900 -0.15035600 2.48726500
 C -0.04553200 -1.56486800 2.94527500
 H 0.07313700 -1.61684100 4.03735300
 H -0.99803300 -2.01934700 2.67450400
 H 0.73106100 -2.14703500 2.45028700
 P -2.29774400 0.10511000 0.54543400
 C -1.19647500 0.58082100 3.03471700
 C -2.50659000 0.12717900 2.39794400
 H -1.03847900 1.64247400 2.82759200
 H -1.23275000 0.45070200 4.12663900
 H -2.77960700 -0.88177000 2.71929600

H -3.31647700 0.78747500 2.71713000
 C -0.01928100 0.07326100 -1.40681300
 O -0.02445400 0.20244100 -2.56162000
 C -3.39137700 -1.31928200 0.01091300
 C -3.17685900 -1.71373600 -1.47757100
 C -4.33019500 -2.59858500 -2.01094600
 C -4.91864400 -3.47717600 -0.90077700
 C -5.56768900 -2.60863800 0.20333500
 C -4.89295000 -1.22027600 0.34026800
 H -3.09810600 -0.82317400 -2.10813900
 H -5.12911200 -1.96937700 -2.42611900
 H -5.65435200 -4.17987000 -1.30845200
 H -6.63299700 -2.46187600 -0.01272000
 H -5.05804800 -0.83312000 1.35104300
 H -2.22305000 -2.24506600 -1.55722200
 H -3.96361800 -3.21464500 -2.84005600
 H -4.11556500 -4.09034300 -0.47165200
 H -5.51695900 -3.13785600 1.16271900
 H -5.36314800 -0.50807500 -0.34766100
 C -3.00175000 1.75669300 -0.02367100
 C -3.17905300 1.87101100 -1.55191900
 C -3.33216900 3.35249000 -1.97348000
 C -4.08452500 4.19534500 -0.91671500
 C -5.04814500 3.31716500 -0.11102700
 C -4.28178700 2.25327300 0.71045800
 H -2.33291300 1.43048200 -2.08522200
 H -2.34100800 3.78616100 -2.15229500
 H -3.36808300 4.66019100 -0.22632600
 H -5.66246900 3.92521800 0.56311700
 H -4.95902500 1.42572700 0.93924000
 H -4.06722500 1.30426100 -1.85424900
 H -3.86475900 3.39061900 -2.93142500
 H -4.62143200 5.01923400 -1.40037000
 H -5.74564900 2.82494400 -0.80101100
 H -3.98734400 2.68857200 1.67228900
 C 2.93762400 1.81578300 0.12338700
 C 2.57875900 2.26449900 -1.32233900
 C 3.44208200 3.45773600 -1.79717300
 C 3.80740100 4.37853200 -0.62806800
 C 4.68700700 3.63134500 0.40311700
 C 4.42327700 2.10471400 0.41449700
 H 2.69840800 1.43750600 -2.02873500
 H 4.36522600 3.09041500 -2.26418100
 H 4.32439900 5.27599500 -0.98605600

H 5.74803500 3.80175400 0.18405400
 H 4.73398500 1.69267600 1.37966400
 H 1.52048300 2.54192300 -1.34595900
 H 2.90461700 4.00997200 -2.57663900
 H 2.88294000 4.72859100 -0.15001500
 H 4.50831000 4.04220900 1.40417900
 H 5.04218000 1.61642900 -0.34673300
 C 3.38446800 -1.24625300 -0.13867600
 C 3.49448300 -1.25879800 -1.67669800
 C 4.01236000 -2.63362500 -2.16376300
 C 5.01390700 -3.27408600 -1.17220600
 C 5.75837200 -2.19765300 -0.37347900
 C 4.78793800 -1.38266600 0.51660900
 H 2.52703800 -1.05078200 -2.14335400
 H 3.16071500 -3.30803800 -2.30886500
 H 4.47798900 -3.92870700 -0.47271400
 H 6.54028300 -2.64479900 0.25127500
 H 5.23196800 -0.40597600 0.72204700
 H 4.17652600 -0.46311200 -2.00062600
 H 4.48375900 -2.50663200 -3.14593100
 H 5.72153200 -3.91507200 -1.71050600
 H 6.27232000 -1.52547800 -1.07328900
 H 4.67398700 -1.88311300 1.48504400
 H -2.97676800 -2.13045200 0.62742500
 H -2.17826900 2.42900700 0.24633400
 H 2.79938900 -2.13042400 0.14332300
 H 2.34633300 2.43130900 0.81597400
 C 0.28853100 -2.96711200 -0.14481600
 O 1.00893800 -3.53291700 0.69186400
 O -0.16052100 -3.28743700 -1.24926600

Cy-TS4_5

Fe -0.01250100 -0.07232500 0.33393100
 H -0.06168200 -1.86954500 0.20687200
 H -0.01243200 1.42175400 0.44381000
 C 1.21471000 0.50939200 3.03142400
 C 2.48890700 -0.01080800 2.37551000
 H 1.25191000 0.36229600 4.12094500
 H 1.11318600 1.58097600 2.84192500
 H 2.66934700 -1.05737300 2.63590200
 H 3.35122200 0.56135200 2.73132600
 P 2.27813300 0.10621600 0.53126100
 N -0.01203900 -0.15035600 2.48726500
 C -0.04553200 -1.56486800 2.94527500

H 0.07313700 -1.61684100 4.03735300
 H -0.99803300 -2.01934700 2.67450400
 H 0.73106100 -2.14703500 2.45028700
 P -2.29774400 0.10511000 0.54543400
 C -1.19647500 0.58082100 3.03471700
 C -2.50659000 0.12717900 2.39794400
 H -1.03847900 1.64247400 2.82759200
 H -1.23275000 0.45070200 4.12663900
 H -2.77960700 -0.88177000 2.71929600
 H -3.31647700 0.78747500 2.71713000
 C -0.01928100 0.07326100 -1.40681300
 O -0.02445400 0.20244100 -2.56162000
 C -3.39137700 -1.31928200 0.01091300
 C -3.17685900 -1.71373600 -1.47757100
 C -4.33019500 -2.59858500 -2.01094600
 C -4.91864400 -3.47717600 -0.90077700
 C -5.56768900 -2.60863800 0.20333500
 C -4.89295000 -1.22027600 0.34026800
 H -3.09810600 -0.82317400 -2.10813900
 H -5.12911200 -1.96937700 -2.42611900
 H -5.65435200 -4.17987000 -1.30845200
 H -6.63299700 -2.46187600 -0.01272000
 H -5.05804800 -0.83312000 1.35104300
 H -2.22305000 -2.24506600 -1.55722200
 H -3.96361800 -3.21464500 -2.84005600
 H -4.11556500 -4.09034300 -0.47165200
 H -5.51695900 -3.13785600 1.16271900
 H -5.36314800 -0.50807500 -0.34766100
 C -3.00175000 1.75669300 -0.02367100
 C -3.17905300 1.87101100 -1.55191900
 C -3.33216900 3.35249000 -1.97348000
 C -4.08452500 4.19534500 -0.91671500
 C -5.04814500 3.31716500 -0.11102700
 C -4.28178700 2.25327300 0.71045800
 H -2.33291300 1.43048200 -2.08522200
 H -2.34100800 3.78616100 -2.15229500
 H -3.36808300 4.66019100 -0.22632600
 H -5.66246900 3.92521800 0.56311700
 H -4.95902500 1.42572700 0.93924000
 H -4.06722500 1.30426100 -1.85424900
 H -3.86475900 3.39061900 -2.93142500
 H -4.62143200 5.01923400 -1.40037000
 H -5.74564900 2.82494400 -0.80101100
 H -3.98734400 2.68857200 1.67228900

C 2.93762400 1.81578300 0.12338700
 C 2.57875900 2.26449900 -1.32233900
 C 3.44208200 3.45773600 -1.79717300
 C 3.80740100 4.37853200 -0.62806800
 C 4.68700700 3.63134500 0.40311700
 C 4.42327700 2.10471400 0.41449700
 H 2.69840800 1.43750600 -2.02873500
 H 4.36522600 3.09041500 -2.26418100
 H 4.32439900 5.27599500 -0.98605600
 H 5.74803500 3.80175400 0.18405400
 H 4.73398500 1.69267600 1.37966400
 H 1.52048300 2.54192300 -1.34595900
 H 2.90461700 4.00997200 -2.57663900
 H 2.88294000 4.72859100 -0.15001500
 H 4.50831000 4.04220900 1.40417900
 H 5.04218000 1.61642900 -0.34673300
 C 3.38446800 -1.24625300 -0.13867600
 C 3.49448300 -1.25879800 -1.67669800
 C 4.01236000 -2.63362500 -2.16376300
 C 5.01390700 -3.27408600 -1.17220600
 C 5.75837200 -2.19765300 -0.37347900
 C 4.78793800 -1.38266600 0.51660900
 H 2.52703800 -1.05078200 -2.14335400
 H 3.16071500 -3.30803800 -2.30886500
 H 4.47798900 -3.92870700 -0.47271400
 H 6.54028300 -2.64479900 0.25127500
 H 5.23196800 -0.40597600 0.72204700
 H 4.17652600 -0.46311200 -2.00062600
 H 4.48375900 -2.50663200 -3.14593100
 H 5.72153200 -3.91507200 -1.71050600
 H 6.27232000 -1.52547800 -1.07328900
 H 4.67398700 -1.88311300 1.48504400
 H -2.97676800 -2.13045200 0.62742500
 H -2.17826900 2.42900700 0.24633400
 H 2.79938900 -2.13042400 0.14332300
 H 2.34633300 2.43130900 0.81597400
 C 0.28853100 -2.96711200 -0.14481600
 O 1.00893800 -3.53291700 0.69186400
 O -0.16052100 -3.28743700 -1.24926600

Cy-5

Fe -0.00894600 0.03088800 0.30287400
 H -0.03069200 1.55701800 0.47198200
 P 2.27713200 0.20550100 0.54247500

P -2.30621700 0.10139600 0.51181700
 C -0.02430500 0.29856200 -1.41410500
 C 2.46992300 0.30893200 2.39638000
 C 3.08684700 1.79642200 -0.03781700
 C 3.30075600 -1.28916100 0.05947600
 C -2.50529900 -0.02312300 2.36032400
 C -3.29183100 -1.35965500 -0.12299900
 C -3.12990100 1.74331800 0.10145100
 O -0.05143700 0.53214100 -2.55559700
 C 1.14498400 0.75683500 3.00759900
 H 2.77067400 -0.66935000 2.77844900
 H 3.25965000 1.01272900 2.67676200
 C 2.76322600 2.13633200 -1.52058500
 C 4.59662800 1.95795000 0.22692200
 H 2.56387400 2.53109700 0.59106400
 C 3.49644700 -1.43334400 -1.46339800
 C 4.64671400 -1.50193900 0.81179900
 H 2.61669500 -2.09265700 0.35943900
 C -1.26367900 0.56980000 3.01993700
 H -2.62810000 -1.07867200 2.62007300
 H -3.39825800 0.49611900 2.71822600
 C -3.17408300 -1.54968500 -1.66107800
 C -4.76265200 -1.49033700 0.32018400
 H -2.73411700 -2.17895200 0.35139000
 C -3.22660500 2.04542600 -1.40807100
 C -4.49015900 2.03362100 0.79868300
 H -2.38656900 2.44154900 0.50857500
 H 1.19103900 0.69594200 4.10600500
 H 0.94734700 1.79649200 2.73641400
 N -0.00641100 -0.05182000 2.50866900
 C 3.74970200 3.16733600 -2.11768100
 H 2.77755300 1.23464200 -2.13953200
 H 1.74361700 2.52979700 -1.57105900
 C 5.02705100 3.43606200 0.05239900
 H 4.86907600 1.62140400 1.23200600
 H 5.15176400 1.32314500 -0.47339300
 C 3.92198600 -2.87764700 -1.81751200
 H 2.57779500 -1.18180700 -2.00257300
 H 4.26019100 -0.72277000 -1.80152800
 C 5.61567500 -2.40978700 0.01828300
 H 5.14351700 -0.55202400 1.02546600
 H 4.43540200 -1.96570700 1.78207500
 H -1.20750700 1.63923800 2.80032500
 H -1.31438600 0.45365100 4.11336800

C -4.26414800 -2.49844500 -2.21551600
 H -3.24240600 -0.59038200 -2.18193100
 H -2.18438700 -1.95729400 -1.88700000
 C -5.27225900 -2.93238200 0.06984500
 H -4.89221200 -1.23738100 1.37762000
 H -5.37524800 -0.78053500 -0.24721200
 C -3.48010100 3.55325900 -1.64595600
 H -2.31761200 1.74342600 -1.93425500
 H -4.04726100 1.46116100 -1.84028500
 C -5.30542100 3.12125000 0.05917600
 H -5.09674600 1.12755300 0.87889000
 H -4.29608700 2.36932100 1.82360600
 C 0.10116100 -1.42804700 3.05525800
 C 4.22382100 4.16200600 -1.05286500
 H 4.62315600 2.65096600 -2.53719800
 H 3.27109700 3.68832000 -2.95488100
 H 6.09792400 3.46355200 -0.18322800
 H 4.90667100 3.96824800 1.00398500
 C 4.85519100 -3.49840900 -0.74793700
 H 3.02686200 -3.50097600 -1.92509200
 H 4.41972600 -2.87026100 -2.79479100
 H 6.34559200 -2.85363100 0.70544400
 H 6.19348700 -1.80646900 -0.69423500
 C -4.63879800 -3.57280500 -1.18833400
 H -5.16301900 -1.92452500 -2.47735500
 H -3.91069700 -2.95543500 -3.14680100
 H -6.36431500 -2.90701800 -0.03051200
 H -5.05605800 -3.55574000 0.94589400
 C -4.38448800 4.18020800 -0.55718200
 H -2.52091100 4.08407900 -1.67856300
 H -3.93892600 3.68057600 -2.63391400
 H -6.01856300 3.57894900 0.75457200
 H -5.90550300 2.66144200 -0.73684200
 H 0.11838800 -1.39590600 4.15477400
 H -0.73432800 -2.03569500 2.71861600
 H 1.00339200 -1.91259900 2.69012500
 H 4.83150100 4.95527900 -1.50290400
 H 3.34705900 4.65864000 -0.61659300
 H 4.26417600 -4.08568700 -0.03315900
 H 5.55345100 -4.20128200 -1.21632000
 H -5.32522900 -4.30694200 -1.62539800
 H -3.73246100 -4.12675600 -0.91171600
 H -3.76676600 4.61799600 0.23821200
 H -4.96911200 5.00566100 -0.97868500

O 0.00745200 -2.00368000 0.31309900
 C 0.15247200 -2.79478900 -0.69062200
 O 0.17640500 -4.02868200 -0.65152000
 H 0.26804500 -2.29014800 -1.68040200

Cy-6

Fe 0.00990400 0.12269000 0.29557100
 H 0.02052500 1.60797000 0.53356100
 C 1.22736500 0.50836300 3.01610800
 C 2.50884000 0.03499500 2.33799000
 H 1.26258400 0.29969200 4.09533500
 H 1.11416500 1.58765600 2.88554500
 H 2.71089200 -1.01413000 2.56693700
 H 3.36182200 0.61350900 2.70543800
 P 2.29771300 0.21791500 0.49782100
 N 0.01242100 -0.13520500 2.42827500
 C 0.00091400 -1.58127100 2.79090400
 H 0.01329800 -1.69481800 3.88425600
 H -0.87205000 -2.07747900 2.37054100
 H 0.85081000 -2.09769800 2.34759600
 P -2.27477600 0.24543900 0.50491800
 C -1.18774600 0.53065000 3.02224300
 C -2.48314600 0.08795700 2.34916000
 H -1.05368900 1.60784500 2.89315800
 H -1.22251900 0.32050400 4.10123700
 H -2.71241100 -0.95652800 2.57762700
 H -3.31714500 0.68700500 2.72272600
 C 0.00604500 0.45255000 -1.42279000
 O 0.00161700 0.70020100 -2.55682300
 C -3.22232000 -1.21164900 -0.17775500
 C -2.93939600 -1.46429700 -1.68570000
 C -3.97076300 -2.43845700 -2.30410900
 C -4.45225100 -3.45350500 -1.26073200
 C -5.24187400 -2.74048500 -0.13836900
 C -4.73293100 -1.29695100 0.11635300
 H -2.93991300 -0.53058800 -2.25640900
 H -4.83388900 -1.87870600 -2.68894300
 H -5.07403000 -4.22778500 -1.72493500
 H -6.30773600 -2.69880300 -0.39543400
 H -4.95823900 -1.00778100 1.14839300
 H -1.93633800 -1.89429100 -1.77468500
 H -3.52304800 -2.94431600 -3.16719300
 H -3.57651300 -3.95952900 -0.83612000
 H -5.16788800 -3.32364200 0.78726800

H -5.27093200 -0.59206700 -0.52862200
C -3.07082000 1.89118800 0.07391700
C -3.20129600 2.14652200 -1.44160000
C -3.48158800 3.64283700 -1.71944900
C -4.37276300 4.29177400 -0.63278800
C -5.26454600 3.24065500 0.03655900
C -4.41729600 2.19216400 0.79452800
H -2.29826500 1.84376800 -1.97734300
H -2.53115900 4.18555900 -1.78889200
H -3.74546900 4.76361700 0.13513300
H -5.96972300 3.71004800 0.73204300
H -5.00879900 1.28174800 0.92395300
H -4.01958500 1.53521500 -1.83919600
H -3.96199800 3.73176200 -2.70114600
H -4.97789900 5.09448400 -1.06859800
H -5.87354500 2.74518300 -0.73064200
H -4.19985500 2.56759500 1.80071500
C 3.10050700 1.87261700 0.13582400
C 2.72891900 2.44526000 -1.25974300
C 3.68069200 3.58780400 -1.69214900
C 4.20677500 4.36585900 -0.48117700
C 5.06649500 3.45207400 0.42292700
C 4.62231700 1.96854700 0.35989400
H 2.75172200 1.66007400 -2.02121200
H 4.53337200 3.17279800 -2.24522700
H 4.78951200 5.23673400 -0.80171700
H 6.11998100 3.51543800 0.12522200
H 4.93216600 1.45817100 1.27707900
H 1.69884500 2.81257600 -1.22046800
H 3.15925000 4.25395700 -2.38885300
H 3.35361200 4.76042800 0.08615000
H 5.01583300 3.80815000 1.45888200
H 5.13509500 1.46136500 -0.46530000
C 3.24315100 -1.21456000 -0.24721300
C 3.37251900 -1.14365200 -1.78321900
C 3.71510800 -2.54290000 -2.35843700
C 4.49971300 -3.41369200 -1.35254400
C 5.42393200 -2.54215600 -0.49296800
C 4.61285500 -1.56140700 0.39488500
H 2.45105500 -0.77588800 -2.24504200
H 2.79114600 -3.06001500 -2.64105400
H 3.79294900 -3.94375500 -0.70227900
H 6.06920300 -3.16210000 0.14011600
H 5.20897700 -0.66239900 0.57343500

H 4.16011300 -0.42675500 -2.04572700
H 4.29735400 -2.41533300 -3.27943300
H 5.07417600 -4.18085600 -1.88461600
H 6.09476400 -1.97747400 -1.15429000
H 4.43607200 -2.02003300 1.37391300
H -2.72858700 -2.02987100 0.36482300
H -2.31647500 2.59504800 0.44915700
H 2.55465100 -2.04088800 -0.02236600
H 2.61505600 2.50462800 0.89324400
C -0.02549800 -4.18547900 0.18801100
O -1.15787700 -3.75343700 0.52759900
O 1.11708300 -3.74519800 0.47919100
H -0.03625900 -5.10350400 -0.47094900
H -0.40880900 -1.52543300 0.13957200
H 0.38720600 -1.53452300 0.11868000

Cy-TS6_7

Fe -0.00202500 0.17376700 0.26150200
H -0.03990200 1.64872300 0.58411400
C 1.19268200 0.55230700 2.99695500
C 2.49962900 0.14092100 2.32564900
H 1.23326100 0.34751400 4.07726000
H 1.02581700 1.62410600 2.86232100
H 2.76368500 -0.88940000 2.57498300
H 3.31679400 0.77420300 2.68450000
P 2.28384700 0.28573400 0.47902000
N 0.01554500 -0.15160300 2.40376900
C 0.08982800 -1.59748600 2.74624300
H 0.13394600 -1.72677900 3.83755900
H -0.77654800 -2.12257500 2.35035900
H 0.95967300 -2.06282400 2.28639200
P -2.29176300 0.18065300 0.48558900
C -1.22079400 0.42742100 3.01198800
C -2.48732900 -0.07056300 2.32173400
H -1.14959100 1.51365700 2.91354400
H -1.24549300 0.18687700 4.08523700
H -2.64732700 -1.13672300 2.50671900
H -3.35770700 0.45548700 2.72116300
C -0.03232400 0.60508700 -1.42865700
O -0.06074800 0.91724200 -2.54822700
C -3.22189400 -1.25632300 -0.26394800
C -2.96632900 -1.40339400 -1.79033600
C -3.97782600 -2.37251300 -2.45054000
C -4.42667000 -3.45667000 -1.46431200

C -5.20733400 -2.83185900 -0.28464100
 C -4.72417200 -1.39663800 0.05195700
 H -3.01887100 -0.43573300 -2.29887900
 H -4.85961400 -1.81598700 -2.79550400
 H -5.04358200 -4.21042000 -1.96703100
 H -6.27843100 -2.79841000 -0.51950700
 H -4.93481800 -1.17843600 1.10436700
 H -1.94806700 -1.78038500 -1.93009700
 H -3.52794100 -2.81887900 -3.34482800
 H -3.53871200 -3.98025600 -1.08893300
 H -5.10348300 -3.47143600 0.59991200
 H -5.29041900 -0.66531500 -0.53682000
 C -3.15246700 1.82278200 0.16022800
 C -3.31238200 2.16259000 -1.33518400
 C -3.63684900 3.66383700 -1.52318800
 C -4.52333100 4.22624300 -0.38599900
 C -5.37902300 3.11604000 0.23432700
 C -4.49539500 2.04396000 0.91486900
 H -2.40860000 1.91399400 -1.89684300
 H -2.70274100 4.23571100 -1.57884400
 H -3.89388700 4.66746800 0.39827000
 H -6.08318400 3.52695400 0.96700400
 H -5.06298200 1.11288500 0.99482600
 H -4.11968900 1.55313100 -1.75727700
 H -4.13842500 3.79475600 -2.48957600
 H -5.15486500 5.03844800 -0.76337500
 H -5.98968100 2.65251500 -0.55135500
 H -4.27426500 2.36185800 1.93996600
 C 3.11975700 1.91969600 0.09045700
 C 2.76305600 2.47355300 -1.31650900
 C 3.73698000 3.58946800 -1.76846300
 C 4.27055500 4.38324800 -0.57110200
 C 5.11051000 3.47393900 0.35569000
 C 4.64121800 1.99714000 0.32193700
 H 2.77069400 1.67346600 -2.06265300
 H 4.58487000 3.14845300 -2.30879900
 H 4.86916200 5.23780400 -0.90618200
 H 6.16624700 3.51334400 0.06153200
 H 4.93531500 1.50243300 1.25279000
 H 1.74055000 2.86221300 -1.28742600
 H 3.23055600 4.25009000 -2.48138900
 H 3.42114900 4.80297500 -0.01635700
 H 5.06167800 3.85279100 1.38366700
 H 5.15155900 1.46321100 -0.48779900

C 3.21515200 -1.17837300 -0.22721500
 C 3.32709500 -1.14692000 -1.76541500
 C 3.66134500 -2.55809300 -2.31304100
 C 4.48609300 -3.39658100 -1.31066600
 C 5.40651300 -2.49282100 -0.48084900
 C 4.59037100 -1.51942700 0.40907200
 H 2.40060200 -0.78752100 -2.22408000
 H 2.73233200 -3.08867200 -2.55166300
 H 3.80747800 -3.93463800 -0.63764000
 H 6.07696500 -3.08964300 0.14847200
 H 5.18271500 -0.61863000 0.58968400
 H 4.11310100 -0.43814300 -2.05396600
 H 4.21139200 -2.45112500 -3.25625000
 H 5.06818100 -4.15734100 -1.84384200
 H 6.05257100 -1.92219200 -1.16157800
 H 4.41855000 -1.98247200 1.38699100
 H -2.70250300 -2.09385100 0.21965000
 H -2.41529400 2.52774400 0.56602100
 H 2.52464500 -1.99453500 0.02857200
 H 2.64092500 2.57241500 0.83444900
 C 0.16728500 -4.28368600 0.51574400
 O -0.78759000 -3.48290600 0.24957100
 O 1.35823100 -4.02231700 0.77236100
 H -0.13112500 -5.36602800 0.51567300
 H -0.17215200 -1.97657000 0.03603600
 H 0.31518600 -1.39030600 -0.25843700

Cy-7

Fe -0.06291900 0.11475200 0.29694000
 H -0.11777700 1.65636600 0.53945400
 C 1.13762200 0.63079900 3.02895600
 C 2.43881700 0.22043000 2.34604100
 H 1.20072800 0.45951400 4.11487400
 H 0.95651600 1.69623300 2.86656500
 H 2.70736700 -0.80921000 2.59608300
 H 3.25865600 0.85570600 2.69541600
 P 2.19723500 0.33504600 0.50046000
 N -0.03944600 -0.10171300 2.47504200
 C 0.03420500 -1.52422600 2.89969500
 H 0.09085300 -1.59582900 3.99669700
 H -0.84711700 -2.06182800 2.55338100
 H 0.89777600 -2.01508400 2.45552200
 P -2.32854400 0.11117200 0.52495100
 C -1.27407300 0.51132600 3.04880100

C -2.54221700 -0.00730800 2.37627900
H -1.19469200 1.59029300 2.89657000
H -1.30892100 0.32412300 4.13322700
H -2.72701500 -1.05508200 2.63212400
H -3.40542100 0.56006200 2.73329200
C -0.08204300 0.28633400 -1.42538600
O -0.09701100 0.38289600 -2.58970000
C -3.29111700 -1.37909800 -0.09050100
C -3.04137900 -1.67467300 -1.59657900
C -4.10634200 -2.62730100 -2.18968000
C -4.60201600 -3.62839100 -1.14004100
C -5.32513300 -2.89705400 0.01607000
C -4.79627800 -1.45598500 0.23124800
H -3.02890200 -0.75036200 -2.18064500
H -4.96223300 -2.04786900 -2.56064200
H -5.26922700 -4.37049500 -1.59317900
H -6.40236700 -2.85061800 -0.18562800
H -5.00335800 -1.14583000 1.26072700
H -2.04623100 -2.11791900 -1.69966400
H -3.68893800 -3.14722100 -3.05956900
H -3.74150400 -4.18808100 -0.75046300
H -5.20907100 -3.47211300 0.94278400
H -5.34073500 -0.76086300 -0.41835900
C -3.22239700 1.70645100 0.06554300
C -3.40020600 1.90031000 -1.45458600
C -3.74158900 3.37309100 -1.78506800
C -4.62622700 4.03579400 -0.70108600
C -5.46042700 2.98372500 0.03751000
C -4.55365800 2.00201500 0.81534200
H -2.49698500 1.60824000 -1.99753500
H -2.81370200 3.94556600 -1.90253700
H -3.99551100 4.56053500 0.02858300
H -6.16466900 3.45824600 0.73094500
H -5.11188900 1.08406300 1.01568400
H -4.20423200 1.24531500 -1.81049500
H -4.25105600 3.40609100 -2.75588600
H -5.27139400 4.79841100 -1.15184300
H -6.07081300 2.43385800 -0.69096800
H -4.31429600 2.43761300 1.79234800
C 2.87477300 2.03978200 0.08756100
C 2.51700700 2.48801700 -1.35834400
C 3.37609600 3.68454700 -1.83335700
C 3.74006000 4.60551300 -0.66396900
C 4.62194700 3.85940800 0.36602000

C 4.35986200 2.33224700 0.37740500
H 2.64077100 1.66149200 -2.06470300
H 4.30041000 3.32105800 -2.30166600
H 4.25459100 5.50482500 -1.02140300
H 5.68265700 4.03234600 0.14626700
H 4.67261500 1.92154100 1.34261700
H 1.45758400 2.75997000 -1.38297800
H 2.83667900 4.23651500 -2.61187600
H 2.81495600 4.95224500 -0.18504500
H 4.44308600 4.26979800 1.36730800
H 4.98061500 1.84571800 -0.38378400
C 3.32741500 -1.00904500 -0.16454200
C 3.43802100 -1.02439300 -1.70256100
C 3.97772900 -2.38944600 -2.19634200
C 4.97332600 -3.02804700 -1.19845900
C 5.71085400 -1.94708400 -0.39966000
C 4.73322700 -1.13750000 0.48749600
H 2.46795000 -0.82601700 -2.16786000
H 3.13748100 -3.07354600 -2.36424100
H 4.43458300 -3.68017500 -0.49869900
H 6.49426800 -2.38959400 0.22654400
H 5.16901600 -0.15716800 0.69176700
H 4.10963800 -0.21923700 -2.02434200
H 4.46229400 -2.24768900 -3.17011200
H 5.68404400 -3.67002600 -1.73168100
H 6.22232400 -1.27348900 -1.10001100
H 4.62460700 -1.63749900 1.45663900
H -2.79730800 -2.17610900 0.48314700
H -2.48082100 2.44766000 0.38846200
H 2.75480600 -1.90000000 0.12029800
H 2.28236200 2.65634100 0.77810800
C 1.23139900 -4.39421700 -0.02572100
O 0.46620100 -3.61159600 -0.77030300
O 1.74033500 -4.11304800 1.04385300
H 1.35820100 -5.37881100 -0.50753900
H 0.33035000 -2.70000600 -0.33728500
H -0.01966400 -1.45895600 0.17897100

Ph-2

Fe 0.01261000 0.13814300 0.20672700
H -0.01852000 1.69698700 0.06977400
H 0.03109400 -1.40171000 0.46874800
C -1.25359200 -0.27840700 2.91949200
C -2.49916600 0.25779500 2.21865800

H -1.31667000 -0.09823900 4.00300600
H -1.18038400 -1.35639400 2.75883600
H -2.66399200 1.31168200 2.45726100
H -3.38154900 -0.29658300 2.55114100
P -2.22116200 0.09880800 0.38190800
N 0.00031400 0.33155100 2.38054900
C 0.08820000 1.74475700 2.83341600
H 0.08971000 1.79880300 3.93242900
H 0.99730000 2.20451700 2.44915300
H -0.75172300 2.31757500 2.44467500
P 2.23451400 0.02068900 0.43368500
C 1.15793100 -0.42928400 2.94376800
C 2.48100100 -0.04248800 2.28537800
H 0.95653200 -1.48772400 2.76894300
H 1.21239800 -0.26604300 4.03076300
H 2.81513700 0.94805000 2.60564900
H 3.26299200 -0.75380500 2.56622800
C 0.07737800 -0.04010900 -1.51447400
O 0.15133400 -0.15244300 -2.67386000
C 3.07945600 -1.48729200 -0.22249800
C 3.00609400 -2.70458600 0.47395000
C 3.72926000 -1.46308400 -1.46641900
C 3.58234400 -3.86194600 -0.05136600
H 2.49144600 -2.75889700 1.42842400
C 4.29804400 -2.62431100 -1.99561000
H 3.80029900 -0.53573300 -2.02668500
C 4.23007100 -3.82607900 -1.28885800
H 3.52173700 -4.79277200 0.50611100
H 4.79772100 -2.58518500 -2.95968500
H 4.67583600 -4.72801300 -1.69890700
C 3.37751000 1.36591700 -0.11135700
C 4.72747700 1.38136000 0.28227200
C 2.89691300 2.39668600 -0.92971200
C 5.57250500 2.41238100 -0.12784700
H 5.12226100 0.58379300 0.90600400
C 3.74709800 3.42509100 -1.34784600
H 1.85354700 2.39330700 -1.22971700
C 5.08320800 3.43612900 -0.94571500
H 6.61244300 2.41616100 0.18712900
H 3.36188600 4.21678600 -1.98454500
H 5.74305300 4.23730700 -1.26721100
C -3.27500700 1.42236900 -0.36694400
C -2.98346700 1.84639800 -1.67369000
C -4.36326300 2.00793900 0.30065200

C -3.76129100 2.82134500 -2.29944300
H -2.13848100 1.41910500 -2.20387100
C -5.13629600 2.99110200 -0.32279000
H -4.61842400 1.70562300 1.31167700
C -4.83930700 3.39878400 -1.62438100
H -3.51851700 3.13467200 -3.31108700
H -5.97109600 3.43687300 0.21123600
H -5.44085500 4.16333300 -2.10810200
C -3.16764400 -1.42918500 -0.08834500
C -4.53254700 -1.56738800 0.21874600
C -2.52516900 -2.46671200 -0.77791700
C -5.23097800 -2.71926400 -0.14268600
H -5.05945600 -0.77221100 0.73848500
C -3.22707200 -3.61798200 -1.14769000
H -1.47063800 -2.37590500 -1.01529500
C -4.57885600 -3.74865400 -0.82830000
H -6.28444100 -2.81175700 0.10733900
H -2.71282400 -4.41189500 -1.68246300
H -5.12386800 -4.64488100 -1.11186100

Ph-3

C -0.29508600 4.24720300 -0.59190300
O -0.09519000 4.11049100 -1.73713000
O -0.49397600 4.42374100 0.54607400
Fe 0.02330300 -0.27550000 0.24853100
H -0.02588500 1.28644100 0.21147700
H 0.08098100 -1.83378100 0.39667500
C -1.17608500 -1.02288500 2.91504500
C -2.47826300 -0.55270000 2.27315200
H -1.24469400 -0.94559000 4.01079100
H -0.99983600 -2.06977800 2.66046400
H -2.78068100 0.42478300 2.65790500
H -3.28214200 -1.25831500 2.50149300
P -2.20745100 -0.38806300 0.42772100
N 0.00926900 -0.25161200 2.43062600
C -0.04179800 1.12336300 2.99238400
H -0.04941700 1.09100500 4.09236400
H 0.81921200 1.69853100 2.65557400
H -0.93442900 1.63823800 2.64168600
P 2.24765700 -0.27529300 0.45431700
C 1.23470600 -0.94038500 2.93942300
C 2.51259000 -0.40422200 2.29904600
H 1.12343800 -1.99969800 2.70121700
H 1.28661300 -0.84064100 4.03414300

H 2.75571700 0.59630200 2.66653500
H 3.35725200 -1.05417400 2.54545100
C 0.05127700 -0.37564500 -1.48091800
O 0.08333200 -0.45608100 -2.64406400
C -3.09967400 -1.83970600 -0.30589500
C -4.20964900 -1.70126200 -1.15305400
C -2.62943700 -3.13415200 -0.02329400
C -4.83746100 -2.82641900 -1.69560600
H -4.59123800 -0.71588600 -1.39733600
C -3.26638900 -4.25648000 -0.55261500
H -1.74825000 -3.26209200 0.59757900
C -4.37267900 -4.10652800 -1.39347700
H -5.69190300 -2.69691800 -2.35439700
H -2.89067200 -5.24853000 -0.31672500
H -4.86246100 -4.98036800 -1.81421800
C -3.28978500 1.03351000 -0.04148900
C -4.51586000 1.28131800 0.59849500
C -2.87936500 1.89502400 -1.06960000
C -5.30481400 2.37163500 0.22571400
H -4.86436600 0.62249500 1.38876800
C -3.67334800 2.98018000 -1.44949300
H -1.92964800 1.72078200 -1.56388400
C -4.88527500 3.22300300 -0.79938900
H -6.24718000 2.55373400 0.73517500
H -3.34181100 3.63740300 -2.24860200
H -5.49958200 4.07120300 -1.08870700
C 3.19963400 -1.68373100 -0.27510900
C 3.85409500 -1.54343500 -1.50874200
C 3.20573200 -2.94125900 0.35033200
C 4.50538500 -2.63020500 -2.09729000
H 3.86393900 -0.58256400 -2.01427000
C 3.86457400 -4.02392300 -0.23396200
H 2.69056800 -3.08442700 1.29546600
C 4.51612200 -3.87233800 -1.46070000
H 5.00745100 -2.50161000 -3.05237200
H 3.86584000 -4.98722700 0.26898500
H 5.02582100 -4.71642700 -1.91681600
C 3.28672800 1.17451800 -0.02885500
C 4.60553300 1.31604600 0.43694000
C 2.75655000 2.15881500 -0.87388900
C 5.36943500 2.42596100 0.07484900
H 5.04039700 0.55726000 1.08206300
C 3.52620900 3.26536400 -1.24525700
H 1.73822300 2.05634500 -1.23374300

C 4.83058000 3.40285100 -0.76818300
H 6.38535000 2.52697300 0.44694900
H 3.10405300 4.01911800 -1.90396300
H 5.42708500 4.26574500 -1.05149600

Ph-TS3_4

Fe -0.05732300 0.02585800 0.22947500
H -0.01120900 -1.57462400 0.12048100
H -0.09371400 1.55244500 0.41281800
C 1.21146300 0.53805400 2.93011600
C 2.44462400 -0.04483800 2.24770700
H 1.26512500 0.38373200 4.01767900
H 1.16754500 1.61401900 2.74357600
H 2.55991600 -1.10641500 2.48174600
H 3.34451800 0.47135400 2.59456900
P 2.19062200 0.13626700 0.41432800
N -0.05674300 -0.05361600 2.40258600
C -0.19314000 -1.44655400 2.90127500
H -0.15531200 -1.46805000 4.00068600
H -1.14218700 -1.86671500 2.57066700
H 0.59380400 -2.07459700 2.49092100
P -2.28786400 0.20215400 0.45042300
C -1.18885800 0.76919400 2.93021200
C -2.52543800 0.39822200 2.29276900
H -0.95298500 1.81174500 2.70964100
H -1.24653900 0.65662600 4.02326100
H -2.90060700 -0.55441200 2.67603300
H -3.27634000 1.15860600 2.52509700
C -0.11581700 0.17316800 -1.49991900
O -0.18639500 0.28474800 -2.65654900
C -3.07384200 1.69330400 -0.30869000
C -2.92909800 2.95591000 0.28893200
C -3.75898300 1.60073000 -1.52987900
C -3.47176200 4.09315200 -0.31081100
H -2.38717500 3.05962400 1.22418000
C -4.29321600 2.74163600 -2.13410000
H -3.88538200 0.63670100 -2.01321800
C -4.15490100 3.98998100 -1.52539800
H -3.35787500 5.06052200 0.17092900
H -4.82109700 2.64993500 -3.07938400
H -4.57480800 4.87607100 -1.99313600
C -3.48389500 -1.13174100 0.00650200
C -4.80279900 -1.11837800 0.49443200
C -3.07713800 -2.18179800 -0.82735400

C	-5.68921200	-2.14289800	0.16314100	H	1.36781900	1.28773900	2.82283600
H	-5.14141500	-0.30577600	1.13162900	H	2.36457500	-1.56715800	2.25874600
C	-3.96986300	-3.20414900	-1.16448700	H	3.38711300	-0.17296000	2.59708200
H	-2.06211800	-2.20382000	-1.20860700	P	2.22568800	-0.08132800	0.38645200
C	-5.27343000	-3.18876800	-0.66734400	N	-0.06148600	-0.18059900	2.35960700
H	-6.70431300	-2.12488300	0.55027300	C	-0.41416900	-1.54103200	2.85187200
H	-3.64090700	-4.01262900	-1.81162200	H	-0.41950300	-1.55732200	3.95096800
H	-5.96509600	-3.98612900	-0.92492900	H	-1.40230900	-1.82526500	2.48992900
C	3.32352800	-1.10645300	-0.35148500	H	0.28937500	-2.27829400	2.46537800
C	3.15322400	-1.41955000	-1.71050600	P	-2.27076100	0.25338100	0.42482400
C	4.36673000	-1.72586500	0.35567500	C	-1.06829500	0.80836800	2.85962500
C	4.00456800	-2.32481800	-2.34541800	C	-2.45303900	0.58582600	2.25331900
H	2.35005700	-0.96059000	-2.27821400	H	-0.70080700	1.79977400	2.58733000
C	5.21388900	-2.63725100	-0.27967500	H	-1.12216100	0.75123300	3.95656900
H	4.52874100	-1.50713800	1.40622400	H	-2.95274300	-0.27803900	2.69856400
C	5.03629400	-2.93813400	-1.63106600	H	-3.08712700	1.45721100	2.43804700
H	3.85560500	-2.55556200	-3.39654400	C	-0.10621600	-0.01342900	-1.53911700
H	6.01281200	-3.11060800	0.28453700	O	-0.16780400	0.13084700	-2.68771900
H	5.69526900	-3.64756200	-2.12374400	C	2.95242500	1.60004000	0.14539800
C	3.06512200	1.71744700	-0.00899600	C	2.77705700	2.22102200	-1.10340200
C	4.41286500	1.90966000	0.34149300	C	3.67505700	2.27717400	1.13816800
C	2.39992900	2.73163600	-0.71112900	C	3.31847100	3.48096700	-1.35424200
C	5.07145200	3.09420800	0.01308900	H	2.21281800	1.72003300	-1.88465100
H	4.95632600	1.12888800	0.86635700	C	4.20899900	3.54538600	0.88874600
C	3.06300500	3.91545300	-1.04850700	H	3.82710500	1.82915300	2.11429400
H	1.35937200	2.59786400	-0.98577000	C	4.03460700	4.14903400	-0.35657700
C	4.39669000	4.10132300	-0.68379000	H	3.17583600	3.94350200	-2.32684700
H	6.11178700	3.22936700	0.29615300	H	4.76253100	4.05702300	1.67131500
H	2.53268500	4.69111900	-1.59419700	H	4.45139500	5.13340600	-0.55001400
H	4.91100600	5.02281200	-0.94241400	C	3.44798500	-1.15198700	-0.48477000
C	0.45211100	-3.18525500	-0.35269400	C	4.80826200	-1.09675600	-0.13377600
O	0.89856900	-3.62383000	0.66010400	C	3.04279400	-2.01210000	-1.51427500
O	0.12984100	-3.24529200	-1.49679700	C	5.74121400	-1.89455500	-0.79461300
Ph-4				H	5.14277800	-0.42321700	0.65039300
C	0.15431000	-3.01560300	-0.14149200	C	3.98176800	-2.80614700	-2.17900300
O	-0.21917700	-3.31805100	-1.28015400	H	1.99685600	-2.08078600	-1.79176200
O	0.77946100	-3.59092400	0.75541700	C	5.32879000	-2.75038000	-1.82074500
Fe	-0.05295900	-0.15294700	0.20580900	H	6.78931100	-1.84578900	-0.51248500
H	-0.19799300	-1.90329700	0.17993000	H	3.65433300	-3.47044000	-2.97373400
H	0.02052300	1.33577700	0.27972900	H	6.05661200	-3.36947400	-2.33791500
C	1.27337000	0.20314800	2.92087100	C	-2.87638900	1.77697100	-0.42094900
C	2.42238200	-0.47751400	2.18162700	C	-3.61047900	1.69348500	-1.61359600
H	1.30254700	-0.03969500	3.99189800	C	-2.54140700	3.04503300	0.08164400
				C	-4.00531800	2.85318500	-2.28532300

H -3.88260300 0.72502200 -2.02157400
C -2.94501500 4.20163400 -0.58625400
H -1.96088200 3.13698400 0.99488000
C -3.67674900 4.10918500 -1.77319800
H -4.57335200 2.77045400 -3.20771800
H -2.68427300 5.17506700 -0.18007000
H -3.98705500 5.01023500 -2.29462500
C -3.58120300 -0.98409000 0.05518700
C -4.89299300 -0.80898800 0.53211500
C -3.27192300 -2.11968900 -0.70710100
C -5.87518800 -1.75926900 0.25673200
H -5.14975300 0.07113800 1.11567900
C -4.26327000 -3.06704800 -0.98444100
H -2.26197100 -2.28070300 -1.07503600
C -5.56081700 -2.89067600 -0.50353300
H -6.88466600 -1.61741500 0.63261300
H -4.01381400 -3.94537200 -1.57325200
H -6.32704300 -3.63063500 -0.71766100

Ph-TS4_5

C 0.04278000 -3.05935000 -0.06961300
O 0.03031300 -2.71692900 -1.29136200
O 0.85250000 -3.77413000 0.54915400
Fe -0.05129100 -0.19003900 0.23988100
H -0.81526300 -2.63227800 0.53090200
H -0.00887300 1.28211800 0.35483100
C 1.23759500 0.33240800 2.93312400
C 2.47290800 -0.23039000 2.23687600
H 1.29371600 0.15971800 4.01705200
H 1.18559500 1.41089600 2.76744600
H 2.58710600 -1.30275000 2.42158800
H 3.37996400 0.25599600 2.60838400
P 2.23930900 -0.02428800 0.41011200
N -0.03544700 -0.25581400 2.40544300
C -0.16794500 -1.65093500 2.90569900
H -0.02956900 -1.67776200 3.99558000
H -1.16082200 -2.03358700 2.67098700
H 0.55492300 -2.30934100 2.42278600
P -2.29109400 0.12681800 0.44946400
C -1.16238400 0.57393200 2.94187900
C -2.50796600 0.24475200 2.29681800
H -0.90902600 1.61752800 2.74527100
H -1.22408100 0.44208500 4.03180200
H -2.88996800 -0.72204100 2.63659000

H -3.24854200 1.00099300 2.57290400
C -0.08419500 0.00742500 -1.50972000
O -0.12565400 0.22497900 -2.64543100
C 3.53031500 -1.09213000 -0.35662800
C 4.88854400 -0.86644400 -0.06731900
C 3.17234400 -2.12599100 -1.23312400
C 5.87327000 -1.66908300 -0.64092200
H 5.18031700 -0.05865700 0.59855000
C 4.16793400 -2.92186300 -1.81039400
H 2.12469800 -2.32629700 -1.44794100
C 5.51305500 -2.69852100 -1.51694100
H 6.91954800 -1.48930200 -0.40918900
H 3.88414700 -3.72304700 -2.48756300
H 6.28097100 -3.32189700 -1.96710400
C 2.85163600 1.66837900 -0.00455600
C 3.27569400 2.59630400 0.95726300
C 2.87006700 2.04472000 -1.35924100
C 3.70857700 3.86955100 0.57361100
H 3.27599100 2.34110500 2.01195700
C 3.30518800 3.31320100 -1.74004000
H 2.54943000 1.34364700 -2.12466300
C 3.72481400 4.23159100 -0.77327400
H 4.03575800 4.57512700 1.33241700
H 3.31587600 3.58367300 -2.79218800
H 4.06223100 5.22070700 -1.06972400
C -3.56058300 -1.08878700 -0.09217600
C -3.20461100 -2.11692100 -0.97834800
C -4.88819100 -0.99534400 0.36256600
C -4.16945200 -3.03737900 -1.40162300
H -2.17538600 -2.21340800 -1.32084900
C -5.84285300 -1.91973300 -0.05940700
H -5.17963300 -0.19818000 1.04117800
C -5.48416100 -2.94187800 -0.94439200
H -3.88673500 -3.83265100 -2.08586700
H -6.86560500 -1.84180900 0.29896500
H -6.22948500 -3.66057800 -1.27378300
C -2.91064800 1.71744000 -0.25100200
C -2.67263000 2.93503100 0.40706600
C -3.56289600 1.73725200 -1.49378500
C -3.09127600 4.14064200 -0.15772400
H -2.15668200 2.95347300 1.36188700
C -3.97339100 2.94598400 -2.06053100
H -3.75938900 0.80989600 -2.02299900
C -3.74179500 4.15026700 -1.39397900

H -2.90578800 5.07272200 0.36894700
H -4.47780000 2.94203500 -3.02272300
H -4.06486700 5.08948200 -1.83393100

Ph-5

C 0.11867200 -2.82096800 -0.72628400
O -0.01836400 -2.01101700 0.26510800
O 0.16890200 -4.05050500 -0.66127100
Fe -0.02460200 0.00805000 0.21709800
H 0.19624700 -2.33131900 -1.72858200
H 0.00449300 1.51593300 0.39193600
C 1.25350000 0.58022000 2.90817100
C 2.46658400 -0.07462200 2.25255500
H 1.30811300 0.47642000 4.00165800
H 1.24194300 1.64764000 2.67235100
H 2.52770600 -1.13349600 2.51501600
H 3.38704700 0.40692900 2.59551200
P 2.24450500 0.07021300 0.41285600
N -0.03220700 0.00055800 2.41143900
C -0.21581300 -1.35042700 3.00109000
H -0.26750300 -1.27938300 4.09715100
H -1.12572500 -1.80861600 2.61994400
H 0.60409200 -2.00303700 2.71276400
P -2.28277700 0.23336700 0.43997100
C -1.14233900 0.88875000 2.87297200
C -2.49014900 0.48446400 2.28010000
H -0.89077700 1.90501200 2.56307300
H -1.19618300 0.87112000 3.97169100
H -2.84143800 -0.45356400 2.71649500
H -3.24095300 1.24947400 2.49646700
C -0.06650200 0.32035800 -1.49598300
O -0.12099300 0.62527900 -2.61755400
C 3.17084400 1.61287000 -0.02442300
C 4.54983900 1.71081900 0.23372700
C 2.51741900 2.69906300 -0.62283300
C 5.25203300 2.87207900 -0.08593800
H 5.08111700 0.87439800 0.67960900
C 3.22375100 3.86097200 -0.94884400
H 1.45462800 2.63758100 -0.82938100
C 4.58933800 3.95141000 -0.67865500
H 6.31651900 2.93318800 0.12307100
H 2.70292800 4.69306800 -1.41458000
H 5.13759700 4.85499300 -0.93055500
C 3.31372700 -1.23633200 -0.32831400

C 4.20790500 -2.01839600 0.41870000
C 3.23120500 -1.44480300 -1.71594600
C 4.99938900 -2.98496300 -0.20812800
H 4.30070400 -1.88100100 1.49095800
C 4.02577500 -2.40567600 -2.34034000
H 2.54295000 -0.85463200 -2.31407700
C 4.91118600 -3.18065500 -1.58677400
H 5.68551400 -3.58304500 0.38522800
H 3.94755000 -2.55383900 -3.41370900
H 5.52592100 -3.93365200 -2.07176800
C -3.08768200 1.71417300 -0.32714900
C -4.29440600 1.62838700 -1.03902400
C -2.47644000 2.97291900 -0.19108100
C -4.87460800 2.77048200 -1.59734600
H -4.78908500 0.67135600 -1.16343400
C -3.06357800 4.11360900 -0.73951900
H -1.53154600 3.05921300 0.33574300
C -4.26414600 4.01611700 -1.44730400
H -5.80660100 2.68164300 -2.14879200
H -2.57672100 5.07769900 -0.61988300
H -4.71680300 4.90319600 -1.88147400
C -3.42587600 -1.14283000 0.00769700
C -4.55284300 -1.47029900 0.77946400
C -3.16602700 -1.88112700 -1.15789800
C -5.39167400 -2.51979900 0.39805000
H -4.79079700 -0.90545700 1.67553600
C -4.00910300 -2.92498300 -1.54181100
H -2.30072200 -1.64099800 -1.76668700
C -5.12085300 -3.24973500 -0.76151100
H -6.25834800 -2.76363700 1.00628600
H -3.79106100 -3.48889400 -2.44429400
H -5.77275700 -4.06771400 -1.05509300

Ph-6

C -0.20366000 -4.55964200 0.11857600
O -0.99287200 -3.93031600 0.88396800
O 0.93819700 -4.24514700 -0.27888900
H -0.59785800 -5.55061800 -0.25278100
H -0.23554000 -1.79455900 -0.01758100
P -2.21082500 -0.09098100 0.32804800
Fe 0.04786400 -0.08501600 0.11207600
C -2.33907900 -0.86568700 2.00561800
P 2.24936500 0.41031100 0.34027000
C -0.02088300 0.32530800 -1.59558300

C -1.24739100 -0.20942400 2.84960600
H -2.16131800 -1.93896000 1.88786400
H -3.32121700 -0.72486800 2.46613600
C 2.41036300 0.63367800 2.18911200
O -0.09033500 0.63999000 -2.70656400
N 0.11115300 -0.37866700 2.23789900
H -1.44199000 0.86384800 2.92990500
H -1.24182500 -0.62395400 3.86613100
C 1.02361900 0.65129600 2.83123600
H 3.01240800 -0.19930800 2.56015600
H 2.95619000 1.55011300 2.43085100
C 0.61739500 -1.74138000 2.57213800
H 1.10927100 0.47947600 3.91368100
H 0.55125000 1.62269700 2.67574100
H 0.67603400 -1.86024100 3.66311600
H -0.02808800 -2.50797400 2.13610700
H 1.61203400 -1.88335800 2.15032800
H -0.03116100 1.37025600 0.39962000
H 0.51176200 -1.68024400 -0.25955800
C 3.63702200 -0.73218700 -0.07383600
C 3.37904600 -2.09379400 -0.29611700
C 4.96713700 -0.27365400 -0.08549200
C 4.43795000 -2.97590900 -0.53444200
H 2.37064300 -2.50115000 -0.26658300
C 6.01718000 -1.15935600 -0.32589600
H 5.18520100 0.77579600 0.08842100
C 5.75379500 -2.51336100 -0.55427800
H 4.22269300 -4.02669100 -0.70468400
H 7.03976000 -0.79233900 -0.33516600
H 6.57238400 -3.20214500 -0.74418800
C 2.72763100 2.00568000 -0.44508300
C 2.52086600 3.22921200 0.21049600
C 3.20539500 2.01643600 -1.76580500
C 2.80266800 4.43520600 -0.43428700
H 2.13415500 3.25333000 1.22466800
C 3.48373200 3.22401300 -2.40884100
H 3.36853600 1.08269300 -2.29573000
C 3.28543900 4.43630000 -1.74465700
H 2.64388300 5.37340800 0.09012800
H 3.85567800 3.21442700 -3.42943400
H 3.50353600 5.37513200 -2.24573400
C -3.29100000 -1.04399600 -0.82081600
C -4.15445800 -0.38421200 -1.71069000
C -3.20257300 -2.44667600 -0.86390200

C -4.92654400 -1.11263500 -2.61816200
H -4.23174100 0.69787700 -1.69995800
C -3.98562000 -3.16651200 -1.76853400
H -2.52025200 -2.98678600 -0.20823700
C -4.84795700 -2.50580500 -2.64673700
H -5.59006800 -0.58754500 -3.29972500
H -3.91420900 -4.25073800 -1.78763600
H -5.45137500 -3.07230600 -3.35065000
C -3.06520400 1.53534900 0.48120600
C -4.32873400 1.61724200 1.09322500
C -2.48485100 2.70345100 -0.03410500
C -4.98389300 2.84366900 1.20433300
H -4.81122900 0.72270900 1.47593000
C -3.14798200 3.92924900 0.06806300
H -1.51162300 2.65461900 -0.51073300
C -4.39404200 4.00275600 0.69224200
H -5.95598200 2.89282600 1.68671800
H -2.68651800 4.82476000 -0.33840000
H -4.90615700 4.95705000 0.77758500

Ph-TS6_7

C 0.27336800 -4.59990500 0.72376200
O -0.57800500 -3.74736400 0.30468400
O 1.47479000 -4.44229300 0.99142400
H -0.15354200 -5.63359700 0.86118500
H 0.00621700 -2.16754900 -0.08558100
P -2.27264700 -0.05591600 0.28915000
Fe 0.00654000 -0.03868400 0.07496800
C -2.43307000 -0.62734200 2.04785400
P 2.23279900 0.38022800 0.30659900
C -0.03481900 0.42958300 -1.61194600
C -1.27360000 -0.00036700 2.81900700
H -2.38704700 -1.71973700 2.05493200
H -3.38772600 -0.33801300 2.49549000
C 2.45161700 0.38349800 2.16034500
O -0.06663100 0.78874600 -2.71413100
N 0.05308400 -0.33937900 2.21549700
H -1.37387300 1.08850000 2.80134500
H -1.28901000 -0.32230800 3.86940000
C 1.07940400 0.57898200 2.80106800
H 2.89078200 -0.57118300 2.45810000
H 3.13330500 1.17683000 2.47862100
C 0.39361100 -1.74360600 2.57080800
H 1.14264600 0.40933400 3.88561800

H 0.73231900 1.60111000 2.63547500
 H 0.51750500 -1.83873900 3.65900100
 H -0.39046200 -2.41282800 2.22650100
 H 1.30318400 -2.06524500 2.06797300
 H -0.14386000 1.39576600 0.42686300
 H 0.42169300 -1.59775100 -0.47871400
 C 3.48046200 -0.80901400 -0.33733400
 C 3.24893800 -1.41534000 -1.58258900
 C 4.65874300 -1.12172100 0.36055300
 C 4.17683300 -2.30759400 -2.12095500
 H 2.33711800 -1.19956500 -2.13119700
 C 5.58339000 -2.01913100 -0.17782200
 H 4.86620100 -0.66597800 1.32375100
 C 5.34496400 -2.61256300 -1.41893000
 H 3.98054000 -2.77195100 -3.08311700
 H 6.48850800 -2.25407400 0.37520400
 H 6.06338700 -3.31335700 -1.83461700
 C 2.86852700 2.02869500 -0.25223600
 C 4.22653100 2.23045100 -0.55319000
 C 1.98976400 3.11966500 -0.34794400
 C 4.69085000 3.49159800 -0.93029400
 H 4.92814200 1.40475100 -0.49995000
 C 2.45749700 4.38130900 -0.72125400
 H 0.93690200 2.97625500 -0.13057900
 C 3.80887600 4.57120500 -1.01413500
 H 5.74357100 3.62743600 -1.16207300
 H 1.76134900 5.21283200 -0.78859000
 H 4.17164000 5.55128900 -1.31093300
 C -3.41760500 -1.10945500 -0.70565600
 C -4.40987100 -0.54687800 -1.52541500
 C -3.25965900 -2.50653900 -0.68637300
 C -5.24167000 -1.36390400 -2.29445200
 H -4.54302300 0.52852300 -1.56802800
 C -4.10167500 -3.31600600 -1.45151500
 H -2.46766700 -2.97432300 -0.10683300
 C -5.09502700 -2.75113500 -2.25484700
 H -6.00439700 -0.91134800 -2.92224500
 H -3.97054500 -4.39449700 -1.42445300
 H -5.74420500 -3.38656900 -2.85101400
 C -3.10501700 1.59418900 0.28360500
 C -4.31848800 1.79007600 0.96643900
 C -2.55414600 2.67063200 -0.42755800
 C -4.95006000 3.03436800 0.95415500
 H -4.78502500 0.96974500 1.50333900

C -3.19149300 3.91360800 -0.44776700
 H -1.62211300 2.54142700 -0.96520000
 C -4.38657600 4.10039100 0.24843100
 H -5.88340400 3.16888600 1.49362800
 H -2.74922200 4.73459900 -1.00501800
 H -4.87861200 5.06886300 0.23914300

Ph-7

C -1.43413700 4.27394800 -0.14378000
 O -0.66585400 3.51538000 -0.91307000
 O -1.77852900 4.04238600 0.99839600
 H -1.72943800 5.18895000 -0.68548900
 H -0.43160300 2.64970700 -0.44876300
 P 2.33798900 -0.06314500 0.42838100
 Fe 0.10905300 -0.13961500 0.19917100
 C 2.56346200 0.11754900 2.27171300
 P -2.11445300 -0.46093300 0.37824200
 C 0.18192100 -0.26059900 -1.52866800
 C 1.33145800 -0.47899700 2.94732200
 H 2.68674100 1.17613600 2.51318900
 H 3.46470500 -0.39862800 2.61345100
 C -2.39090000 -0.42246200 2.22088100
 O 0.25850100 -0.31312900 -2.69131800
 N 0.06029200 0.05219000 2.36710900
 H 1.32471900 -1.56177900 2.80157600
 H 1.35440000 -0.28161300 4.02935500
 C -1.06810500 -0.77169700 2.89690900
 H -2.72114400 0.58114800 2.49930600
 H -3.16750800 -1.12469400 2.53606100
 C -0.11890500 1.46053500 2.81127400
 H -1.14841000 -0.63190300 3.98541200
 H -0.82121100 -1.81806700 2.70454000
 H -0.22060800 1.50644200 3.90576700
 H 0.74030300 2.05813300 2.51071300
 H -0.99192500 1.90828000 2.34158900
 H 0.21823800 -1.66668300 0.44998200
 H 0.01790000 1.41674500 0.09646500
 C -3.36580300 0.72042000 -0.30366300
 C -3.16959900 1.23021400 -1.59733100
 C -4.51327200 1.11129900 0.40581500
 C -4.09453100 2.10721700 -2.16642000
 H -2.28811200 0.94735200 -2.16423100
 C -5.43590100 1.99272100 -0.16232600
 H -4.69758800 0.73479700 1.40702300

C -5.22921800 2.49303200 -1.44922300
H -3.92384200 2.49231600 -3.16794900
H -6.31553400 2.28753400 0.40344800
H -5.94645300 3.18015600 -1.88945600
C -2.83557600 -2.08434400 -0.16199800
C -4.13126800 -2.46910100 0.22392800
C -2.10177600 -2.93919600 -0.99540500
C -4.67003500 -3.68354300 -0.20112100
H -4.72982400 -1.81877700 0.85567600
C -2.64486800 -4.15125400 -1.43062500
H -1.09845700 -2.65955300 -1.29554100
C -3.92735200 -4.52836800 -1.03122100
H -5.67070400 -3.96851500 0.11227900
H -2.06097400 -4.80040400 -2.07749100
H -4.34804800 -5.47300000 -1.36475000
C 3.30064100 1.33752600 -0.30531400
C 4.19668700 1.14875900 -1.36862400
C 3.06293900 2.64694100 0.14678100
C 4.84795100 2.23814900 -1.95397300
H 4.39387000 0.15078000 -1.74586900
C 3.72222600 3.73209900 -0.43008400
H 2.35092800 2.82610900 0.94689700
C 4.61790000 3.53138800 -1.48397800
H 5.53708900 2.07058200 -2.77717700
H 3.53027600 4.73581100 -0.06063700
H 5.12698300 4.37737100 -1.93717800
C 3.37713100 -1.53434500 0.00742700
C 4.69875800 -1.64098700 0.47691900
C 2.86082900 -2.56566900 -0.78850600
C 5.47665600 -2.75622200 0.16592800
H 5.12911600 -0.84765500 1.08187400
C 3.64274000 -3.67969200 -1.10706900
H 1.84120300 -2.50188600 -1.15120500
C 4.94929000 -3.77923000 -0.62778700
H 6.49417000 -2.82538500 0.54066900
H 3.22606800 -4.46970700 -1.72569600
H 5.5522000 -4.64791600 -0.87011800