

Supporting Information

Mechanistic Insights into CO Hydrogenation to Methanol Mediated by a Manganese Pincer Catalyst: A DFT Study

Shuqi Zhang^a, Zhexuan Zhang^a, Lei Qin^a, Qin Ma^a, Yonghong Hu^{b,c}, Yuanxin Cao,^{a} Lili Zhao^{a*}*

^aState Key Laboratory of Materials-Oriented Chemical Engineering, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China.

Email: 202510007743@njtech.edu.cn; ias_llzhao@njtech.edu.cn

^bCollege of chemical engineering, Nanjing Tech University, Nanjing 211816, China.

^cCollege of Food Science and Light Industry, Nanjing Tech University, Nanjing, 211816, China.

Table of Contents

1. Optimized geometries of Structure	S3
(1) Optimized geometries of intermediates and transition states in Stage I	S3
(2) Optimized geometries of intermediates and transition states in Stage II	S3
(3) Optimized geometries of intermediates and transition states in Stage III	S5
(4) Optimized geometries of intermediates and transition states in Stage IV	S5
(5) Optimized geometric structures of manganese catalysts with different ligands ...	S6
2. Benchmark of different thermotical levels in this study	S7
3. The calculated NPA charge(q) and Wiberg bond order	S8
4. Supplementary reaction energy barrier diagram	S10
5. Supplementary weak interaction and bonding analysis	S11
6. Supplementary relaxed scan diagram	S13
7. Supplementary conformational search via kinetic simulation	S14
8. Cartesian coordinates of All the Structures	S15

1. Optimized geometries of Structure

(1) Optimized geometries of intermediates and transition states in Stage I

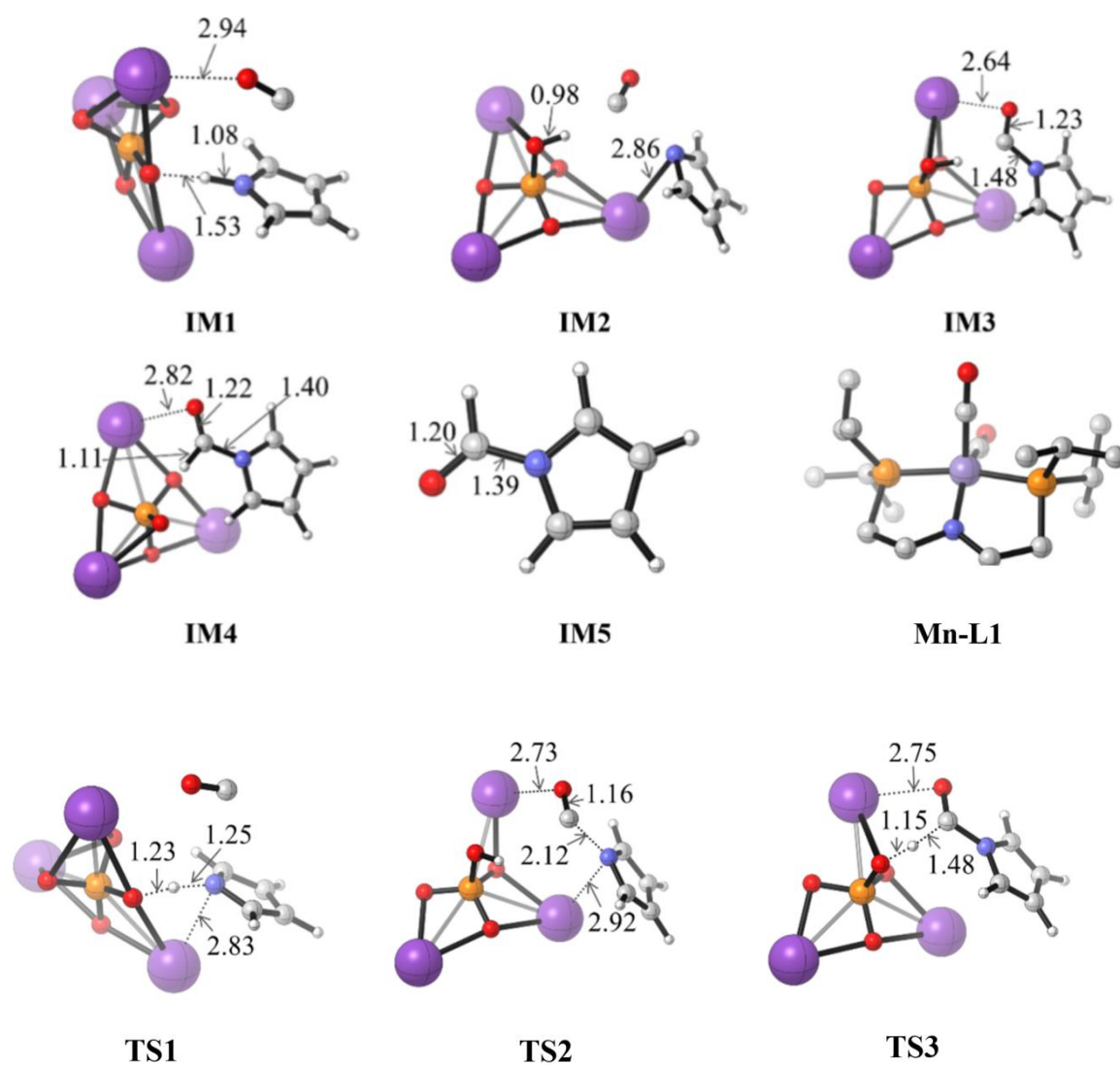


Figure S1: Optimized geometries of Stage I. selected bond distance is given in Å (color code, C: grey, H: white, O: red, P: yellow, N: blue.).

(2) Optimized geometries of intermediates and transition states in Stage II

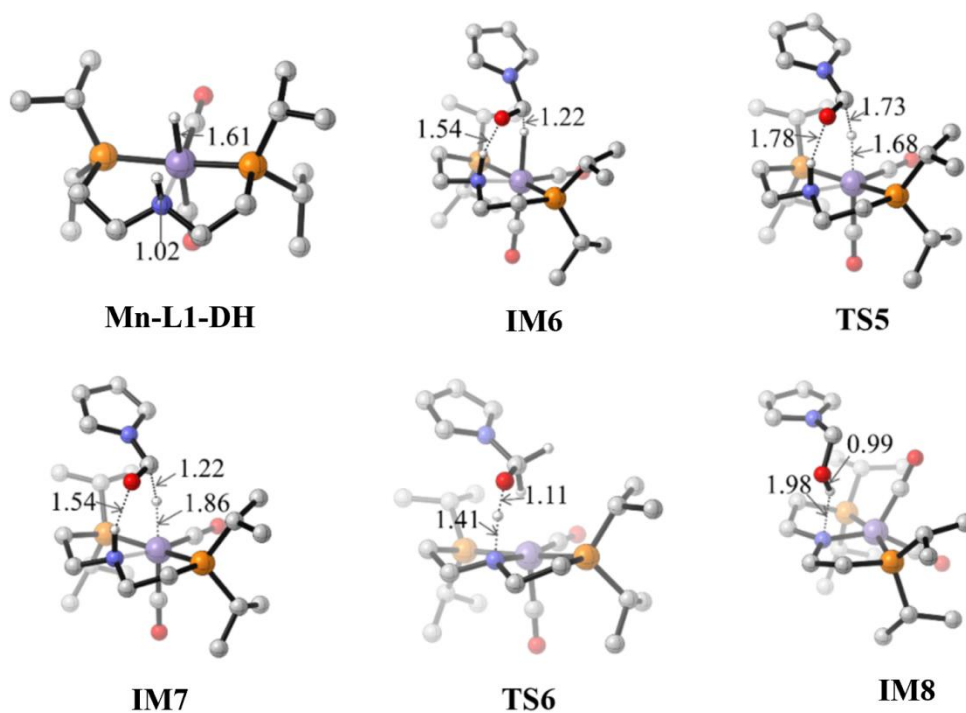


Figure S2: Optimized geometries of Stage II. hydrogen atoms have been omitted for clarity, selected bond distance is given in Å (color code, C: grey, H: white, O: red, P: yellow, Mn: purple ,N: blue.).

(3) Optimized geometries of intermediates and transition states in Stage III

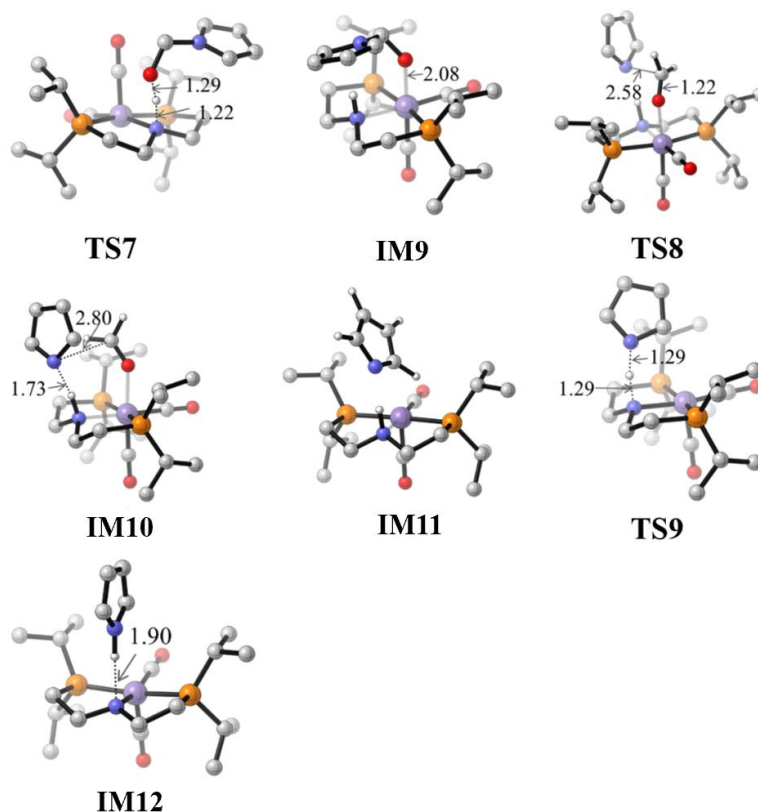


Figure S3: Optimized geometries of Stage III. hydrogen atoms have been omitted for clarity ,selected bond distance is given in Å (color code, C: grey, H: white, O: red, P: yellow, Mn: purple ,N: blue.).

(4) Optimized geometries of intermediates and transition states in Stage IV

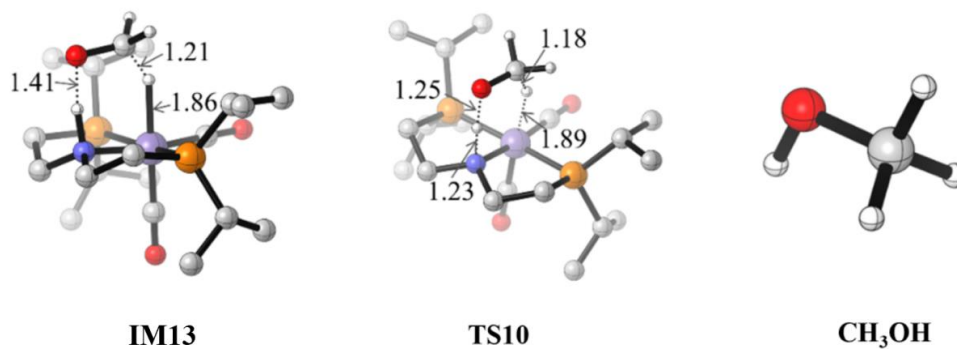


Figure S4: Optimized geometries of figure 6. hydrogen atoms have been omitted for clarity ,selected bond distance is given in Å (color code, C: grey, H: white, O: red, P: yellow, Mn: purple ,N: blue.).

(5) Optimized geometric structures of manganese catalysts with different ligands

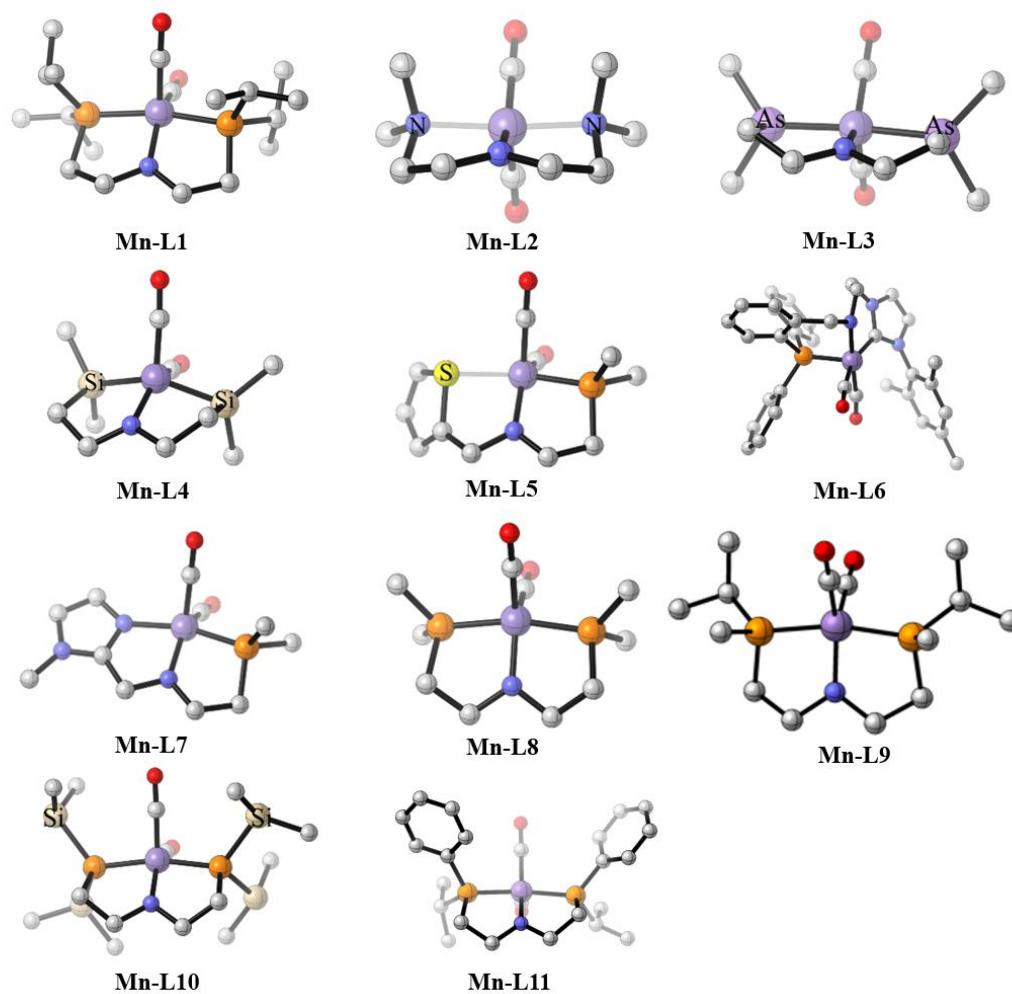


Figure S5: Optimized geometries of design of catalysts. (Color code, C: grey, H: white, O: red, P: yellow, Mn: purple.).

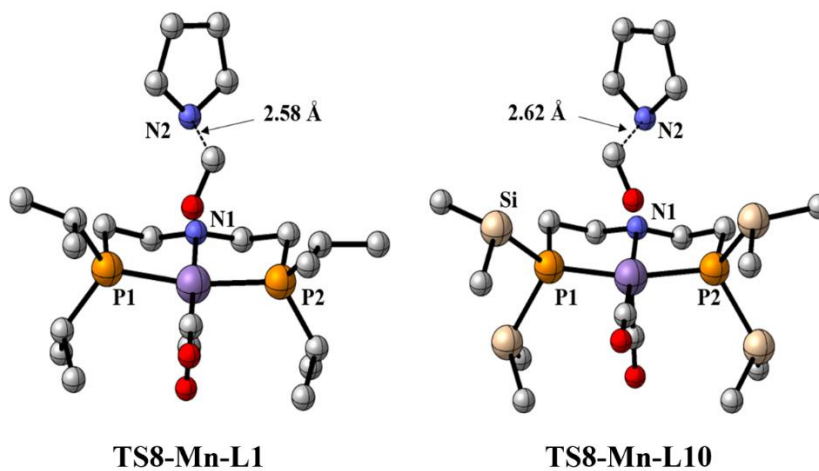
2. Benchmark of different thermotical levels in this study

Table S1: Computed the corresponding free energy barriers ($\Delta\Delta G^\ddagger$) and electronic energy($\Delta\Delta E^\ddagger$) are given in kcal/mol using different levels of theories.

Methods and Basis	$\Delta\Delta G^\ddagger$	$\Delta\Delta E^\ddagger$
M062x+D3/6-311++G(d,p)//M062x+D3/6-31G(d,p)	21.5	12.1
M062x+D3/def2-TZVPP//M062x+D3/6-31G(d,p)	22.2	12.8
B3LYP+D3(BJ)/6-311++G(d,p)//B3LYP+D3(BJ)/6-31G(d,p)	26.1	16.5
B3LYP+D3(BJ) /def2-TZVPP//B3LYP+D3(BJ) /6-31G(d,p)	26.7	17.0
BP86+D3/def2-TZVPP//BP86+D3/def2-SVP	26.2	15.2
PBE0+D3(BJ)/def2-TZVPP//PBE0+D3(BJ)/def2-SVP	21.5	10.7

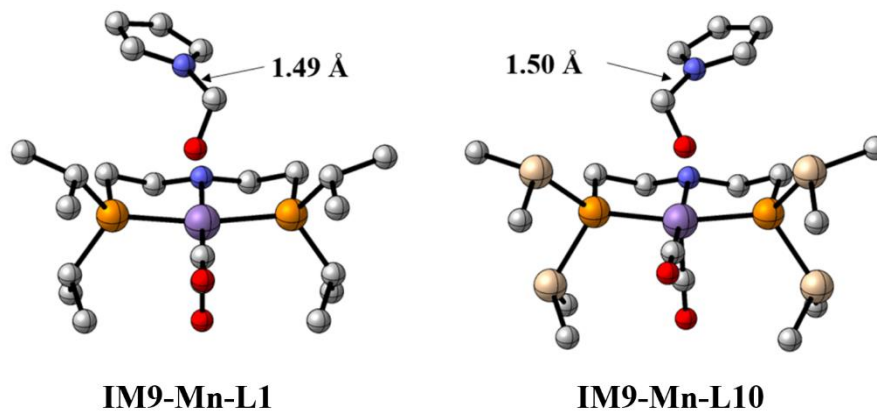
3. The calculated NPA charge(q) and Wiberg bond order

Table S2. The calculated NPA charge(q) and Wiberg bond order(P) of the optimized structures of **TS8-Mn-L1** and **TS8-Mn-L10** at the PBE0+D3(BJ)/def2-SVP (SMD,solvent= cyclohexane) level.



Natural charge q			Wiberg bond order		
	TS8-Mn-L1	TS8-Mn-L10		TS8-Mn-L1	TS8-Mn-L10
Mn	0.16	0.23	Mn-P1	0.72	0.69
P1	0.93	-0.08	Mn-P2	0.71	0.69
P2	0.95	-0.10	Mn-N1	0.50	0.49
N1	-0.67	-0.80	Mn-C1	1.10	1.06
C1	0.43	0.46	Mn-C2	1.05	1.11
C2	0.46	0.42	C3-N2	0.08	0.07
C3	0.28	0.29			
N2	-0.67	-0.67			

Table S3. The calculated NPA charge(q) , Wiberg bond order(P) and N3-C2 BDE of the optimized structures of **IM9-Mn-L1** and **IM9-Mn-L10** at the PBE0+D3(BJ)/def2-SVP (SMD,solvent= cyclohexane) level.



N3-C2 BDE **IM9-Mn-L1** 117.432 Kcal/mol

N3-C2 BDE **IM9-Mn-L10** 114.865 Kcal/mol

Natural charge q			Wiberg bond order		
	IM9-Mn-L1	IM9-Mn-L10		IM9-Mn-L1	IM9-Mn-L10
Mn	0.16	0.24	Mn-P1	0.52	0.48
P1	0.95	-0.05	Mn-P2	0.51	0.47
P2	0.97	-0.08	Mn-N1	0.22	0.20
N1	-0.74	-0.75	Mn-C1	1.22	1.14
C1	0.40	0.49	Mn-C2	1.12	1.24
C2	0.49	0.38	C3-N2	0.83	0.83
C3	0.17	0.17			
N2	-0.45	-0.45			

4. Supplementary reaction energy barrier diagram

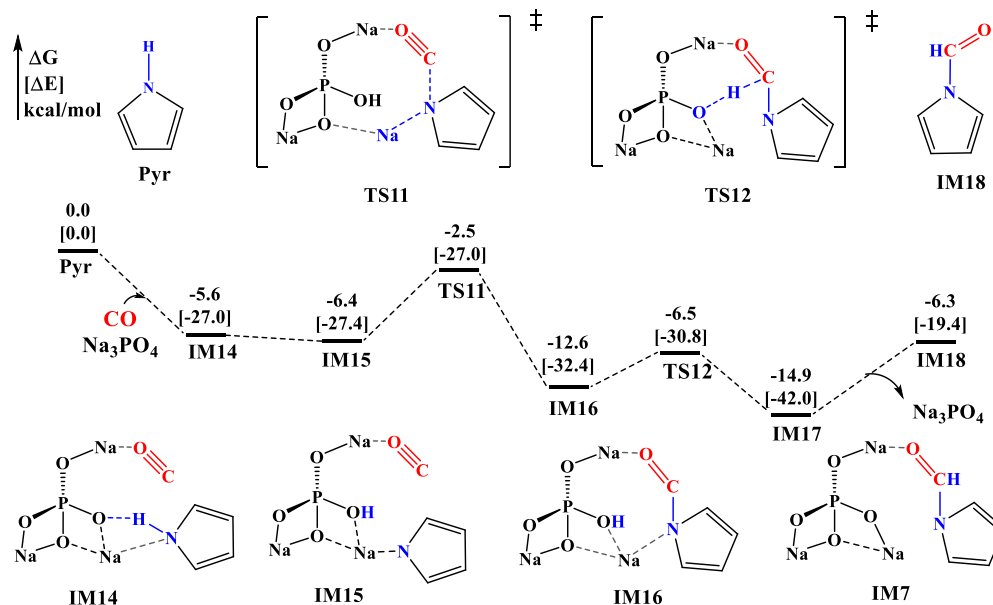


Figure S6: Using Na_3PO_4 as a reaction cocatalyst computed free energy profile (in kcal/mol) for stage I

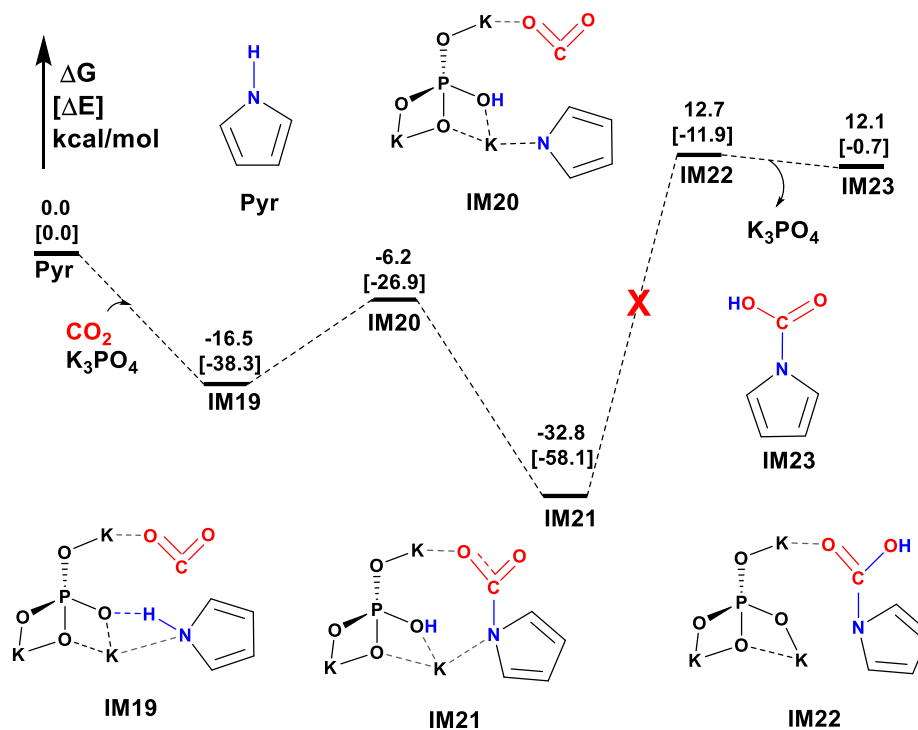


Figure S7: Computed free energy profile (in kcal/mol) for CO_2 system

5. Supplementary weak interaction and bonding analysis

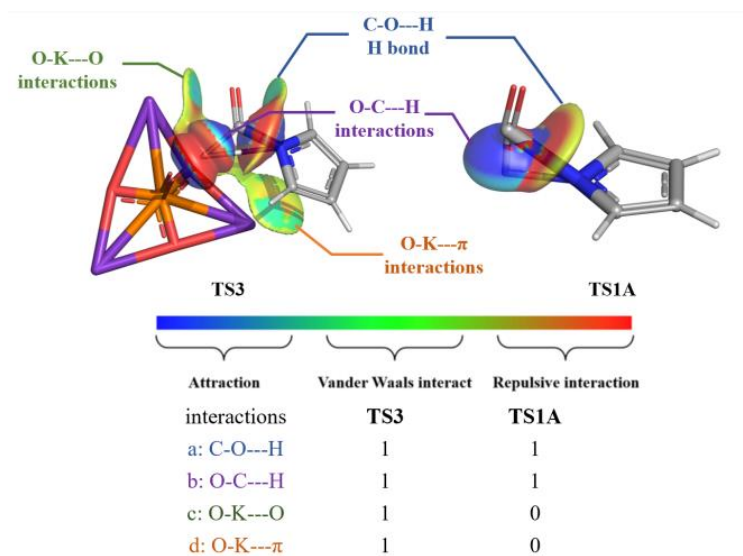


Figure S8. Independent Gradient Model based on Hirshfeld partitioning analysis for TS3 and TS1A.

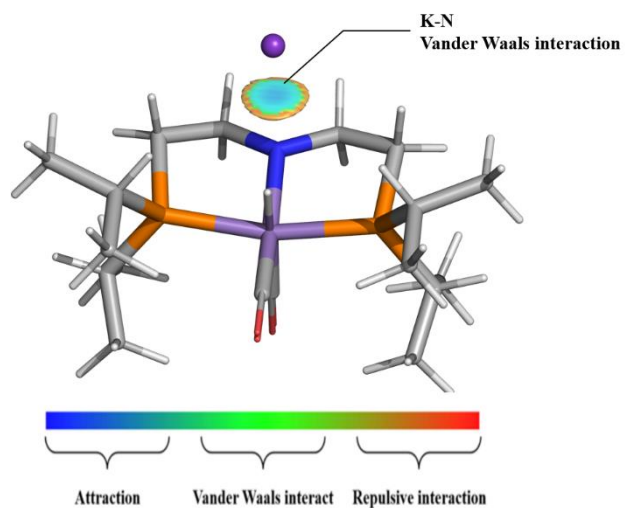


Figure S9 Independent Gradient Model based on Hirshfeld partitioning analysis for MnH-NK

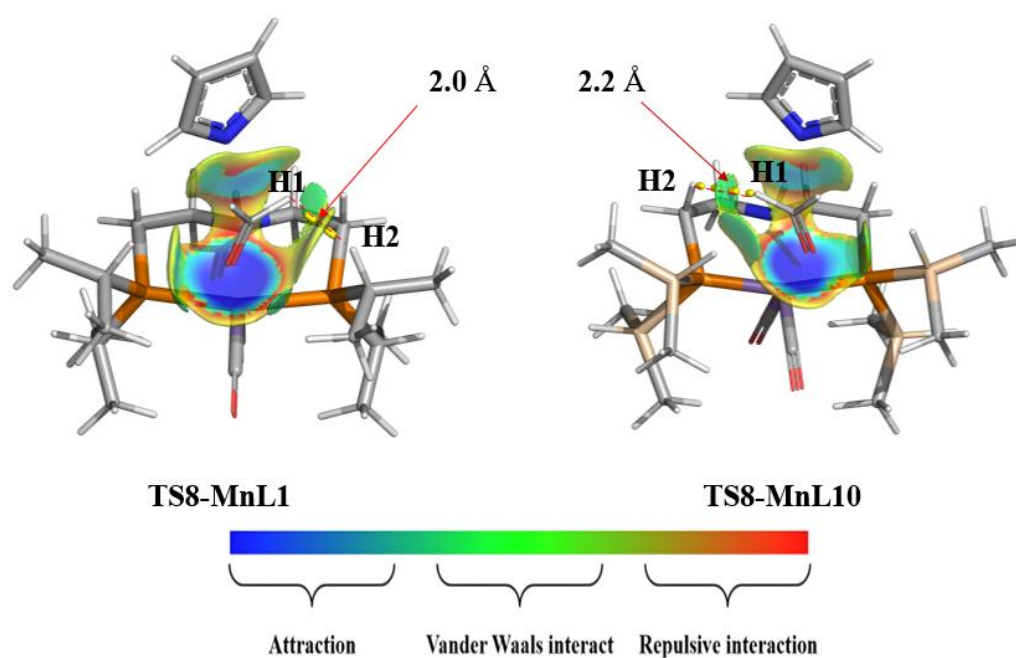


Figure S10: Independent Gradient Model based on Hirshfeld partitioning analysis for **TS8-ML1** and **TS8-ML10**

Table S4. The EDA-NOCV results of **TS1A** and **TS3** compound at the BP86/TZ2P//BP86/def2-SVP level of theory. Energy values are given in kcal/mol.

	TS1A	TS3
Fragments	pyrrole(S) + CO(S)	K ₃ PO ₄ +pyrrole(S) + CO(S)
ΔE_{int}	-8.2	-38.9
ΔE_{Pauli}	260.7	579.4
$\Delta E_{\text{disp}}^{[a]}$	-2.2(0.8%)	-6.1(1.0%)
$\Delta E_{\text{elstat}}^{[a]}$	-84.9(31.6%)	-246.3(39.8%)
$\Delta E_{\text{orb}}^{[a]}$	-181.8(67.6%)	-366.0(59.2%)

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$.

6. Supplementary relaxed scan diagram

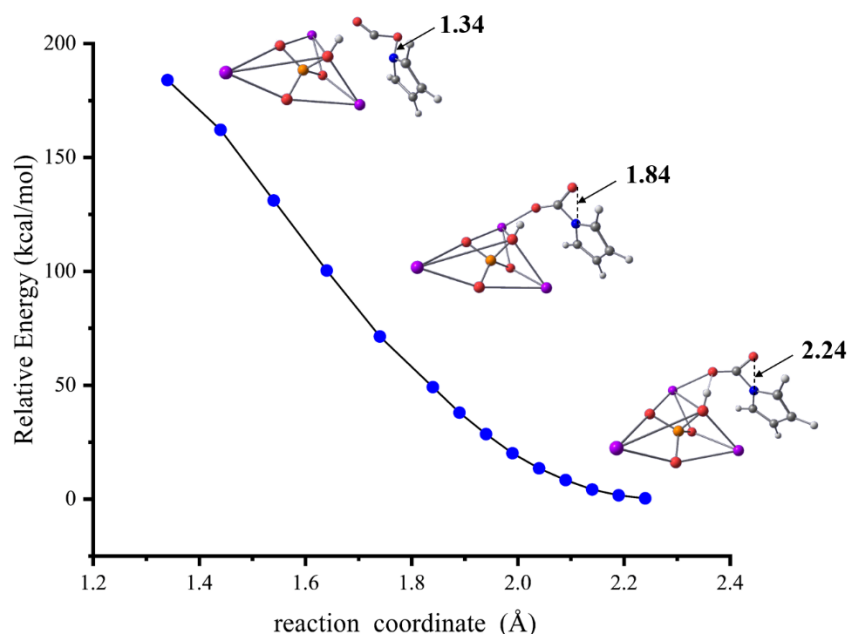


Figure S11: Flexible scan of the attack process of the O atom in CO₂ on the N atom in pyrrole

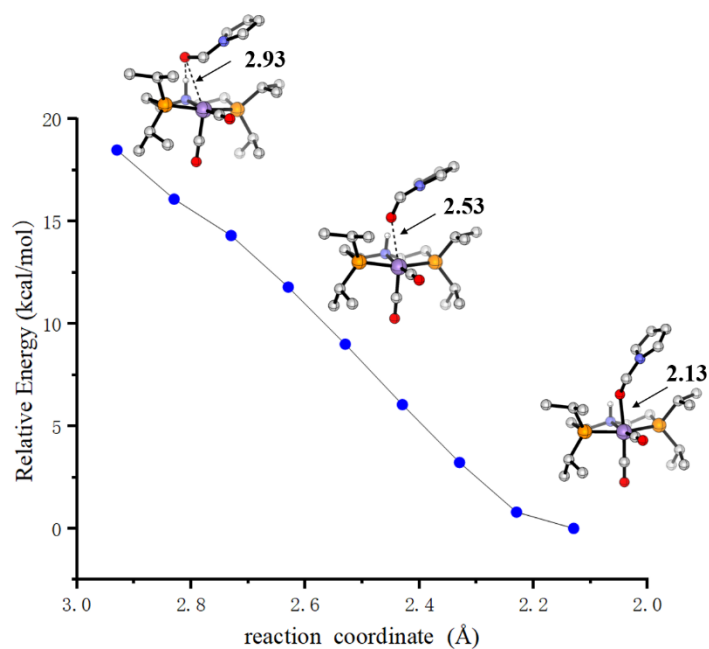


Figure S12: Relax scan of O-Mn bond formation during the IM7→IM9 transformation

7. Supplementary conformational search via kinetic simulation

Table S5: Energy comparison of different conformations of **IM1**

	$\Delta\Delta E(\text{Kcal}\cdot\text{mol}^{-1})$	$\Delta\Delta G(\text{Kcal}\cdot\text{mol}^{-1})$
IM1	0	0
IM1D	10.6	10.0
IM1E	7.7	7.9
IM1F	13	10.8

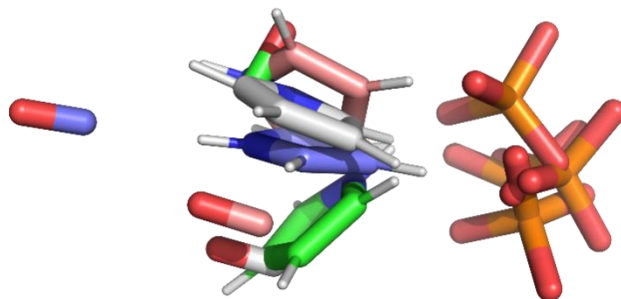


Figure S13: Structural comparison of different conformations of **IM1**. All structures were generated through an initial xTB-GFN1 conformational search followed by geometric optimization at the DFT level of theory.

8. Cartesian coordinates of All the Structures

Table S1: Atomic cartesian coordinates (Å) and transition states

Pyrrole				P	1.2086400	-0.4031700	-0.3485800
C	-0.9756000	-0.0441000	0.0000000	O	0.9702200	-1.9416000	-0.2896800
N	-0.1556000	-1.1337000	0.0000000	O	2.5976100	-0.0466000	-0.9472200
C	1.1485000	-0.7357000	0.0000000	O	0.0728900	0.3004600	-1.2577100
C	-0.1819000	1.0742000	0.0000000	O	1.1339600	0.2300400	1.0789800
C	1.1655000	0.6354000	0.0000000	K	3.1733000	-1.6178800	1.2125600
H	-2.0482000	-0.1502000	0.0000000	K	-1.3789700	-2.1373300	-1.1367800
H	-0.4661000	-2.0873000	0.0000000	K	1.6524700	2.4009600	-0.4378700
H	1.9530000	-1.4530000	0.0000000	C	-1.9079600	3.0908200	0.9506700
H	-0.5310000	2.0947000	0.0000000	O	-0.9317400	3.4339400	0.4875900
H	2.0485000	1.2548000	0.0000000				
CO				IM2			
C	0.0000000	0.0000000	-0.6444500	P	-1.4396100	-0.1053800	-0.0182700
O	0.0000000	0.0000000	0.4833400	O	-1.2378800	0.7067900	1.4231200
				O	-0.9432200	-1.5558200	0.1411600
K ₃ PO ₄				O	-2.9737000	-0.0131300	-0.2009200
P	0.0313800	0.0000100	0.0005500	O	-0.6444400	0.7216400	-1.0479000
O	0.9304400	-1.2935800	0.0009600	K	1.3590300	-1.0213200	-1.1128200
O	-0.9208900	0.0000500	1.2530800	K	-2.3915400	2.5920300	-0.4440000
O	0.9303700	1.2936300	0.0007900	K	-3.2990400	-2.4609700	0.4409300
O	-0.9197100	-0.0001100	-1.2529300	C	1.3872900	2.0122800	1.1698200
K	-1.5427700	-2.2793900	-0.0001600	O	1.8344700	2.9519800	0.7077600
K	3.0525100	0.0001200	-0.0004400	C	3.7952800	0.4910000	-0.4362200
K	-1.5430200	2.2792700	-0.0006500	N	3.0840300	0.3445600	0.7083100
				C	3.2594100	-0.9385500	1.1095000
IM1				C	4.4305000	-0.7063600	-0.7949100
C	-3.3116300	0.2732600	-0.6946600	C	4.0801800	-1.6404700	0.2152300
N	-2.0967400	0.3909800	-0.0867900	H	3.8238800	1.4539300	-0.9552100
C	-2.1762400	-0.2183500	1.1303500	H	-0.2931800	0.9273500	1.5498200
C	-4.1899300	-0.4142900	0.1388200	H	2.7867300	-1.3096600	2.0231500
C	-3.4565900	-0.7311500	1.3152700	H	5.0879600	-0.8725300	-1.6503800
H	-3.4864300	0.6960800	-1.6856700	H	4.4102100	-2.6775500	0.3006100
H	-0.9869700	0.4742400	-0.6623400				
H	-1.2823900	-0.2614700	1.7554400	IM3			
H	-5.2384900	-0.6349800	-0.0634800	P	-1.5830400	0.2864100	-0.1696200
H	-3.8261900	-1.2525100	2.1985800	O	-1.0746600	1.0026000	1.2324800

O	-1.3992500	-1.2557400	-0.0055000	N	0.2652200	0.1898000	0.0002000
O	-3.0576900	0.6781600	-0.2859100	C	-0.3005100	-1.0716600	-0.0001200
O	-0.6384700	0.8303300	-1.2765100	C	-1.9372000	0.4912100	-0.0000200
K	0.7495100	-1.3342800	-1.4366800	C	-1.6589900	-0.9160700	0.0000000
K	-0.1335600	3.0936600	-0.2281500	C	1.6256500	0.4625400	0.0004100
K	-3.8740300	-1.5253900	0.5339000	O	2.4791300	-0.3808000	-0.0004400
C	1.7064200	1.0462700	1.0309300	H	-0.4939100	2.2063200	0.0002400
O	2.1779400	2.0453500	0.4937400	H	0.3358400	-1.9530300	-0.0002200
C	3.5227500	-0.3032600	-0.1678100	H	-2.9194500	0.9608600	-0.0000400
N	2.4942100	-0.1736400	0.7312900	H	-2.3908600	-1.7224300	-0.0000500
C	2.1922200	-1.4032600	1.2518500	H	1.8298200	1.5567800	-0.0002400
C	3.8762100	-1.6364000	-0.2325400				
C	3.0277300	-2.3409600	0.6786400	TS1			
H	3.9047000	0.5800400	-0.6753900	C	-3.3429900	0.0014900	-0.5689200
H	-0.0708200	0.8694300	1.3649800	N	-2.0649400	-0.0454400	-0.0919500
H	1.3845300	-1.4991000	1.9755700	C	-2.0826100	-0.4068500	1.2229900
H	4.6675900	-2.0623900	-0.8498400	C	-4.2064400	-0.3452300	0.4601500
H	3.0417100	-3.4085800	0.8962100	C	-3.4023900	-0.6050200	1.6018600
				H	-3.5498000	0.2860900	-1.6005000
IM4				H	-1.1444800	0.1306500	-0.6351700
P	1.3843300	-0.1584800	0.3517400	H	-1.1308000	-0.4699900	1.7530300
O	1.5323100	0.7131400	-0.9674700	H	-5.2932900	-0.3930800	0.3977400
O	0.8498700	-1.5888500	-0.0682300	H	-3.7500900	-0.8931300	2.5934200
O	2.7748300	-0.2875800	1.0137700	P	1.3736300	-0.3434500	-0.4247300
O	0.3116800	0.5331800	1.2839900	O	1.4766100	-1.9055600	-0.3941000
K	-0.8473600	-1.6235200	1.8280700	O	2.7110400	0.3088200	-0.8943200
K	1.0126600	2.8297200	0.4330000	O	0.1825100	0.1047200	-1.3863400
K	3.2508300	-1.3956900	-1.2991300	O	1.0829700	0.2108300	1.0160600
C	-1.3639200	1.2921300	-0.8763400	K	3.4551000	-1.1574700	1.2392200
O	-1.5871400	2.4583700	-0.6261200	K	-0.6633100	-2.3637300	-1.5829500
C	-3.6595900	0.4965000	-0.3833500	K	1.2140000	2.4740100	-0.4516900
N	-2.3447700	0.3091500	-0.7561500	C	-2.4029400	2.6249400	0.9430500
C	-2.1028100	-1.0352500	-0.9719500	O	-1.4719600	3.1397400	0.5496400
C	-4.2638300	-0.7334100	-0.3619800				
C	-3.2750000	-1.7077800	-0.7295000	TS2			
H	-4.0322800	1.4973500	-0.1807700	P	-1.7200400	0.2051600	-0.2339600
H	-0.3709700	0.9041800	-1.2163600	O	-1.3191700	1.2498800	1.0384400
H	-1.0764200	-1.3722400	-1.1626600	O	-1.5083700	-1.2207600	0.3399700
H	-5.3082500	-0.9250700	-0.1191200	O	-3.1791700	0.5208200	-0.5386400
H	-3.4206200	-2.7842300	-0.8143800	O	-0.6923300	0.5555800	-1.3311200
				K	0.8037700	-1.5622700	-0.8840400
IM5				K	-0.0510500	2.8948700	-0.6689900
C	-0.7374600	1.1455400	0.0001300	K	-4.0444400	-1.5725500	0.5339700

C	1.8045000	1.4368400	1.7868700	H	-3.1214100	-1.3599700	-0.0067800
O	1.9303100	2.3857100	1.1324600	H	-3.1201200	1.3617000	-0.0067700
C	3.3629900	-0.0655400	-0.5055000	C	1.3241700	-0.1766700	-0.5096400
N	2.7676200	-0.1134400	0.7110200	O	1.9323300	-0.3806500	-1.6882900
C	2.9206400	-1.3714800	1.1893400	H	0.8402900	0.0749200	0.4396700
C	3.8967500	-1.3155300	-0.8373200				
C	3.6093200	-2.1648100	0.2653800	Mn-L1			
H	3.3894800	0.8641300	-1.0809700	C	-3.0929000	1.8192000	0.4377000
H	-0.7129500	0.7909700	1.6378000	N	-1.6102000	1.8197700	0.4690100
H	2.5314700	-1.6419700	2.1740000	C	-1.2189000	3.2458000	0.5774000
H	4.4498200	-1.5732700	-1.7421700	C	0.2342000	3.3628000	0.9984000
H	3.8967500	-3.2108400	0.3842500	P	1.1232000	1.9218000	0.2996000
				Mn	-0.5410000	0.4587300	0.0123900
TS3				C	-0.1238000	0.0395300	-1.6321100
P	1.4333400	0.1918300	0.0825800	H	-3.5081000	2.5260000	1.1717000
O	0.8866200	0.6065500	-1.3801700	H	-3.4531000	2.1673000	-0.5437000
O	1.7337000	-1.3415200	0.1241900	H	0.6799000	4.3148000	0.6998000
O	2.7169800	1.0343600	0.3079700	H	-1.3764000	3.7591000	-0.3847000
O	0.3050700	0.5562900	1.0941100	H	-1.8504000	3.7790000	1.3039000
K	-0.6049800	-1.7857300	1.2478300	O	0.1245000	-0.2021700	-2.7389100
K	0.4930200	2.9622900	0.1033100	H	0.3026000	3.2878000	2.0859000
K	4.2297000	-0.9339400	0.0293200	C	0.4575000	-0.8894700	0.5630900
C	-1.6513100	1.0670200	-1.0428600	C	2.0672000	2.6254000	-1.1211000
O	-2.0424800	2.1340400	-0.5895100	C	2.4395000	1.5249000	1.5397000
C	-3.5221300	-0.1458500	0.1764600	C	3.4777000	2.6196000	1.7411000
N	-2.5048600	-0.0791600	-0.7400200	H	3.0113000	3.5515000	2.0737000
C	-2.2953600	-1.3228400	-1.2785000	H	4.0476000	2.8310000	0.8352000
C	-3.9666000	-1.4506300	0.2348600	H	4.1903000	2.3189000	2.5146000
C	-3.1876800	-2.2035700	-0.7008100	C	1.8179000	1.1222000	2.8719000
H	-3.8226900	0.7528700	0.7103500	H	1.3966000	1.9869000	3.3909000
H	-0.2525300	0.7327100	-1.4028800	H	2.5826000	0.6917000	3.5234000
H	-1.5209700	-1.4641400	-2.0312800	H	1.0232000	0.3857000	2.7487000
H	-4.7711700	-1.8274100	0.8664500	H	2.9290000	0.6382000	1.1212000
H	-3.2898900	-3.2625700	-0.9373000	C	3.0141000	1.5959000	-1.7223000
				H	3.7466000	1.2342000	-0.9975000
TS1A				H	3.5651000	2.0392000	-2.5565000
C	-0.9261500	-1.0844200	0.0027000	H	2.4673000	0.7343000	-2.1080000
N	-0.1019400	-0.0005800	0.0064300	C	1.1175000	3.1924000	-2.1679000
C	-0.9251200	1.0840600	0.0027000	H	0.4413800	2.3979200	-2.5749400
C	-2.2603300	-0.7053000	-0.0031200	H	1.6903000	3.6162000	-2.9975000
C	-2.2596600	0.7062100	-0.0031200	H	0.4876000	3.9857000	-1.7606000
H	-0.5229400	-2.0916400	0.0047300	H	2.6560000	3.4525000	-0.7086000
H	-0.5209700	2.0909100	0.0047400	H	-3.7015000	0.2835000	1.8064000

H	-4.6219000	0.2683000	0.3010000	C	0.0000000	-1.2699900	1.2159200
C	-3.1884000	-1.4832000	-1.4134000	O	-0.0001100	-2.0887000	2.0504200
H	-4.1677000	-1.8567000	-1.0936000	C	0.0000200	1.2865900	1.2556100
C	-3.4101000	-0.3987000	-2.4590000	O	0.0000000	2.1419100	2.0452700
H	-2.4402800	0.0465800	-2.7942600	C	2.9918400	1.6125800	-0.9917100
H	-4.0302000	0.4148000	-2.0771000	C	4.4206800	1.4276100	-1.4859100
H	-3.9172000	-0.8210000	-3.3311000	C	2.8770200	2.8057900	-0.0524600
C	-2.3715000	-2.6420000	-1.9663000	H	2.3347300	1.8099700	-1.8574800
H	-1.3672000	-2.3188000	-2.2442000	H	4.5260200	0.5847100	-2.1858400
H	-2.8507000	-3.0446000	-2.8631000	H	4.7587200	2.3348100	-2.0136000
H	-2.2761000	-3.4583000	-1.2475000	H	5.1232600	1.2641200	-0.6533000
C	-3.6284000	0.4285000	0.7264000	H	1.8506800	2.9435000	0.3140300
P	-2.3994000	-0.7762000	0.0982000	H	3.5424600	2.7041300	0.8191300
C	-2.4536000	-2.1794000	1.3060000	H	3.1744200	3.7281000	-0.5778800
H	-1.6961000	-2.8758000	0.9290000	C	3.3898400	-0.5423700	0.9853200
C	-1.7703000	-1.4729400	2.4685000	C	3.3994900	-2.0620300	1.1089700
H	-0.9410000	-0.9682100	2.9829400	C	3.0640900	0.0986200	2.3317400
H	-1.6606900	-2.0855100	3.3664400	H	4.3935600	-0.2141600	0.6644600
H	-2.3343300	-1.0015400	3.2822500	H	3.7225300	-2.5641000	0.1851000
C	-3.7950000	-2.8936000	1.3867000	H	4.1018400	-2.3650400	1.9029500
H	-4.5952000	-2.2010000	1.6636000	H	2.4090000	-2.4499200	1.3889900
H	-3.7583000	-3.6718000	2.1544000	H	3.0023700	1.1944800	2.2808500
H	-4.0734000	-3.3730000	0.4471000	H	2.0988400	-0.2656100	2.7139400
O	1.1085000	-1.7696700	0.9396900	H	3.8380100	-0.1602400	3.0730300
Mn-L1-DH				C	-2.9918100	1.6126800	-0.9916300
P	2.1916400	0.0661600	-0.3148300	C	-2.8769400	2.8059200	-0.0524200
C	2.4165600	-1.0934600	-1.7538900	C	-4.4206600	1.4277500	-1.4858200
C	1.2278600	-2.0346400	-1.7922900	H	-2.3347100	1.8100300	-1.8574200
H	3.3686700	-1.6431100	-1.7300800	H	-1.8506000	2.9435700	0.3141100
H	2.4253700	-0.4752500	-2.6680200	H	-3.1742500	3.7282300	-0.5778900
H	1.2305500	-2.6359100	-2.7219500	H	-3.5424300	2.7043200	0.8191400
H	1.2565900	-2.7371400	-0.9443900	H	-4.5260300	0.5848800	-2.1857700
N	-0.0000400	-1.2490500	-1.6798400	H	-5.1232200	1.2642400	-0.6531900
H	-0.0000400	-0.5595100	-2.4324700	H	-4.7587100	2.3349800	-2.0134600
C	-1.2279700	-2.0346000	-1.7922700	C	-3.3898000	-0.5423400	0.9853600
C	-2.4166400	-1.0933700	-1.7538400	C	-3.0638300	0.0983900	2.3318500
H	-1.2567100	-2.7371100	-0.9443700	C	-3.3996100	-2.0620200	1.1087600
H	-1.2307100	-2.6358600	-2.7219400	H	-4.3935100	-0.2139700	0.6646200
H	-2.4254600	-0.4751700	-2.6679800	H	-3.0020300	1.1942600	2.2811500
H	-3.3687700	-1.6429900	-1.7300000	H	-3.8376700	-0.1605400	3.0732100
P	-2.1916400	0.0662200	-0.3147800	H	-2.0985500	-0.2659800	2.7138500
Mn	0.0000000	0.0360500	0.0362100	H	-3.7227800	-2.5638900	0.1848200
				H	-2.4091500	-2.4500800	1.3886400

H	-4.1019500	-2.3650700	1.9027400	H	1.8481700	2.8904300	-2.3235900
H	0.0000200	1.2365000	-1.0432200	H	0.4443100	3.5908600	-1.4986100
IM6				C	-2.7351700	-2.2831900	-0.4416600
P	1.6935200	1.2463900	0.1175400	C	-2.4476400	-2.4903500	-1.9224800
C	1.9930800	0.9025400	1.9071700	C	-4.0813900	-2.8704500	-0.0365700
C	0.6691300	0.9554500	2.6426700	H	-1.9587000	-2.7998700	0.1467200
H	2.7385800	1.5720400	2.3612900	H	-1.4801600	-2.0626900	-2.2226000
H	2.4017500	-0.1208500	1.9473000	H	-2.4266100	-3.5670700	-2.1562600
H	0.7883500	0.5700500	3.6727600	H	-3.2246300	-2.0363400	-2.5574600
H	0.3158300	1.9961900	2.7299400	H	-4.3031300	-2.7207700	1.0309600
N	-0.3471400	0.1804500	1.9279000	H	-4.9127500	-2.4471800	-0.6218500
H	-0.0779200	-0.8669300	1.9379000	H	-4.0820700	-3.9572900	-0.2197500
C	-1.6491400	0.2636300	2.5998100	C	-4.0002100	0.3808300	-0.4592600
C	-2.6174000	-0.7064600	1.9506600	C	-3.8040200	0.9286300	-1.8699900
H	-2.0188400	1.3009300	2.5347200	C	-4.4604800	1.4722600	0.5010200
H	-1.5401400	0.0255800	3.6746200	H	-4.7887500	-0.3891000	-0.4919600
H	-2.2917700	-1.7342300	2.1718100	H	-3.4368800	0.1687600	-2.5741500
H	-3.6421900	-0.5763600	2.3254500	H	-4.7606900	1.3115500	-2.2608400
P	-2.4722000	-0.5244300	0.1163100	H	-3.0861700	1.7616800	-1.8801700
Mn	-0.4261600	0.4577600	-0.1257100	H	-4.7108900	1.0797000	1.4969000
C	-1.1147100	2.0505700	-0.0866500	H	-3.7088500	2.2647700	0.6188800
O	-1.5716500	3.1204900	-0.0543800	H	-5.3721100	1.9471700	0.1030600
C	-0.4228200	0.4465700	-1.8893900	H	0.4246900	-1.1942100	-0.1492100
O	-0.4278100	0.4515000	-3.0484500	C	2.4755300	-2.9655900	-1.0609300
C	3.1220400	0.3694700	-0.6871400	N	1.8957100	-2.6754200	0.1415700
C	4.4811200	0.7299900	-0.1019200	C	2.8320700	-2.7401500	1.1317400
C	3.1236600	0.4665500	-2.2069600	C	3.8169300	-3.2177900	-0.8418800
H	2.9139100	-0.6779600	-0.4247800	C	4.0435700	-3.0752600	0.5553400
H	4.5236100	0.5862900	0.9873500	C	0.4878400	-2.3047100	0.3542600
H	5.2510400	0.0761900	-0.5415400	O	0.0936600	-2.3516200	1.5801600
H	4.7709900	1.7694700	-0.3256400	H	1.8903300	-2.9566600	-1.9794100
H	2.1423100	0.2365100	-2.6446000	H	2.5311400	-2.5830800	2.1642700
H	3.4296300	1.4651300	-2.5565200	H	4.5486500	-3.4864600	-1.6026200
H	3.8460200	-0.2572200	-2.6161900	H	4.9836100	-3.2236500	1.0849100
C	2.0685400	3.0554700	-0.1409200	H	-0.0833100	-2.8857300	-0.4047200
C	1.5774300	3.9460900	0.9947600	IM7			
C	1.5417500	3.5375700	-1.4907400	P	1.6935200	1.2463900	0.1175400
H	3.1707000	3.1084900	-0.1582200	C	1.9930800	0.9025400	1.9071700
H	2.0285100	3.6823900	1.9624500	C	0.6691300	0.9554500	2.6426700
H	1.8510500	4.9929700	0.7846500	H	2.7385800	1.5720400	2.3612900
H	0.4836000	3.9141600	1.0990200	H	2.4017500	-0.1208500	1.9473000
H	1.9221000	4.5507000	-1.6998100	H	0.7883500	0.5700500	3.6727600

H	0.3158300	1.9961900	2.7299400	H	-4.9127500	-2.4471800	-0.6218500
N	-0.3471400	0.1804500	1.9279000	H	-4.0820700	-3.9572900	-0.2197500
H	-0.0779200	-0.8669300	1.9379000	C	-4.0002100	0.3808300	-0.4592600
C	-1.6491400	0.2636300	2.5998100	C	-3.8040200	0.9286300	-1.8699900
C	-2.6174000	-0.7064600	1.9506600	C	-4.4604800	1.4722600	0.5010200
H	-2.0188400	1.3009300	2.5347200	H	-4.7887500	-0.3891000	-0.4919600
H	-1.5401400	0.0255800	3.6746200	H	-3.4368800	0.1687600	-2.5741500
H	-2.2917700	-1.7342300	2.1718100	H	-4.7606900	1.3115500	-2.2608400
H	-3.6421900	-0.5763600	2.3254500	H	-3.0861700	1.7616800	-1.8801700
P	-2.4722000	-0.5244300	0.1163100	H	-4.7108900	1.0797000	1.4969000
Mn	-0.4261600	0.4577600	-0.1257100	H	-3.7088500	2.2647700	0.6188800
C	-1.1147100	2.0505700	-0.0866500	H	-5.3721100	1.9471700	0.1030600
O	-1.5716500	3.1204900	-0.0543800	H	0.4246900	-1.1942100	-0.1492100
C	-0.4228200	0.4465700	-1.8893900	C	2.4755300	-2.9655900	-1.0609300
O	-0.4278100	0.4515000	-3.0484500	N	1.8957100	-2.6754200	0.1415700
C	3.1220400	0.3694700	-0.6871400	C	2.8320700	-2.7401500	1.1317400
C	4.4811200	0.7299900	-0.1019200	C	3.8169300	-3.2177900	-0.8418800
C	3.1236600	0.4665500	-2.2069600	C	4.0435700	-3.0752600	0.5553400
H	2.9139100	-0.6779600	-0.4247800	C	0.4878400	-2.3047100	0.3542600
H	4.5236100	0.5862900	0.9873500	O	0.0936600	-2.3516200	1.5801600
H	5.2510400	0.0761900	-0.5415400	H	1.8903300	-2.9566600	-1.9794100
H	4.7709900	1.7694700	-0.3256400	H	2.5311400	-2.5830800	2.1642700
H	2.1423100	0.2365100	-2.6446000	H	4.5486500	-3.4864600	-1.6026200
H	3.4296300	1.4651300	-2.5565200	H	4.9836100	-3.2236500	1.0849100
H	3.8460200	-0.2572200	-2.6161900	H	-0.0833100	-2.8857300	-0.4047200
C	2.0685400	3.0554700	-0.1409200				
C	1.5774300	3.9460900	0.9947600	IM8			
C	1.5417500	3.5375700	-1.4907400	P	1.4051500	1.4948100	0.1870400
H	3.1707000	3.1084900	-0.1582200	C	2.1916200	0.4948100	1.5093700
H	2.0285100	3.6823900	1.9624500	C	1.0879100	-0.0805200	2.3810400
H	1.8510500	4.9929700	0.7846500	H	2.9339100	1.0573800	2.0965400
H	0.4836000	3.9141600	1.0990200	H	2.7281900	-0.3174100	0.9926100
H	1.9221000	4.5507000	-1.6998100	H	1.4283000	-1.0434400	2.8120300
H	1.8481700	2.8904300	-2.3235900	H	0.9037400	0.5777600	3.2545200
H	0.4443100	3.5908600	-1.4986100	N	-0.1501700	-0.2834500	1.6374100
C	-2.7351700	-2.2831900	-0.4416600	H	0.3423300	-1.9655500	0.7338700
C	-2.4476400	-2.4903500	-1.9224800	C	-1.1037600	-0.9713000	2.5018000
C	-4.0813900	-2.8704500	-0.0365700	C	-2.2233800	-1.6225500	1.7059000
H	-1.9587000	-2.7998700	0.1467200	H	-1.5154900	-0.2605400	3.2468800
H	-1.4801600	-2.0626900	-2.2226000	H	-0.5855000	-1.7509200	3.0938700
H	-2.4266100	-3.5670700	-2.1562600	H	-1.8909600	-2.6145100	1.3626200
H	-3.2246300	-2.0363400	-2.5574600	H	-3.1388100	-1.7561800	2.3023400
H	-4.3031300	-2.7207700	1.0309600	P	-2.5102700	-0.6244600	0.1850300

Mn	-0.5365400	0.4142000	-0.0887800	H	-2.9282100	2.2039700	1.1883900
C	-1.2386700	1.7021300	-1.0565700	H	-4.4885800	1.9945100	2.0144500
O	-1.7148800	2.5508200	-1.6939100	H	0.9575800	-3.0771000	-1.2491300
C	-0.0534900	-0.4092900	-1.5369400	C	3.3248500	-2.1342200	-1.1122500
O	0.3037000	-1.0152600	-2.4677000	N	2.6587900	-2.8168700	-0.1310200
C	2.6779900	1.5140700	-1.1592800	C	3.4671000	-2.9423800	0.9659800
C	3.9929800	2.1649100	-0.7573300	C	4.5831600	-1.8172600	-0.6395200
C	2.1550800	2.0237000	-2.4973300	C	4.6704100	-2.3263000	0.6860200
H	2.8574300	0.4302100	-1.2651000	C	1.3148300	-3.3554600	-0.2431000
H	4.3865000	1.7604400	0.1875800	O	0.4815100	-2.9397400	0.7719800
H	4.7562400	1.9829000	-1.5319600	H	2.8411000	-1.9273800	-2.0650600
H	3.8936500	3.2563100	-0.6515500	H	3.1119900	-3.4504500	1.8601200
H	1.2017200	1.5536000	-2.7754800	H	5.3513800	-1.2718700	-1.1855600
H	2.0043000	3.1122500	-2.5019200	H	5.5210900	-2.2520100	1.3618300
H	2.8826300	1.7908600	-3.2917600	H	1.3670500	-4.4549200	-0.1873700
C	1.3213300	3.2166300	0.9024800				
C	0.2956600	3.2583700	2.0310000	IM9			
C	1.0151700	4.2752600	-0.1546500	C	-1.2724500	0.3138000	-2.3166100
H	2.3229200	3.4112800	1.3259700	N	-0.1382700	0.7608800	-1.5035300
H	0.5402400	2.5698500	2.8516600	C	1.0395000	1.1341900	-2.2901100
H	0.2426500	4.2738000	2.4563800	C	2.1642500	1.5772600	-1.3664700
H	-0.7071800	2.9924100	1.6628100	P	2.3742600	0.3116600	-0.0274900
H	0.8789300	5.2554100	0.3310200	Mn	0.2908700	-0.5450400	0.1148100
H	1.8337900	4.3839600	-0.8796400	C	0.7008400	-1.8508700	-0.9581600
H	0.0920400	4.0526300	-0.7086100	H	-1.5318400	1.0750800	-3.0758200
C	-3.0570800	-1.9000900	-1.0510600	H	-0.9699600	-0.5996800	-2.8532500
C	-3.1675900	-1.3670600	-2.4757600	H	3.0864700	1.7894600	-1.9275900
C	-4.2979700	-2.6747800	-0.6265000	H	1.3441500	0.2557700	-2.8803300
H	-2.1885700	-2.5836400	-1.0200800	H	0.7893200	1.9376700	-3.0085800
H	-2.3083900	-0.7421900	-2.7549200	O	0.9627700	-2.7174300	-1.6965200
H	-3.2095200	-2.2087400	-3.1857300	H	1.8771600	2.5129300	-0.8601200
H	-4.0785400	-0.7705200	-2.6237200	C	0.6063800	-1.5328300	1.5398500
H	-4.1931800	-3.1164700	0.3759400	C	3.8112500	-0.7612400	-0.5568900
H	-5.1947300	-2.0355600	-0.6246400	C	3.0884900	1.3038700	1.3805300
H	-4.4905200	-3.5009000	-1.3305600	C	3.4568000	0.4309300	2.5746500
C	-4.0054900	0.3974300	0.6304000	H	4.3570700	-0.1723400	2.3791500
C	-4.7053000	1.0303700	-0.5664400	H	2.6408000	-0.2480000	2.8600500
C	-3.5977400	1.4597900	1.6465400	H	3.6791500	1.0675400	3.4461000
H	-4.7035900	-0.3058300	1.1179800	C	4.2352400	2.2238300	0.9832100
H	-5.1782800	0.2830400	-1.2177800	H	3.9561300	2.9324200	0.1894200
H	-5.5021800	1.7055700	-0.2138200	H	5.1180700	1.6609800	0.6390500
H	-4.0146700	1.6296000	-1.1775300	H	4.5562800	2.8198400	1.8534000
H	-3.0811000	1.0362600	2.5203700	H	2.2297400	1.9219500	1.6818900

C	3.8053500	-2.0898900	0.1968000	H	-4.2290700	3.9337300	-0.5862600
H	3.6885500	-1.9682000	1.2817200	H	-2.1460500	4.8766200	-2.0888300
H	4.7535900	-2.6235800	0.0204900	H	-0.4908600	2.6890200	2.4384300
H	2.9906900	-2.7405300	-0.1507800	H	0.6960300	2.7786000	1.1172600
C	3.8841300	-0.9956700	-2.0618400	H	-0.4565000	1.5913200	-0.9972800
H	3.0026400	-1.5383600	-2.4328900				
H	4.7654800	-1.6157100	-2.2939600	IM10			
H	3.9882000	-0.0619900	-2.6332500	C	-1.2420800	0.2149200	-2.3719700
H	4.7108100	-0.1942400	-0.2598500	N	-0.1415700	0.6669400	-1.5101000
H	-2.7709900	1.0002500	-0.9412100	C	1.0538000	0.9739900	-2.2875700
H	-3.3233900	-0.3351600	-1.9678000	C	2.1758300	1.4131900	-1.3675200
C	-2.4963200	-2.7776600	-0.4670300	P	2.3349000	0.1507500	-0.0238800
H	-3.5532000	-2.8102300	-0.1470200	Mn	0.2137200	-0.6449700	0.1152600
C	-2.4486200	-3.0847300	-1.9600800	C	0.5769000	-1.9883400	-0.9462200
H	-3.0639000	-2.3946600	-2.5555300	H	-1.4481000	0.9775400	-3.1456200
H	-2.8355300	-4.1010900	-2.1403900	H	-0.9455100	-0.7111500	-2.8841000
H	-1.4195200	-3.0580600	-2.3472200	H	3.1104800	1.5864100	-1.9205100
C	-1.7140400	-3.8271500	0.3240700	H	1.3477000	0.0815500	-2.8692300
H	-2.1742700	-4.8196500	0.1880600	H	0.8310600	1.7762500	-3.0241300
H	-1.6798300	-3.6213000	1.4043000	O	0.8056700	-2.8894200	-1.6348700
H	-0.6750700	-3.8934000	-0.0287400	H	1.8970300	2.3596700	-0.8731100
C	-2.4594000	0.0503900	-1.4071200	C	0.4946600	-1.7090400	1.5075400
P	-1.9132200	-1.0587500	-0.0262600	C	3.7522400	-0.9569900	-0.5145500
C	-3.0022400	-0.5568600	1.3893900	C	3.0090700	1.1741800	1.3865800
H	-2.5245400	0.4005900	1.6528400	C	2.8731600	0.4956100	2.7417900
C	-4.4610400	-0.3431900	1.0150600	H	3.5190900	-0.3948500	2.8286600
H	-4.5888200	0.4085600	0.2226000	H	1.8331200	0.1733000	2.9445900
H	-5.0273000	0.0103000	1.8930600	H	3.1653600	1.1856500	3.5435200
H	-4.9441900	-1.2758300	0.6788300	C	4.4162200	1.7052700	1.1566400
C	-2.8542200	-1.4810900	2.5931300	H	4.5415500	2.1703300	0.1665000
H	-3.3164000	-2.4666300	2.4223600	H	5.1743500	0.9134400	1.2560700
H	-3.3608100	-1.0354800	3.4647500	H	4.6542600	2.4783900	1.9110800
H	-1.8012400	-1.6340600	2.8689800	H	2.3160700	2.0338900	1.3695800
O	0.8146900	-2.1733400	2.4814800	C	3.7740000	-2.2144900	0.3403800
C	-2.6152000	3.0630300	0.6413200	H	3.7738000	-1.9989600	1.4165000
N	-1.2560600	3.0959800	0.5274200	H	4.6802200	-2.8030700	0.1241900
C	-0.9226300	3.8288100	-0.5799500	H	2.9059200	-2.8665900	0.1354200
C	-3.1662300	3.7721100	-0.4108000	C	3.7639500	-1.3015300	-2.0087000
C	-2.0851400	4.2604600	-1.1928000	H	2.8874600	-1.8777200	-2.3102300
C	-0.2854700	2.3264300	1.4041700	H	4.6545900	-1.9250200	-2.2192500
O	-0.3847600	1.0058000	1.3099200	H	3.8347200	-0.4095800	-2.6393300
H	-3.0915000	2.5348000	1.4644600	H	4.6633000	-0.3736100	-0.3048000
H	0.1204600	4.0212900	-0.8267000	H	-2.8099600	0.9781000	-1.1357300

H	-3.3140100	-0.4162600	-2.1125600	C	2.3384860	-0.3282770	-1.9417880
C	-2.6793700	-2.7533100	-0.3988000	P	2.1287190	-0.4823780	-0.1119100
H	-3.7448300	-2.7072400	-0.1153700	Mn	-0.1332360	-0.2634430	0.1267130
C	-2.6029000	-3.1593700	-1.8668700	C	-0.3615990	-1.9833490	0.0706200
H	-3.1800300	-2.4923600	-2.5229200	H	-1.2883770	-0.0389250	-3.7247390
H	-3.0203300	-4.1722500	-1.9877000	H	-1.5221550	-1.4200680	-2.6351760
H	-1.5657500	-3.1923200	-2.2298600	H	3.1980940	-0.8942080	-2.3282880
C	-1.9854700	-3.7828800	0.4892000	H	0.8853700	-1.8271260	-2.5406810
H	-2.4982100	-4.7550100	0.4076100	H	1.0843560	-0.4939970	-3.6963830
H	-1.9783200	-3.4972500	1.5499300	O	-0.5180580	-3.1360510	0.0406340
H	-0.9406400	-3.9346300	0.1812500	H	2.5228570	0.7411780	-2.1292110
C	-2.4816600	0.0048000	-1.5250700	C	-0.1267980	-0.2859600	1.8940780
P	-2.0203200	-1.0401300	-0.0635900	C	2.9589140	-2.0865070	0.3730330
C	-3.1173700	-0.3626700	1.2783800	C	3.2816750	0.8222080	0.5262450
H	-2.7646300	0.6763200	1.3450700	C	3.3102130	0.8898880	2.0468540
C	-4.5964400	-0.3380500	0.9173000	H	3.8741330	0.0514150	2.4863690
H	-4.7902100	0.1754800	-0.0362800	H	2.3010040	0.8931000	2.4813960
H	-5.1621200	0.1981800	1.6967000	H	3.8065390	1.8206600	2.3650190
H	-5.0237900	-1.3513500	0.8519400	C	4.6863460	0.7528850	-0.0584470
C	-2.8668700	-1.0218200	2.6279900	H	4.6888810	0.7651620	-1.1583180
H	-3.2364700	-2.0589600	2.6542500	H	5.2399110	-0.1399750	0.2752430
H	-3.3998300	-0.4698000	3.4190200	H	5.2633570	1.6310340	0.2747010
H	-1.7987500	-1.0197900	2.8866500	H	2.7996110	1.7442620	0.1621560
O	0.6976100	-2.4209400	2.3902100	C	2.5002440	-2.5415900	1.7565160
C	-2.1192200	3.4159600	0.0946600	H	2.5541340	-1.7416740	2.5074370
N	-1.1901200	3.1345700	-0.9104700	H	3.1342450	-3.3720420	2.1077980
C	-0.5850700	4.2979000	-1.1870600	H	1.4634400	-2.9068990	1.7364590
C	-2.1240900	4.7881700	0.4207200	C	2.8034080	-3.2032490	-0.6531470
C	-1.1230000	5.3568000	-0.4018800	H	1.7524370	-3.4934170	-0.7916350
C	-0.2737100	2.1121100	1.6290000	H	3.3417240	-4.0998130	-0.3043390
O	-0.3137800	0.9008800	1.4280400	H	3.2233820	-2.9370130	-1.6337650
H	-2.8009500	2.6385500	0.4455000	H	4.0311940	-1.8323270	0.4310830
H	0.2161700	4.3508500	-1.9553700	H	-2.3346800	1.4953510	-2.1062330
H	-2.7762200	5.2988700	1.1400100	H	-3.4562960	0.1527230	-2.4116250
H	-0.8252700	6.4127500	-0.4327700	C	-3.6214800	-1.2308210	0.2456450
H	-0.7499700	2.5320400	2.5696600	H	-4.5946000	-0.7120070	0.2671420
H	0.2664100	2.8259400	0.9170600	C	-3.7010130	-2.3234780	-0.8149460
H	-0.5077600	1.6084000	-1.1428800	H	-3.9837850	-1.9323410	-1.8029610
				H	-4.4706780	-3.0572370	-0.5253490
IM11				H	-2.7538750	-2.8718870	-0.9140160
C	-1.3464150	-0.3315940	-2.6595220	C	-3.3548670	-1.8161350	1.6302690
N	-0.0814070	-0.0518060	-1.9828100	H	-4.1884390	-2.4741790	1.9244550
C	1.0452050	-0.7386280	-2.6180630	H	-3.2507370	-1.0445830	2.4056390

H	-2.4376990	-2.4216980	1.6401470	C	3.0079500	0.6990300	2.2560800
C	-2.4794300	0.4095290	-1.9761480	H	3.4718700	-0.1746000	2.7401500
P	-2.3836800	0.1027550	-0.1552590	H	1.9583900	0.7466300	2.5750500
C	-3.1516230	1.6662170	0.5224740	H	3.5143000	1.5946300	2.6506700
H	-2.4758590	2.4407980	0.1191700	C	4.6243100	0.6203700	0.3299400
C	-4.5528740	1.9500610	-0.0029690	H	5.1490800	-0.2520200	0.7506900
H	-4.6071070	1.9279820	-1.1015920	H	5.1379900	1.5188200	0.7092300
H	-4.8721190	2.9547160	0.3184950	H	4.7609500	0.6052800	-0.7618800
H	-5.2954200	1.2380120	0.3904670	H	2.7122400	1.5872600	0.3464200
C	-3.0888130	1.7476670	2.0422680	C	2.5658700	-2.8390800	1.5573600
H	-3.7880260	1.0437970	2.5196130	H	2.6602100	-2.1232600	2.3854900
H	-3.3709910	2.7599750	2.3727160	H	3.1968900	-3.7110500	1.7945200
H	-2.0812340	1.5424850	2.4314220	H	1.5216700	-3.1835800	1.5361200
O	-0.1235530	-0.3247950	3.0509200	C	2.7642600	-3.2531600	-0.9165500
C	0.2856220	2.2289070	0.0091690	H	1.7006000	-3.4947700	-1.0529500
N	0.6484090	2.4809030	-1.2806960	H	3.2838200	-4.1952100	-0.6769400
C	1.5192390	3.5047020	-1.2231670	H	3.1627600	-2.8982500	-1.8781200
C	0.9019090	3.1198780	0.9024520	H	4.0540400	-2.0033900	0.2490900
C	1.7078160	3.9467940	0.1010580	H	-2.2766300	1.7632500	-1.8791500
H	-0.6313530	1.6534380	0.2370270	H	-3.3900800	0.4770400	-2.3804400
H	1.9885400	3.8959900	-2.1295960	C	-3.6666100	-1.1925600	0.0528400
H	0.7645250	3.1606600	1.9830860	H	-4.6216800	-0.6398600	0.0514100
H	2.3508630	4.7635820	0.4312640	C	-3.6956300	-2.1785700	-1.1109400
H	0.1290260	0.9837220	-2.0174770	H	-2.7491700	-2.7292900	-1.2061400
				H	-3.9083500	-1.6897300	-2.0725500
IM12				H	-4.4899100	-2.9240300	-0.9419800
C	-1.2645100	0.0146900	-2.6413200	C	-3.5242900	-1.9206700	1.3870400
N	-0.0525000	0.0150100	-1.8392600	H	-3.4648700	-1.2364200	2.2442300
C	1.0728700	-0.4472400	-2.6309800	H	-2.6213600	-2.5484400	1.4033400
C	2.3832200	-0.2288400	-1.8878000	H	-4.3900500	-2.5832500	1.5489500
P	2.1089000	-0.6359200	-0.1024700	C	-2.4190000	0.6700300	-1.9001800
Mn	-0.1598200	-0.4703200	0.0542900	P	-2.3445000	0.1034500	-0.1447200
C	-0.4479400	-2.1669900	-0.0391400	C	-3.0036600	1.6029400	0.7541300
H	-1.0937200	0.5438100	-3.6021700	H	-2.2731400	2.3732700	0.4509100
H	-1.5519300	-1.0202700	-2.9269600	C	-4.3785100	2.0526300	0.2748300
H	3.2130900	-0.7960900	-2.3341400	H	-4.4383600	2.1510800	-0.8191200
H	0.9638000	-1.5212100	-2.8955600	H	-4.6188000	3.0384400	0.7049800
H	1.1088500	0.0862600	-3.6040700	H	-5.1724200	1.3606800	0.5990500
O	-0.6364800	-3.3088000	-0.1712900	C	-2.9501700	1.5028000	2.2734800
H	2.6605800	0.8373500	-1.9269300	H	-3.6930800	0.7907500	2.6650600
C	-0.1818200	-0.5469400	1.8244400	H	-3.1792100	2.4838700	2.7196000
C	2.9789100	-2.2499500	0.2123100	H	-1.9637800	1.1921700	2.6442700
C	3.1576500	0.6569900	0.7416200	O	-0.2040400	-0.6686300	2.9782800

C	1.3963100	3.6480400	-1.3781500	C	-3.3256800	1.4208700	0.3445600
N	0.6487200	2.6047300	-0.9247600	C	-3.3053000	2.5306900	-0.7009600
C	0.4793100	2.7086900	0.4163300	C	-2.9522200	1.9576900	1.7228100
C	1.7059400	4.4565900	-0.2970700	H	-4.3507800	1.0163500	0.3888900
C	1.1213000	3.8548200	0.8516500	H	-3.6596400	2.1918000	-1.6850000
H	1.6496400	3.7465000	-2.4323400	H	-3.9721300	3.3478200	-0.3805600
H	-0.0614100	1.9373400	0.9677900	H	-2.3016000	2.9613000	-0.8237700
H	2.2827400	5.3799700	-0.3305400	H	-2.9262000	1.1734800	2.4924000
H	1.1622400	4.2166200	1.8779900	H	-1.9620000	2.4367500	1.7069700
H	0.3577700	1.7385000	-1.4296500	H	-3.6836400	2.7171700	2.0436100
IM13				C	3.1370800	-1.4816300	0.8313800
P	-2.2466100	-0.0308300	-0.1074000	C	3.1944000	-1.2497600	2.3360300
C	-2.4605500	-0.3042800	-1.9235000	C	4.5103200	-1.8201900	0.2652300
C	-1.1925700	0.1592000	-2.6157700	H	2.4694400	-2.3406600	0.6509200
H	-3.3610700	0.1703700	-2.3377600	H	2.2156900	-0.9827600	2.7582400
H	-2.5477100	-1.3945600	-2.0492700	H	3.5349200	-2.1686300	2.8401000
H	-1.1817900	-0.2039800	-3.6612100	H	3.9099900	-0.4556500	2.5999900
H	-1.1380800	1.2611500	-2.6578200	H	4.4781300	-2.0669800	-0.8059600
N	-0.0347800	-0.3624000	-1.8866000	H	5.2287400	-0.9964800	0.4041000
H	-0.1970600	-1.4739200	-1.8070400	H	4.9238300	-2.6970800	0.7897000
C	1.2071300	-0.1423300	-2.6257000	C	3.3815100	1.3439300	0.0551500
C	2.3758200	-0.7157400	-1.8468300	C	3.0869300	2.1251100	1.3337700
H	1.3430800	0.9389900	-2.7984000	C	3.3397100	2.2570700	-1.1651100
H	1.1483600	-0.6204600	-3.6221900	H	4.3977600	0.9194800	0.1280800
H	2.2715700	-1.8130700	-1.8088300	H	3.0561200	1.4878700	2.2277000
H	3.3423800	-0.4864500	-2.3195200	H	3.8669000	2.8871800	1.4942300
P	2.2493800	-0.1296300	-0.0987200	H	2.1230700	2.6489900	1.2683300
Mn	0.0090800	0.1014300	0.1225700	H	3.6463800	1.7431200	-2.0876300
C	0.0366300	1.8249800	-0.0787400	H	2.3387100	2.6851000	-1.3204400
O	0.0598900	2.9799700	-0.2244800	H	4.0331400	3.1009100	-1.0168100
C	0.0107000	0.2539500	1.8792300	H	0.0397800	-1.7463000	0.3302100
O	0.0142300	0.3789900	3.0326500	C	-0.1028200	-2.8280800	-0.1899400
C	-3.1185600	-1.5246200	0.5851300	O	-0.4629700	-2.8063900	-1.4493400
C	-4.5939000	-1.6080400	0.2157300	H	0.8948100	-3.2819600	0.0411400
C	-2.8941000	-1.7176600	2.0782700	H	-0.8280300	-3.2644900	0.5384400
H	-2.5880200	-2.3271400	0.0447100	CH3OH			
H	-4.7678400	-1.4649400	-0.8616300	C	0.6439000	-0.0196000	0.0000000
H	-4.9894400	-2.6022300	0.4804000	H	1.0892100	0.9875500	0.0000000
H	-5.1992100	-0.8668800	0.7613700	H	1.0305100	-0.5477900	-0.8947000
H	-1.8293400	-1.6674900	2.3461900	H	1.0305100	-0.5477900	0.8947000
H	-3.4277400	-0.9615000	2.6753500	O	-0.7448800	0.1250600	0.0000000
H	-3.2730300	-2.7040200	2.3915900	H	-1.1341000	-0.7555400	0.0000000

				C	-3.0289500	1.5859300	-0.9875700
TS4				C	-2.9504200	2.7747700	-0.0384600
P	2.2282000	0.0367300	-0.3189400	C	-4.4491700	1.3766100	-1.4982100
C	2.4206800	-1.1217000	-1.7477300	H	-2.3744000	1.8011300	-1.8516600
C	1.1944400	-2.0193200	-1.7764900	H	-1.9336100	2.9401100	0.3432400
H	3.3629900	-1.6887700	-1.7259400	H	-3.2671000	3.6926200	-0.5600400
H	2.4301100	-0.4937300	-2.6541600	H	-3.6213300	2.6494500	0.8257000
H	1.1918800	-2.5955800	-2.7271300	H	-4.5252100	0.5455200	-2.2148600
H	1.2782000	-2.7818000	-0.9649500	H	-5.1534900	1.1794000	-0.6744400
N	0.0000000	-1.2319000	-1.6544400	H	-4.8038700	2.2859300	-2.0106800
H	0.0000000	0.3523200	-1.6821200	C	-3.3795500	-0.5541000	1.0227900
C	-1.1944400	-2.0193200	-1.7764900	C	-3.0197000	0.0905400	2.3586600
C	-2.4206800	-1.1216900	-1.7477300	C	-3.4099900	-2.0737100	1.1453700
H	-1.2782000	-2.7818000	-0.9649500	H	-4.3854800	-0.2129300	0.7228500
H	-1.1918800	-2.5955800	-2.7271400	H	-2.9387300	1.1846000	2.2990200
H	-2.4301100	-0.4937300	-2.6541600	H	-3.7883300	-0.1485700	3.1116500
H	-3.3629900	-1.6887600	-1.7259400	H	-2.0581400	-0.2892700	2.7344000
P	-2.2282000	0.0367300	-0.3189400	H	-3.7581300	-2.5666200	0.2265100
Mn	0.0000000	0.0762000	-0.0162400	H	-2.4212300	-2.4814800	1.4005800
C	0.0000000	-1.1947100	1.2005000	H	-4.1009800	-2.3639800	1.9537100
O	0.0000000	-2.0476100	1.9887000	H	0.0000000	1.1914700	-1.3256600
C	0.0000000	1.3572100	1.1928300				
O	0.0000000	2.1822900	2.0107200	TS5			
C	3.0289500	1.5859300	-0.9875700	P	1.6222000	1.3017800	0.1098400
C	4.4491800	1.3766100	-1.4982100	C	1.9390700	1.0188600	1.9126500
C	2.9504100	2.7747700	-0.0384700	C	0.6122200	1.0571400	2.6447500
H	2.3744000	1.8011200	-1.8516700	H	2.6631000	1.7234400	2.3482000
H	4.5252200	0.5455100	-2.2148500	H	2.3778800	0.0098600	1.9900200
H	4.8038700	2.2859300	-2.0106800	H	0.7389600	0.7407600	3.6975900
H	5.1534900	1.1794100	-0.6744300	H	0.2068600	2.0812600	2.6610000
H	1.9336000	2.9401200	0.3432200	N	-0.3588200	0.1985900	1.9636900
H	3.6213100	2.6494600	0.8256900	H	-0.0213800	-0.7788700	2.0139900
H	3.2670900	3.6926200	-0.5600500	C	-1.6726800	0.2184100	2.6152100
C	3.3795500	-0.5541000	1.0227900	C	-2.5817000	-0.7930000	1.9432400
C	3.4099800	-2.0737100	1.1453800	H	-2.0823400	1.2379700	2.5313300
C	3.0197000	0.0905400	2.3586500	H	-1.5742500	-0.0091200	3.6937100
H	4.3854800	-0.2129400	0.7228500	H	-2.2139500	-1.8076600	2.1618300
H	3.7581200	-2.5666200	0.2265100	H	-3.6143200	-0.7194700	2.3132600
H	4.1009800	-2.3639800	1.9537100	P	-2.4326800	-0.5690500	0.1079200
H	2.4212300	-2.4814800	1.4005900	Mn	-0.4585800	0.4919200	-0.1244200
H	2.9387300	1.1846000	2.2990200	C	-1.1961400	2.0766000	-0.0532100
H	2.0581400	-0.2892600	2.7344000	O	-1.6737400	3.1418200	-0.0531100
H	3.7883300	-0.1485700	3.1116500	C	-0.4532300	0.4760100	-1.8764600

O	-0.4449600	0.4481900	-3.0384900	N	1.9857300	-2.7211200	0.2024300
C	3.0696400	0.4266200	-0.6653400	C	2.9950700	-2.6929600	1.1361000
C	4.4262900	0.8133700	-0.0921200	C	3.8752000	-3.1078100	-0.9037400
C	3.0706400	0.4842700	-2.1871500	C	4.1799000	-2.9315500	0.4813600
H	2.8625500	-0.6133200	-0.3763600	C	0.6109300	-2.5519100	0.4870000
H	4.4715000	0.7043100	1.0013600	O	0.2233600	-2.5104700	1.6546100
H	5.2050300	0.1575700	-0.5138400	H	1.8729600	-3.0088900	-1.9203400
H	4.7053900	1.8490800	-0.3449500	H	2.7590900	-2.5411100	2.1858500
H	2.0930700	0.2230600	-2.6153500	H	4.5803000	-3.3119000	-1.7077800
H	3.3539500	1.4808600	-2.5608900	H	5.1636900	-2.9866900	0.9446000
H	3.8094100	-0.2318100	-2.5812800	H	-0.0052200	-2.9185800	-0.3518600
C	1.9956600	3.1091400	-0.1882200				
C	1.4997400	4.0228800	0.9268500	TS6			
C	1.4478300	3.5544100	-1.5424700	P	1.6241800	1.3168500	0.1137000
H	3.0969300	3.1761100	-0.2164900	C	1.9702900	0.9399900	1.8849700
H	1.9591000	3.7918500	1.8992300	C	0.6476800	0.8808700	2.6244100
H	1.7560100	5.0684800	0.6890900	H	2.6774700	1.6425200	2.3504600
H	0.4066700	3.9766500	1.0363600	H	2.4445600	-0.0549700	1.8872700
H	1.8106000	4.5679000	-1.7804700	H	0.8008900	0.4170900	3.6199500
H	1.7511900	2.8914100	-2.3640900	H	0.2771400	1.9062500	2.8216000
H	0.3493800	3.5894500	-1.5354200	N	-0.3419300	0.1283400	1.8632600
C	-2.6474000	-2.3315600	-0.4742500	H	0.0487000	-1.2279600	1.7833100
C	-2.2711800	-2.5260900	-1.9370100	C	-1.5971300	0.0839100	2.6093400
C	-4.0001400	-2.9521000	-0.1484000	C	-2.5716300	-0.8764800	1.9501200
H	-1.8967300	-2.8444600	0.1495200	H	-2.0400200	1.0975400	2.6776000
H	-1.2932100	-2.0822300	-2.1729700	H	-1.4131200	-0.2406600	3.6530900
H	-2.2282000	-3.6005400	-2.1802600	H	-2.2379600	-1.9108300	2.1229500
H	-3.0118700	-2.0717100	-2.6133800	H	-3.5903800	-0.7770100	2.3507000
H	-4.2955500	-2.7938000	0.9002600	P	-2.4721900	-0.6013900	0.1266100
H	-4.8016900	-2.5564400	-0.7914800	Mn	-0.4787400	0.4706100	-0.1050500
H	-3.9641000	-4.0409600	-0.3169800	C	-1.2191100	2.0301000	-0.0728300
C	-4.0159400	0.2708500	-0.4245700	O	-1.7183600	3.0799500	-0.0123300
C	-3.8762800	0.8155500	-1.8429100	C	-0.4859100	0.4693900	-1.8728700
C	-4.4806400	1.3576200	0.5386800	O	-0.5109000	0.5080800	-3.0324600
H	-4.7818600	-0.5219300	-0.4271700	C	3.0625400	0.4989400	-0.7415800
H	-3.5198400	0.0581300	-2.5556000	C	4.4216900	0.9054900	-0.1868400
H	-4.8502400	1.1832100	-2.2053700	C	3.0263300	0.6045400	-2.2603600
H	-3.1692100	1.6573900	-1.8773100	H	2.9020300	-0.5581000	-0.4810400
H	-4.6819100	0.9699200	1.5478600	H	4.4905600	0.7717000	0.9023600
H	-3.7534100	2.1769900	0.6190000	H	5.2036700	0.2744600	-0.6384100
H	-5.4224400	1.7955200	0.1688700	H	4.6716900	1.9523200	-0.4234100
H	0.3321800	-0.9911000	-0.2125300	H	2.0446000	0.3432900	-2.6788700
C	2.5151100	-2.9727800	-1.0422700	H	3.2880300	1.6158000	-2.6088700

H	3.7662500	-0.0884700	-2.6913200	H	0.1075500	-3.0361300	-0.3422100
C	1.9303800	3.1416500	-0.1126000				
C	1.4082500	3.9841000	1.0460200	TS7			
C	1.3792000	3.6332200	-1.4490200	C	1.2670700	-0.3015300	-2.2594600
H	3.0296000	3.2374400	-0.1315600	N	0.0396400	-0.6062500	-1.5264500
H	1.8772900	3.7177600	2.0041500	C	-1.0074000	-1.0092100	-2.4666700
H	1.6331900	5.0466600	0.8577700	C	-2.2063600	-1.5689800	-1.7209400
H	0.3181300	3.8990200	1.1578800	P	-2.5092300	-0.5230500	-0.2298400
H	1.7191100	4.6649000	-1.6360100	Mn	-0.5359600	0.5735600	0.0465300
H	1.7057600	3.0177600	-2.2980800	C	-0.0640100	-0.3256300	1.4561400
H	0.2805000	3.6443100	-1.4510000	H	1.6695600	-1.2205000	-2.7261000
C	-2.6510200	-2.3462600	-0.5134800	H	1.0330200	0.3852600	-3.0931700
C	-2.3434500	-2.4904400	-1.9975300	H	-3.0953300	-1.6452900	-2.3651800
C	-3.9724400	-3.0075600	-0.1415600	H	-1.2978800	-0.1495200	-3.1005400
H	-1.8556700	-2.8547600	0.0570000	H	-0.6149900	-1.7814200	-3.1560900
H	-1.3826700	-2.0324700	-2.2717400	O	0.2697600	-0.9067400	2.4021000
H	-2.2985200	-3.5572300	-2.2708600	H	-1.9398900	-2.5668900	-1.3423400
H	-3.1225900	-2.0292800	-2.6241500	H	0.9440300	-4.4790300	0.3253000
H	-4.2146300	-2.8956000	0.9262300	C	-3.9929000	0.4924800	-0.7090600
H	-4.8138000	-2.6052200	-0.7270900	C	-3.0175800	-1.7615000	1.0486100
H	-3.9223100	-4.0879100	-0.3539800	C	-3.1523600	-1.1896000	2.4556400
C	-4.0521900	0.2506500	-0.3785200	H	-4.1052900	-0.6591900	2.5957200
C	-3.9268800	0.8342800	-1.7828400	H	-2.3420300	-0.4928100	2.7091200
C	-4.5132000	1.3045700	0.6226400	H	-3.1238200	-2.0087800	3.1917700
H	-4.8120300	-0.5480700	-0.3982300	C	-4.2370700	-2.5783100	0.6427200
H	-3.5609100	0.1023300	-2.5165300	H	-5.1523500	-1.9649600	0.6223700
H	-4.9096000	1.1924600	-2.1300500	H	-4.4060600	-3.3898600	1.3692200
H	-3.2379800	1.6912400	-1.8005200	H	-4.1169700	-3.0461100	-0.3458600
H	-4.7138600	0.8813400	1.6170800	H	-2.1216000	-2.4097100	1.0166300
H	-3.7833500	2.1180200	0.7334100	C	-4.6548700	1.1891000	0.4725600
H	-5.4534900	1.7573500	0.2679100	H	-5.1150500	0.4770900	1.1708200
H	0.5118500	-1.3063800	-0.2417900	H	-5.4544800	1.8566300	0.1118100
C	2.6886600	-2.9429400	-1.0582900	H	-3.9408900	1.8061100	1.0386100
N	2.0796300	-2.6480000	0.1297400	C	-3.5669700	1.5002000	-1.7725400
C	3.0077400	-2.6354600	1.1317200	H	-2.8369200	2.2180600	-1.3621600
C	4.0376700	-3.1201300	-0.8167800	H	-4.4352700	2.0812800	-2.1230600
C	4.2399700	-2.9262800	0.5768700	H	-3.1159800	1.0204300	-2.6543500
C	0.6665400	-2.3183200	0.2880900	H	-4.7132500	-0.2141000	-1.1577300
O	0.2771100	-2.2877100	1.5658100	H	2.7872000	-0.4758500	-0.7375700
H	2.1160900	-2.9902900	-1.9833500	H	3.1296700	0.7805300	-1.9386500
H	2.6959000	-2.4568400	2.1570900	C	1.5752800	3.1331100	-1.0134500
H	4.7908600	-3.3724100	-1.5617500	H	2.5996600	3.2482600	-1.4090300
H	5.1795100	-3.0097500	1.1209000	C	0.5909300	3.1409800	-2.1792600

H	-0.4394300	2.9658700	-1.8253500	H	-1.4481000	0.9861400	-3.1370200
H	0.8250700	2.3812400	-2.9378600	H	-0.9455100	-0.7025500	-2.8841000
H	0.6000700	4.1215500	-2.6819800	H	3.1276800	1.5520100	-1.9377100
C	1.2808700	4.2797900	-0.0539200	H	1.3391000	0.0901500	-2.8692300
H	1.2237300	5.2275800	-0.6136300	H	0.8310600	1.7848500	-3.0155300
H	2.0620200	4.3987800	0.7089500	O	0.8056700	-2.8980200	-1.6348700
H	0.3187900	4.1436300	0.4638200	H	1.9486300	2.3682700	-0.8989100
C	2.3231200	0.3078100	-1.3571300	C	0.5032600	-1.7090400	1.5075400
P	1.5134200	1.4690600	-0.1803700	C	3.7522400	-0.9655900	-0.5231500
C	2.6923100	1.4955100	1.2504600	C	3.0348700	1.1655800	1.3865800
H	2.8059800	0.4120000	1.4327100	C	2.8817600	0.4870100	2.7417900
C	4.0615600	2.0551900	0.8871900	H	3.5104900	-0.4120500	2.8286600
H	4.4987600	1.5466000	0.0148500	H	1.8417200	0.1905000	2.9359900
H	4.7599800	1.9167500	1.7284700	H	3.1911600	1.1770500	3.5435200
H	4.0210800	3.1346100	0.6717300	C	4.4506300	1.6794700	1.1566400
C	2.1192300	2.1164200	2.5190700	H	4.5759500	2.1445300	0.1665000
H	1.1433400	1.6884900	2.7855900	H	5.2001500	0.8790400	1.2560700
H	1.9962300	3.2055500	2.4380300	H	4.6972600	2.4439900	1.9110800
H	2.8030400	1.9256700	3.3618700	H	2.3676700	2.0424900	1.3781800
C	-1.1695200	1.8361000	1.0894700	C	3.7740000	-2.2230900	0.3403800
H	0.1917200	-1.6128100	-0.8602400	H	3.7738000	-1.9989600	1.4165000
O	-1.5913300	2.6807900	1.7662500	H	4.6802200	-2.8116700	0.1241900
C	3.0169100	-3.1687700	-0.9779000	H	2.9059200	-2.8665900	0.1354200
N	2.3522400	-2.9613800	0.1953800	C	3.7639500	-1.3101300	-2.0087000
C	3.1840400	-2.3371900	1.0790800	H	2.8788600	-1.8863200	-2.3102300
C	4.2996500	-2.6656700	-0.8508000	H	4.6459900	-1.9336200	-2.2278500
C	4.4079500	-2.1355100	0.4641200	H	3.8347200	-0.4181800	-2.6479300
C	0.9595300	-3.3742700	0.4684300	H	4.6633000	-0.3822100	-0.3134000
O	0.0387500	-2.7581400	-0.2904800	H	-2.8099600	0.9781000	-1.1185300
H	2.5208600	-3.6603300	-1.8127600	H	-3.3140100	-0.4076600	-2.1039600
H	2.8364300	-2.0902600	2.0806300	C	-2.6793700	-2.7533100	-0.3988000
H	5.0731500	-2.6830000	-1.6176000	H	-3.7448300	-2.7072400	-0.1153700
H	5.2795300	-1.6605000	0.9127300	C	-2.6029000	-3.1593700	-1.8668700
H	0.8438400	-3.1972700	1.5605800	H	-3.1800300	-2.4923600	-2.5229200
				H	-3.0203300	-4.1722500	-1.9877000
TS8				H	-1.5657500	-3.1923200	-2.2298600
C	-1.2420800	0.2235200	-2.3633700	C	-1.9854700	-3.7828800	0.4892000
N	-0.1415700	0.6669400	-1.5015000	H	-2.4982100	-4.7550100	0.4076100
C	1.0538000	0.9825900	-2.2875700	H	-1.9783200	-3.4972500	1.5499300
C	2.1930300	1.4045900	-1.3761200	H	-0.9406400	-3.9346300	0.1812500
P	2.3435000	0.1507500	-0.0238800	C	-2.4816600	0.0048000	-1.5164700
Mn	0.2223200	-0.6535700	0.1152600	P	-2.0203200	-1.0401300	-0.0635900
C	0.5769000	-1.9883400	-0.9462200	C	-3.1173700	-0.3626700	1.2783800

H	-2.7560300	0.6763200	1.3450700	C	2.9769000	0.5729300	2.3381100
C	-4.5964400	-0.3380500	0.9173000	H	3.4417000	-0.3237000	2.7780000
H	-4.7902100	0.1754800	-0.0362800	H	1.9213900	0.5953900	2.6427100
H	-5.1621200	0.1981800	1.6967000	H	3.4678400	1.4500900	2.7890700
H	-5.0237900	-1.3513500	0.8519400	C	4.6076300	0.5986700	0.4150500
C	-2.8668700	-1.0218200	2.6279900	H	5.1296200	-0.2989700	0.7839500
H	-3.2364700	-2.0589600	2.6542500	H	5.1230700	1.4725900	0.8451900
H	-3.3998300	-0.4698000	3.4190200	H	4.7424400	0.6485800	-0.6758000
H	-1.7987500	-1.0283900	2.8866500	H	2.6956500	1.5690400	0.4767500
O	0.6976100	-2.4209400	2.3988100	C	2.4307600	-2.9154600	1.4842700
C	-2.2224200	3.4761600	0.0860600	H	2.4871200	-2.2384800	2.3478200
N	-1.1643200	3.1173700	-0.7040700	H	3.0390200	-3.8048300	1.7158100
C	-0.5248700	4.2721000	-1.0236600	H	1.3857000	-3.2455900	1.3911000
C	-2.2616800	4.8569700	0.2745200	C	2.7641200	-3.2195600	-0.9906300
C	-1.1574000	5.3740000	-0.4448800	H	1.7093000	-3.4604500	-1.1849200
C	-0.2049100	2.1121100	1.4742000	H	3.2791200	-4.1688900	-0.7705700
O	-0.3481800	0.9008800	1.3936400	H	3.2036700	-2.8205200	-1.9158300
H	-2.9213500	2.7245500	0.4627000	H	3.9958400	-2.0357300	0.3011100
H	0.3623700	4.2648500	-1.6629700	H	-2.1662700	1.9643300	-1.7057000
H	-2.9998200	5.4192700	0.8476100	H	-3.3456900	0.7893200	-2.3279000
H	-0.8682700	6.4213500	-0.5445700	C	-3.6956200	-1.1112100	-0.0530400
H	-0.7757700	2.6868400	2.2256600	H	-4.6381700	-0.5425500	0.0167500
H	0.5502100	2.6711400	0.8998600	C	-3.7571600	-1.9646500	-1.3154500
H	-0.4991600	1.5912000	-1.0998800	H	-2.8312200	-2.5355600	-1.4725600
				H	-3.9553600	-1.3688600	-2.2180100
TS9				H	-4.5771100	-2.6952200	-1.2222200
C	-1.2472000	0.2431200	-2.6105000	C	-3.5546400	-1.9773700	1.1955000
N	-0.0227300	0.2314000	-1.8205500	H	-3.4760100	-1.3857100	2.1180400
C	1.0827800	-0.3217000	-2.5972500	H	-2.6651600	-2.6210500	1.1381000
C	2.3910000	-0.1582400	-1.8421100	H	-4.4327500	-2.6357100	1.2954700
P	2.0949400	-0.6231600	-0.0791800	C	-2.3735600	0.8875900	-1.8226100
Mn	-0.1682900	-0.4357700	0.1021500	P	-2.3561800	0.1815300	-0.1171000
C	-0.4619300	-2.1001300	-0.2446800	C	-3.0163800	1.6127700	0.8854200
H	-1.0904500	0.8016200	-3.5549300	H	-2.2943900	2.4071200	0.6276900
H	-1.5228100	-0.7880600	-2.9039300	C	-4.3988900	2.0811300	0.4483000
H	3.2099700	-0.7248500	-2.3073500	H	-4.4631200	2.2597300	-0.6355300
H	0.8957000	-1.3903400	-2.8189000	H	-4.6449500	3.0306500	0.9506400
H	1.1565300	0.1890200	-3.5781400	H	-5.1847000	1.3603300	0.7239700
O	-0.6488400	-3.2175500	-0.5098000	C	-2.9455000	1.3938600	2.3908800
H	2.6846200	0.9028400	-1.8314900	H	-3.6747900	0.6430200	2.7320300
C	-0.2395900	-0.7737000	1.8371600	H	-3.1805900	2.3341600	2.9148100
C	2.9231600	-2.2701900	0.1921200	H	-1.9491500	1.0697300	2.7224400
C	3.1412500	0.6212000	0.8257300	O	-0.2997600	-1.0447400	2.9622600

C	1.6152100	3.4702500	-1.3277100	C	-3.3259200	1.4224000	0.3131500
N	0.6805100	2.5506600	-0.9756600	C	-3.2896500	2.5178000	-0.7473200
C	0.4567000	2.6848700	0.3588600	C	-2.9640500	1.9745700	1.6885200
C	1.9933500	4.2142800	-0.2110700	H	-4.3536000	1.0240800	0.3518600
C	1.2476300	3.7043400	0.8805800	H	-3.6340800	2.1656100	-1.7302100
H	1.9645300	3.5513200	-2.3582400	H	-3.9579300	3.3408500	-0.4456200
H	-0.2552800	2.0366900	0.8836800	H	-2.2837700	2.9439200	-0.8654200
H	2.7122200	5.0337300	-0.1900000	H	-2.9538900	1.2005300	2.4687900
H	1.2728400	4.0428000	1.9162300	H	-1.9700000	2.4456200	1.6788500
H	0.3000000	1.4387700	-1.5169200	H	-3.6931600	2.7439800	1.9903400
TS10				C	3.1491800	-1.4672600	0.8279800
P	-2.2511400	-0.0404300	-0.1111600	C	3.2003600	-1.2428200	2.3339800
C	-2.4606900	-0.3439200	-1.9213600	C	4.5277400	-1.7866400	0.2633400
C	-1.1902200	0.1163100	-2.6128000	H	2.4937700	-2.3341000	0.6415900
H	-3.3623700	0.1211000	-2.3444200	H	2.2176400	-0.9895300	2.7554500
H	-2.5458000	-1.4358000	-2.0333300	H	3.5513900	-2.1597700	2.8343900
H	-1.1696300	-0.2746100	-3.6489100	H	3.9053900	-0.4411400	2.6032700
H	-1.1595800	1.2190400	-2.6917700	H	4.5009100	-2.0254000	-0.8098100
N	-0.0307600	-0.3679700	-1.8665700	H	5.2366300	-0.9561600	0.4103800
H	-0.1818300	-1.5844000	-1.7699700	H	4.9495800	-2.6627900	0.7824400
C	1.2000100	-0.1396000	-2.6168200	C	3.3637100	1.3644000	0.0697700
C	2.3830700	-0.6968300	-1.8473800	C	3.0573400	2.1352400	1.3519400
H	1.3325800	0.9411300	-2.8078700	C	3.3193000	2.2834500	-1.1460500
H	1.1391400	-0.6282200	-3.6091300	H	4.3835200	0.9490900	0.1447400
H	2.2941900	-1.7954700	-1.8112300	H	3.0259000	1.4920100	2.2415500
H	3.3451600	-0.4510900	-2.3208600	H	3.8317400	2.9010700	1.5213100
P	2.2487600	-0.1204400	-0.0987300	H	2.0907700	2.6537600	1.2852800
Mn	0.0035500	0.0909100	0.1161200	H	3.6345700	1.7766000	-2.0695000
C	0.0263000	1.8124500	-0.0698800	H	2.3153800	2.7030400	-1.3045500
O	0.0447900	2.9671400	-0.2181400	H	4.0046300	3.1325200	-0.9899500
C	0.0031600	0.2323800	1.8754500	H	0.0362000	-1.7832300	0.3432800
O	0.0056300	0.3610200	3.0288400	C	-0.0764000	-2.8339000	-0.1856700
C	-3.1308100	-1.5185200	0.6090700	O	-0.3641400	-2.7819300	-1.4809500
C	-4.6107900	-1.5908900	0.2560100	H	0.8960100	-3.3150400	0.0774100
C	-2.8917500	-1.7024100	2.1010500	H	-0.8479500	-3.3015100	0.4663700
H	-2.6162700	-2.3350100	0.0745800	TS4B			
H	-4.7951400	-1.4505300	-0.8200300	P	2.2282000	0.0367300	-0.3189400
H	-5.0128000	-2.5799500	0.5299400	C	2.4206800	-1.1217000	-1.7477300
H	-5.2025500	-0.8414100	0.8048700	C	1.1944400	-2.0193200	-1.7764900
H	-1.8230000	-1.6725400	2.3553000	H	3.3629900	-1.6887700	-1.7259400
H	-3.4011200	-0.9297400	2.6977800	H	2.4301100	-0.4937300	-2.6541600
H	-3.2878500	-2.6775000	2.4282100	H	1.1918800	-2.5955800	-2.7271300

H	1.2782000	-2.7818000	-0.9649500	H	-5.1534900	1.1794000	-0.6744400
N	0.0000000	-1.2319000	-1.6544400	H	-4.8038700	2.2859300	-2.0106800
H	0.0000000	0.3523200	-1.6821200	C	-3.3795500	-0.5541000	1.0227900
C	-1.1944400	-2.0193200	-1.7764900	C	-3.0197000	0.0905400	2.3586600
C	-2.4206800	-1.1216900	-1.7477300	C	-3.4099900	-2.0737100	1.1453700
H	-1.2782000	-2.7818000	-0.9649500	H	-4.3854800	-0.2129300	0.7228500
H	-1.1918800	-2.5955800	-2.7271400	H	-2.9387300	1.1846000	2.2990200
H	-2.4301100	-0.4937300	-2.6541600	H	-3.7883300	-0.1485700	3.1116500
H	-3.3629900	-1.6887600	-1.7259400	H	-2.0581400	-0.2892700	2.7344000
P	-2.2282000	0.0367300	-0.3189400	H	-3.7581300	-2.5666200	0.2265100
Mn	0.0000000	0.0762000	-0.0162400	H	-2.4212300	-2.4814800	1.4005800
C	0.0000000	-1.1947100	1.2005000	H	-4.1009800	-2.3639800	1.9537100
O	0.0000000	-2.0476100	1.9887000	H	0.0000000	1.1914700	-1.3256600
C	0.0000000	1.3572100	1.1928300	P	-0.3290500	-5.8613900	-0.4443300
O	0.0000000	2.1822900	2.0107200	O	0.9628900	-5.8444600	0.4196500
C	3.0289500	1.5859300	-0.9875700	O	-0.3814600	-7.1579000	-1.3005000
C	4.4491800	1.3766100	-1.4982100	O	-1.5931300	-5.7647900	0.4550200
C	2.9504100	2.7747700	-0.0384700	O	-0.3066300	-4.6849200	-1.4604500
H	2.3744000	1.8011200	-1.8516700	K	1.9220500	-6.0325000	-2.0733800
H	4.5252200	0.5455100	-2.2148500	K	-0.2820300	-5.6637800	2.5695200
H	4.8038700	2.2859300	-2.0106800	K	-2.6304900	-5.8917000	-2.0096900
H	5.1534900	1.1794100	-0.6744300				
H	1.9336000	2.9401200	0.3432200	K			
H	3.6213100	2.6494600	0.8256900	K	0.0000000	0.0000000	0.0000000
H	3.2670900	3.6926200	-0.5600500				
C	3.3795500	-0.5541000	1.0227900	IM1B			
C	3.4099800	-2.0737100	1.1453800	C	0.813568	-1.061216	0.961906
C	3.0197000	0.0905400	2.3586500	N	0.577640	-1.349657	-0.353603
H	4.3854800	-0.2129400	0.7228500	C	1.391485	-0.599216	-1.156293
H	3.7581200	-2.5666200	0.2265100	C	1.789940	-0.081789	1.008977
H	4.1009800	-2.3639800	1.9537100	C	2.157948	0.211002	-0.337014
H	2.4212300	-2.4814800	1.4005900	H	0.296166	-1.591179	1.759659
H	2.9387300	1.1846000	2.2990200	H	1.389255	-0.721020	-2.237588
H	2.0581400	-0.2892600	2.7344000	H	2.218290	0.346370	1.914274
H	3.7883300	-0.1485700	3.1116500	H	2.925864	0.907903	-0.670425
C	-3.0289500	1.5859300	-0.9875700	C	-2.804389	-1.338553	-0.009406
C	-2.9504200	2.7747700	-0.0384600	O	-2.714165	-0.210596	0.008861
C	-4.4491700	1.3766100	-1.4982100	H	-0.021601	-2.100726	-0.681425
H	-2.3744000	1.8011300	-1.8516600	K	-0.485760	1.658403	-0.025746
H	-1.9336100	2.9401100	0.3432400				
H	-3.2671000	3.6926200	-0.5600400	TS1B			
H	-3.6213300	2.6494500	0.8257000	C	0.157790	0.865783	-1.106428
H	-4.5252100	0.5455200	-2.2148600	N	-0.599292	0.577775	0.000152

C	0.158068	0.865088	1.106677				
C	1.414484	1.308083	-0.711786	IM15			
C	1.414642	1.307642	0.711995	P	-1.639240	0.016413	0.206879
H	-0.245939	0.755549	-2.114737	O	-1.609986	0.981651	1.515436
H	-0.245230	0.753748	2.115040	O	-1.051113	-1.367402	0.571805
H	2.225491	1.622768	-1.368827	O	-3.142473	-0.116066	-0.175245
H	2.225919	1.621718	1.368996	O	-0.838093	0.702501	-0.926052
C	-2.774552	0.249782	0.000026	C	1.100113	2.194050	1.154039
O	-3.173670	-0.804237	-0.000022	O	1.607497	3.110546	0.727368
H	-2.170811	1.202339	0.000185	C	3.214415	0.311375	-0.832734
K	1.345914	-1.639206	-0.000234	N	2.930558	0.322480	0.495457
				C	3.057495	-0.962086	0.917498
Na3PO4				C	3.503190	-0.985856	-1.285870
P	0.045482	0.000063	-0.000526	C	3.400532	-1.819190	-0.140019
O	0.940333	1.290729	-0.000819	H	3.191443	1.235456	-1.417378
O	-0.925177	0.000724	-1.238184	H	-0.694628	1.285948	1.664613
O	0.941093	-1.290166	-0.002485	H	2.886685	-1.227376	1.964404
O	-0.921842	-0.001320	1.239655	H	3.790413	-1.283120	-2.295891
Na	-1.399815	-1.979889	0.000572	H	3.588525	-2.892640	-0.083348
Na	-1.400926	1.979331	0.000713	Na	0.929444	-0.793252	-0.491429
Na	2.713698	0.000496	0.000765	Na	-3.099210	-2.216725	0.637030
				Na	-2.745586	1.324393	-1.871761
IM14							
C	-3.325907	0.313052	-0.894393	IM16			
N	-2.193534	0.621628	-0.194008	P	2.589999	-0.186060	-0.075277
C	-2.384251	0.362188	1.129831	O	2.153797	-1.327081	1.086938
C	-4.278322	-0.141978	0.006230	O	2.183790	1.223266	0.457929
C	-3.677334	-0.109604	1.295441	O	4.106591	-0.267252	-0.223750
H	-3.381517	0.471788	-1.970820	O	1.648704	-0.608506	-1.213479
H	-1.238877	0.757863	-0.616104	C	-1.846308	-0.170604	-0.184525
H	-1.549696	0.497706	1.817677	O	-1.597570	-1.378506	-0.029473
H	-5.299002	-0.437098	-0.234788	C	-4.258184	-0.720987	0.307679
H	-4.140415	-0.392780	2.239714	N	-3.233235	0.144066	-0.005183
P	1.073607	-0.377011	-0.003297	C	-3.743247	1.414842	-0.125519
O	0.689900	-1.880976	0.338401	C	-5.422542	0.003180	0.386178
O	2.627049	-0.381723	-0.345094	C	-5.095295	1.368924	0.109405
O	0.181902	0.039030	-1.224641	H	-4.046276	-1.778154	0.444184
O	0.868863	0.615101	1.174792	H	2.878900	-1.486605	1.702457
C	0.364290	2.794811	-0.705061	H	-3.082328	2.243939	-0.371260
O	1.473864	3.034570	-0.645293	H	-6.410508	-0.395019	0.617322
Na	2.847044	1.468233	0.845981	H	-5.781192	2.214893	0.087404
Na	2.733482	-2.533741	-0.027573	Na	4.332684	1.820529	0.431704
Na	-1.222648	-1.690178	-0.746205	Na	0.189381	1.122657	-0.660956

Na	0.428393	-2.172651	-0.216139	O	-0.851820	0.344398	-1.249117
				C	2.693579	1.694845	1.119376
IM17				O	2.344463	2.464732	0.290768
P	1.620772	-0.537039	0.145031	C	2.673438	-0.356191	-0.932398
O	1.999513	0.775154	-0.693941	N	2.525573	-0.000751	0.372788
O	0.587525	-1.425191	-0.613832	C	2.586766	-1.127728	1.128181
O	2.949626	-1.267204	0.455254	C	2.798883	-1.741148	-1.032023
O	0.860082	-0.001791	1.442517	C	2.739764	-2.241247	0.301838
C	-1.080300	1.239086	-0.680922	H	2.698434	0.397307	-1.722828
O	-0.976587	2.343559	-0.186352	H	-2.186030	1.903694	1.345251
C	-3.346606	0.809928	0.200013	H	2.528272	-1.064144	2.215887
N	-2.215404	0.463853	-0.519329	H	2.952382	-2.316597	-1.945645
C	-2.338705	-0.837368	-0.989326	H	2.838597	-3.279838	0.619930
C	-4.186736	-0.269144	0.192549	Na	-3.943573	-1.436152	0.485530
C	-3.546437	-1.316393	-0.556525	Na	0.281277	-1.387187	-0.216806
H	-3.429957	1.798247	0.644435	Na	0.322436	2.087933	-0.597387
H	-0.273298	0.735973	-1.252293				
H	-1.499612	-1.287771	-1.521840	TS12			
H	-5.165410	-0.316309	0.667722	P	-1.719070	0.110195	-0.077719
H	-3.945908	-2.308899	-0.759618	O	-1.266355	1.034974	1.166608
Na	-0.660746	-1.578872	1.174790	O	-1.254862	-1.378521	0.162298
Na	4.014596	-0.068434	-0.965037	O	-3.246129	0.148786	-0.205732
Na	1.113594	2.104988	0.831840	O	-0.897676	0.669835	-1.293720
				C	1.289445	1.235718	0.895349
IM18				O	1.571966	2.311278	0.369680
C	0.737145	1.144946	-0.000006	C	3.163757	0.155280	-0.397670
N	-0.265975	0.189659	-0.000329	N	2.171179	0.147934	0.559733
C	0.301548	-1.071241	-0.000341	C	2.001988	-1.134323	1.031908
C	1.938032	0.491688	0.000210	C	3.620108	-1.134469	-0.546627
C	1.660523	-0.915559	0.000198	C	2.881558	-1.958552	0.366347
C	-1.626635	0.462170	-0.000633	H	3.435918	1.088232	-0.885224
O	-2.480240	-0.381097	0.000581	H	-0.097690	0.993419	1.283571
H	0.493326	2.205397	0.000001	H	1.235959	-1.341488	1.776047
H	-0.334289	-1.952670	-0.000623	H	4.408494	-1.460082	-1.224761
H	2.919840	0.961887	0.000458	H	2.999608	-3.029886	0.523647
H	2.392780	-1.721361	0.000405	Na	-3.393247	-1.936486	0.374907
H	-1.831582	1.555880	0.000847	Na	0.464976	-1.121667	-1.232432
				Na	-0.561836	2.675299	-0.407435
TS11				CO ₂			
P	-1.950290	0.277330	-0.172584	C	0.000000	0.000000	0.000025
O	-1.492666	1.612887	0.741687	O	0.000000	0.000000	-1.159077
O	-1.762996	-1.002963	0.698537	O	0.000000	0.000000	1.159059
O	-3.421032	0.446341	-0.535363				

				C	-2.357058	2.617391	0.499710
IM19				O	-1.412302	2.975754	-0.082251
C	2.051043	-2.147150	1.227138	O	-3.316116	2.384155	1.098203
N	1.711516	-0.851942	1.451570	IM21			
C	2.770605	-0.100774	1.052838	P	-1.763438	0.246566	-0.236406
C	3.330008	-2.240692	0.667833	O	-1.435586	1.110273	1.151421
C	3.799206	-0.905350	0.553849	O	-1.587943	-1.261812	0.123491
H	1.353061	-2.953415	1.464282	O	-3.214673	0.599309	-0.548089
H	0.230219	-0.337322	1.569189	O	-0.687237	0.691852	-1.256641
H	2.753641	0.987230	1.156623	K	0.583673	-1.552954	-1.230932
H	3.866889	-3.154291	0.407327	K	0.018791	2.972782	-0.330805
H	4.771170	-0.574092	0.185349	K	-4.109151	-1.479050	0.497284
P	-1.282148	-0.079492	-0.046803	C	2.089095	1.150760	0.624993
O	-1.191363	-1.538756	-0.552951	O	2.488534	1.965615	-0.211952
O	-0.748226	0.009480	1.498994	C	3.488670	-0.605299	-0.503859
O	-0.379326	0.884509	-0.861324	N	2.639554	-0.198751	0.492856
O	-2.742354	0.431581	0.059924	C	2.333737	-1.264211	1.299015
K	-3.683684	-1.895979	-0.274027	C	3.721527	-1.956109	-0.344519
K	1.316935	-1.066311	-1.433113	C	2.985235	-2.375941	0.806241
K	-1.396289	2.616903	0.948043	H	3.848349	0.120033	-1.229443
C	1.521609	2.398290	-0.990437	H	-0.520587	0.934777	1.455995
O	1.119837	3.148352	-0.194131	H	1.666819	-1.125603	2.146139
O	2.058873	1.780370	-1.811288	H	4.367655	-2.571437	-0.969637
IM20				H	2.951995	-3.377071	1.234327
C	-3.106313	-0.691756	-0.701731	O	1.259145	1.287525	1.540781
N	-2.036729	-0.113451	-0.086331	IM22			
C	-1.898761	-0.732997	1.119348	P	-1.746596	-0.063611	-0.160634
C	-3.658309	-1.693959	0.099134	O	-2.652093	-1.208527	-0.736443
C	-2.872013	-1.720112	1.283180	O	-2.635549	1.170302	0.254224
H	-3.434111	-0.356246	-1.688984	O	-1.021855	-0.663551	1.094848
H	-0.681237	0.216799	-0.819083	O	-0.674634	0.384787	-1.233089
H	-1.066276	-0.456872	1.770269	K	-1.572119	2.710693	-1.378022
H	-4.536270	-2.301958	-0.124721	K	-0.179935	-2.269238	-0.937896
H	-3.015304	-2.359736	2.155368	K	-3.603420	-0.815627	1.749371
P	1.485355	-0.200619	-0.349709	C	3.289888	-1.064245	-0.211759
O	1.541385	-1.742227	-0.211221	O	2.419405	-1.726891	-0.729125
O	2.742781	0.396534	-1.019503	C	1.925610	0.915992	0.270812
O	0.222821	0.213550	-1.325333	N	3.122702	0.205714	0.294522
O	1.263775	0.501872	1.017300	C	4.106611	0.959914	0.932248
K	3.669037	-0.924293	1.231706	C	2.163413	2.110440	0.890795
K	-0.755740	-2.545701	-0.902453	C	3.536411	2.140356	1.308797
K	1.282805	2.656992	-0.595479				

H	1.005334	0.531688	-0.201377	H	3.302013	-1.398575	1.978230
H	5.112070	0.569529	1.055476	H	2.654548	0.169131	2.504938
H	1.417301	2.886850	1.053388	C	-3.333058	1.862460	-1.611514
H	4.043769	2.946555	1.836692	H	-2.332694	2.066671	-2.022647
O	4.540975	-1.493441	-0.067651	H	-3.960915	2.744561	-1.816690
H	4.573959	-2.387363	-0.439408	H	-3.759947	1.017155	-2.171388
IM23				C	-4.633413	-1.282277	-0.432500
C	-0.787726	1.128377	0.000191	H	-4.905827	-1.356498	0.633173
N	-0.022011	-0.026624	0.000176	H	-5.078112	-2.153814	-0.940651
C	-0.855191	-1.131178	-0.000209	H	-5.117913	-0.385235	-0.844177
C	-2.102516	0.752924	-0.000117	C	1.134749	-1.342790	2.310790
C	-2.145387	-0.679475	-0.000293	H	1.135692	-2.427822	2.075032
C	1.364807	-0.119706	0.000429	H	1.054799	-1.287671	3.415282
O	1.967485	-1.158452	-0.000080	C	-1.199162	-1.036045	2.459652
H	-0.314060	2.105662	0.000434	H	-1.012312	-0.861834	3.538932
H	-0.428974	-2.130761	-0.000306	H	-1.415305	-2.121661	2.377378
H	-2.954929	1.430267	-0.000164	C	4.768444	1.193926	0.235947
H	-3.036765	-1.304362	-0.000513	H	4.992363	0.727125	1.209379
O	1.927316	1.087419	0.000021	H	5.315643	2.150452	0.201937
H	2.886481	0.948173	-0.000217	H	5.188153	0.552082	-0.551930
Mn-L1				C	0.120125	1.666661	-0.811971
Mn	0.001822	0.104969	-0.022287	C	-3.123605	-1.281372	-0.626729
P	-2.219745	0.105000	0.231305	H	-2.898126	-1.110807	-1.693769
P	2.225881	-0.098567	0.157072	C	2.492688	-2.702652	-0.799714
N	-0.011772	-0.693828	1.691340	H	2.440964	-3.068340	0.236812
O	0.228430	2.707978	-1.321548	H	3.076506	-3.436558	-1.378983
O	-0.271330	-1.172480	-2.618855	H	1.471415	-2.695496	-1.207499
C	-3.268421	1.599774	-0.110106	C	-0.134763	-0.639075	-1.591988
H	-4.280261	1.356114	0.258707	C	2.773059	2.488769	1.052429
C	3.142838	-1.327045	-0.894303	H	1.682135	2.614828	1.011135
H	4.155590	-1.393952	-0.459763	H	3.234198	3.464812	0.832986
C	-2.412772	-0.230402	2.025642	H	3.041113	2.228742	2.088889
H	-2.407968	0.748930	2.528183	C	3.253387	-0.849775	-2.337363
H	-3.364093	-0.726336	2.275406	H	2.262187	-0.733841	-2.799676
C	3.274859	1.438818	0.065461	H	3.812883	-1.585489	-2.937918
H	3.082541	1.817308	-0.953956	H	3.780526	0.112362	-2.422617
C	-2.764016	2.825259	0.643609	C	-2.513158	-2.624045	-0.232118
H	-2.730834	2.669103	1.732004	H	-1.413479	-2.593192	-0.231758
H	-3.434889	3.679479	0.456856	H	-2.834035	-3.410469	-0.933585
H	-1.756962	3.117316	0.312787	H	-2.842299	-2.928356	0.773852
C	2.447335	-0.711542	1.878190	Mn-L2			
				C	1.1922700	2.4581100	-0.0771900

N	0.0000600	1.6255300	-0.1459200	H	1.0541100	3.3809100	-0.6756800
C	-1.1920500	2.4582100	-0.0764400	H	1.3760800	2.8101500	0.9610900
C	-2.4083900	1.7031000	-0.5876000	H	-3.3628600	2.1618700	-0.2826800
Mn	0.0000100	-0.2596300	-0.0450300	H	-1.3754300	2.8098700	0.9620400
C	0.0000000	-1.4021300	1.2834800	H	-1.0540300	3.3812100	-0.6746400
H	1.0541100	3.3809100	-0.6756800	O	-0.0000400	-2.1118100	2.2048200
H	1.3760800	2.8101500	0.9610900	H	-2.3804900	1.6574100	-1.6888700
H	-3.3628600	2.1618700	-0.2826800	C	-0.0000300	-1.5516200	-1.2336000
H	-1.3754300	2.8098700	0.9620400	H	2.3799300	1.6564200	-1.6897500
H	-1.0540300	3.3812100	-0.6746400	H	3.3629600	2.1615800	-0.2842500
O	-0.0000400	-2.1118100	2.2048200	C	2.4083400	1.7027000	-0.5885100
H	-2.3804900	1.6574100	-1.6888700	O	-0.0000500	-2.3590500	-2.0690800
C	-0.0000300	-1.5516200	-1.2336000	C	-3.3354100	-1.0274000	-1.0167500
H	2.3799300	1.6564200	-1.6897500	H	-3.3026700	-2.0700500	-0.6655500
H	3.3629600	2.1615800	-0.2842500	H	-4.3726600	-0.6613700	-0.9620900
C	2.4083400	1.7027000	-0.5885100	H	-2.9972900	-1.0116900	-2.0633800
O	-0.0000500	-2.3590500	-2.0690800	C	-3.0011000	-0.0479400	1.6453700
C	-3.3354100	-1.0274000	-1.0167500	H	-4.0589200	0.2546900	1.5996100
H	-3.3026700	-2.0700500	-0.6655500	H	-2.9331800	-1.0635400	2.0639100
H	-4.3726600	-0.6613700	-0.9620900	H	-2.4559900	0.6288700	2.3202600
H	-2.9972900	-1.0116900	-2.0633800	C	3.3355600	-1.0280800	-1.0159400
C	-3.0011000	-0.0479400	1.6453700	H	4.3729000	-0.6623600	-0.9609100
H	-4.0589200	0.2546900	1.5996100	H	3.3023400	-2.0706200	-0.6644800
H	-2.9331800	-1.0635400	2.0639100	H	2.9979100	-1.0125400	-2.0627300
H	-2.4559900	0.6288700	2.3202600	C	3.0008600	-0.0469500	1.6455400
C	3.3355600	-1.0280800	-1.0159400	H	2.9329900	-1.0623100	2.0646700
H	4.3729000	-0.6623600	-0.9609100	H	4.0586400	0.2557800	1.5997500
H	3.3023400	-2.0706200	-0.6644800	H	2.4555700	0.6301900	2.3199600
H	2.9979100	-1.0125400	-2.0627300	As	-2.2022200	-0.0200800	-0.0008500
C	3.0008600	-0.0469500	1.6455400	As	2.2022200	-0.0201600	-0.0008200
H	2.9329900	-1.0623100	2.0646700				
H	4.0586400	0.2557800	1.5997500	Mn-L4			
H	2.4555700	0.6301900	2.3199600	C	-0.2652000	-1.3065000	-2.1010500
N	-2.2022200	-0.0200800	-0.0008500	N	-0.4373300	-0.0439000	-1.3669900
N	2.2022200	-0.0201600	-0.0008200	C	-0.2830700	1.1221600	-2.2482900
				C	-0.2721500	2.4167500	-1.4523100
Mn-L3				Mn	0.7177200	0.0380300	0.3795900
C	1.1922700	2.4581100	-0.0771900	C	2.1363400	0.2565300	-0.6282800
N	0.0000600	1.6255300	-0.1459200	H	-1.1440800	-1.4789500	-2.7487300
C	-1.1920500	2.4582100	-0.0764400	H	0.6056200	-1.1972400	-2.7706800
C	-2.4083900	1.7031000	-0.5876000	H	-0.0344800	3.2668600	-2.1133800
Mn	0.0000100	-0.2596300	-0.0450300	H	0.6669000	1.0138900	-2.7990600
C	0.0000000	-1.4021300	1.2834800	H	-1.0921100	1.1239700	-3.0013700

O	3.0615200	0.3921400	-1.3207600	C	-2.9713600	-0.3324800	-0.2068300
H	-1.2743100	2.6129200	-1.0353200	C	-4.4596800	1.2896200	-0.3077200
C	1.6699500	0.1340900	1.8783200	H	-5.4371300	1.7587700	-0.3842500
C	2.5379400	3.2769600	-0.2842400	C	-3.1953000	1.8196800	-0.2031300
C	0.1082300	2.9764400	1.5662300	H	-2.8866300	2.8619200	-0.1764800
H	-0.8016700	2.4053600	1.8043300	C	2.8213400	0.3099100	-1.6621700
H	2.3219200	4.3583800	-0.2795800	H	3.2287700	1.2637300	-1.3992400
H	-0.9243300	-2.6527600	-0.5314000	H	3.6183100	-0.3761500	-1.8598100
H	0.1317900	-3.4020300	-1.7310600	H	2.2125700	0.4108100	-2.5363100
C	3.0636100	-2.6090800	-0.9114100	C	3.0090500	-0.5987100	1.0519400
H	3.1112600	-3.7096300	-0.9704100	H	3.9174200	-0.9864700	0.6403500
C	-0.0322400	-2.4747800	-1.1545400	H	3.2099300	0.3260500	1.5512900
C	1.3718000	-3.0824000	1.5778200	H	2.6057800	-1.3012700	1.7510000
H	0.4647100	-2.8315600	2.1477700	C	-4.3087600	-0.0859600	-0.3164700
O	2.3143200	0.2047500	2.8295800	H	-5.0888300	-0.8142200	-0.3940800
Si	1.4739800	-2.1289700	-0.0411500	S	-2.2359300	0.7888300	-0.1349700
Si	0.9492700	2.3312800	0.0078000				
H	1.3610500	-4.1663400	1.3696400	Mn-L6			
H	2.2438300	-2.8722600	2.2169500	Mn	0.2208600	-0.0552000	-1.0606200
H	-0.1846300	4.0285500	1.3998500	P	-1.5143000	0.3266400	0.1425900
H	0.7800700	2.9434300	2.4377300	O	1.7107300	2.0593700	0.3177800
H	3.9503200	-2.2655800	-0.3556500	O	-0.3212700	2.0818100	-2.9867100
H	3.1296400	-2.2067700	-1.9324500	N	-0.7329000	-1.4514200	-1.9879400
H	3.2688500	3.0774000	0.5158200	N	0.8095900	-2.7619500	0.1729800
H	3.0052800	3.0217300	-1.2460500	N	2.5714000	-1.5628800	0.2762200
				C	-0.7692400	-2.8647100	-1.6760400
Mn-L5				H	-0.0384500	-3.4335400	-2.2923000
P	1.8082200	-0.3171400	-0.2863900	H	-1.7596000	-3.2957100	-1.9128500
C	1.4338500	-2.0549200	-0.9282000	C	-0.5117500	-3.2025700	-0.2240800
C	0.0703800	-2.5214400	-0.4156800	H	-1.2617200	-2.7265000	0.4234300
H	2.2149500	-2.7894500	-0.6783900	H	-0.5630800	-4.2892400	-0.0669300
H	1.4039400	-1.9852800	-2.0290000	C	1.2652100	-1.5220200	-0.1146600
H	-0.2273100	-3.4708200	-0.9062600	C	1.7794400	-3.5559100	0.7410300
H	0.1068900	-2.7118000	0.6689900	H	1.5928300	-4.5838100	1.0404600
N	-0.8949900	-1.3920200	-0.6215800	C	2.9043200	-2.7982800	0.8031600
C	-2.2505600	-1.6425100	-0.1254300	H	3.9074200	-3.0257000	1.1527200
H	-2.1688600	-1.9665300	0.9289100	C	3.5380900	-0.5382200	0.0418900
H	-2.7780200	-2.4473900	-0.6752700	C	4.0549600	0.1857500	1.1223700
Mn	-0.3346400	0.4486600	0.0030000	C	5.0256000	1.1549100	0.8551200
C	-0.4013200	0.1661800	1.7771700	H	5.4245200	1.7414800	1.6897100
O	-0.3917000	0.0595900	2.9411600	C	5.4632800	1.4246400	-0.4417500
C	0.0725500	2.1677900	0.1307600	C	4.9088800	0.6897000	-1.4950100
O	0.3097100	3.3076900	0.1461700	H	5.2244500	0.9009800	-2.5196600

C	3.9509200	-0.3000800	-1.2799900	H	-2.5148700	5.1086200	-0.5690800
C	3.5185700	0.0204500	2.5123400	C	-2.1898200	4.7072500	1.5308000
H	4.2439400	0.3602800	3.2599000	H	-2.3294600	5.7474900	1.8352100
H	3.2284500	-1.0072900	2.7407300	C	-1.9075800	3.7305800	2.4821000
H	2.6181400	0.6530800	2.6268700	H	-1.8268300	3.9998500	3.5382800
C	6.4913200	2.4820100	-0.7215700	C	-1.7288900	2.4018300	2.0952100
H	7.5460700	1.9244100	-1.0805300	H	-1.5164900	1.6466600	2.8543200
H	6.6679000	3.1342200	0.3065400				
H	6.0848100	3.2148200	-1.6412400	Mn-L7			
C	3.3510400	-1.0547800	-2.4263200	P	1.8082200	-0.3171400	-0.2863900
H	2.2942000	-0.7659700	-2.5740000	C	1.4338500	-2.0549200	-0.9282000
H	3.3578100	-2.1418600	-2.2517300	C	0.0703800	-2.5214400	-0.4156800
H	3.8916100	-0.8385700	-3.3599300	H	2.2149500	-2.7894500	-0.6783900
C	-3.0890000	-0.0317200	-0.7427500	H	1.4039400	-1.9852800	-2.0290000
C	-3.1230000	-0.6836900	-1.9913700	H	-0.2273100	-3.4708200	-0.9062600
C	-1.8750400	-1.0742400	-2.7737100	H	0.1068900	-2.7118000	0.6689900
H	-2.1714200	-1.8776000	-3.4764600	N	-0.8949900	-1.3920200	-0.6215800
H	-1.6284400	-0.2114000	-3.4162400	C	-2.2505600	-1.6425100	-0.1254300
C	1.1903800	1.1869600	-0.2461200	H	-2.1688600	-1.9665300	0.9289100
C	-0.1950500	1.2227300	-2.2157800	H	-2.7780200	-2.4473900	-0.6752700
C	-4.2908000	0.4003400	-0.1577200	Mn	-0.3346400	0.4486600	0.0030000
H	-4.2583700	0.9424100	0.7910800	C	-0.4013200	0.1661800	1.7771700
C	-5.5194100	0.1635900	-0.7639000	O	-0.3917000	0.0595900	2.9411600
H	-6.4407600	0.5047200	-0.2859000	C	0.0725500	2.1677900	0.1307600
C	-5.5582500	-0.5071900	-1.9854700	O	0.3097100	3.3076900	0.1461700
H	-6.5148200	-0.7066800	-2.4754200	C	-2.9713600	-0.3324800	-0.2068300
C	-4.3719600	-0.9153000	-2.5848100	C	-4.4596800	1.2896200	-0.3077200
H	-4.4033000	-1.4271200	-3.5514200	H	-5.4371300	1.7587700	-0.3842500
C	-1.6264100	-0.6527500	1.7033600	N	-2.2359300	0.7888300	-0.1349700
C	-2.7545800	-1.3735600	2.1118400	N	-4.3087600	-0.0859600	-0.3164700
H	-3.6624300	-1.3597500	1.5061100	C	-3.1953000	1.8196800	-0.2031300
C	-2.7227800	-2.1333100	3.2815700	H	-2.8866300	2.8619200	-0.1764800
H	-3.6094300	-2.6971600	3.5823600	C	-5.3807300	-1.0632500	-0.3487400
C	-1.5688700	-2.1769700	4.0617700	H	-6.2774200	-0.6021000	-0.7838300
H	-1.5473400	-2.7732900	4.9773500	H	-5.0986800	-1.9216700	-0.9754000
C	-0.4405600	-1.4579200	3.6659000	H	-5.6277200	-1.4287000	0.6616500
H	0.4703600	-1.4866100	4.2691600	C	2.8213400	0.3099100	-1.6621700
C	-0.4673600	-0.7105500	2.4917400	H	3.2287700	1.2637300	-1.3992400
H	0.4253800	-0.1699400	2.1693700	H	3.6183100	-0.3761500	-1.8598100
C	-1.8278600	2.0366800	0.7492900	H	2.2125700	0.4108100	-2.5363100
C	-2.1113700	3.0267200	-0.2027800	C	3.0090500	-0.5987100	1.0519400
H	-2.1941000	2.7609200	-1.2589000	H	3.9174200	-0.9864700	0.6403500
C	-2.2935000	4.3500800	0.1857300	H	3.2099300	0.3260500	1.5512900

H	2.6057800	-1.3012700	1.7510000	C	1.0794400	0.9188800	-2.3057000
				C	2.2717800	1.2046300	-1.4092000
Mn-L8				P	2.4041900	-0.1993200	-0.1958700
C	-0.2881400	1.1236300	2.2048600	Mn	0.2874000	-0.9617300	-0.0762900
N	-0.2426300	-0.0433100	1.2014100	C	0.6029300	-2.1442600	-1.3179500
C	-0.3051600	-1.2969000	2.0939100	H	-1.4486500	1.0472100	-3.0885200
C	-0.3512400	-2.4916200	1.1554900	H	-0.9339000	-0.6546400	-3.0384300
P	0.9285600	-2.2145100	-0.1444300	H	3.1876300	1.3458600	-1.9926600
Mn	1.0520100	0.0235100	-0.2605000	H	1.3231800	0.0810800	-2.9884700
C	2.4032600	0.0296100	0.8465000	H	0.8599300	1.7910600	-2.9391500
H	-1.1081500	1.0905800	2.9455300	O	0.8149500	-2.9379400	-2.1389000
H	0.6623100	1.1022900	2.7661400	H	2.0928000	2.1266400	-0.8376200
H	-0.2050400	-3.4420800	1.6924400	C	0.5713200	-2.1953300	1.1459400
H	0.6244800	-1.3134000	2.6895800	C	3.6355000	-1.3165100	-0.9487700
H	-1.1465000	-1.3397100	2.8101500	C	3.3024400	0.5194000	1.2667700
O	3.3031500	0.0409900	1.5800800	C	3.3280000	-0.4717200	2.4153300
H	-1.3344700	-2.5409800	0.6588500	H	3.8601600	-1.3962400	2.1445300
C	2.1589900	0.0947300	-1.6405300	H	2.3074600	-0.7608700	2.7274600
H	-1.4031100	2.4500300	0.9297100	H	3.8346100	-0.0408000	3.2887800
H	-0.2357500	3.2960400	1.9720300	C	4.6801900	1.0756300	0.9381800
C	-0.3948500	2.3879900	1.3700100	H	4.6600300	1.7922400	0.1042200
P	0.8141700	2.2452500	-0.0155400	H	5.3928600	0.2794900	0.7009600
O	2.8965000	0.1396000	-2.5299100	H	5.0846700	1.6199000	1.8114200
C	0.4193700	-3.2479200	-1.5636400	H	2.6606100	1.3680400	1.5738600
H	1.2139200	-3.2129700	-2.3247900	H	4.6064600	-0.8240500	-1.1113700
H	0.2582900	-4.2945000	-1.2617700	H	-2.8151900	0.7788200	-1.0766800
H	-0.5034400	-2.8654500	-2.0206600	H	-3.2698400	-0.5210100	-2.2019700
C	2.3966800	-3.1191400	0.4590600	C	-2.4895600	-2.9591100	-0.8497300
H	2.1944900	-4.1967000	0.5578800	H	-3.5748100	-3.0034900	-1.0219600
H	3.2270600	-2.9712900	-0.2483700	C	-2.4522700	-0.1378500	-1.5789900
H	2.7102300	-2.7184800	1.4335100	P	-1.9420500	-1.3180300	-0.2643100
C	0.1084600	3.2363600	-1.3727900	C	-3.0402900	-0.9167800	1.1647100
H	-0.1538900	4.2531100	-1.0421600	H	-2.7769200	0.1326200	1.3800800
H	0.8446000	3.2993200	-2.1887400	C	-4.5229900	-0.9881400	0.8288400
H	-0.7845600	2.7280500	-1.7612400	H	-4.7886500	-0.3941200	-0.0522000
C	2.2566200	3.2331000	0.5102500	H	-5.1222300	-0.6133000	1.6744800
H	3.0388600	3.1689900	-0.2617900	H	-4.8529600	-2.0253300	0.6412700
H	1.9893200	4.2896300	0.6656400	C	-2.6815600	-1.7532400	2.3832600
H	2.6696900	2.8235800	1.4434500	H	-2.8237500	-2.8310100	2.2011900
				H	-3.3210000	-1.4701500	3.2381500
Mn-L9				H	-1.6361500	-1.5910300	2.6798100
C	-1.2251000	0.2041000	-2.4091500	O	0.7697600	-3.0485900	1.9125100
N	-0.1058800	0.5406900	-1.5264400	H	-1.9713200	-3.1934600	-1.7908500

H	-2.2156300	-3.7272400	-0.1147200	C	2.4926900	-2.7026500	-0.7997100
H	3.7699500	-2.1991900	-0.3056000	H	2.4409600	-3.0683400	0.2368100
H	3.2614300	-1.6700200	-1.9201000	H	3.0765100	-3.4365600	-1.3789800
Mn-L10				H	1.4714200	-2.6955000	-1.2075000
Mn	0.0018200	0.1049700	-0.0222900	C	-0.1347600	-0.6390800	-1.5919900
P	-2.2197500	0.1050000	0.2313100	C	2.7730600	2.4887700	1.0524300
P	2.2258800	-0.0985700	0.1570700	H	1.6821400	2.6148300	1.0111300
N	-0.0117700	-0.6938300	1.6913400	H	3.2342000	3.4648100	0.8329900
O	0.2284300	2.7079800	-1.3215500	H	3.0411100	2.2287400	2.0888900
O	-0.2713300	-1.1724800	-2.6188600	C	3.2533900	-0.8497800	-2.3373600
H	-4.2802600	1.3561100	0.2587100	H	2.2621900	-0.7338400	-2.7996800
H	4.1555900	-1.3939500	-0.4597600	H	3.8128800	-1.5854900	-2.9379200
C	-2.4127700	-0.2304000	2.0256400	H	3.7805300	0.1123600	-2.4226200
H	-2.4079700	0.7489300	2.5281800	C	-2.5131600	-2.6240500	-0.2321200
H	-3.3640900	-0.7263400	2.2754100	H	-1.4134800	-2.5931900	-0.2317600
H	3.0825400	1.8173100	-0.9539600	H	-2.8340400	-3.4104700	-0.9335900
C	-2.7640200	2.8252600	0.6436100	H	-2.8423000	-2.9283600	0.7738500
H	-2.7308300	2.6691000	1.7320000	Si	-3.1236000	-1.2813700	-0.6267300
H	-3.4348900	3.6794800	0.4568600	Si	-3.2684200	1.5997700	-0.1101100
H	-1.7569600	3.1173200	0.3127900	Si	3.1428400	-1.3270500	-0.8943000
C	2.4473400	-0.7115400	1.8781900	Si	3.2748600	1.4388200	0.0654600
H	3.3020100	-1.3985800	1.9782300	Mn-L11			
H	2.6545500	0.1691300	2.5049400	C	-1.122615	-2.016049	-2.217333
C	-3.3330600	1.8624600	-1.6115100	N	0.063169	-1.208259	-1.925790
H	-2.3326900	2.0666700	-2.0226500	C	1.290385	-1.926887	-2.271799
H	-3.9609200	2.7445600	-1.8166900	C	2.500201	-1.061959	-1.966321
H	-3.7599500	1.0171600	-2.1713900	P	2.303231	-0.425409	-0.243029
C	-4.6334100	-1.2822800	-0.4325000	Mn	0.060937	-0.415146	0.038747
H	-4.9058300	-1.3565000	0.6331700	C	0.014786	-2.008219	0.758014
H	-5.0781100	-2.1538100	-0.9406500	H	-1.118425	-2.330351	-3.277346
H	-5.1179100	-0.3852400	-0.8441800	H	-1.100432	-2.933731	-1.604037
C	1.1347500	-1.3427900	2.3107900	H	3.443530	-1.607806	-2.118900
H	1.1356900	-2.4278200	2.0750300	H	1.329926	-2.867399	-1.696403
H	1.0548000	-1.2876700	3.4152800	H	1.283626	-2.202379	-3.342877
C	-1.1991600	-1.0360500	2.4596500	O	-0.066051	-3.054845	1.255094
H	-1.0123100	-0.8618300	3.5389300	H	2.508015	-0.191407	-2.641507
H	-1.4153100	-2.1216600	2.3773800	C	0.057074	0.301184	1.653323
C	4.7684400	1.1939300	0.2359500	C	3.444650	-1.458722	0.807605
H	4.9923600	0.7271300	1.2093800	C	3.237556	-1.110885	2.275903
H	5.3156400	2.1504500	0.2019400	H	3.324970	-0.029784	2.463381
H	5.1881500	0.5520800	-0.5519300	H	3.993256	-1.617923	2.896822
C	0.1201300	1.6666600	-0.8119700	H	2.245649	-1.435933	2.625855
H	-2.8981300	-1.1108100	-1.6937700				

C	3.317521	-2.954345	0.550619
H	2.325675	-3.338458	0.826015
H	4.057601	-3.493646	1.163669
H	3.513045	-3.220001	-0.498804
H	4.455785	-1.134413	0.503932
H	-2.413814	-0.364932	-2.654675
H	-3.283149	-1.796814	-2.053370
C	-3.211154	-1.585801	0.847269
H	-2.766432	-2.581729	0.670223
C	-3.017530	-1.222939	2.314175
H	-1.965658	-1.280554	2.625030
H	-3.590807	-1.914987	2.951426
H	-3.381016	-0.204455	2.525632
C	-4.685953	-1.623169	0.473355
H	-5.207753	-2.379210	1.082004
H	-4.853439	-1.882876	-0.582761
H	-5.169821	-0.652568	0.663092
C	-2.368683	-1.197366	-1.935931
P	-2.192924	-0.477433	-0.247975
O	0.057329	0.749548	2.721624
C	3.201195	1.173138	-0.243491
C	4.317129	1.381090	-1.066009
C	2.778048	2.208647	0.599598
C	4.990161	2.600578	-1.049994
H	4.666105	0.588408	-1.732712
C	3.457336	3.425934	0.619851
H	1.905822	2.067903	1.240631
C	4.560963	3.625605	-0.207199
H	5.853873	2.751884	-1.702000
H	3.115031	4.224842	1.281907
H	5.087123	4.583211	-0.197973
C	-3.128722	1.089942	-0.281853
C	-4.128069	1.343734	-1.230032
C	-2.838836	2.068943	0.677905
C	-4.824164	2.551362	-1.217100
H	-4.368239	0.599645	-1.992510
C	-3.542487	3.270838	0.695399
H	-2.048931	1.895485	1.411148
C	-4.534090	3.515938	-0.253797
H	-5.596155	2.738685	-1.967343
H	-3.305345	4.025655	1.449073
H	-5.078248	4.463551	-0.246385