

**Electronic Supplementary Information to:**

**Reaction mechanism for the *Pu*DddK dimethylsulfoniopropionate lyase and cofactor effects of various transition metal ions**

Ying Wang and Shi-Lu Chen\*

*Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China*

\*E-mail: shlchen@bit.edu.cn

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1. Supplementary tables, figures, and scheme
2. Cartesian coordinates of optimized structures

*1. Supplementary tables and figures*

**Table S1** Properties of the enzyme-substrate complexes with various divalent transition metal ions as cofactors in different electronic states.

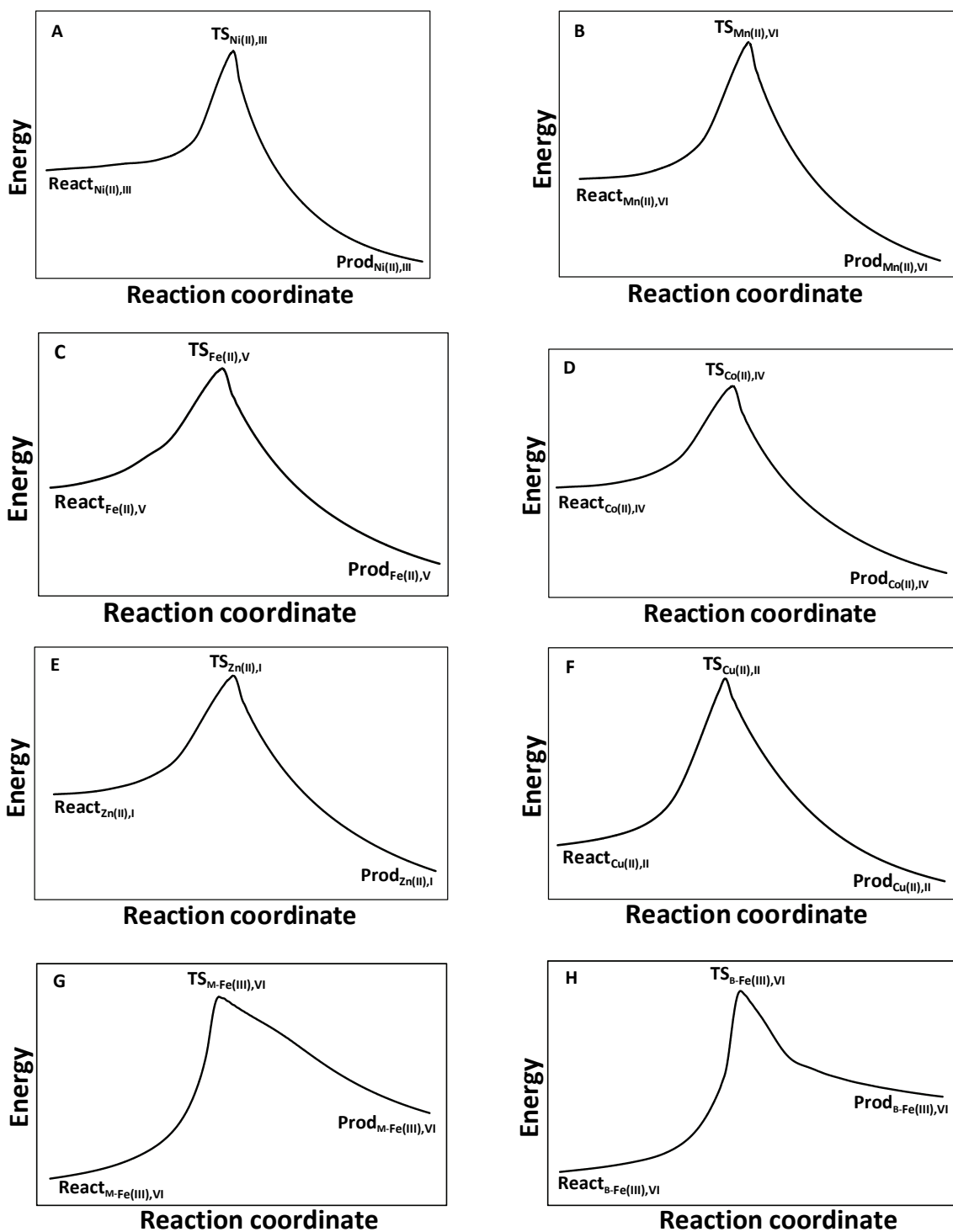
metal	multiplicity	spin in metal	energy (kcal/mol)
Ni <sup>2+</sup>	3	1.69	0.0
	1	-0.02	19.1
Mn <sup>2+</sup>	6	4.82	0.0
	4	2.98	37.9
	2	1.04	52.6
Fe <sup>2+</sup>	5	3.76	0.0
	3	1.99	18.9
	1	0.00	32.6
Co <sup>2+</sup>	4	2.75	0.0
	2	0.97	20.4

**Table S2** Properties of the enzyme-substrate complexes with a ferric ion as the cofactor in various electronic states. Both monodentate ( $\text{Fe}_M^{3+}$ ) and bidentate ( $\text{Fe}_B^{3+}$ ) bindings of DMSP were obtained.

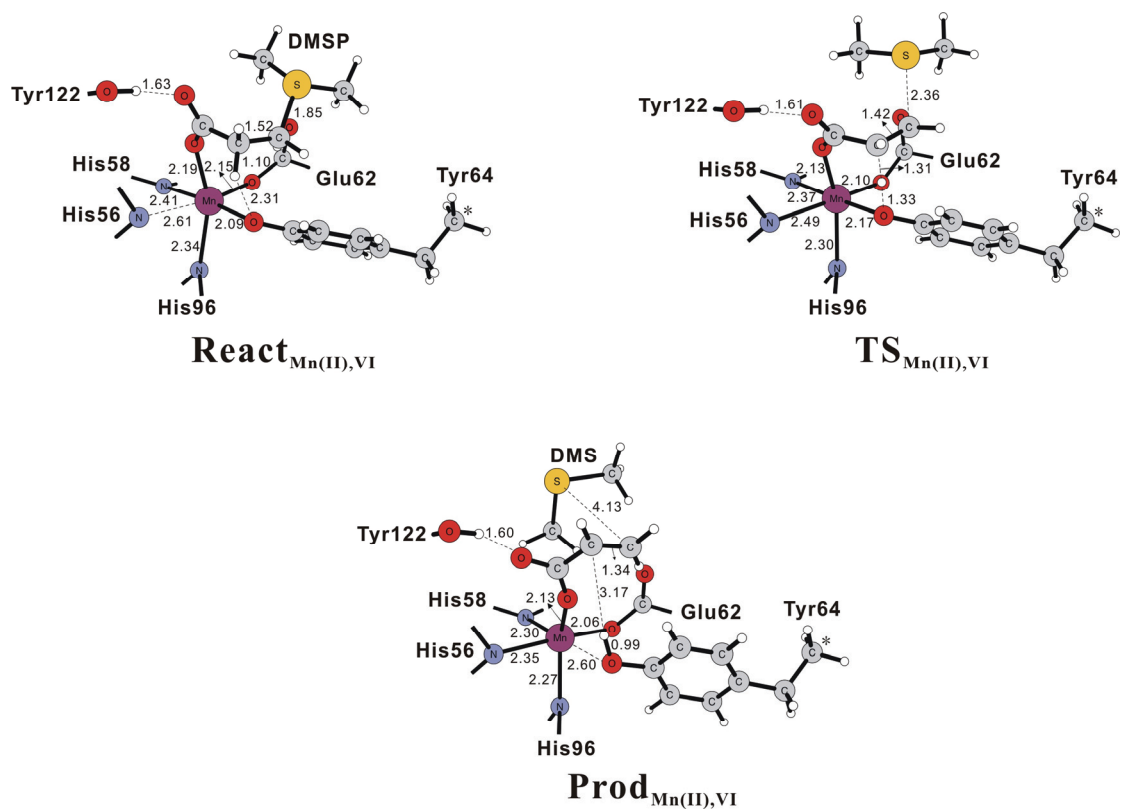
multiplicity	spin		energy (kcal mol <sup>-1</sup> )
	$\text{Fe}_M^{3+}$	Tyr64	
6	3.97	0.57	0
4	3.76	-0.97	9.5
2	0.91	0.09	28.9

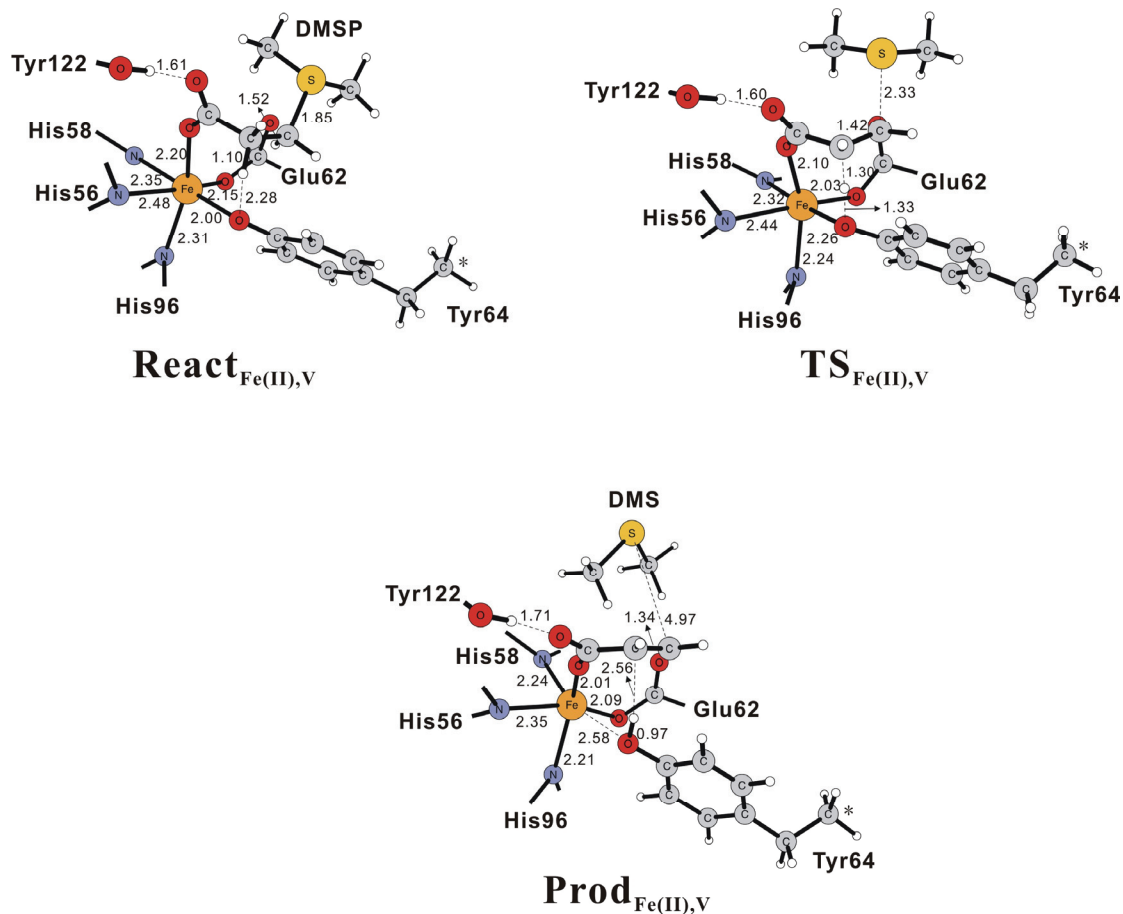
multiplicity	spin		energy (kcal mol <sup>-1</sup> )
	$\text{Fe}_B^{3+}$	Tyr64	
6	3.76	1.01	10.7
4	3.76	-1.01	10.8
4	1.99	1.01	30.1
2	1.99	-1.01	30.5
2	-0.00	1.01	32.0



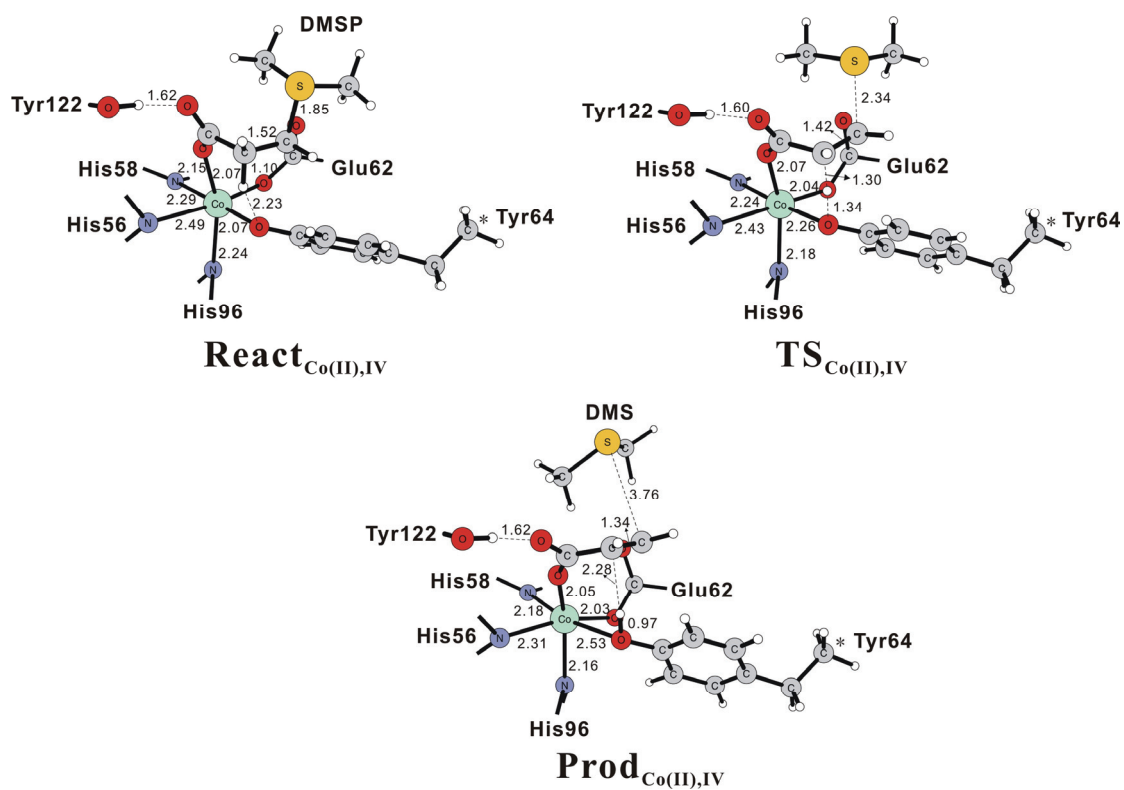
**Fig. S1** Schematic potential energy surfaces obtained by the IRC (intrinsic reaction coordinate) calculations with the transition state structures as the starting points. The results with various metal ions are given, including  $\text{Ni}^{2+}$  (A),  $\text{Mn}^{2+}$  (B),  $\text{Fe}^{2+}$  (C),  $\text{Co}^{2+}$  (D),  $\text{Zn}^{2+}$  (E),  $\text{Cu}^{2+}$  (F),  $\text{Fe}_M^{3+}$  (G), and  $\text{Fe}_B^{3+}$  (H).



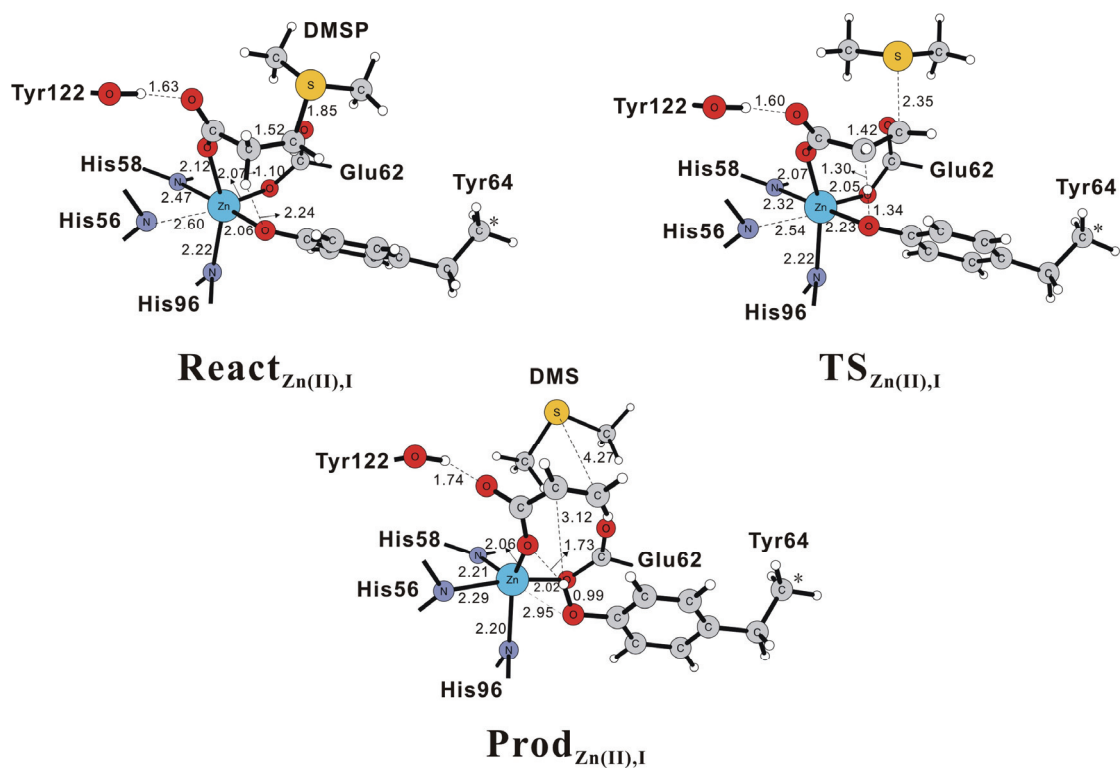
**Fig. S2** Optimized structures of stationary points in the  $\text{Mn}^{2+}$ -dependent *PuDddK*-catalyzed decomposition of DMSP.



**Fig. S3** Optimized structures of stationary points in the  $\text{Fe}^{2+}$ -dependent *Pu*DddK-catalyzed decomposition of DMSP.

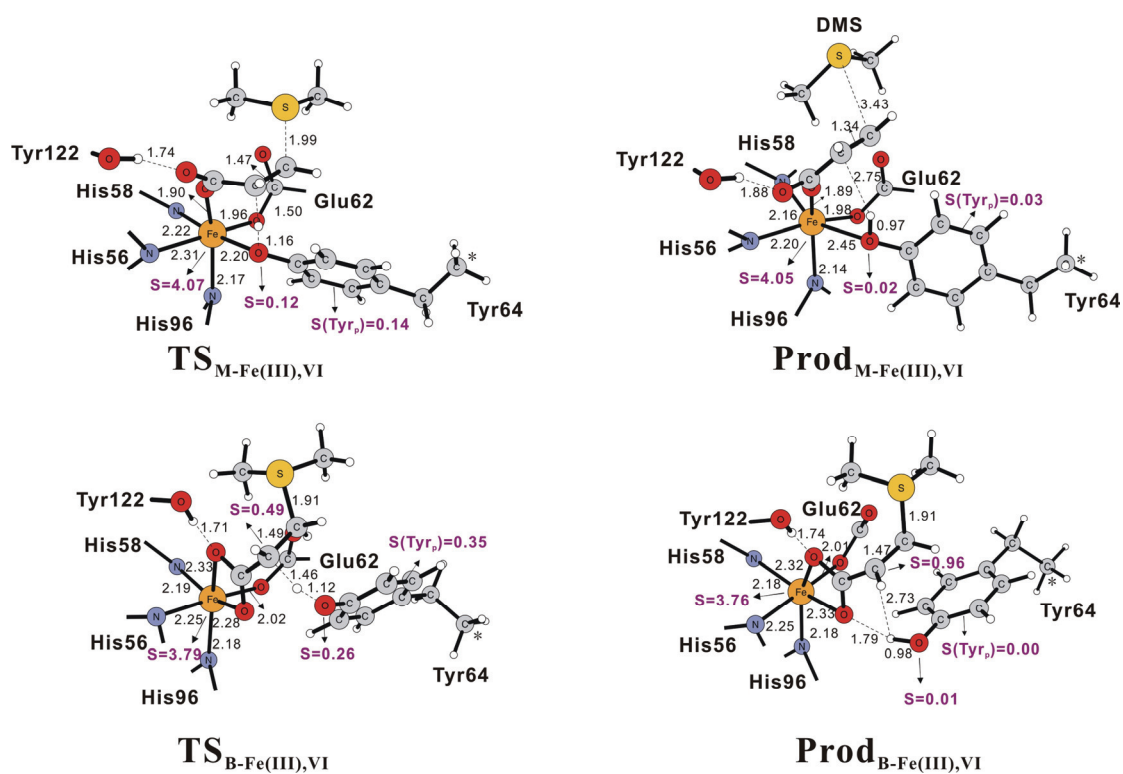


**Fig. S4** Optimized structures of stationary points in the  $\text{Co}^{2+}$ -dependent *Pu*DddK-catalyzed decomposition of DMSP.

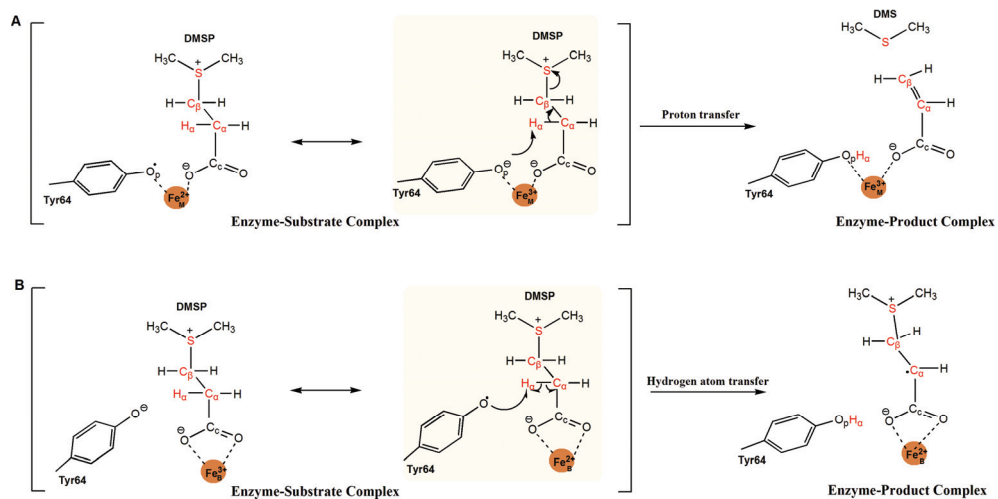


**Fig. S5** Optimized structures of stationary points in the Zn<sup>2+</sup>-dependent *Pu*DddK-catalyzed decomposition of DMSP.





**Fig. S6** Optimized structures of stationary points in the  $\text{Fe}^{3+}$ -dependent *Pu*DddK-catalyzed decomposition of DMSP.



**Scheme S1** Possible reaction mechanisms for  $\text{Fe}^{3+}$ -dependent *Pu*DddK. (A) A monodentate DMSP coordination with  $\text{Fe}_M^{3+}$ . (B) A bidentate DMSP coordination with  $\text{Fe}_B^{3+}$ .

## 2. Cartesian coordinates of optimized structures

The abbreviations used here are consistent with those in the text.

### React<sub>Ni(II),III</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.1610471129	-35.8835948910	19.3940518877
C	-5.5113866992	-34.8144760147	18.4045777177
N	-5.2618840027	-34.9226640178	17.0464836950
C	-5.9850239465	-33.5353385983	18.5660988236
C	-5.5638874436	-33.7306862478	16.4637426791
N	-5.9988404308	-32.8583191941	17.3580504153
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.6468651623	-33.2813323942	19.4444356361
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N	-1.8205282749	-31.0333008990	19.6258160493
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N	-3.5959324007	-31.2558950244	18.3396795565
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C	-3.3172666983	-26.4573258093	18.8584367558
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C	-8.6185845571	-26.5911295463	14.9532104944
C	-7.0784971861	-27.3578641117	17.1308026975
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### TS<sub>Ni(II),III</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
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H	-4.3853450000	-33.7293550000	13.5276040000
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H	-9.0926180000	-33.6820020000	21.2160290000
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C	-2.5094840000	-27.3119460000	12.8678250000
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Ni	-5.3238320000	-30.5135640000	17.2279540000

### TS<sub>Ni(II),III</sub>

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N	-5.1796707627	-34.9425403089	16.9562009782
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C	-5.4452266129	-33.7228525531	16.4264871888
N	-5.7770983304	-32.8629934589	17.3781932846
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N	-1.7245538357	-30.8685631116	19.6523881100
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C	-2.8951874674	-30.3492725805	19.2080294438
N	-3.5184881694	-31.2219199650	18.4393174074
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C	-3.2547863866	-26.4884996613	18.9412395817
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C	-3.7279328602	-28.1612854814	17.1729962640
O	-2.7037889853	-28.6906612464	16.7103852420
O	-4.8097216330	-28.7687500250	17.5277835791
C	-8.1409660000	-23.1040170000	14.9750030000
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C	-8.3392118122	-25.5612746776	15.8468835622
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C	-8.2507676521	-26.3150762463	14.6675493296
C	-7.5337145481	-27.5287181492	17.0725044283
C	-7.8248129260	-27.6452641409	14.6793502641



C	-7.4633934129	-28.2563789773	15.8857709343
O	-7.0639923927	-29.5857572619	15.9245474145
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.7776138617	-31.8707160521	20.3178246007
C	-8.4531563831	-31.2713500164	19.9613208201
N	-7.4389927423	-31.0513404945	20.8857867028
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C	-6.3331982154	-30.6218025548	20.2173690906
N	-6.5809870370	-30.5644178627	18.9242725800
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8255372241	-36.6725817586	17.4908336919
C	-1.7188926253	-36.1555098353	16.3813681172
C	-1.6978842077	-34.8011100248	16.0106751881
C	-2.5786800613	-37.0031713771	15.6723461654
C	-2.5162169059	-34.2958748160	15.0059786087
C	-3.4058079840	-36.5207616911	14.6539406744
C	-3.3947582982	-35.1562875376	14.3178312165
O	-4.2655834074	-34.7206211400	13.3917360168
C	-4.6203202846	-28.6832890456	13.9299467552
C	-5.0529668960	-29.8783999214	13.5083938504
C	-4.6552199212	-31.1632465096	14.1746091731
O	-4.4847874477	-31.2028601100	15.4376761183
O	-4.4887772893	-32.1393012424	13.3961884759
H	-4.9857516881	-35.5908277412	20.2805607537
H	-3.9214827809	-36.2741302869	19.0616507949
H	-5.9288444088	-33.1032179352	19.5134888170
H	-5.3459587555	-33.4905591091	15.3800109504
H	-5.5191612537	-38.0057363156	19.8755075990
H	0.5147688044	-32.5398690961	18.9427601774
H	-0.5217252915	-33.9518311854	18.8801678511
H	-2.9909893127	-33.1952947267	17.7779926089
H	-3.2459533024	-29.3549632664	19.4282823988
H	0.7638885104	-33.8888031424	21.0295290656
H	-3.9735527352	-26.9870342697	19.6069750020
H	-2.2907673420	-27.0026616007	19.0611271571
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H	-2.3752732089	-24.5169874951	18.6995189291
H	-8.9139345631	-23.7751033543	16.8821708249
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H	-8.0198432847	-25.6465938655	17.9760502293
H	-8.5386588163	-25.8669279151	13.7190352866
H	-7.2014902178	-27.9991668754	17.9896757875
H	-7.7789482134	-28.2130919356	13.7542317156

H	-8.1286256073	-23.4051083745	13.9222102256
H	-10.1263385937	-31.4737090554	21.2804436038
H	-10.5099201418	-31.5491564169	19.5699602814
H	-8.3212861495	-30.9956647300	17.7622945743
H	-5.3881640287	-30.3945260501	20.6857836398
H	-10.7158552680	-33.8254839426	20.6079551868
H	-1.0475372898	-36.1400560416	18.4279796297
H	-1.0575274606	-37.7271717847	17.6841265858
H	-2.6083983502	-38.0626870705	15.9202678665
H	-1.0340329959	-34.1130961790	16.5292131953
H	-4.0736894658	-37.1815084660	14.1088325457
H	-2.5210263125	-33.2356806794	14.7732264757
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H	-4.8370224277	-27.7741732470	13.3769796499
H	-6.5702037193	-29.7625252967	15.1030001526
H	-5.5909239366	-29.9926844537	12.5693922401
H	-4.7894851342	-35.7167616099	16.4278376109
H	-7.5214505119	-31.1579241166	21.8858686023
H	-1.0409578505	-30.3767810850	20.2074703337
H	-8.6275926011	-22.1255974694	15.0408905197
H	-7.1012413817	-22.9955014783	15.3009952867
H	-4.0603653445	-24.4909749666	19.2327484740
H	-2.7771833295	-24.9131246794	20.3775409595
H	0.9298989831	-37.0802923691	16.2649252058
H	1.2905626231	-36.9124124500	17.9949512533
H	-5.8309136109	-37.6728661681	18.1653215452
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H	-9.4103457735	-33.8160092829	19.4017969243
H	-9.0211653936	-33.7619617517	21.1251564745
S	-1.0533827919	-28.8484907918	13.3314496110
C	-1.3932167342	-30.4205312615	14.2031099077
C	-0.2932227740	-27.9100745139	14.7050947649
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H	-0.0923506515	-26.8997617645	14.3354757241
H	-0.9858484244	-27.8714654200	15.5495888207
H	-2.0147414249	-30.2427784653	15.0833253266
H	-1.9294709278	-31.0660636059	13.5032977946
H	-0.4567094907	-30.9105879509	14.4923744114
H	0.0695847410	-32.3161651728	21.4360285056
H	-0.9737900841	-33.7436351239	21.3610750883
Ni	-5.2174064491	-30.7012079406	17.2983300848

**React<sub>Mn(II),VI</sub>**

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N	-5.0995437319	-34.9737081245	16.9028911066
C	-5.8810908061	-33.6321184606	18.4358321670
C	-5.4395725588	-33.7853235739	16.3356108138
N	-5.9121464293	-32.9402200973	17.2376915471
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.4933019401	-33.2290512735	19.3992624131
C	-1.5808484208	-32.2604775307	19.0453028569
N	-1.5192731793	-30.9075022990	19.3562183024
C	-2.7660092102	-32.4019292230	18.3634888361
C	-2.6318180116	-30.3021381122	18.8578146565
N	-3.4087508756	-31.1825599325	18.2534125583
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2463244516	-26.3917884145	18.6701143312
C	-3.5788710531	-26.2815460248	17.1821470085
C	-3.8042540460	-27.6197090384	16.4758553008
O	-3.6111580680	-27.6627646018	15.2360509734
O	-4.2076414045	-28.5852153875	17.2020804424
C	-8.1409660000	-23.1040170000	14.9750030000
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C	-8.4114591919	-25.5063515864	15.9593250378
C	-7.4758667268	-25.8937687634	16.9342742341
C	-8.8885894418	-26.5244440527	15.1190200637
C	-7.0257706969	-27.2076715371	17.0602674688
C	-8.4490754532	-27.8460243195	15.2292029829
C	-7.4784459190	-28.2360863692	16.1912450493
O	-7.0385573137	-29.4814825368	16.2518870847
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.6367528792	-31.8726728422	20.4571466830
C	-8.2918496305	-31.3227005910	20.0882036537
N	-7.1900848839	-31.3535508682	20.9385704694
C	-7.8129578108	-30.7725896429	18.9257988857
C	-6.1181968248	-30.8424755339	20.2671776395
N	-6.4652094052	-30.4908156941	19.0455694724
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8341969125	-36.7348623006	17.4085073662
C	-1.6938818956	-36.1794995576	16.2900104859
C	-1.7102375459	-34.8063775109	15.9980993427
C	-2.4881191959	-37.0160222402	15.4950386939
C	-2.4905383484	-34.2777626339	14.9738146871
C	-3.2741680217	-36.5093899339	14.4574315564
C	-3.2860771833	-35.1316895894	14.1866250274

O	-4.1017235980	-34.6854425567	13.2118179281
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C	-6.1264148179	-30.5194983304	13.5063722844
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O	-4.3697328065	-32.0868441768	13.0788254008
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H	-6.2043061908	-33.1782722985	19.3581933982
H	-5.2960187086	-33.5791124470	15.2895009357
H	-5.5225496376	-37.9769717114	19.9075717434
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H	-0.8266080364	-34.2240638267	19.0900922265
H	-3.1817483226	-33.2953202522	17.9272572573
H	-2.8388187445	-29.2449750422	18.9136026914
H	0.6716636907	-33.9882793816	21.0820646020
H	-4.0290406914	-26.9807250800	19.1610127725
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H	-2.8015470333	-25.7306057286	16.6408793428
H	-2.3171657491	-24.4281647847	18.8665252499
H	-8.9805018225	-23.6574034847	16.8864955231
H	-9.9766935176	-24.1070203840	15.5170730595
H	-7.1006482317	-25.1445381444	17.6321366912
H	-9.6464267629	-26.2838758080	14.3731545117
H	-6.3019251695	-27.4760423270	17.8220616406
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H	-8.1165608255	-23.4606729442	13.9387122169
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H	-10.3727393341	-31.4247415852	19.7813981243
H	-8.3144010558	-30.5681235267	17.9918573725
H	-5.1225073040	-30.7774651363	20.6798297974
H	-10.7394457075	-33.7551269782	20.6202766217
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H	-2.4943495603	-38.0873388426	15.6875965374
H	-1.1151896566	-34.1224754896	16.5982959610
H	-3.8903187512	-37.1624615645	13.8465888679
H	-2.5359659198	-33.2058956912	14.8022863162
H	-4.1019333118	-33.6897286431	13.1641328919
H	0.9153373811	-35.4645350612	17.0878810605
H	-5.3265476626	-28.7192028869	14.4501729772
H	-6.7236842832	-28.4238202304	13.3816035932
H	-6.9145644927	-30.6416380798	14.2573212990

H	-6.4786806465	-30.8584343432	12.5282150121
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H	-8.5914690570	-22.1047793428	14.9826832576
H	-7.1044803339	-23.0156087219	15.3200392103
H	-4.0406431284	-24.4530048961	19.2564154157
H	-2.8660227986	-25.1131720348	20.4034888923
H	0.9897002723	-37.0161380554	16.2471629917
H	1.2631025369	-36.9433220499	18.0002008258
H	-5.8044904698	-37.7041287837	18.1805138759
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H	-9.0265049889	-33.8945223306	21.0548831078
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H	-5.5523332682	-26.2859882165	12.4617441077
H	-4.1758755909	-26.6426481117	13.5817298343
H	-2.9466895177	-28.9135784036	13.7169476520
H	-3.0740205958	-30.2011627372	12.4440631000
H	-2.3374328656	-28.6117602234	12.0345051352
H	0.2599228731	-32.2774824102	21.2312664612
H	-0.9817514120	-33.5062553465	21.5120213049
Mn	-5.3235842931	-30.4088841596	17.0085809677

### TS<sub>Mn(II),VI</sub>

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N	-5.2538830000#	-34.9491730000#	17.0909220000#
C	-5.9174890000#	-33.5196540000#	18.6019940000#
C	-5.5352100000#	-33.7614760000#	16.4934170000#
N	-5.9331420000#	-32.8650510000	17.3811450000
C	-0.1150060000	-33.2509900000	20.8939940000
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C	-1.5947880000	-32.2647230000	19.0650970000
N	-1.5437840000	-30.9150910000	19.3904950000
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C	-3.4830620000	-35.1780160000	14.3945860000
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C	-5.0557650000	-31.3120440000	13.9999410000
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H	-5.7284470000	-28.0697460000	12.9450260000
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C	-2.7011750000	-27.2691820000	12.5440740000
H	-1.6832200000	-27.1495950000	12.1634270000
H	-3.3454940000	-26.5113380000	12.0913050000
H	-2.7217810000	-27.1929070000	13.6350040000
H	-2.4377920000	-29.7429070000	14.1180730000
H	-2.6194790000	-31.0144850000	12.8646240000
H	-1.2552110000	-29.8591320000	12.7596300000
H	0.2536120000	-32.2773680000	21.2365390000
H	-0.9789120000	-33.5157820000	21.5115150000
Mn	-5.2929990000	-30.4824050000	17.0185230000

**Prod<sub>Mn(II),VI</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-4.8228215581	-36.0967869062	19.2296835908
C	-5.1000867358	-34.9365665543	18.3210209219
N	-4.8643579371	-34.9655198390	16.9548640529
C	-5.5334881240	-33.6564629051	18.5676671596
C	-5.1352385780	-33.7398624634	16.4410236186
N	-5.5407729791	-32.9151042958	17.3980460052
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.1402279713	-32.9529723910	19.3819111682
C	-1.2686276424	-32.0562360169	18.9811127608
N	-1.2620575732	-30.6842392083	19.2038212090
C	-2.4935062508	-32.3090259327	18.4172147980
C	-2.4388750563	-30.1691204564	18.7630719411
N	-3.2096092193	-31.1324601353	18.2874952779
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2788046215	-26.3825278637	18.6579189975
C	-4.1253673116	-26.3179205890	17.3793583577
C	-4.2337883220	-27.6789312835	16.6874438443
O	-3.9851170506	-27.7818274409	15.4776656956
O	-4.5742479806	-28.6494658629	17.4751713490
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.9935288287	-24.0765919300	15.8133950517
C	-8.4675740229	-25.5013136294	15.8820173580
C	-8.1989616594	-26.1244728066	17.1087854127
C	-8.2781365578	-26.2609332097	14.7184108917
C	-7.7744615401	-27.4530932008	17.1839466947
C	-7.8597097497	-27.5889794647	14.7730638058
C	-7.6136519286	-28.1915410543	16.0112796376
O	-7.2596654270	-29.5149683120	16.1096646972
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.6624312749	-31.8771650688	20.4966889661
C	-8.3341231449	-31.3190382531	20.0886507561



N	-7.2546718602	-31.1951923848	20.9548778527
C	-7.8465724214	-30.9220430067	18.8697482275
C	-6.1856471272	-30.7375324222	20.2448638320
N	-6.5163245312	-30.5717453215	18.9795708535
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8406489447	-36.5749887648	17.4502851193
C	-1.6660123164	-36.1331441914	16.2593462220
C	-1.6032787847	-34.8107186383	15.7912008893
C	-2.4900904697	-37.0267742958	15.5634921403
C	-2.3393480271	-34.3868947192	14.6899590522
C	-3.2483425768	-36.6172647776	14.4618052313
C	-3.1878797612	-35.2872627364	14.0191142401
O	-3.9565472875	-34.9224171339	12.9713327784
C	-5.1021183396	-29.0380932515	12.8357735501
C	-5.0129547017	-30.3693844177	12.7277824585
C	-4.9570219815	-31.2807605756	13.9098057415
O	-5.2983028151	-30.7970812713	15.0555168145
O	-4.5998681696	-32.4679952653	13.7362612673
H	-4.7654797763	-35.7109473360	20.2541313990
H	-3.8262051960	-36.4976055473	18.9966879557
H	-5.8124027273	-33.2188074928	19.5139143800
H	-4.9952121594	-33.4598901635	15.4031658533
H	-5.5846084596	-38.0439415142	19.8611408233
H	0.8162960337	-32.5102564390	19.0732611569
H	-0.2359391575	-33.8890250433	18.8226141365
H	-2.8931779996	-33.2524359273	18.0812562095
H	-2.7062850022	-29.1242445016	18.7653894703
H	0.7223307847	-33.9085634131	21.1484593724
H	-3.7495604297	-27.0929280822	19.3479183697
H	-2.2858103739	-26.7876109419	18.4099157008
H	-5.1439873685	-25.9899117697	17.6268509534
H	-3.7063407218	-25.5993248640	16.6682376987
H	-2.6169671172	-24.3059130207	18.6708605652
H	-9.0892165445	-23.6828153991	16.8328959946
H	-10.0128178888	-24.0933735924	15.4011944353
H	-8.3271210115	-25.5603054019	18.0306951793
H	-8.4784178234	-25.8150134385	13.7467755226
H	-7.5473084264	-27.9268330121	18.1333144148
H	-7.7301873125	-28.1674782682	13.8622125502
H	-8.0569268382	-23.4402052909	13.9363150544
H	-9.8953697543	-31.5764168012	21.5268760307
H	-10.4323376392	-31.4225829490	19.8641680130
H	-8.3454839044	-30.8650122174	17.9146392818
H	-5.2074416434	-30.5588078307	20.6657742463

H	-10.7178248380	-33.7851902252	20.6601757571
H	-1.0702175474	-35.9400125412	18.3189250216
H	-1.1280167617	-37.5939396507	17.7380146654
H	-2.5490297918	-38.0635572321	15.8898134256
H	-0.9692769674	-34.0886170642	16.3018875533
H	-3.8958497813	-37.3108421809	13.9338005428
H	-2.2921924609	-33.3594737479	14.3456935815
H	-4.1021845766	-33.9487402163	12.9969558358
H	0.9940751159	-35.5149377181	16.9142903899
H	-5.1023336923	-28.5513915741	13.8070108904
H	-5.1081285994	-28.4079072697	11.9491747707
H	-6.7375303797	-29.8151971813	15.3295834893
H	-4.9248560614	-30.8676724877	11.7655509135
H	-4.4577596957	-35.7287409965	16.4237650546
H	-7.2739698248	-31.3739360083	21.9479809082
H	-0.4920525509	-30.1499283190	19.5783724463
H	-8.5861606969	-22.1033260126	14.9691033171
H	-7.1261266817	-23.0273296305	15.3795658690
H	-4.0802088787	-24.6001407606	19.6170839341
H	-2.5032178772	-25.0989135215	20.2495677375
H	0.9313408210	-37.1814784461	16.3349680659
H	1.2473247498	-36.8520168326	18.0507101066
H	-5.9186796622	-37.6631928669	18.1631666365
H	-6.8532911078	-36.8740527142	19.4402652035
H	-9.5370868232	-33.7180237994	19.3344229641
H	-8.9813112533	-33.8964225553	21.0031419156
S	-1.3559108492	-30.5295729172	13.7117226183
C	-1.9733323327	-30.4947345138	15.4268932424
C	-1.4384437313	-28.7387243340	13.3564825894
H	-0.7151312000	-28.1825954791	13.9619791138
H	-1.1966372559	-28.6043729653	12.2984611428
H	-2.4440177292	-28.3629787856	13.5596267367
H	-2.8505211602	-29.8470451023	15.4873468759
H	-2.2569958578	-31.5105433913	15.7049847711
H	-1.2081287049	-30.1365341099	16.1239609101
H	-0.0113953983	-32.3303307646	21.4789393027
H	-1.0440293493	-33.7400749002	21.2037528675
Mn	-5.1469712399	-30.6068196745	17.1709596571

### React<sub>Fe(II),V</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.1587119644	-35.8824193760	19.3823273018
C	-5.4842756849	-34.8249361470	18.3711446737
N	-5.2013397419	-34.9475775469	17.0200884169

C	-5.9583825767	-33.5426424374	18.5077484613
C	-5.4859862268	-33.7613744953	16.4184483252
N	-5.9403528633	-32.8778795701	17.2927159248
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.6036076846	-33.2540327254	19.4293958239
C	-1.7222000641	-32.3021863788	19.1139971106
N	-1.7365204872	-30.9754220036	19.5272096103
C	-2.8537502346	-32.4316214528	18.3425440353
C	-2.8367765135	-30.3720747877	18.9990338311
N	-3.5343651988	-31.2299845778	18.2765803058
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2935146850	-26.4206574547	18.7476165132
C	-3.5758336382	-26.3785061555	17.2460231603
C	-3.8023918046	-27.7499965961	16.6070867052
O	-3.4917707455	-27.8827186376	15.3960216746
O	-4.3258307740	-28.6349600825	17.3543389818
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.9420804550	-24.1926807677	15.7379328538
C	-8.3472481692	-25.5967891092	15.8212891942
C	-7.5073444598	-25.9878761900	16.8797213342
C	-8.7053004331	-26.6083534465	14.9153660381
C	-7.0440049130	-27.2962494598	17.0302969674
C	-8.2511078961	-27.9239988509	15.0490187558
C	-7.3881747494	-28.3153022862	16.1052767052
O	-6.9595146819	-29.5698886043	16.2021650114
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.7156710053	-31.8668567835	20.3934798228
C	-8.3842249661	-31.2664174462	20.0547132607
N	-7.3153869587	-31.2138606942	20.9444443735
C	-7.8831543047	-30.7482509717	18.8869928127
C	-6.2399239753	-30.6871567726	20.2875531742
N	-6.5524637810	-30.4067050944	19.0390098562
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8145056460	-36.7813130467	17.4744489557
C	-1.7304292368	-36.2564484739	16.3874651760
C	-1.7405838393	-34.8945964149	16.0470751390
C	-2.5761766806	-37.1075870541	15.6653535128
C	-2.5560430135	-34.3915210080	15.0389119589
C	-3.4008909697	-36.6266299438	14.6448087034
C	-3.3972589484	-35.2611839252	14.3186886118
O	-4.2402952961	-34.8322682008	13.3588138689
C	-5.5567773368	-29.0758342767	13.4923353530
C	-5.9479311616	-30.5457489482	13.4794298578
C	-4.8126268893	-31.4280581350	14.0131676018

O	-4.4546169209	-31.2655487018	15.2140331847
O	-4.2763256087	-32.2291476556	13.1916409581
H	-5.4172863431	-35.4837566133	20.3700557995
H	-4.0697828295	-36.0404762762	19.3924655785
H	-6.2772087098	-33.0543539777	19.4133716397
H	-5.3198412517	-33.5863716213	15.3705791741
H	-5.5668439102	-37.9501497472	19.9512157796
H	0.2531042972	-33.0458465980	18.7711952266
H	-0.9481057383	-34.2574998660	19.1614647642
H	-3.2014311080	-33.3009928297	17.8093253704
H	-3.0901441634	-29.3302036426	19.1169770665
H	0.6768446591	-33.9930338743	21.0323428678
H	-4.1188177785	-26.9431009173	19.2440140560
H	-2.3896198248	-27.0206502889	18.9296435189
H	-4.4955798604	-25.8049363689	17.0607129137
H	-2.7689604046	-25.8701365048	16.7062310753
H	-2.2725125052	-24.4976391048	18.8605947931
H	-9.1145727572	-23.8300121744	16.7602230480
H	-9.9366237597	-24.2655549066	15.2780003338
H	-7.2248681623	-25.2483775524	17.6295049059
H	-9.3875073750	-26.3715464233	14.0988300903
H	-6.3975598442	-27.5659042642	17.8573886815
H	-8.5824169672	-28.6889309612	14.3488920822
H	-7.9898149580	-23.3904666070	13.9279091860
H	-10.0500375806	-31.5111954144	21.3779135633
H	-10.4428604811	-31.4855247569	19.6691197342
H	-8.3580449581	-30.6138658666	17.9272092129
H	-5.2654936448	-30.5609758314	20.7352770358
H	-10.7335467585	-33.7947686610	20.5844885363
H	-1.0685681015	-36.3191565450	18.4399167902
H	-0.9828661415	-37.8572514351	17.6050747907
H	-2.5889983751	-38.1708965302	15.8979380369
H	-1.1068413036	-34.1997494105	16.5931556103
H	-4.0520993978	-37.2919641198	14.0855471804
H	-2.5903454405	-33.3276075073	14.8240762483
H	-4.1930880365	-33.8394891305	13.2693146514
H	0.8817029837	-35.4581963709	17.0808927216
H	-5.1356528277	-28.7756835006	14.4545847183
H	-6.3897407092	-28.4210531914	13.2261509794
H	-6.7839508742	-30.6081331757	14.1845379673
H	-6.2569730856	-30.8886160822	12.4882616574
H	-4.7554589198	-35.7307653232	16.5554476448
H	-7.3431760487	-31.4823495878	21.9165534647
H	-1.0378618805	-30.5246586459	20.0978907730

H	-8.6737282438	-22.1467829922	14.9956438271
H	-7.1527323534	-22.9571126167	15.4252619203
H	-4.0069470378	-24.4137938329	19.1885346623
H	-2.9062959739	-25.0582887311	20.4152268655
H	0.9627766803	-37.0049438853	16.2325885538
H	1.3118835072	-36.9267605796	17.9716756296
H	-5.5858725023	-37.6764180761	18.2034775485
H	-6.9456591211	-37.1261386071	19.1924937563
H	-9.4200323366	-33.7809817418	19.3847852964
H	-9.0409881526	-33.8287227729	21.1101337681
S	-4.2631719986	-28.6636985490	12.2341680160
C	-2.7347385640	-29.3988583401	12.9117384175
C	-4.0125441964	-26.8995775789	12.6219308197
H	-3.2187578594	-26.5275909149	11.9703208483
H	-4.9508005640	-26.3867810983	12.3993651790
H	-3.7530186905	-26.8257264576	13.6844648793
H	-2.7181962844	-29.1937496377	13.9858909751
H	-2.7729943402	-30.4673796964	12.6948480083
H	-1.9034605092	-28.9225324154	12.3867599634
H	0.2969690458	-32.2768192010	21.1830672112
H	-0.9331614534	-33.4869860139	21.5820291201
Fe	-5.3895210061	-30.4761212946	17.0387869343

### TS<sub>Fe(II),V</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
C	-5.1787990000#	-35.8859580000#	19.4510650000#
C	-5.4967650000#	-34.8032170000#	18.4662570000#
N	-5.3068200000#	-34.9450100000#	17.1008200000#
C	-5.8873670000#	-33.4952920000#	18.6258760000#
C	-5.5617160000#	-33.7496250000#	16.5086790000#
N	-5.9086370000	-32.8398910000	17.4047830000
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.5141010000	-33.2062030000	19.4070010000
C	-1.6290650000	-32.2568250000	19.0915920000
N	-1.6255110000	-30.9300390000	19.5007720000
C	-2.7903300000	-32.3917040000	18.3677470000
C	-2.7467270000	-30.3305780000	19.0159280000
N	-3.4726100000	-31.1904110000	18.3259740000
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2444310000	-26.4522250000	18.8160540000
C	-3.5590120000	-26.4986750000	17.3166430000
C	-3.6804460000	-27.9253950000	16.7902950000
O	-3.0103760000	-28.2794370000	15.8004830000
O	-4.5049690000	-28.6629950000	17.4456840000

C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.9225250000	-24.1742550000	15.7712800000
C	-8.3424120000	-25.5818340000	15.7732580000
C	-7.6640590000	-26.0991120000	16.8896430000
C	-8.5299060000	-26.4563480000	14.6926540000
C	-7.1998370000	-27.4143610000	16.9401660000
C	-8.0798240000	-27.7794790000	14.7263580000
C	-7.4071880000	-28.2959910000	15.8581430000
O	-6.9924730000	-29.5810100000	15.8869180000
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.8561140000	-31.8973090000	20.0960270000
C	-8.5475150000	-31.2365360000	19.7912330000
N	-7.5616080000	-31.0218310000	20.7499300000
C	-7.9829770000	-30.8135960000	18.6148690000
C	-6.4665690000	-30.5023050000	20.1265880000
N	-6.6913640000	-30.3752750000	18.8341230000
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8145070000	-36.7376540000	17.5072370000
C	-1.7564780000	-36.2122650000	16.4422670000
C	-1.7797150000	-34.8528500000	16.0912490000
C	-2.6340470000	-37.0661180000	15.7612160000
C	-2.6418810000	-34.3530030000	15.1179070000
C	-3.5009880000	-36.5902670000	14.7747830000
C	-3.5165520000	-35.2245070000	14.4395870000
O	-4.4071410000	-34.8119720000	13.5213880000
C	-5.0699030000	-28.9081450000	13.5672320000
C	-5.7898320000	-30.1333300000	13.6211170000
C	-5.0025770000	-31.3347450000	14.1094640000
O	-4.5503570000	-31.3313010000	15.3017490000
O	-4.8054240000	-32.2599420000	13.2778260000
H	-5.4622590000	-35.5252120000	20.4459160000
H	-4.0893190000	-36.0350440000	19.4781500000
H	-6.1181380000	-32.9813300000	19.5451750000
H	-5.4591340000	-33.5831480000	15.4514630000
H	-5.5854440000	-37.9736470000	19.9351370000
H	0.3712200000	-32.9552720000	18.8051000000
H	-0.8273500000	-34.2012390000	19.0798710000
H	-3.1646120000	-33.2654900000	17.8605200000
H	-2.9941940000	-29.2918070000	19.1604430000
H	0.6828110000	-33.9816840000	21.0563690000
H	-4.0387720000	-26.9832850000	19.3527030000
H	-2.3093710000	-26.9995480000	19.0060220000
H	-4.5225410000	-26.0041400000	17.1337510000
H	-2.7901270000	-25.9725480000	16.7425800000

H	-2.3038560000	-24.4889430000	18.8200350000
H	-9.0190170000	-23.8337470000	16.8098860000
H	-9.9456410000	-24.2170100000	15.3742290000
H	-7.5068990000	-25.4577420000	17.7559180000
H	-9.0702150000	-26.1086020000	13.8135020000
H	-6.6663410000	-27.7853830000	17.8057470000
H	-8.2788280000	-28.4422870000	13.8885460000
H	-8.0538020000	-23.3876800000	13.9205210000
H	-10.3386850000	-31.4074460000	20.9527370000
H	-10.5157540000	-31.7327760000	19.2383330000
H	-8.3849330000	-30.8118990000	17.6131700000
H	-5.5418170000	-30.2633690000	20.6297830000
H	-10.7147830000	-33.8590160000	20.5417920000
H	-1.0338760000	-36.2582740000	18.4723900000
H	-1.0038630000	-37.8069720000	17.6593070000
H	-2.6398680000	-38.1272570000	16.0022460000
H	-1.1214150000	-34.1551680000	16.6026460000
H	-4.1743150000	-37.2582720000	14.2462860000
H	-2.6887140000	-33.2876500000	14.9129080000
H	-4.4503150000	-33.8121440000	13.4517110000
H	0.9047410000	-35.4655100000	17.0553250000
H	-4.4595900000	-28.6447660000	14.4273140000
H	-5.5189750000	-28.0734130000	13.0345020000
H	-6.5058560000	-29.8553220000	14.6717150000
H	-6.4066400000	-30.3657130000	12.7523890000
H	-4.9190280000	-35.7471470000	16.6174460000
H	-7.6550300000	-31.1928090000	21.7396160000
H	-0.9025120000	-30.4775360000	20.0382160000
H	-8.6459400000	-22.1335810000	15.0276070000
H	-7.1262100000	-22.9868050000	15.3704190000
H	-4.0341880000	-24.4601280000	19.1770880000
H	-2.8862330000	-25.0017810000	20.4108350000
H	0.9330620000	-37.0296630000	16.2371610000
H	1.3156510000	-36.9265860000	17.9681140000
H	-5.5483430000	-37.6418120000	18.2001810000
H	-6.9465720000	-37.1373350000	19.1596280000
H	-9.2621980000	-33.9159270000	19.5160540000
H	-9.1110310000	-33.6076990000	21.2494650000
S	-3.1553830000	-29.0018740000	12.2469540000
C	-2.1849740000	-30.1567080000	13.2771620000
C	-2.4485410000	-27.4122700000	12.7988530000
H	-1.4165700000	-27.3325860000	12.4469690000
H	-3.0452060000	-26.6153980000	12.3479210000
H	-2.4944740000	-27.3599580000	13.8903960000

H	-2.3673860000	-29.9397620000	14.3318730000
H	-2.5266380000	-31.1625030000	13.0286290000
H	-1.1278380000	-30.0438820000	13.0232270000
H	0.2557220000	-32.2808170000	21.2441800000
H	-0.9690150000	-33.5276490000	21.5200660000
Fe	-5.3023850000	-30.4948110000	17.0852880000

**Prod<sub>Fe(II),V</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-4.7126384854	-36.2313678579	18.9413290542
C	-5.0238167884	-35.1118574016	17.9924773157
N	-4.8911376944	-35.2179893813	16.6154202915
C	-5.3888032456	-33.8043483155	18.2017736512
C	-5.1376333719	-34.0026745380	16.0620431409
N	-5.4421446855	-33.1195874026	17.0001299171
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.2090736711	-33.1110669407	19.3605316117
C	-1.3435912573	-32.2409869262	18.9186642110
N	-1.4385136230	-30.9027975201	19.2762586386
C	-2.4744655105	-32.4819050272	18.1779402755
C	-2.5819927209	-30.3949582297	18.7485347078
N	-3.2343735354	-31.3279513039	18.0802105017
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.1981274653	-26.4342768780	18.7505575850
C	-4.3101427456	-26.5737881413	17.6954713059
C	-4.2518414060	-27.9573881015	17.0515159837
O	-3.5650540782	-28.1206218846	16.0276843577
O	-4.8794289196	-28.8930368356	17.6829588267
C	-8.1409660000	-23.1040170000	14.9750030000
C	-9.0298389976	-24.2913842367	15.3948142618
C	-8.3398104730	-25.6456314998	15.3823944079
C	-8.2231042606	-26.4216036947	16.5437480747
C	-7.8302926315	-26.1872543992	14.1938336433
C	-7.6422604438	-27.6911055455	16.5303604055
C	-7.2488381012	-27.4538476107	14.1583437535
C	-7.1620949288	-28.2136975617	15.3300401769
O	-6.6420895045	-29.4874267195	15.3277445725
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.9932920492	-32.1171348735	19.5752516856
C	-8.7240988212	-31.4372827045	19.1662332722
N	-8.1062583055	-30.4433591248	19.9144153210
C	-7.8639924415	-31.6730405440	18.1246343827
C	-6.9320864395	-30.1161918471	19.3107074114
N	-6.7599700122	-30.8545914903	18.2303577049



C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8417168510	-36.7197202477	17.3514644563
C	-1.6231719690	-36.2996533344	16.1249741512
C	-1.6081038410	-34.9646727897	15.6924381455
C	-2.3586138813	-37.2182984634	15.3664117379
C	-2.3162446607	-34.5491422678	14.5710090302
C	-3.0788498658	-36.8208727092	14.2360157880
C	-3.0753954310	-35.4769123021	13.8341358353
O	-3.8201005464	-35.1278223155	12.7640396438
C	-4.1117286322	-29.0589230091	13.1063436553
C	-4.3931575377	-30.3212281851	12.7540945644
C	-4.4517845077	-31.4595848750	13.7301709759
O	-4.4097340794	-31.1783606192	14.9805664352
O	-4.5444633709	-32.6174841005	13.2597548186
H	-4.4285322877	-35.7845608645	19.9012211257
H	-3.8231209275	-36.7631937423	18.5765854096
H	-5.5734680450	-33.2973879129	19.1370823024
H	-5.0484836896	-33.7776689448	15.0088778967
H	-5.5528707135	-38.0158298088	19.8800547292
H	0.7380818559	-32.7175840492	18.9665944542
H	-0.3427162262	-34.0969473510	18.9041853648
H	-2.7855471989	-33.3981080192	17.7046812904
H	-2.9097411850	-29.3750922719	18.8562077230
H	0.7178227545	-33.9039632951	21.1733601550
H	-3.3774178232	-27.1592523350	19.5575964114
H	-2.2372869657	-26.7006944649	18.2897753599
H	-5.2911668181	-26.4197605412	18.1575916774
H	-4.1717941492	-25.8217424615	16.9124064385
H	-2.8964806582	-24.2882833498	18.5536906752
H	-9.4292326337	-24.1034227308	16.3990674877
H	-9.9015071830	-24.3302835527	14.7264744102
H	-8.5993568773	-26.0265393250	17.4855148428
H	-7.9038535675	-25.6183002781	13.2696293578
H	-7.5304116708	-28.2782881456	17.4333091120
H	-6.8736794496	-27.8631509577	13.2239097069
H	-7.7517995226	-23.2387189358	13.9604303756
H	-10.6135818064	-31.4315472443	20.1670004500
H	-10.5703524885	-32.3494525873	18.6735511930
H	-7.9456141855	-32.3852807058	17.3191677677
H	-6.2598307595	-29.3330319744	19.6247447837
H	-10.6706710424	-33.9049370417	20.6389963887
H	-1.1817500341	-36.1431411408	18.2246682380
H	-1.0546616474	-37.7708179429	17.5823242418
H	-2.3760778799	-38.2650242193	15.6642963824

H	-1.0398618512	-34.2241544436	16.2504765097
H	-3.6561121807	-37.5338455485	13.6549821829
H	-2.3248485275	-33.5041898284	14.2800482967
H	-3.9884419226	-34.1585288606	12.7836714614
H	0.9185786274	-35.4808884550	16.9744307148
H	-3.9106856340	-28.7842895445	14.1405232606
H	-4.0597643358	-28.2742625525	12.3548450786
H	-6.0862142792	-29.6115565550	14.5428799765
H	-4.5665041441	-30.6073404986	11.7190814318
H	-4.5155314597	-36.0097543596	16.1051499801
H	-8.4819219294	-30.0143894570	20.7468530543
H	-0.7566536172	-30.3828263029	19.8077788471
H	-8.7072912272	-22.1668986572	14.9970348407
H	-7.2822368660	-23.0027469623	15.6470426139
H	-4.0510282262	-24.7341064291	19.8167101213
H	-2.3139492167	-24.9490417042	20.0897524188
H	1.0398613585	-37.1197188025	16.3295715182
H	1.2213386939	-36.8372943788	18.0724769273
H	-6.1464333800	-37.7274023362	18.2344540134
H	-6.7419215111	-36.7338051700	19.5713517433
H	-9.1364439770	-34.1106616276	19.7691278515
H	-9.1756834653	-33.2055983233	21.2881410619
S	0.2507803564	-29.6598389102	15.4129222413
C	-1.2694429448	-30.6693921077	15.2624248843
C	-0.3101836526	-28.4296544377	16.6442806942
H	-0.4430237907	-28.8868489562	17.6300074643
H	0.4660563810	-27.6617243470	16.7106785370
H	-1.2541837487	-27.9802675045	16.3268327854
H	-2.1545519286	-30.0317927777	15.2568558513
H	-1.2102625743	-31.2071737987	14.3126280264
H	-1.3547251638	-31.3918467058	16.0761857223
H	0.0487024502	-32.2806422947	21.3765736407
H	-1.0382032415	-33.6746816757	21.3018432615
Fe	-5.0325760938	-30.8095444766	16.8570519586

### React<sub>Co(II),IV</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.2109057219	-35.8665037996	19.4368617118
C	-5.5388594179	-34.8007895290	18.4357277724
N	-5.2522324488	-34.9126071325	17.0851372228
C	-6.0230475864	-33.5228499406	18.5793638629
C	-5.5466327550	-33.7243990273	16.4905852092
N	-6.0100730246	-32.8504750426	17.3688370683
C	-0.1150060000	-33.2509900000	20.8939940000

C	-0.6636438874	-33.2614353328	19.4493423977
C	-1.7950399352	-32.3117991224	19.1667657617
N	-1.8170630137	-30.9985277677	19.6199113965
C	-2.9262448255	-32.4249156611	18.3907692575
C	-2.9219683705	-30.3865413564	19.1124903996
N	-3.6161790436	-31.2258248931	18.3651265861
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.3492355314	-26.4213815053	18.7694215940
C	-3.6602023828	-26.3836743306	17.2741985752
C	-3.9327357534	-27.7465441471	16.6400331316
O	-3.7345981274	-27.8613661120	15.4074567581
O	-4.3700614071	-28.6527501209	17.4238008493
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.8645318066	-24.1125294253	15.9093267267
C	-8.3340525150	-25.5435348219	15.9751645043
C	-7.5024984829	-25.9824149801	17.0207714743
C	-8.7461852035	-26.5343042471	15.0671159222
C	-7.0822429652	-27.3083602691	17.1492864017
C	-8.3348744948	-27.8649317763	15.1782641182
C	-7.4551918571	-28.3056780524	16.2078265682
O	-7.0429723078	-29.5643617686	16.2505940066
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.7468066369	-31.8666541835	20.4059859009
C	-8.4238741977	-31.2420188554	20.0784987678
N	-7.3637461352	-31.1746657457	20.9782210812
C	-7.9177953209	-30.7270798204	18.9118168719
C	-6.2856698932	-30.6475765984	20.3298681126
N	-6.5909048870	-30.3764992942	19.0768516249
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8088832370	-36.7842368482	17.5014618784
C	-1.7470403063	-36.2546001480	16.4356800226
C	-1.7597545378	-34.8921597699	16.0971781879
C	-2.6103003552	-37.1018136929	15.7300710945
C	-2.5907860795	-34.3858838640	15.1034012107
C	-3.4523294086	-36.6173416832	14.7255065457
C	-3.4477816601	-35.2524861210	14.3986919276
O	-4.3031217380	-34.8196584497	13.4498715179
C	-5.7779959485	-29.1427150307	13.5549120720
C	-6.0867643425	-30.6301659837	13.6139440352
C	-4.8941438204	-31.4172186480	14.1655180428
O	-4.5344618689	-31.2021930689	15.3581935460
O	-4.3087410884	-32.2056896582	13.3651622146
H	-5.5147086867	-35.4981778820	20.4234753052
H	-4.1183099715	-35.9904049201	19.4802505562

H	-6.3476186089	-33.0443032352	19.4881765230
H	-5.3809938485	-33.5470734631	15.4432016625
H	-5.5720475282	-37.9583121811	19.9455982183
H	0.1671634726	-33.0554288982	18.7580793189
H	-1.0140584119	-34.2674598132	19.1997834224
H	-3.2656132842	-33.2785004272	17.8278219165
H	-3.1753309520	-29.3480686440	19.2591332567
H	0.6790083373	-33.9954581128	21.0024463510
H	-4.1806867305	-26.9105152138	19.2891920367
H	-2.4626351095	-27.0490925234	18.9401250155
H	-4.5678072271	-25.7886879371	17.0995547937
H	-2.8523997946	-25.8986550797	16.7141406346
H	-2.2649634030	-24.5313636387	18.8384944786
H	-8.8585302388	-23.6955835143	16.9251815439
H	-9.9212643275	-24.1475070826	15.6102557147
H	-7.1868489220	-25.2643487883	17.7785530571
H	-9.4347510652	-26.2652436237	14.2655341154
H	-6.4401185432	-27.6041281983	17.9705909640
H	-8.7081327465	-28.6092472932	14.4763477157
H	-8.1642022115	-23.4480079150	13.9345409364
H	-10.0920244407	-31.5248635666	21.3916597328
H	-10.4772185952	-31.4932873007	19.6807920735
H	-8.3794999471	-30.6023547406	17.9443985983
H	-5.3159186445	-30.5134940778	20.7846214160
H	-10.7268370614	-33.8162041820	20.5765244379
H	-1.0448258995	-36.3282324492	18.4743416352
H	-0.9736528686	-37.8611229719	17.6291213316
H	-2.6228408184	-38.1651678494	15.9622404975
H	-1.1131195932	-34.2000067994	16.6313478422
H	-4.1160806173	-37.2802182297	14.1782154035
H	-2.6211769014	-33.3229095934	14.8839060241
H	-4.2569462486	-33.8279320301	13.3709494438
H	0.8794588764	-35.4574995087	17.0839670337
H	-5.3607613224	-28.7832445850	14.4974333558
H	-6.6503970099	-28.5470192155	13.2784814174
H	-6.9052592751	-30.6976884933	14.3390376691
H	-6.3895572589	-31.0367059459	12.6450916099
H	-4.8026344094	-35.6907816238	16.6160010302
H	-7.3986137745	-31.4372866126	21.9517893066
H	-1.1194355026	-30.5610122434	20.2018223765
H	-8.6216007137	-22.1204532129	15.0215427912
H	-7.0901374851	-22.9881066690	15.2637575312
H	-3.9893449129	-24.3866921715	19.1971099385
H	-2.8873818689	-25.0513985483	20.4116358845

H	0.9450084179	-36.9987642941	16.2243356713
H	1.3266827143	-36.9315913971	17.9570405649
H	-5.5368350988	-37.6457932474	18.2050882418
H	-6.9487856168	-37.1612148267	19.1550172318
H	-9.4075719021	-33.7667011005	19.3835439977
H	-9.0362669355	-33.8207229209	21.1103453854
S	-4.5357181400	-28.6952554943	12.2575184122
C	-2.9529702727	-29.3387306127	12.9022246189
C	-4.3681290510	-26.9150802988	12.6185921722
H	-3.6172554840	-26.5070955529	11.9385104345
H	-5.3398924211	-26.4560578384	12.4246141599
H	-4.0799647195	-26.8131723306	13.6704548830
H	-2.9157321464	-29.1157884343	13.9719682052
H	-2.9425822260	-30.4120659319	12.7073416833
H	-2.1621868133	-28.8301037282	12.3456717694
H	0.3133404268	-32.2771938055	21.1593428105
H	-0.9042989477	-33.4802023496	21.6170760162
Co	-5.4073159159	-30.4247536514	17.1758533414

### TS<sub>Co(II),IV</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
C	-5.1508950000#	-35.9010150000#	19.4508540000#
C	-5.4603950000#	-34.8100060000#	18.4733800000#
N	-5.2646190000#	-34.9406940000#	17.1079120000#
C	-5.8519510000#	-33.5032510000#	18.6417350000#
C	-5.5177240000#	-33.7388100000#	16.5251550000#
N	-5.8671930000	-32.8376370000	17.4272000000
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.5246780000	-33.1974330000	19.4092820000
C	-1.6429130000	-32.2493340000	19.0972220000
N	-1.6412630000	-30.9197940000	19.5001340000
C	-2.8009840000	-32.3881450000	18.3699850000
C	-2.7578770000	-30.3210060000	19.0081550000
N	-3.4822300000	-31.1859280000	18.3204830000
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2432240000	-26.4495900000	18.8095230000
C	-3.4983020000	-26.4904270000	17.3001400000
C	-3.6610590000	-27.9100800000	16.7596320000
O	-3.0343680000	-28.2495380000	15.7338390000
O	-4.4763120000	-28.6398080000	17.4261130000
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.8571780000	-24.1526610000	15.8582110000
C	-8.2831950000	-25.5637010000	15.8569090000
C	-7.5877360000	-26.0783100000	16.9643420000

C	-8.5018880000	-26.4480140000	14.7902240000
C	-7.1337250000	-27.3971430000	17.0188660000
C	-8.0616700000	-27.7745440000	14.8283050000
C	-7.3663710000	-28.2877660000	15.9493020000
O	-6.9645830000	-29.5765430000	15.9773130000
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.8490660000	-31.9026670000	20.0615380000
C	-8.5378900000	-31.2483290000	19.7515200000
N	-7.5641650000	-30.9981420000	20.7141370000
C	-7.9628890000	-30.8606000000	18.5683780000
C	-6.4650570000	-30.4918090000	20.0875980000
N	-6.6771150000	-30.4078440000	18.7893130000
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8184310000	-36.7291590000	17.4938950000
C	-1.7467940000	-36.1865310000	16.4258720000
C	-1.7540380000	-34.8241630000	16.0863010000
C	-2.6257000000	-37.0265310000	15.7292870000
C	-2.6034880000	-34.3080010000	15.1106300000
C	-3.4807740000	-36.5338020000	14.7406880000
C	-3.4819970000	-35.1648190000	14.4190560000
O	-4.3627130000	-34.7341400000	13.4994780000
C	-5.1522080000	-28.8622310000	13.5765430000
C	-5.8274210000	-30.1098460000	13.6757680000
C	-4.9846520000	-31.2782530000	14.1483890000
O	-4.5551450000	-31.2881290000	15.3489170000
O	-4.7264030000	-32.1722270000	13.2996260000
H	-5.4185400000	-35.5395710000	20.4498210000
H	-4.0640830000	-36.0699610000	19.4668300000
H	-6.0873270000	-32.9975950000	19.5649390000
H	-5.4102840000	-33.5628930000	15.4699870000
H	-5.5904450000	-37.9842090000	19.9267560000
H	0.3568060000	-32.9421380000	18.8036880000
H	-0.8376570000	-34.1914850000	19.0788420000
H	-3.1704710000	-33.2630670000	17.8623750000
H	-3.0057830000	-29.2807910000	19.1413200000
H	0.6869550000	-33.9795940000	21.0439180000
H	-4.0657350000	-26.9695120000	19.3133780000
H	-2.3244230000	-27.0105150000	19.0370440000
H	-4.4345350000	-25.9593520000	17.0792580000
H	-2.6906460000	-25.9926560000	16.7545180000
H	-2.2787760000	-24.4981090000	18.8509530000
H	-8.8735190000	-23.7837540000	16.8914150000
H	-9.9082920000	-24.2025570000	15.5428660000
H	-7.4077150000	-25.4307470000	17.8215640000

H	-9.0598380000	-26.1059950000	13.9198270000
H	-6.5856320000	-27.7634890000	17.8764340000
H	-8.2863690000	-28.4431320000	14.0016600000
H	-8.1356720000	-23.4146580000	13.9245690000
H	-10.3370370000	-31.3929200000	20.9034220000
H	-10.5022540000	-31.7558160000	19.1957360000
H	-8.3519540000	-30.8909660000	17.5627680000
H	-5.5481820000	-30.2299300000	20.5935190000
H	-10.7178740000	-33.8511060000	20.5440820000
H	-1.0417410000	-36.2566600000	18.4616160000
H	-1.0174990000	-37.7982390000	17.6347010000
H	-2.6424680000	-38.0898340000	15.9600860000
H	-1.0922740000	-34.1374130000	16.6078640000
H	-4.1562070000	-37.1907470000	14.2011780000
H	-2.6362030000	-33.2411120000	14.9113880000
H	-4.3951700000	-33.7335420000	13.4438270000
H	0.9142890000	-35.4663260000	17.0676560000
H	-4.5202900000	-28.5632040000	14.4089400000
H	-5.6457320000	-28.0551110000	13.0412500000
H	-6.5112430000	-29.8484080000	14.7462690000
H	-6.4644720000	-30.3758220000	12.8313060000
H	-4.8759430000	-35.7390360000	16.6191060000
H	-7.6693320000	-31.1328450000	21.7081250000
H	-0.9200120000	-30.4643590000	20.0376410000
H	-8.6426440000	-22.1327880000	15.0415180000
H	-7.0988210000	-22.9765470000	15.2872060000
H	-4.0205180000	-24.4485420000	19.1433860000
H	-2.9260280000	-25.0044980000	20.4184770000
H	0.9361310000	-37.0223430000	16.2341590000
H	1.3066100000	-36.9396070000	17.9687610000
H	-5.5684220000	-37.6406200000	18.1935630000
H	-6.9445170000	-37.1167050000	19.1735980000
H	-9.2580770000	-33.9360150000	19.5305810000
H	-9.1181840000	-33.5902920000	21.2580380000
S	-3.2729570000	-28.9079570000	12.1889530000
C	-2.2308930000	-30.0345290000	13.1789850000
C	-2.6039920000	-27.2986750000	12.7318690000
H	-1.5925390000	-27.1731430000	12.3365330000
H	-3.2510330000	-26.5199320000	12.3203580000
H	-2.6041900000	-27.2634130000	13.8252600000
H	-2.3853990000	-29.8264150000	14.2401950000
H	-2.5486050000	-31.0494380000	12.9364850000
H	-1.1868620000	-29.8842520000	12.8920820000
H	0.2541540000	-32.2817510000	21.2484630000

H	-0.9630930000	-33.5362290000	21.5242150000
Co	-5.2555130000	-30.5048960000	17.1302080000

**Prod<sub>Co(m),IV</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-4.5956625813	-36.3724658527	18.9913517376
C	-4.8324688340	-35.1471171352	18.1674209277
N	-4.9856290851	-35.1851130502	16.7909526978
C	-4.9691214319	-33.8220899930	18.4947289218
C	-5.1741978451	-33.9199563481	16.3397764364
N	-5.1723895719	-33.0662653143	17.3501413001
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.0407952245	-32.8221644095	19.4161818661
C	-1.2153634372	-31.9926269514	19.0104737657
N	-1.4576274557	-30.7218492374	19.5206093104
C	-2.2926713450	-32.2561160499	18.2063658671
C	-2.6309191845	-30.2693391874	19.0119477418
N	-3.1614385143	-31.1807524912	18.2173637824
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2294944270	-26.4576303463	18.8132229277
C	-4.1805158558	-26.5922988904	17.6079415348
C	-4.1205422569	-28.0223219878	17.0669683131
O	-3.2518809305	-28.3138415585	16.2301789021
O	-4.9487139583	-28.8536161315	17.6143789811
C	-8.1409660000	-23.1040170000	14.9750030000
C	-9.1175624211	-24.2043690184	14.5256819373
C	-8.6658668721	-25.6140390185	14.8598210495
C	-9.4241926430	-26.4509277790	15.6875448386
C	-7.4858569941	-26.1436878403	14.3161103283
C	-9.0447354668	-27.7692690015	15.9414603433
C	-7.0880000374	-27.4558027731	14.5603511204
C	-7.8808197214	-28.2894776178	15.3633152849
O	-7.5937135265	-29.5959230468	15.5871804472
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.9512641151	-31.9174491396	20.1056589094
C	-8.7710977719	-31.2955348211	19.4278115662
N	-8.6485048695	-29.9313369381	19.1921385857
C	-7.6167301559	-31.8385535328	18.9294204983
C	-7.4620392712	-29.7016113329	18.5801318037
N	-6.8097009267	-30.8403801804	18.4134894324
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8446792138	-36.6884069919	17.3712754857
C	-1.6574296665	-36.2407272944	16.1726432801
C	-1.6149131092	-34.9049616513	15.7439079188



C	-2.4732566517	-37.1215630939	15.4523582572
C	-2.3814377922	-34.4506264047	14.6775329248
C	-3.2507931814	-36.6855037325	14.3729174564
C	-3.2290304981	-35.3363548342	13.9906830726
O	-4.0394163369	-34.9325659220	12.9857978657
C	-4.0454009262	-29.0098983122	13.1929263044
C	-4.4788732210	-30.2554593458	12.9660714240
C	-4.7851598746	-31.2223090751	14.0644991315
O	-5.1653116408	-30.7328081384	15.1986886056
O	-4.6462140763	-32.4420854273	13.8232971782
H	-4.2195687622	-36.0587030900	19.9715392051
H	-3.7975869214	-36.9685385889	18.5278825764
H	-4.9045130686	-33.3579246927	19.4677690209
H	-5.2506777358	-33.6338345824	15.3000229824
H	-5.6405979639	-38.1251519291	19.7764318100
H	0.8942208335	-32.2769216753	19.2294853875
H	-0.0140962474	-33.7072900234	18.7715523344
H	-2.5052008287	-33.1400020782	17.6292301916
H	-3.0625040516	-29.3036026207	19.2165493132
H	0.7479830370	-33.8669628684	21.1662414964
H	-3.5868456800	-27.1117196901	19.6216616604
H	-2.2372434599	-26.8237025002	18.5157572670
H	-5.2040543534	-26.3400455394	17.9052663187
H	-3.8653865280	-25.9072987586	16.8143503142
H	-2.7236116363	-24.3547996399	18.5598967353
H	-10.0998539789	-24.0234447652	14.9795230720
H	-9.2669679016	-24.1213658836	13.4399064207
H	-10.3435295527	-26.0707052518	16.1294977439
H	-6.8698872713	-25.5235527995	13.6678435625
H	-9.6541276194	-28.4238978285	16.5587601029
H	-6.1826575196	-27.8535978905	14.1131812082
H	-7.1574334833	-23.2330890737	14.5111965093
H	-10.1457510000	-31.4011865996	21.0567104707
H	-10.8533184223	-31.7777306922	19.4930509097
H	-7.3152770449	-32.8716315232	18.8991994648
H	-7.1059712830	-28.7402938165	18.2479375455
H	-10.5975155252	-33.8510622345	20.8701440330
H	-1.1539769466	-36.1109753442	18.2556601748
H	-1.0746626398	-37.7367230613	17.5985956728
H	-2.5115811359	-38.1705696072	15.7405433319
H	-0.9691670886	-34.1964045575	16.2582560439
H	-3.8853719171	-37.3732316316	13.8213713770
H	-2.3646866987	-33.4075461623	14.3867107861
H	-4.1598502318	-33.9587790186	13.0357983870

H	0.9410570354	-35.4849167033	16.9807058798
H	-3.9223208629	-28.6357839111	14.2060770830
H	-3.7576074316	-28.3621880028	12.3682341369
H	-6.6948031723	-29.8412337378	15.2721420274
H	-4.5362280525	-30.6720840890	11.9629487066
H	-4.7798718117	-35.9747317890	16.1899938237
H	-9.3369111634	-29.2254189405	19.4059821179
H	-0.8477694105	-30.2036354490	20.1352735046
H	-8.5134029050	-22.1108117652	14.7009298366
H	-7.9984155415	-23.1284070786	16.0608775225
H	-4.0825964011	-24.6359438002	19.6565055033
H	-2.4278872442	-24.9662780637	20.1954382293
H	1.0176109394	-37.1198499246	16.3204074788
H	1.2231616403	-36.8580326427	18.0634669930
H	-6.2432178661	-37.5757384842	18.2031895672
H	-6.6495180078	-36.6681977304	19.6653652553
H	-9.5756816744	-33.9533686311	19.4281976338
H	-8.8513318019	-33.5711526742	20.9985274112
S	0.1081425643	-29.9021022168	15.0262283372
C	-1.4593684357	-30.8430307536	15.0464437488
C	-0.0691580446	-29.0024210041	16.6088630824
H	-0.0396047148	-29.6935765943	17.4572093301
H	0.7746266725	-28.3100544030	16.6837688332
H	-1.0106745419	-28.4480714675	16.6154704239
H	-2.2847642032	-30.1875323212	15.3311269378
H	-1.6274063918	-31.2142283992	14.0330625040
H	-1.4016622628	-31.6851777097	15.7396806057
H	-0.1292550337	-32.3826626744	21.5625162565
H	-1.0249718317	-33.8299522233	21.0808590247
Co	-5.0241837169	-30.8511369898	17.2471102927

### React<sub>Zn(II),I</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.1777408150	-35.8828040527	19.4224552841
C	-5.5277407557	-34.8253780687	18.4240564735
N	-5.2213916265	-34.9237667495	17.0773641900
C	-6.0846569406	-33.5773036037	18.5608581435
C	-5.5751947296	-33.7533195391	16.4792733876
N	-6.0962593227	-32.9066056278	17.3511780288
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.6396968655	-33.2706699949	19.4415332955
C	-1.7490728455	-32.3044907349	19.1369698361
N	-1.7138731672	-30.9660962628	19.5059428252
C	-2.9195023933	-32.4305440372	18.4234754281

C	-2.8268995431	-30.3554372872	19.0092213928
N	-3.5780757856	-31.2171590851	18.3481794929
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.3319489830	-26.4218340794	18.7687716675
C	-3.7285280961	-26.3784593179	17.2942114747
C	-4.0158895782	-27.7438565610	16.6775588893
O	-3.8005087471	-27.8884792553	15.4498018204
O	-4.4941028651	-28.6243401060	17.4650210866
C	-8.1409660000	-23.1040170000	14.9750030000
C	-9.0003436757	-24.0881269629	15.8087356139
C	-8.4987277832	-25.5229668473	15.9170477859
C	-7.6462123909	-25.9359183160	16.9554465440
C	-8.9334421414	-26.5300691241	15.0401096848
C	-7.2324292250	-27.2599886901	17.1077505272
C	-8.5302877782	-27.8605741228	15.1763442085
C	-7.6394987036	-28.2777165775	16.2033461680
O	-7.2432526792	-29.5384199654	16.2853183850
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.7063411209	-31.8822944837	20.5773766681
C	-8.4000923644	-31.2640872184	20.1842388327
N	-7.2824454782	-31.2381925416	21.0137626345
C	-7.9565748902	-30.7531802120	18.9916942243
C	-6.2326361247	-30.7384937032	20.3028681246
N	-6.6127832282	-30.4461620985	19.0753397555
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8160618739	-36.7686670789	17.4801554955
C	-1.7380207117	-36.2236135777	16.4075314666
C	-1.7685512033	-34.8534460672	16.1028245701
C	-2.5754835631	-37.0670895814	15.6664499967
C	-2.5957483629	-34.3363129878	15.1101166476
C	-3.4104759501	-36.5716824276	14.6620429946
C	-3.4272735413	-35.1986097725	14.3709692246
O	-4.2788868282	-34.7602229105	13.4222331932
C	-5.8953233870	-29.0643683988	13.5900709207
C	-6.2248272896	-30.5493251509	13.6162955411
C	-5.0513144037	-31.3724437684	14.1584442473
O	-4.7010649972	-31.1935081933	15.3623485055
O	-4.4736851208	-32.1513724926	13.3478458340
H	-5.4493700964	-35.5079602016	20.4158779595
H	-4.0864117638	-36.0222393200	19.4347221711
H	-6.4527024315	-33.1231187063	19.4656659433
H	-5.4072486455	-33.5664730957	15.4339691046
H	-5.5668322546	-37.9705792284	19.9325470298
H	0.2045595224	-33.0896939362	18.7594165691

H	-1.0062789584	-34.2727796896	19.1998704942
H	-3.3096107959	-33.3108153466	17.9395133939
H	-3.0489622349	-29.3049851839	19.1138061714
H	0.6684354079	-34.0031912373	21.0261205767
H	-4.1153326289	-26.9451763403	19.3276132036
H	-2.4146574545	-27.0181123147	18.8812383461
H	-4.6558522280	-25.7990619816	17.1777685110
H	-2.9624344838	-25.8771413844	16.6923221114
H	-2.3139132615	-24.4956485788	18.7965106165
H	-9.1050569667	-23.6751422468	16.8211508019
H	-10.0137615497	-24.1002661644	15.3854977589
H	-7.3103466262	-25.1989505049	17.6858106809
H	-9.6318657279	-26.2733432368	14.2431713033
H	-6.5732959891	-27.5398815283	17.9216053877
H	-8.9184067143	-28.6206571597	14.5000561042
H	-8.0529157238	-23.4459506625	13.9371880120
H	-9.9401339722	-31.6440532206	21.6239455769
H	-10.4942708204	-31.4189773086	19.9744138723
H	-8.4765771430	-30.5988787680	18.0585089130
H	-5.2306487777	-30.6372828042	20.6905609304
H	-10.7081157863	-33.8277437314	20.6351708701
H	-1.0594509743	-36.3164845701	18.4527283947
H	-0.9939610928	-37.8444649847	17.5991066191
H	-2.5751060409	-38.1357950308	15.8731215984
H	-1.1437521016	-34.1640347105	16.6654333575
H	-4.0572669750	-37.2306615393	14.0904835926
H	-2.6444048809	-33.2677789288	14.9214266158
H	-4.2767889336	-33.7657503033	13.3763206832
H	0.8903837095	-35.4591397365	17.0885771023
H	-5.4630577554	-28.7297565283	14.5348223948
H	-6.7637321789	-28.4515054248	13.3388175031
H	-7.0515463225	-30.6214440230	14.3319226347
H	-6.5279251398	-30.9290186459	12.6367652878
H	-4.7299113753	-35.6796318795	16.6142493895
H	-7.2613525809	-31.5176255737	21.9830210229
H	-0.9791762697	-30.5146882545	20.0286541002
H	-8.5867160131	-22.1027242595	14.9691149266
H	-7.1279364352	-23.0263656729	15.3860771017
H	-4.0183269286	-24.4179219637	19.2560535487
H	-2.8241386788	-25.0529746418	20.3966417569
H	0.9534890845	-36.9998980945	16.2272945877
H	1.3113498727	-36.9395425525	17.9654470498
H	-5.5744720320	-37.6461895497	18.1936234951
H	-6.9468538879	-37.1377419055	19.1863432755

H	-9.5202437408	-33.6576561961	19.3219992184
H	-8.9707237685	-33.9078980976	20.9818421636
S	-4.6593071549	-28.6064860107	12.2912736465
C	-3.0831017280	-29.3036094007	12.8955572479
C	-4.4454774959	-26.8411020921	12.6968668256
H	-3.6940551594	-26.4331463941	12.0173327375
H	-5.4085791417	-26.3544098099	12.5286407746
H	-4.1404578162	-26.7754915667	13.7470167465
H	-3.0236675487	-29.1101911076	13.9698396231
H	-3.1005715076	-30.3713778233	12.6727565104
H	-2.2884786775	-28.7990953766	12.3407666848
H	0.3182560015	-32.2785563579	21.1563754137
H	-0.9198599745	-33.4619871781	21.6052937681
Zn	-5.5553444328	-30.3732565334	17.1255380460

### TS<sub>Zn(II),I</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
C	-5.1490050000#	-35.8974320000#	19.4230110000#
C	-5.4778580000#	-34.8270630000#	18.4309630000#
N	-5.2412060000#	-34.9582490000#	17.0720570000#
C	-5.9444320000#	-33.5426340000#	18.5774270000#
C	-5.5457670000#	-33.7752870000#	16.4732970000#
N	-5.9678520000#	-32.8883510000	17.3577660000
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.5855080000	-33.2601350000	19.4263410000
C	-1.6857250000	-32.2932000000	19.1047560000
N	-1.6566920000	-30.9583320000	19.4870950000
C	-2.8464870000	-32.4178370000	18.3780840000
C	-2.7616440000	-30.3442590000	18.9860000000
N	-3.5041440000	-31.2033480000	18.3095480000
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2340340000	-26.4406620000	18.7871020000
C	-3.5167720000	-26.4597470000	17.2825630000
C	-3.7099030000	-27.8693790000	16.7286840000
O	-3.1625570000	-28.1853900000	15.6515940000
O	-4.4637550000	-28.6223650000	17.4409440000
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.9517520000	-24.1795530000	15.7346110000
C	-8.3720190000	-25.5872260000	15.7487680000
C	-7.6374860000	-26.0723030000	16.8439490000
C	-8.6124890000	-26.4920690000	14.7044650000
C	-7.1676460000	-27.3850480000	16.9071060000
C	-8.1586330000	-27.8135010000	14.7528870000
C	-7.4268870000	-28.2960350000	15.8616800000

O	-7.0113130000	-29.5821850000	15.9030420000
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.8439410000	-31.8950580000	20.1017120000
C	-8.5350030000	-31.2452950000	19.7740840000
N	-7.5351060000	-31.0253140000	20.7173090000
C	-7.9852600000	-30.8365520000	18.5862680000
C	-6.4470110000	-30.5154430000	20.0754600000
N	-6.6899830000	-30.3990240000	18.7849120000
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8194260000	-36.7396600000	17.4819940000
C	-1.7413580000	-36.1949250000	16.4097090000
C	-1.7596190000	-34.8291270000	16.0846020000
C	-2.5999520000	-37.0380090000	15.6915800000
C	-2.5982540000	-34.3133930000	15.0991560000
C	-3.4447730000	-36.5451830000	14.6945840000
C	-3.4548310000	-35.1736300000	14.3845510000
O	-4.3232990000	-34.7457470000	13.4521870000
C	-5.2299020000	-28.8864660000	13.4965200000
C	-5.8725360000	-30.1479260000	13.6099250000
C	-5.0035450000	-31.2940940000	14.0999970000
O	-4.5708890000	-31.2754600000	15.2982770000
O	-4.7282550000	-32.1899600000	13.2597230000
H	-5.4064630000	-35.5206260000	20.4189080000
H	-4.0615200000	-36.0622720000	19.4283130000
H	-6.2313060000	-33.0462920000	19.4911220000
H	-5.4199910000	-33.6011180000	15.4193330000
H	-5.5792090000	-37.9758630000	19.9311330000
H	0.2785700000	-33.0681550000	18.7739340000
H	-0.9426350000	-34.2591080000	19.1619820000
H	-3.2325280000	-33.2936480000	17.8841130000
H	-2.9862650000	-29.2964600000	19.1020870000
H	0.6648350000	-34.0019280000	21.0497250000
H	-4.0405000000	-26.9784030000	19.2970280000
H	-2.3057460000	-26.9957470000	18.9880880000
H	-4.4507940000	-25.9156690000	17.0834780000
H	-2.7168400000	-25.9628910000	16.7248390000
H	-2.2959550000	-24.4764880000	18.8456110000
H	-9.0849520000	-23.8453470000	16.7713570000
H	-9.9595840000	-24.2199190000	15.3008010000
H	-7.4405480000	-25.4077580000	17.6841260000
H	-9.1989310000	-26.1702480000	13.8453240000
H	-6.5928350000	-27.7295930000	17.7569590000
H	-8.4002890000	-28.5005650000	13.9464680000
H	-8.0199000000	-23.3778840000	13.9213270000

H	-10.3055760000	-31.4018870000	20.9679450000
H	-10.5175230000	-31.7216080000	19.2567320000
H	-8.4023560000	-30.8430780000	17.5913180000
H	-5.5152390000	-30.2741710000	20.5639950000
H	-10.7170330000	-33.8477930000	20.5565100000
H	-1.0518360000	-36.2746770000	18.4509060000
H	-1.0137290000	-37.8107270000	17.6140660000
H	-2.6084960000	-38.1035660000	15.9120660000
H	-1.1156790000	-34.1402890000	16.6253070000
H	-4.1058410000	-37.2037470000	14.1396460000
H	-2.6387850000	-33.2451860000	14.9081350000
H	-4.3685420000	-33.7458560000	13.4040470000
H	0.9080530000	-35.4642140000	17.0749510000
H	-4.6038850000	-28.5586560000	14.3236650000
H	-5.7379510000	-28.1006500000	12.9435380000
H	-6.5649750000	-29.8742920000	14.6779440000
H	-6.5050340000	-30.4396820000	12.7706850000
H	-4.8061340000	-35.7425410000	16.5996600000
H	-7.6142600000	-31.1893640000	21.7093510000
H	-0.9279860000	-30.5109010000	20.0211650000
H	-8.6444890000	-22.1325210000	15.0211570000
H	-7.1395460000	-22.9941160000	15.4050280000
H	-4.0319710000	-24.4578890000	19.1716540000
H	-2.9055470000	-25.0210760000	20.4150230000
H	0.9458100000	-37.0155980000	16.2333860000
H	1.3035950000	-36.9399910000	17.9710050000
H	-5.5837920000	-37.6508650000	18.1934760000
H	-6.9443360000	-37.1165420000	19.1883530000
H	-9.2816660000	-33.9191540000	19.5076270000
H	-9.0993970000	-33.6168850000	21.2390630000
S	-3.3274700000	-28.9043760000	12.1096290000
C	-2.2715940000	-29.9936760000	13.1259020000
C	-2.7025430000	-27.2727200000	12.6383240000
H	-1.6880250000	-27.1298550000	12.2567900000
H	-3.3601490000	-26.5150060000	12.2048900000
H	-2.7204090000	-27.2194650000	13.7307420000
H	-2.4402110000	-29.7744040000	14.1824570000
H	-2.5667470000	-31.0185130000	12.8965310000
H	-1.2277700000	-29.8274250000	12.8471230000
H	0.3068000000	-32.2804220000	21.1796340000
H	-0.9445150000	-33.4686130000	21.5739360000
Zn	-5.3070520000	-30.4538760000	17.0508160000

**Prod<sub>Zn(II),I</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-4.8143094729	-36.1117489391	19.2956289138
C	-5.0667706431	-34.9295829360	18.4108944714
N	-4.8363451722	-34.9416300862	17.0440695374
C	-5.4956558404	-33.6525765695	18.6778228313
C	-5.1053672715	-33.7084337331	16.5491755181
N	-5.5047059607	-32.8968876278	17.5178158308
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.1345779148	-32.9277753749	19.3863663056
C	-1.2642808742	-32.0291981426	18.9915495087
N	-1.2843092447	-30.6668059731	19.2661710618
C	-2.4709399030	-32.2785639062	18.3885373797
C	-2.4588961811	-30.1518900273	18.8197122202
N	-3.2017141698	-31.1087988122	18.2888408612
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.3435422516	-26.3963011842	18.7153847831
C	-4.3557465584	-26.3682481962	17.5618483651
C	-4.4824016425	-27.7458737024	16.9152406255
O	-4.2599885852	-27.8879376886	15.7045118026
O	-4.7827269053	-28.6913337264	17.7481722910
C	-8.1409660000	-23.1040170000	14.9750030000
C	-9.1222244626	-23.9847460353	15.7726355193
C	-8.6946241275	-25.4359334226	15.9060054636
C	-8.4462778321	-26.0199869482	17.1551708051
C	-8.5604218369	-26.2516953083	14.7731137894
C	-8.0802076496	-27.3621482092	17.2788748156
C	-8.2031843123	-27.5938732974	14.8786059925
C	-7.9563861578	-28.1569451601	16.1372503532
O	-7.6483337390	-29.4814434160	16.2867860134
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.6316706744	-31.9035602874	20.6664130758
C	-8.3152422164	-31.3335032574	20.2381844578
N	-7.2362136102	-31.1560687411	21.0938153304
C	-7.8357558913	-30.9993570668	18.9978530787
C	-6.1722010395	-30.7289366091	20.3578530820
N	-6.5089404480	-30.6375603750	19.0862354925
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8469204867	-36.5784949999	17.4071727418
C	-1.6442574035	-36.0540620320	16.2303339008
C	-1.5296362320	-34.7146689056	15.8253203493
C	-2.5069668608	-36.8787375617	15.4965485826
C	-2.2622783363	-34.2056337930	14.7592029482
C	-3.2620438829	-36.3826805258	14.4279697011
C	-3.1601886153	-35.0329118764	14.0600675002



O	-3.9391965708	-34.5739441106	13.0569378488
C	-5.4977709015	-28.9216888445	13.0640771684
C	-5.2824684561	-30.2406221511	12.9959345003
C	-5.0806722826	-31.0937697383	14.2034582727
O	-5.5432161836	-30.6635003138	15.3289642002
O	-4.4727306915	-32.1798539316	14.0694722572
H	-4.7824017925	-35.7551302476	20.3313988775
H	-3.8147124093	-36.5139803291	19.0781632364
H	-5.7779318763	-33.2298436053	19.6297755803
H	-4.9532865778	-33.4038908894	15.5220888995
H	-5.6135664656	-38.0703074913	19.8404757720
H	0.8225251576	-32.4781066382	19.0896142803
H	-0.2256698003	-33.8556160202	18.8124215087
H	-2.8462824391	-33.2145565906	18.0082088613
H	-2.7478161217	-29.1138981594	18.8654744679
H	0.7227703838	-33.9111510557	21.1397597865
H	-3.7054863383	-27.0975996621	19.4769148368
H	-2.3868446624	-26.7922450716	18.3417675052
H	-5.3425379739	-26.0696991721	17.9381073179
H	-4.0529447860	-25.6486544020	16.7952290238
H	-2.7224767231	-24.3140439050	18.5968822692
H	-9.2602622637	-23.5563347135	16.7730280538
H	-10.1073520811	-23.9426239368	15.2866965539
H	-8.5398147615	-25.4131029666	18.0539219919
H	-8.7572684314	-25.8356233096	13.7871353591
H	-7.8685767330	-27.8072778671	18.2460215444
H	-8.1224707620	-28.2182399643	13.9933824259
H	-8.0078262105	-23.4825584190	13.9562918691
H	-9.7921898770	-31.7182464959	21.7364306054
H	-10.4324096661	-31.3726254978	20.1399985679
H	-8.3417437699	-30.9798950120	18.0455677043
H	-5.1983281771	-30.5086558635	20.7683854210
H	-10.7028532110	-33.8109281768	20.6770731033
H	-1.0927001308	-35.9971655628	18.3088947502
H	-1.1490727915	-37.6107102097	17.6232406083
H	-2.6016656112	-37.9287051035	15.7679656794
H	-0.8583445555	-34.0461666202	16.3602047302
H	-3.9423973993	-37.0223220113	13.8736681314
H	-2.1779153173	-33.1647607053	14.4677864421
H	-4.0586772347	-33.6008471541	13.1610590362
H	1.0109473105	-35.5038175471	16.9900883508
H	-5.5284276868	-28.4099664959	14.0203097364
H	-5.5819606229	-28.3240036375	12.1592289122
H	-7.0062521745	-29.7884683080	15.6034831798

H	-5.1565668678	-30.7569121871	12.0475239841
H	-4.4282596280	-35.6948679168	16.5001190830
H	-7.2537767361	-31.2785987917	22.0952252314
H	-0.5325241490	-30.1363532198	19.6808976789
H	-8.5056862914	-22.0732068798	14.9072500405
H	-7.1553626610	-23.0899448763	15.4521298493
H	-4.0414875353	-24.6074822048	19.7354618848
H	-2.3861507757	-25.0680724261	20.1624325915
H	0.9494206512	-37.1281866661	16.3016642943
H	1.2202631004	-36.9135708184	18.0429663807
H	-5.8956247468	-37.6285033033	18.1481753857
H	-6.8563156826	-36.8714125240	19.4244285776
H	-9.6069435213	-33.5984303158	19.2962284845
H	-8.9485992112	-33.9699094377	20.8937630203
S	-1.4642978730	-30.1355438551	13.7384811867
C	-2.0140992527	-30.2864368802	15.4704567650
C	-1.7236373838	-28.3388725307	13.5215075578
H	-1.0386664104	-27.7616567104	14.1517127429
H	-1.5226066239	-28.1064445481	12.4719670911
H	-2.7536819919	-28.0759474080	13.7724102292
H	-2.9577426193	-29.7544422155	15.6071401801
H	-2.1629170470	-31.3449247207	15.6851222595
H	-1.2683770694	-29.8819963505	16.1640622052
H	-0.0148134882	-32.3405094251	21.4954146188
H	-1.0442883766	-33.7467536688	21.1920085920
Zn	-5.1561255624	-30.6378566112	17.3569213261

### React<sub>Cu(II),II</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-6.4848756052	-37.5340268738	17.7974643509
C	-7.4006097284	-36.4390400414	17.3304159688
N	-7.2872268572	-35.8539810749	16.0845647393
C	-8.4452319838	-35.7727376944	17.9309523751
C	-8.2175157318	-34.8709352472	15.9928390700
N	-8.9491190983	-34.7920694553	17.0939336535
C	-0.1150060000	-33.2509900000	20.8939940000
C	-1.6554866200	-33.2727860225	20.8252750086
C	-2.2408512866	-32.1282417145	20.0510176210
N	-1.7126528157	-30.8448433204	20.1202917167
C	-3.3165671075	-32.0151924052	19.2008373351
C	-2.4496843088	-30.0259438506	19.3311022315
N	-3.4288498678	-30.7073347487	18.7665795196
C	-3.1080190000	-25.0239970000	19.3379980000
C	-2.9422066850	-26.3580447669	18.6096755457

C	-3.1388018635	-26.2401605949	17.0941586696
C	-2.8574744436	-27.5390429371	16.3445637904
O	-2.3360043865	-27.5004187088	15.2165839970
O	-3.1488199227	-28.6425696316	16.9627400368
C	-8.1437350000	-23.1303020000	14.9325590000
C	-7.0295149205	-23.5519802899	15.9120279119
C	-6.7507854347	-25.0437370188	15.9380639784
C	-7.0166479486	-25.8300960193	17.0694906263
C	-6.1875857212	-25.6907943637	14.8254604416
C	-6.7302959925	-27.1946519041	17.0998305869
C	-5.8843960041	-27.0481994311	14.8434282256
C	-6.1458726580	-27.8395011891	15.9864862595
O	-5.8496936258	-29.1358193099	15.9895618615
C	-9.7309990000	-33.4130130000	20.3670160000
C	-8.1963135289	-33.2426340718	20.4451770353
C	-7.6056115687	-32.2787670116	19.4538722268
N	-7.9809965155	-32.2707965039	18.1214950868
C	-6.6068960901	-31.3364476820	19.5459922137
C	-7.2214596804	-31.3682791910	17.4653630490
N	-6.3754012887	-30.7769856757	18.2986770812
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.6200204021	-36.6400690586	18.0026882018
C	-1.8380908771	-36.3237460494	17.1642344791
C	-2.4883781981	-35.0880644706	17.2488795796
C	-2.2950756753	-37.2356681062	16.2023087595
C	-3.5495636691	-34.7537117943	16.4055226121
C	-3.3395059317	-36.9183314354	15.3379286370
C	-3.9627955171	-35.6667822531	15.4246938316
O	-4.9673481830	-35.3969127527	14.5430569587
C	-3.7332594122	-30.0622576291	13.9160274247
C	-4.8999500417	-31.0204465851	13.7582988845
C	-5.0950017451	-31.9854095097	14.9357109287
O	-4.4763092583	-31.7410089440	16.0107141763
O	-5.8678243887	-32.9646145655	14.7326903814
H	-5.6842216161	-37.6651318217	17.0602403265
H	-7.0274356952	-38.4883381603	17.8401179045
H	-8.8651574383	-35.9433567541	18.9120898938
H	-8.2788403995	-34.2171871943	15.1345443202
H	-5.2121345940	-38.0644438016	19.4903166649
H	-1.9954237405	-34.2042849532	20.3604479538
H	-2.0605832465	-33.2772509272	21.8471455195
H	-4.0092185417	-32.7703110673	18.8623768527
H	-2.2478949814	-28.9830138580	19.1537003064
H	0.2551830142	-34.1335841519	21.4236867932

H	-3.6603473223	-27.0898563146	18.9978035658
H	-1.9376586465	-26.7578826648	18.8147392245
H	-4.1756521137	-25.9548583691	16.8785109433
H	-2.4976867721	-25.4602140997	16.6699101858
H	-2.3782917642	-24.2855025777	18.9854253482
H	-6.1069931948	-23.0177235844	15.6441353130
H	-7.2923000009	-23.2157340579	16.9227015928
H	-7.4532407137	-25.3615730198	17.9502431842
H	-5.9574710008	-25.1099930585	13.9338158444
H	-6.9336115316	-27.7940197384	17.9839533851
H	-5.4194254081	-27.5238235371	13.9845015433
H	-9.0945310837	-23.6051471435	15.1971768508
H	-7.7287485457	-34.2257785698	20.2936918586
H	-7.9065231465	-32.9144458180	21.4496409293
H	-6.0403848356	-31.0303677682	20.4127503053
H	-7.2734602545	-31.1715013706	16.4076744340
H	-10.0688039012	-34.1309139018	21.1210375800
H	-0.5676649064	-35.9556812777	18.8597522777
H	-0.6978078051	-37.6531959572	18.4183252712
H	-1.8117774937	-38.2071359879	16.1165732977
H	-2.1588372738	-34.3567050552	17.9846850774
H	-3.6768080861	-37.6181243510	14.5788580061
H	-4.0419860833	-33.7896829203	16.4913377891
H	-5.2779918981	-34.4460878744	14.6387950925
H	0.7879317978	-35.5157029732	16.7740604635
H	-3.8096075377	-29.4542632632	14.8132888507
H	-3.6204251296	-29.4057424146	13.0481281442
H	-5.8022160232	-30.4001457148	13.7119141570
H	-4.8470267013	-31.5999147052	12.8306012646
H	-6.5290541372	-35.9891706948	15.4145079738
H	-8.5872415116	-32.9800726870	17.6891060475
H	-0.9016307361	-30.5683266653	20.6519953060
H	-8.2869153655	-22.0440768292	14.9435272137
H	-7.8988140646	-23.4298376476	13.9080033277
H	-4.1077094636	-24.6089099905	19.1629926746
H	-2.9760588316	-25.1346910356	20.4204631593
H	0.6486916431	-37.2180842696	16.3244022502
H	1.5592995432	-36.7623996185	17.7768409449
H	-6.6279662769	-37.0960134255	19.9349909866
H	-5.2507895676	-36.3285610931	19.1230763906
H	-10.2409118608	-32.4609994066	20.5470395153
H	-10.0389022413	-33.7825223743	19.3843644629
S	-2.1003427550	-30.9466889666	13.9951975845
C	-1.6548261317	-31.0738500026	15.7598005032

C	-0.9819535447	-29.6008542740	13.4859226805
H	0.0417631509	-29.9482419761	13.6411188070
H	-1.1522854861	-29.4177964026	12.4229315063
H	-1.2298364334	-28.7212837751	14.0924965301
H	-1.9741428332	-30.1573681943	16.2670704696
H	-2.1875775919	-31.9335633645	16.1604604176
H	-0.5719982452	-31.2230075778	15.7823240058
H	0.3245064010	-33.2470611516	19.8911543687
H	0.2596644816	-32.3738594341	21.4345559006
Cu	-4.7199245740	-29.8421088116	17.3875227080

### TS<sub>Cu(II),II</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
C	-5.7636830000#	-36.8493940000#	17.6949590000#
C	-7.0470560000#	-36.2912390000#	17.1621080000#
N	-7.1595810000#	-35.7514740000#	15.8962860000#
C	-8.3003690000#	-36.1474420000#	17.7173340000#
C	-8.4355120000#	-35.3041250000#	15.7483410000#
N	-9.1626030000	-35.5154250000	16.8369690000
C	-0.1150060000	-33.2509900000	20.8939940000
C	-1.5974750000	-33.5063610000	20.5590980000
C	-2.2785230000	-32.3681290000	19.8576150000
N	-2.0457240000	-31.0389700000	20.1867350000
C	-3.2307400000	-32.3191460000	18.8667650000
C	-2.8258640000	-30.2530070000	19.4051270000
N	-3.5556690000	-31.0028190000	18.6001970000
C	-3.1080190000	-25.0239970000	19.3379980000
C	-2.9804920000	-26.4663150000	18.8612200000
C	-2.6594940000	-26.5875390000	17.3647010000
C	-2.8260280000	-28.0178360000	16.8481310000
O	-1.9969770000	-28.5358000000	16.0823330000
O	-3.9085020000	-28.5646700000	17.2816130000
C	-8.1437350000	-23.1303020000	14.9325590000
C	-6.8036520000	-23.6395670000	15.4978010000
C	-6.6995500000	-25.1495560000	15.6075770000
C	-6.5802690000	-25.7948680000	16.8478020000
C	-6.7018370000	-25.9590570000	14.4633820000
C	-6.4399900000	-27.1784410000	16.9466600000
C	-6.5672270000	-27.3452750000	14.5438590000
C	-6.4148160000	-27.9791450000	15.7931100000
O	-6.2545950000	-29.3248260000	15.8759310000
C	-9.7309990000	-33.4130130000	20.3670160000
C	-8.1993000000	-33.5305850000	20.3228580000
C	-7.5708920000	-32.7764700000	19.1954210000

N	-7.9108420000	-32.9794740000	17.8694690000
C	-6.5819650000	-31.8263440000	19.1656610000
C	-7.1347100000	-32.1905410000	17.0955690000
N	-6.3195820000	-31.4745300000	17.8559660000
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.7138590000	-36.8611140000	17.7492170000
C	-1.8331670000	-36.4143630000	16.8357470000
C	-2.2305460000	-35.0709980000	16.7941160000
C	-2.4670000000	-37.3062460000	15.9610670000
C	-3.2369500000	-34.6230020000	15.9375430000
C	-3.4660170000	-36.8802860000	15.0871150000
C	-3.8662290000	-35.5377210000	15.0770810000
O	-4.8990210000	-35.1899720000	14.2621800000
C	-3.9983250000	-29.5083170000	13.7873780000
C	-5.1147610000	-30.3882690000	13.7644240000
C	-4.9679000000	-31.6968950000	14.4972920000
O	-4.3286730000	-31.6758860000	15.5984110000
O	-5.5114510000	-32.7192340000	13.9889110000
H	-4.9620410000	-36.1141620000	17.5581210000
H	-5.4587970000	-37.7185180000	17.0986190000
H	-8.6290940000	-36.4536660000	18.7002160000
H	-8.7785790000	-34.8259200000	14.8409800000
H	-4.9037510000	-37.6456290000	19.5210800000
H	-1.6895680000	-34.3914380000	19.9214610000
H	-2.1381240000	-33.7430780000	21.4861050000
H	-3.6998680000	-33.1263840000	18.3274720000
H	-2.8389220000	-29.1765510000	19.4293950000
H	0.3264620000	-34.1360110000	21.3601090000
H	-3.9202580000	-26.9945410000	19.0474190000
H	-2.1989510000	-26.9780910000	19.4427540000
H	-3.3732480000	-25.9721940000	16.8001870000
H	-1.6507970000	-26.2329560000	17.1335060000
H	-2.1868380000	-24.4557600000	19.1633290000
H	-5.9907270000	-23.2681160000	14.8586990000
H	-6.6373950000	-23.1949100000	16.4864690000
H	-6.5843670000	-25.2002390000	17.7592970000
H	-6.8103100000	-25.4991360000	13.4832130000
H	-6.3107400000	-27.6572470000	17.9108860000
H	-6.5891490000	-27.9453190000	13.6402370000
H	-8.9780520000	-23.4389050000	15.5709140000
H	-7.9215010000	-34.5899310000	20.2427760000
H	-7.7638530000	-33.1615150000	21.2576650000
H	-6.0343400000	-31.3865230000	19.9845200000
H	-7.1539410000	-32.1846430000	16.0170800000

H	-10.1358920000	-33.9619330000	21.2227840000
H	-0.8191990000	-36.3805840000	18.7317720000
H	-0.7874470000	-37.9408210000	17.9266440000
H	-2.1758140000	-38.3544620000	15.9644190000
H	-1.7471960000	-34.3505760000	17.4514860000
H	-3.9600390000	-37.5756100000	14.4153940000
H	-3.5569930000	-33.5842130000	15.9427260000
H	-5.0595920000	-34.1864330000	14.2317030000
H	0.7766690000	-35.4500920000	17.0162170000
H	-3.4853290000	-29.3605070000	14.7332610000
H	-4.0372270000	-28.6225550000	13.1561680000
H	-5.8046010000	-29.7650210000	14.7544930000
H	-5.6786020000	-30.4629840000	12.8353570000
H	-6.4005740000	-35.6444710000	15.2123110000
H	-8.5681620000	-33.6792280000	17.5221110000
H	-1.3782570000	-30.7074640000	20.8658880000
H	-8.1500720000	-22.0374080000	14.8618840000
H	-8.3274050000	-23.5348310000	13.9317950000
H	-3.9165450000	-24.5135760000	18.8019030000
H	-3.3323940000	-24.9724040000	20.4089680000
H	0.8171410000	-37.0187840000	16.2065530000
H	1.4753690000	-36.8542300000	17.8468400000
H	-6.6293660000	-37.9972260000	19.3373380000
H	-6.1025290000	-36.3695940000	19.7911890000
H	-10.0411280000	-32.3667980000	20.4500510000
H	-10.1823180000	-33.8301370000	19.4606650000
S	-2.0816530000	-30.3440130000	12.8772640000
C	-1.4991920000	-31.2999370000	14.3204120000
C	-1.0602870000	-28.8431060000	13.0594290000
H	-0.0082970000	-29.1017510000	12.9134420000
H	-1.3693310000	-28.1413530000	12.2810280000
H	-1.2203190000	-28.4185920000	14.0537850000
H	-1.6108010000	-30.6892260000	15.2184490000
H	-2.1268890000	-32.1869970000	14.4008150000
H	-0.4577120000	-31.5849330000	14.1506210000
H	0.4587080000	-33.0166590000	19.9921100000
H	0.0073140000	-32.4221600000	21.6009490000
Cu	-4.8790810000	-30.2261420000	17.1884650000

### **Prod<sub>Cu(II),II</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.7576121669	-37.0720983786	17.6521877888
C	-7.0124974882	-36.5108969223	17.0563328527
N	-7.0732615602	-36.0025450883	15.7734506973

C	-8.2794552042	-36.3267631068	17.5655868078
C	-8.3328281530	-35.5300423594	15.5736643271
N	-9.0983659228	-35.6986223336	16.6424080455
C	-0.1150060000	-33.2509900000	20.8939940000
C	-1.6320212786	-33.4381076026	20.6912835766
C	-2.2765658986	-32.3640610281	19.8662918367
N	-1.9441897172	-31.0215546210	19.9933105448
C	-3.2641195036	-32.3881895581	18.9107871135
C	-2.7015981268	-30.2969927100	19.1363307043
N	-3.5121391668	-31.1011542878	18.4711269242
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.1168114588	-26.4219705188	18.7076178211
C	-3.4180797231	-26.4137371497	17.1997656152
C	-3.4554714597	-27.8130841430	16.5783514162
O	-2.9003224816	-28.0630485846	15.5056474697
O	-4.1280843708	-28.6673896967	17.2966594340
C	-8.1437350000	-23.1303020000	14.9325590000
C	-7.1964280369	-23.7060462925	16.0022693809
C	-6.9700947402	-25.2000694978	15.8698985655
C	-7.4107467258	-26.1058699015	16.8451381155
C	-6.2953144644	-25.7189873635	14.7561281111
C	-7.1849774628	-27.4778130969	16.7253494744
C	-6.0597669538	-27.0843710147	14.6189303682
C	-6.5105627173	-27.9615215479	15.6076736984
O	-6.2822681330	-29.3214066284	15.5228742267
C	-9.7309990000	-33.4130130000	20.3670160000
C	-8.2063175688	-33.5658761721	20.1827588721
C	-7.5947654827	-32.8532472803	19.0103886615
N	-7.8801864801	-33.1647163666	17.6907013868
C	-6.5913853529	-31.9174983976	18.9385973771
C	-7.0561748832	-32.4609938548	16.8844130848
N	-6.2615687506	-31.6863560458	17.6136420609
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.7007778296	-36.6222133801	17.8590482740
C	-1.8204803657	-36.2777565149	16.9032455917
C	-2.2768187438	-34.9609806992	16.7700369551
C	-2.3733374734	-37.2485798005	16.0580149318
C	-3.2703298774	-34.6114165292	15.8532000616
C	-3.3535306036	-36.9214527679	15.1248951084
C	-3.8158162294	-35.6038250587	15.0257346380
O	-4.8307492702	-35.3616916797	14.1467004610
C	-4.0777986710	-29.7611012453	13.0608051012
C	-4.8734830598	-30.8388442433	13.0050496168
C	-4.9620533678	-31.8364647343	14.1245719863



O	-4.3970220891	-31.5570503862	15.2319748959
O	-5.6039692577	-32.8989443257	13.8918612554
H	-4.9165022785	-36.4135421922	17.4102814417
H	-5.5157173736	-38.0367758241	17.1856653104
H	-8.6467274920	-36.5986316440	18.5454423856
H	-8.6346505173	-35.0649709797	14.6449075442
H	-4.9239950440	-37.6426904584	19.5755330327
H	-1.8278893335	-34.3949944149	20.1969541254
H	-2.1229420427	-33.4949490385	21.6732053064
H	-3.8005110409	-33.2297227134	18.5016008525
H	-2.6543374812	-29.2288401049	19.0073107054
H	0.2973738101	-34.0882888041	21.4640158398
H	-3.8657373531	-27.0488967205	19.2043707942
H	-2.1388865360	-26.8982672285	18.8757491068
H	-4.4054838208	-25.9656709833	17.0259198435
H	-2.6820307907	-25.8199955901	16.6490932849
H	-2.3491476624	-24.3826623326	18.8748620420
H	-6.2295599844	-23.1885929474	15.9367414307
H	-7.5949772970	-23.4848101066	16.9996142523
H	-7.9342013726	-25.7318398204	17.7220842003
H	-5.9282742563	-25.0425599329	13.9878986620
H	-7.5108526611	-28.1770685299	17.4891212438
H	-5.5056971323	-27.4680487025	13.7681264972
H	-9.1320008629	-23.5977560614	14.9955828606
H	-7.9673811596	-34.6344417965	20.0901311577
H	-7.6898697746	-33.2116389362	21.0816350375
H	-6.0659174052	-31.4202349558	19.7393812878
H	-7.0126702200	-32.5617964776	15.8093818464
H	-10.0626644356	-33.9690547339	21.2492265725
H	-0.7227599059	-35.9425925046	18.7218180234
H	-0.8446884852	-37.6349975991	18.2569203696
H	-2.0305975513	-38.2788545000	16.1309680577
H	-1.8444668222	-34.1851974979	17.3978988427
H	-3.7855926630	-37.6744192350	14.4724163985
H	-3.6239237106	-33.5866122070	15.7732334013
H	-5.0524890616	-34.3848667845	14.0909559039
H	0.8458948905	-35.5171820368	16.7926238027
H	-3.4788921272	-29.5410760713	13.9401912721
H	-4.0055472910	-29.0757799085	12.2190659504
H	-5.8454931719	-29.5200713326	14.6741421551
H	-5.4636203128	-31.0781050191	12.1237454084
H	-6.2956509715	-35.9132020103	15.1092785470
H	-8.5324779916	-33.8834024026	17.3692013775
H	-1.2310249987	-30.6453625930	20.5994963147

H	-8.2668529602	-22.0494802846	15.0593070403
H	-7.7558120163	-23.3102482295	13.9246113868
H	-4.0795865011	-24.5326357706	19.2087931128
H	-2.8964370848	-25.0711579756	20.4119482190
H	0.7267379582	-37.2153220846	16.3234258139
H	1.4860324126	-36.7786891369	17.8669882211
H	-6.6671780275	-37.9213746017	19.4491905023
H	-6.0492225856	-36.2751288574	19.6546217333
H	-10.0083457718	-32.3619400754	20.4955086135
H	-10.2735443222	-33.8033692472	19.4992083763
S	-0.6253006451	-31.2017034610	14.3542428628
C	-1.3320138326	-31.0712950812	16.0289491215
C	-0.0975675046	-29.4632321471	14.1450318171
H	0.7111959498	-29.2092975094	14.8391983143
H	0.2725089791	-29.3557509564	13.1215440124
H	-0.9418469713	-28.7884237185	14.3058136654
H	-2.0627305395	-30.2626591879	16.0563703394
H	-1.8434232268	-32.0100214589	16.2407933294
H	-0.5523093566	-30.9007386478	16.7810583090
H	0.4073858995	-33.2014022706	19.9333873889
H	0.1138736666	-32.3371425513	21.4547260162
Cu	-4.7644628211	-30.4464186766	16.9543473775

### React<sub>M-Fe(III),VI</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.2078650532	-35.8632805845	19.4255907800
C	-5.5005051916	-34.7992538993	18.4072247958
N	-5.2727302359	-34.9572532073	17.0505585763
C	-5.8800696089	-33.4860991282	18.5398629362
C	-5.4938883707	-33.7702768948	16.4340464399
N	-5.8575569027	-32.8426879522	17.3098790993
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.6101520729	-33.2771361094	19.4290217537
C	-1.7316021150	-32.3281322924	19.1024612882
N	-1.7971905042	-31.0388111769	19.6114828856
C	-2.8141747216	-32.4183488831	18.2565125078
C	-2.8727944427	-30.4116549794	19.0721574190
N	-3.5131588242	-31.2213441488	18.2434814061
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.3063532069	-26.4665327506	18.8724525462
C	-3.5801580436	-26.5419144511	17.3659357535
C	-3.7232844360	-27.9626439315	16.8403759111
O	-3.0943372949	-28.3089490863	15.8200127423
O	-4.5300139741	-28.7176112493	17.5034815007

C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.7592906234	-24.1717929105	15.9171055107
C	-8.1478251184	-25.5683890523	15.9222332128
C	-7.5692813589	-26.1086128484	17.0888142521
C	-8.2428505621	-26.4270816114	14.8046520360
C	-7.1112870479	-27.4201671041	17.1571110112
C	-7.7947705618	-27.7416303330	14.8495479704
C	-7.1951821807	-28.2813194550	16.0267121897
O	-6.7425442771	-29.5196905885	16.0364788802
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.8016481165	-31.8788044984	20.1896254626
C	-8.4878023037	-31.2578725002	19.8210799319
N	-7.4733363787	-31.0046898109	20.7382572980
C	-7.9518997188	-30.8986754650	18.6112510905
C	-6.3906978733	-30.5258402098	20.0707503922
N	-6.6510712390	-30.4599606556	18.7771858716
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.7936652658	-36.8363736289	17.5213468534
C	-1.7602098733	-36.3560128060	16.4577508443
C	-1.7519720498	-35.0204967223	16.0290443248
C	-2.6655540400	-37.2267263796	15.8374877286
C	-2.6046909044	-34.5632275844	15.0296104448
C	-3.5328991560	-36.7898248012	14.8320233117
C	-3.5069452277	-35.4505195391	14.4182659957
O	-4.3955685007	-35.0545160637	13.4759981266
C	-4.8796470954	-28.9555070487	13.4223226568
C	-5.5610569420	-30.3137910611	13.3108424164
C	-4.7808122655	-31.4113505309	14.0387409966
O	-4.5560560295	-31.2603610838	15.2915753816
O	-4.3565410207	-32.3647512679	13.3555855725
H	-5.5236291358	-35.4788545309	20.4019450376
H	-4.1173044972	-35.9931599294	19.4878437844
H	-6.1286591686	-32.9643937116	19.4486389257
H	-5.3539310911	-33.6245529110	15.3779109742
H	-5.5927277839	-37.9376851778	19.9698964751
H	0.2416300564	-33.0693974763	18.7654428818
H	-0.9484520055	-34.2852065826	19.1710528782
H	-3.1190829864	-33.2522481767	17.6452227672
H	-3.1517477816	-29.3910509004	19.2777616542
H	0.6705140506	-33.9976701781	21.0364541449
H	-4.1411075926	-26.9350224606	19.4073773651
H	-2.4072072341	-27.0542999845	19.1068614266
H	-4.5213525531	-26.0203962652	17.1428704297
H	-2.7816618909	-26.0463309484	16.8050188866

H	-2.2586389511	-24.5570526087	18.8269105851
H	-8.7404192320	-23.7843845195	16.9421715831
H	-9.8214623226	-24.2785187616	15.6565254511
H	-7.4978291305	-25.4844723363	17.9770561513
H	-8.7097130971	-26.0596463536	13.8933664726
H	-6.6701025903	-27.8158828912	18.0624033568
H	-7.9157589270	-28.3903586562	13.9865823989
H	-8.1768048372	-23.4266092000	13.9291310507
H	-10.1889980299	-31.4146382963	21.1060102046
H	-10.5178958037	-31.6354787370	19.3982062366
H	-8.3897945591	-30.9507734766	17.6274158706
H	-5.4528334929	-30.2667625925	20.5374054097
H	-10.7198987218	-33.8168258167	20.6018198505
H	-1.0403145387	-36.3794364280	18.4915527535
H	-0.9167353411	-37.9163665197	17.6627518510
H	-2.6896961998	-38.2726512711	16.1357629716
H	-1.0653781926	-34.3126006151	16.4870730490
H	-4.2245258518	-37.4723825708	14.3473165737
H	-2.6068665627	-33.5192930860	14.7340966002
H	-4.3334734729	-34.0822695415	13.3500459898
H	0.8503509131	-35.4517264356	17.0907180544
H	-4.6242643312	-28.7155626815	14.4546759488
H	-5.4813738106	-28.1581721989	12.9774899787
H	-6.5228696609	-30.2060316537	13.8195495440
H	-5.7263643717	-30.6126830248	12.2730697420
H	-4.9003750395	-35.7790737665	16.5853488006
H	-7.5433003690	-31.1245917668	21.7387250738
H	-1.1466158290	-30.6300696450	20.2657305871
H	-8.6981347285	-22.1672937814	15.0615106878
H	-7.0949891463	-22.9093357178	15.2329579325
H	-3.9960215790	-24.4175053374	19.1250495843
H	-2.9186466413	-24.9695064143	20.4152237039
H	0.9472871502	-36.9848111942	16.2186601061
H	1.3485634074	-36.9170255362	17.9449361406
H	-5.5128767322	-37.6716459841	18.2248853026
H	-6.9475113084	-37.1591829084	19.1277768061
H	-9.3666848887	-33.8894448239	19.4518636760
H	-9.0508448484	-33.6878797278	21.1808723871
S	-3.2890812168	-28.8757605564	12.4734477481
C	-2.1480642678	-29.9595072707	13.4029772420
C	-2.6912664618	-27.2283334191	12.9760928728
H	-1.7133094876	-27.0821330933	12.5127144804
H	-3.3974244298	-26.4927533861	12.5850802007
H	-2.6387896447	-27.2050960260	14.0688067308

H	-2.3099852365	-29.7986911233	14.4708239606
H	-2.3618354951	-30.9855091221	13.1026049335
H	-1.1403110202	-29.6734093063	13.0936853757
H	0.3120820911	-32.2780075954	21.1634414496
H	-0.9291135538	-33.4711321398	21.5917166202
Fe	-5.3344198997	-30.5217519888	17.0128323959

### T<sub>SM-Fe(III),VI</sub>

C	-5.8569950000#	-37.2389910000#	19.1709910000#
C	-5.2210220000#	-35.8762240000#	19.5071520000#
C	-5.4805850000#	-34.7716530000#	18.5243540000#
N	-5.2957690000#	-34.9114540000#	17.1578680000#
C	-5.7846420000#	-33.4432750000#	18.6964720000#
C	-5.4662200000#	-33.7066710000#	16.5678020000#
N	-5.7571220000	-32.7814520000	17.4751810000
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.4859270000	-33.1028040000	19.4063680000
C	-1.6508960000	-32.1974860000	19.1433630000
N	-1.7547310000	-30.9281630000	19.6969580000
C	-2.7638940000	-32.3220400000	18.3484850000
C	-2.8783930000	-30.3388010000	19.2268840000
N	-3.5154100000	-31.1602780000	18.4061980000
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2579820000	-26.4863660000	18.9215610000
C	-3.5162180000	-26.6311770000	17.4136680000
C	-3.5608690000	-28.0863250000	16.9815690000
O	-2.7305960000	-28.5508220000	16.1906630000
O	-4.5319950000	-28.7665870000	17.5265180000
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.7380090000	-24.1345570000	15.9631210000
C	-8.1621650000	-25.5459280000	15.9379970000
C	-7.5894810000	-26.1222640000	17.0828980000
C	-8.2718570000	-26.3709250000	14.8060680000
C	-7.1410000000	-27.4468390000	17.1136880000
C	-7.8340790000	-27.6972600000	14.8159300000
C	-7.2505230000	-28.2500830000	15.9714160000
O	-6.7945220000	-29.5549440000	15.9491630000
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.8829900000	-31.9137200000	20.0234790000
C	-8.5830550000	-31.2448840000	19.6971060000
N	-7.6371670000	-30.9035280000	20.6584170000
C	-7.9922450000	-30.9234900000	18.5029810000
C	-6.5373370000	-30.4126590000	20.0338730000
N	-6.7226650000	-30.4210530000	18.7238830000

C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8017160000	-36.7064170000	17.5753430000
C	-1.7756450000	-36.2358320000	16.5136460000
C	-1.7797120000	-34.9054890000	16.0669850000
C	-2.6877730000	-37.1175630000	15.9176960000
C	-2.6563300000	-34.4612900000	15.0786090000
C	-3.5731870000	-36.6956450000	14.9226840000
C	-3.5670200000	-35.3587510000	14.4934680000
O	-4.4741800000	-34.9917110000	13.5616280000
C	-4.8323130000	-28.7967060000	13.7345060000
C	-5.5986760000	-30.0432280000	13.6591150000
C	-5.0095110000	-31.2490060000	14.2450460000
O	-4.5284840000	-31.1127950000	15.4791190000
O	-4.9976410000	-32.3492950000	13.6672540000
H	-5.5680770000	-35.5342650000	20.4880890000
H	-4.1332620000	-36.0083460000	19.5976340000
H	-5.9822510000	-32.9212090000	19.6184570000
H	-5.3595140000	-33.5328830000	15.5106230000
H	-5.6211300000	-37.9683550000	19.9502450000
H	0.3891520000	-32.7400000000	18.8498250000
H	-0.7279560000	-34.0815420000	18.9839270000
H	-3.0569660000	-33.1526920000	17.7278620000
H	-3.1880390000	-29.3356830000	19.4689080000
H	0.7208710000	-33.9459540000	21.0082790000
H	-4.0860630000	-26.9562110000	19.4663900000
H	-2.3437360000	-27.0367780000	19.1852110000
H	-4.4817120000	-26.1729380000	17.1661780000
H	-2.7305950000	-26.1257400000	16.8445780000
H	-2.2684670000	-24.5511750000	18.8174310000
H	-8.6445670000	-23.7402170000	16.9815760000
H	-9.8168710000	-24.2072390000	15.7704080000
H	-7.5011680000	-25.5249520000	17.9877030000
H	-8.7355920000	-25.9813930000	13.9029530000
H	-6.6885170000	-27.8597160000	18.0041250000
H	-7.9618160000	-28.3177380000	13.9342550000
H	-8.2492260000	-23.4377710000	13.9377280000
H	-10.3752570000	-31.3892060000	20.8521790000
H	-10.5404110000	-31.8007530000	19.1561530000
H	-8.3675300000	-31.0354580000	17.4983570000
H	-5.6429060000	-30.0869490000	20.5414740000
H	-10.7090380000	-33.8609220000	20.5617560000
H	-0.9862120000	-36.1698860000	18.5176140000
H	-0.9920920000	-37.7627670000	17.7961250000
H	-2.7028770000	-38.1593550000	16.2291760000

H	-1.0816440000	-34.1926590000	16.4991080000
H	-4.2688830000	-37.3862360000	14.4562670000
H	-2.6635360000	-33.4190120000	14.7742520000
H	-4.5389210000	-34.0147210000	13.5014200000
H	0.9115990000	-35.4763650000	16.9899610000
H	-4.4077110000	-28.5933100000	14.7135500000
H	-5.3475310000	-27.9257470000	13.3278910000
H	-6.4513090000	-29.7807580000	14.8597340000
H	-6.1157560000	-30.2356380000	12.7204120000
H	-4.9741260000	-35.7403830000	16.6680200000
H	-7.7647080000	-30.9747840000	21.6577130000
H	-1.0911740000	-30.5050620000	20.3288560000
H	-8.6541670000	-22.1436130000	15.0758060000
H	-7.0744290000	-22.9467090000	15.1664880000
H	-4.0117900000	-24.4533940000	19.0970700000
H	-2.9299530000	-24.9290490000	20.4137680000
H	0.8934340000	-37.0828230000	16.2576410000
H	1.3404500000	-36.8911620000	17.9634930000
H	-5.4745460000	-37.6339400000	18.2234690000
H	-6.9450870000	-37.1599300000	19.0893980000
H	-9.2580550000	-33.9507810000	19.5400390000
H	-9.1109700000	-33.5558020000	21.2587450000
S	-3.1756460000	-28.7884400000	12.6300580000
C	-2.2298620000	-30.1309980000	13.4189120000
C	-2.3240640000	-27.3191690000	13.2919730000
H	-1.3517680000	-27.2334800000	12.8023990000
H	-2.9372590000	-26.4516970000	13.0374440000
H	-2.2222650000	-27.4292020000	14.3747570000
H	-2.3114500000	-30.0357200000	14.5034810000
H	-2.6577650000	-31.0712870000	13.0687070000
H	-1.1958320000	-30.0463410000	13.0782980000
H	0.1960300000	-32.2970370000	21.3346970000
H	-0.9602960000	-33.6315790000	21.4752460000
Fe	-5.2427980000	-30.5563890000	17.1463680000

### **Prod<sub>M-Fe(III),VI</sub>**

C	-5.8569950000	-37.2389910000	19.1709910000
C	-4.7687149547	-36.1497208994	19.2043845021
C	-4.9919320228	-35.0223895819	18.2446222779
N	-4.8852027051	-35.1669064596	16.8680580331
C	-5.2671954271	-33.6933277265	18.4342268136
C	-5.0613001306	-33.9650395824	16.2821426108
N	-5.2921842304	-33.0404726922	17.2097938681
C	-0.1150060000	-33.2509900000	20.8939940000

C	-0.2019598978	-33.0140950802	19.3713560717
C	-1.3729521985	-32.1699450719	18.9733221269
N	-1.5826808635	-30.9003775217	19.4996490286
C	-2.4306817529	-32.3740430308	18.1249571957
C	-2.7160084340	-30.3886142490	18.9762335702
N	-3.2593711776	-31.2604975184	18.1378277417
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.1070271520	-26.4410084414	18.7608392603
C	-4.3342566456	-26.7260832222	17.8711447653
C	-4.1790367529	-28.0761643251	17.1929501580
O	-3.3725882557	-28.2294024514	16.2767036273
O	-4.8961045024	-29.0534339887	17.7083234921
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.4797609708	-24.1789021408	16.0197471446
C	-7.9101018587	-25.5718592626	15.7843271109
C	-8.4855585821	-26.6718648486	16.4455794715
C	-6.8131065916	-25.8247630777	14.9516723299
C	-7.9951822286	-27.9666097181	16.2945653126
C	-6.2992800914	-27.1150519937	14.7946858262
C	-6.8948321199	-28.1836370380	15.4645490484
O	-6.4277409435	-29.4790038123	15.3185588714
C	-9.7309990000	-33.4130130000	20.3670160000
C	-10.0596845579	-32.3254380521	19.3227555858
C	-8.8407161329	-31.5701151151	18.8945703152
N	-8.3517709439	-30.4586570316	19.5726989734
C	-7.9079873734	-31.8225774687	17.9237808984
C	-7.1819054323	-30.0785013883	19.0125230726
N	-6.8816082798	-30.8988970390	18.0140872737
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8402267402	-36.6479399132	17.4214618130
C	-1.6641771062	-36.2576250087	16.2119864208
C	-1.5714945569	-34.9682837187	15.6674050873
C	-2.5180199896	-37.1683040163	15.5747816359
C	-2.3178478023	-34.5864439299	14.5567296686
C	-3.2847685877	-36.8008429436	14.4642888240
C	-3.2023990941	-35.4970047359	13.9551727543
O	-3.9937840995	-35.1727740878	12.9048144674
C	-3.2303077691	-29.3023918190	13.3435072294
C	-3.7247464278	-30.5053089742	13.0119315624
C	-4.2504329845	-31.4777533796	13.9953715382
O	-4.2795622028	-31.0913445958	15.2590528907
O	-4.6441928691	-32.5925749587	13.6323007160
H	-4.7006907428	-35.7237200249	20.2111237586
H	-3.7896530320	-36.6014472950	18.9924814035



H	-5.4150627169	-33.1571863977	19.3588056677
H	-5.0003411981	-33.7701360302	15.2217596139
H	-5.6297479323	-38.0304231203	19.8908155484
H	0.7269483090	-32.5468183313	19.0167451817
H	-0.2819038602	-33.9702581827	18.8453814361
H	-2.6405619722	-33.2269129365	17.5011771546
H	-3.1191539834	-29.4199066937	19.2135469086
H	0.7409497334	-33.8883676401	21.1316623766
H	-3.0777312325	-27.1682894253	19.5860773055
H	-2.2010347340	-26.6003854258	18.1637906106
H	-5.2588279979	-26.6929699924	18.4551623044
H	-4.4009261925	-25.9703199825	17.0822918968
H	-3.0866907516	-24.2774423864	18.5366158681
H	-8.1444505697	-23.8324459516	17.0083265740
H	-9.5707416808	-24.2677797957	16.0989900299
H	-9.3505117421	-26.5088406141	17.0849934416
H	-6.3422656381	-25.0107808497	14.4096378685
H	-8.4625422518	-28.8125501840	16.7876994914
H	-5.4377977893	-27.2889152977	14.1545757110
H	-8.4461563734	-23.4186366648	13.9718965138
H	-10.8084893375	-31.6303865056	19.7224077687
H	-10.5096466322	-32.7857535336	18.4372641749
H	-7.8876500436	-32.6103536897	17.1888334564
H	-6.5932753380	-29.2223778070	19.2986393685
H	-10.6358099730	-33.9543127059	20.6579920417
H	-1.1217544526	-36.0178938007	18.2791358576
H	-1.0829852535	-37.6765948991	17.7128193868
H	-2.5891575833	-38.1867994291	15.9507865829
H	-0.8946076005	-34.2428918921	16.1134952632
H	-3.9455801339	-37.5095088594	13.9742822841
H	-2.2312594131	-33.5824444673	14.1541367219
H	-4.0820249686	-34.2037688408	12.8418250791
H	0.9586833505	-35.5022670310	16.9224524795
H	-3.1910424159	-28.9666192071	14.3742477504
H	-2.8441074138	-28.6355149189	12.5787307364
H	-5.7322001163	-29.4818866800	14.6433814309
H	-3.7551490507	-30.8574950278	11.9846682946
H	-4.5826686330	-35.9968679046	16.3655640728
H	-8.8063420766	-29.9975071608	20.3484137169
H	-0.9821576877	-30.4300995240	20.1618408950
H	-8.6608662133	-22.1714814202	15.2115139629
H	-7.0684544832	-22.8846354755	14.9488488060
H	-4.0041669687	-24.8392715299	19.9411227192
H	-2.2344244989	-24.8549501522	19.9756705585

H	0.9794841215	-37.1695828279	16.3426077711
H	1.2414385977	-36.8265262587	18.0623966798
H	-5.9303660329	-37.6979254960	18.1792089832
H	-6.8369218028	-36.8190943947	19.4189237666
H	-9.0151150925	-34.1326828127	19.9577361775
H	-9.2917494763	-32.9763437222	21.2702798491
S	-0.0559170776	-29.3975423155	14.6627582193
C	-0.9278582720	-30.6523750541	15.6575549828
C	-0.0720415935	-28.0244659748	15.8680445546
H	0.4895019139	-28.2917856589	16.7701830935
H	0.4195221405	-27.1714080467	15.3931817215
H	-1.0999202225	-27.7581233509	16.1251787790
H	-1.9093983945	-30.2899688741	15.9670267370
H	-1.0600700808	-31.5369337677	15.0289812045
H	-0.3393549486	-30.9353254205	16.5363791276
H	0.0134600477	-32.3123756111	21.4444429960
H	-1.0213569807	-33.7387176801	21.2654300191
Fe	-5.0313884397	-30.8697283296	16.9596236719

### React<sub>B-Fe(III),VI</sub>

C	-5.8570000000	-37.2390000000	19.1710000000
C	-4.7017448353	-36.3975323428	18.6038469385
C	-5.1238431685	-35.0605369700	18.0822061609
N	-6.0057780762	-34.8996418126	17.0249748001
C	-4.7613431898	-33.7818637677	18.4244683517
C	-6.1282724225	-33.5728852234	16.7607514015
N	-5.3745475111	-32.8687114354	17.5867476078
C	-0.1150000000	-33.2510000000	20.8940000000
C	0.1187707540	-32.4039268893	19.6276380015
C	-1.0934656696	-31.6124468179	19.2551802820
N	-1.4868308977	-30.4591118484	19.9186136546
C	-2.0965946336	-31.8556459355	18.3517335648
C	-2.6796779114	-30.0539401698	19.4086206357
N	-3.0804087502	-30.8901695969	18.4663965049
C	-3.1080000000	-25.0240000000	19.3380000000
C	-3.4484009532	-26.4005017451	18.7532305181
C	-4.1701534728	-26.3199021058	17.4009391501
C	-4.4372183687	-27.6788464071	16.7448614388
O	-4.3795236796	-27.7705888883	15.4993456075
O	-4.7223750182	-28.6384338146	17.5502271325
C	-8.1410000000	-23.1040000000	14.9750000000
C	-7.1063000514	-24.2287764995	15.1873098810
C	-7.5424553509	-25.5535838177	14.6104801210
C	-7.6924154511	-26.7040138502	15.4196207121

C	-7.8117980566	-25.6606905851	13.2182311361
C	-8.0806767396	-27.9142899886	14.8858848930
C	-8.2076164933	-26.8493654808	12.6550498155
C	-8.3391927201	-28.0484349997	13.4640095570
O	-8.6019703957	-29.1636489048	12.9368907546
C	-9.7310000000	-33.4130000000	20.3670000000
C	-9.7419009839	-31.8801868381	20.2013440751
C	-8.3730816567	-31.3330562763	19.9506931290
N	-7.3952769628	-31.2735235915	20.9343980171
C	-7.7405364181	-30.9159503427	18.8073903514
C	-6.2397793346	-30.8386338308	20.3663659400
N	-6.4192767472	-30.6158127600	19.0791535191
C	0.6730000000	-36.5290000000	17.1750000000
C	-0.4126373244	-37.0461391488	16.2138979724
C	-1.1273988678	-35.9186042147	15.4999414981
C	-0.8077133244	-35.5546527056	14.1850532780
C	-2.1038696553	-35.1635252494	16.1615442618
C	-1.4220974724	-34.4736493232	13.5520019376
C	-2.7383552097	-34.0890772220	15.5416336736
C	-2.3862718956	-33.7282936158	14.2343906185
O	-2.9709524636	-32.6632546798	13.6079383768
C	-5.4711298202	-29.2678620599	13.0165570251
C	-5.8520880635	-30.6990282136	13.4250267667
C	-5.5885502712	-30.8804315732	14.9113359953
O	-6.5138902653	-30.6755403634	15.7427849872
O	-4.4037313503	-31.1738494667	15.2943242303
H	-3.9476975596	-36.2273781216	19.3802064563
H	-4.1950121491	-36.9527308543	17.8023321328
H	-4.0789426893	-33.4631511271	19.1967136149
H	-6.7539898878	-33.1585552629	15.9853276113
H	-5.4886710946	-38.1991659949	19.5439725625
H	0.9788179496	-31.7376902414	19.7737603414
H	0.3711102212	-33.0566536928	18.7853367981
H	-2.1638443971	-32.6526053432	17.6286819205
H	-3.2023431547	-29.1550463518	19.6966383146
H	0.7798688992	-33.8265058143	21.1493402400
H	-4.0828163767	-26.9613301243	19.4496903888
H	-2.5265433530	-26.9856571650	18.6288489939
H	-5.1441592436	-25.8263039422	17.5341299590
H	-3.6060485744	-25.7071283906	16.6899084204
H	-2.4493489042	-24.4599086527	18.6677980070
H	-6.1577099260	-23.9335156681	14.7159770016
H	-6.8970577701	-24.3436936212	16.2565023248
H	-7.4718632898	-26.6335271360	16.4822282352

H	-7.7024315490	-24.7775266435	12.5931490021
H	-8.1390939414	-28.8146503597	15.4886180352
H	-8.4217620659	-26.9407727442	11.5936119541
H	-9.0954478400	-23.3589142973	15.4460600929
H	-10.1828989154	-31.4104038785	21.0904396724
H	-10.3802800718	-31.6012776233	19.3569789554
H	-8.1241753383	-30.8371800265	17.8014463437
H	-5.3120746474	-30.7124561762	20.9043281053
H	-10.7423748280	-33.7945983425	20.5365793192
H	-1.1382556043	-37.6459447127	16.7793914695
H	0.0418928516	-37.7223174433	15.4804780414
H	-2.3768526838	-35.4156349688	17.1841240205
H	-0.0577029333	-36.1261245330	13.6427807790
H	-3.5035703470	-33.5212437015	16.0567896201
H	-1.1643891768	-34.1982617220	12.5337224265
H	-3.5156782655	-32.1628146463	14.2661724208
H	0.2362110864	-35.8694738649	17.9345659170
H	-5.5797344214	-28.5728382213	13.8515921910
H	-6.0768498817	-28.9429143302	12.1675706707
H	-6.9261389349	-30.7873541692	13.2440271309
H	-5.3197647039	-31.4549537788	12.8381648553
H	-6.4531218230	-35.6446690757	16.5107053587
H	-7.5295260167	-31.4923919427	21.9108128039
H	-0.9578708645	-29.9812015486	20.6337523672
H	-7.7817157528	-22.1681640648	15.4140369257
H	-8.3293474447	-22.9245411822	13.9121657174
H	-4.0133153517	-24.4255111687	19.4924699787
H	-2.6007761304	-25.1147580812	20.3043865098
H	1.4292625615	-35.9528830292	16.6313501586
H	1.1766669658	-37.3535748548	17.6907423210
H	-6.6133020105	-37.4512789484	18.4065016875
H	-6.3533806304	-36.7171497177	19.9952390327
H	-9.3261229243	-33.8925648745	19.4701383416
H	-9.1102595581	-33.7171938695	21.2171762405
S	-3.7571678202	-29.0114201078	12.3680517924
C	-2.5620958488	-29.4468792962	13.6735132707
C	-3.7202252464	-27.1902943597	12.4823169339
H	-2.7592627867	-26.8534483000	12.0889761267
H	-4.5322881173	-26.8068629271	11.8616504031
H	-3.8576606135	-26.9181114029	13.5326081985
H	-2.3709599820	-30.5169097953	13.6002538158
H	-1.6590891099	-28.8805135143	13.4297933311
H	-2.9816607594	-29.1580066181	14.6376929760
H	-0.3674018717	-32.6211852664	21.7540964249

H	-0.9410726542	-33.9523136031	20.7385503553
Fe	-4.9908909506	-30.6316652590	17.4280253292

**TS<sub>B-Fe(III),VI</sub>**

C	-5.8570000000#	-37.2390000000#	19.1710000000#
C	-4.6876500000#	-36.3768980000#	18.6655600000#
C	-5.0900830000#	-35.0493270000#	18.1048330000#
N	-5.9221860000#	-34.9054470000#	17.0053270000#
C	-4.7325040000#	-33.7654960000#	18.4347580000#
C	-6.0221570000#	-33.5846270000#	16.7060510000#
N	-5.3026640000	-32.8670160000	17.5513130000
C	-0.1150000000	-33.2510000000	20.8940000000
C	0.1337430000	-32.3556730000	19.6649020000
C	-1.0818980000	-31.5725320000	19.2872120000
N	-1.5021240000	-30.4369920000	19.9640940000
C	-2.0707070000	-31.8163290000	18.3676690000
C	-2.6940700000	-30.0407590000	19.4447980000
N	-3.0692800000	-30.8667210000	18.4827120000
C	-3.1080000000	-25.0240000000	19.3380000000
C	-3.3778590000	-26.4205410000	18.7654750000
C	-3.9320470000	-26.3805100000	17.3350300000
C	-4.1336770000	-27.7560990000	16.6979430000
O	-3.7843140000	-27.9281730000	15.5112600000
O	-4.6729130000	-28.6502500000	17.4491770000
C	-8.1410000000	-23.1040000000	14.9750000000
C	-6.8533970000	-23.9485420000	15.0281870000
C	-7.0732330000	-25.3531640000	14.5200090000
C	-7.2151770000	-26.4378960000	15.4038360000
C	-7.1867010000	-25.5966250000	13.1375340000
C	-7.4536430000	-27.7241180000	14.9394500000
C	-7.4152360000	-26.8763950000	12.6519540000
C	-7.5585350000	-27.9575290000	13.5506130000
O	-7.7723860000	-29.1904200000	13.0674670000
C	-9.7310000000	-33.4130000000	20.3670000000
C	-9.7394740000	-31.8938570000	20.1062850000
C	-8.3689880000	-31.3491280000	19.8608540000
N	-7.4018690000	-31.2742150000	20.8539710000
C	-7.7287120000	-30.9317990000	18.7217760000
C	-6.2449370000	-30.8330920000	20.2951130000
N	-6.4117010000	-30.6197480000	19.0037760000
C	0.6730000000	-36.5290000000	17.1750000000
C	-0.4827120000	-37.0905420000	16.3296300000
C	-1.2057380000	-36.0077690000	15.5598870000
C	-0.9819310000	-35.7958280000	14.1927650000

C	-2.0904160000	-35.1417720000	16.2151060000
C	-1.6082560000	-34.7596160000	13.4990050000
C	-2.7292380000	-34.1040030000	15.5395110000
C	-2.4829820000	-33.9041440000	14.1742090000
O	-3.0843720000	-32.8886650000	13.4819630000
C	-4.7815210000	-29.2505300000	12.9911430000
C	-5.5682830000	-30.4522830000	13.3786420000
C	-5.4393380000	-30.8319180000	14.8296010000
O	-6.4030970000	-30.6969300000	15.6294040000
O	-4.2885190000	-31.2208200000	15.2258350000
H	-3.9849290000	-36.1884020000	19.4840230000
H	-4.1236900000	-36.9287930000	17.9013450000
H	-4.0830130000	-33.4338670000	19.2292060000
H	-6.6063280000	-33.1828060000	15.8930290000
H	-5.4887850000	-38.1861320000	19.5744450000
H	0.9771860000	-31.6805220000	19.8558910000
H	0.4191080000	-32.9741440000	18.8078510000
H	-2.1194720000	-32.6061480000	17.6353630000
H	-3.2312010000	-29.1543240000	19.7436040000
H	0.7834910000	-33.8202450000	21.1493190000
H	-4.0918000000	-26.9596500000	19.3993020000
H	-2.4463200000	-27.0037410000	18.7711410000
H	-4.9073030000	-25.8754560000	17.3376340000
H	-3.2764280000	-25.7993850000	16.6795760000
H	-2.3788940000	-24.4810030000	18.7267440000
H	-6.0779570000	-23.4594560000	14.4254800000
H	-6.4769660000	-23.9820720000	16.0569050000
H	-7.1327020000	-26.2670330000	16.4737530000
H	-7.0900120000	-24.7658790000	12.4429480000
H	-7.5252810000	-28.5693670000	15.6139300000
H	-7.5042920000	-27.0735570000	11.5878160000
H	-8.9261090000	-23.5516630000	15.5922870000
H	-10.2078760000	-31.3734540000	20.9517500000
H	-10.3538030000	-31.6699480000	19.2289140000
H	-8.1084150000	-30.8574170000	17.7135430000
H	-5.3249120000	-30.6973820000	20.8430270000
H	-10.7466130000	-33.7850750000	20.5291690000
H	-1.1892350000	-37.6123960000	16.9884500000
H	-0.0942650000	-37.8444030000	15.6356520000
H	-2.2878690000	-35.2770780000	17.2762610000
H	-0.3023620000	-36.4540140000	13.6569160000
H	-3.4192090000	-33.4459560000	16.0523420000
H	-1.4312610000	-34.6048480000	12.4394030000
H	-3.5743800000	-32.3213540000	14.1226030000

H	0.3033740000	-35.7927160000	17.8985900000
H	-4.7901680000	-28.4981280000	13.7830610000
H	-5.1398260000	-28.8328480000	12.0450160000
H	-6.9062210000	-29.8681790000	13.2817190000
H	-5.6095320000	-31.2793570000	12.6680210000
H	-6.3469620000	-35.6589560000	16.4849270000
H	-7.5435570000	-31.4922930000	21.8292490000
H	-0.9901590000	-29.9641070000	20.6946110000
H	-7.9556650000	-22.0884430000	15.3379490000
H	-8.5210200000	-23.0358710000	13.9508270000
H	-4.0258080000	-24.4259190000	19.3668060000
H	-2.7143610000	-25.0783150000	20.3581690000
H	1.4095570000	-36.0268220000	16.5395050000
H	1.1841120000	-37.3222490000	17.7303830000
H	-6.5604010000	-37.4764490000	18.3653410000
H	-6.4135720000	-36.7220030000	19.9584520000
H	-9.2986720000	-33.9466660000	19.5149970000
H	-9.1377530000	-33.6621740000	21.2535310000
S	-2.9311480000	-29.4228380000	12.5616250000
C	-1.9852830000	-29.8801750000	14.0531180000
C	-2.5730550000	-27.6333840000	12.5166580000
H	-1.5210190000	-27.5084190000	12.2541640000
H	-3.2012550000	-27.1869720000	11.7436200000
H	-2.7994570000	-27.2179900000	13.5023280000
H	-1.9331790000	-30.9650350000	14.0770410000
H	-0.9919210000	-29.4496000000	13.9003110000
H	-2.4881590000	-29.4591430000	14.9241130000
H	-0.3972530000	-32.6566780000	21.7694510000
H	-0.9248210000	-33.9594400000	20.6939940000
Fe	-4.9477570000	-30.6462100000	17.3876530000

### **Prod<sub>B-Fe(III),VI</sub>**

C	-5.8570000000	-37.2390000000	19.1710000000
C	-4.7287761880	-36.4027293041	18.5399340592
C	-5.1495768706	-35.0505383624	18.0511324939
N	-6.0230737488	-34.8536648947	16.9921594168
C	-4.7808998140	-33.7834939697	18.4299565371
C	-6.1365413065	-33.5189563910	16.7647486727
N	-5.3878349817	-32.8426143131	17.6185659562
C	-0.1150000000	-33.2510000000	20.8940000000
C	0.1226619756	-32.2873135209	19.7166956591
C	-1.1206713271	-31.5271875028	19.3918579841
N	-1.5567993481	-30.4339389267	20.1256973570
C	-2.1327424581	-31.7809185781	18.5020938832

C	-2.7828769578	-30.0694913464	19.6686490964
N	-3.1612094010	-30.8774955125	18.6933874709
C	-3.1080000000	-25.0240000000	19.3380000000
C	-3.4920717067	-26.4216319167	18.8345115391
C	-3.7160777464	-26.4676777692	17.3202220733
C	-4.2215381892	-27.7997795820	16.7552159052
O	-4.1735773441	-27.9783062846	15.5202404775
O	-4.6965303960	-28.6408760107	17.6041436275
C	-8.1410000000	-23.1040000000	14.9750000000
C	-6.9965613532	-24.0098903740	14.4970257605
C	-7.3982618878	-25.4674024993	14.5125068134
C	-7.1063855991	-26.2878475876	15.6069222278
C	-8.1444498021	-26.0239971404	13.4614107115
C	-7.4929717911	-27.6265150302	15.6453365651
C	-8.5458479774	-27.3591727002	13.4823607735
C	-8.1972632410	-28.1758191090	14.5661471848
O	-8.5093130019	-29.5042359503	14.5035786493
C	-9.7310000000	-33.4130000000	20.3670000000
C	-9.7601782272	-31.8736910923	20.2900447387
C	-8.3959566275	-31.3163843520	20.0437932457
N	-7.3951379245	-31.3403035497	21.0049070405
C	-7.7800208638	-30.8430443401	18.9137172541
C	-6.2431131657	-30.8992084002	20.4386969167
N	-6.4454476741	-30.5921226729	19.1713341997
C	0.6730000000	-36.5290000000	17.1750000000
C	-0.4231906281	-36.9618088853	16.1847260299
C	-1.0316160727	-35.7652044715	15.4895704809
C	-0.4963754942	-35.2629858884	14.2957315922
C	-2.0875792221	-35.0594124311	16.0752308230
C	-0.9713325889	-34.0860649220	13.7193614982
C	-2.5887579452	-33.8897138209	15.5065234805
C	-2.0096552950	-33.3824700338	14.3342459319
O	-2.4346008221	-32.2087857195	13.7746784042
C	-5.6694948803	-29.2846237815	12.9749123107
C	-5.3081264155	-30.6069626332	13.5058194440
C	-5.2662097865	-30.7942808785	14.9740572469
O	-6.3061878954	-30.5991048808	15.6771885700
O	-4.1631656901	-31.1299247187	15.5051136884
H	-3.9276278144	-36.2509817626	19.2713050759
H	-4.2778651242	-36.9599793085	17.7074183088
H	-4.0991854866	-33.4900476934	19.2124683026
H	-6.7487877913	-33.0791196549	15.9923306837
H	-5.4739296130	-38.2055865158	19.5104359843
H	0.9448290920	-31.5984046540	19.9482761026



H	0.4266116803	-32.8499427058	18.8281028440
H	-2.1811958644	-32.5438394487	17.7406772745
H	-3.3408825749	-29.2126578160	20.0136674491
H	0.7962713611	-33.8059905394	21.1372903787
H	-4.4032565614	-26.7693551027	19.3349390259
H	-2.7020694243	-27.1387384742	19.0957679441
H	-4.4506483813	-25.7052601947	17.0258682282
H	-2.7979734171	-26.2111391235	16.7777079212
H	-2.1867175441	-24.6674453807	18.8622599943
H	-6.6989266492	-23.7131113029	13.4828036000
H	-6.1172576329	-23.8612202394	15.1363011951
H	-6.5554873137	-25.8773217974	16.4484160738
H	-8.4148187346	-25.4011009960	12.6109037653
H	-7.2005453654	-28.2553082204	16.4802656766
H	-9.1091599378	-27.7927944488	12.6610655843
H	-8.4417720770	-23.3664231454	15.9947345185
H	-10.1841227150	-31.4578337182	21.2133752407
H	-10.4159264117	-31.5507803675	19.4754650654
H	-8.1950090841	-30.6854253073	17.9296417991
H	-5.2991789289	-30.8331246602	20.9581616705
H	-10.7351436732	-33.8156259008	20.5309550057
H	-1.2011821111	-37.5194434668	16.7220763052
H	0.0017310060	-37.6524617639	15.4470521465
H	-2.5254759376	-35.4216072247	17.0021985287
H	0.3206818278	-35.7954145893	13.8139573458
H	-3.4162623635	-33.3615633564	15.9661514029
H	-0.5400292341	-33.6947106207	12.8031256503
H	-3.0174557182	-31.7564285478	14.4294449475
H	0.2619470605	-35.8531387998	17.9343335435
H	-5.9723709380	-28.6014380371	13.7670282591
H	-6.4215462844	-29.3124327515	12.1805177654
H	-7.8399673720	-29.9966217320	15.0265981564
H	-4.9144210372	-31.3921875989	12.8668757379
H	-6.4699025885	-35.5811921751	16.4529102091
H	-7.5132751468	-31.6166728400	21.9688717553
H	-1.0339451530	-29.9664594444	20.8523087944
H	-7.8469826487	-22.0487809814	14.9662981810
H	-9.0197972924	-23.2176338796	14.3316433205
H	-3.8967283819	-24.2953179875	19.1169292922
H	-2.9465880179	-25.0197506310	20.4212603636
H	1.4743294573	-35.9936985869	16.6548050584
H	1.1151536971	-37.3899879844	17.6883779982
H	-6.6615141460	-37.4348788630	18.4532600922
H	-6.2946130264	-36.7209246086	20.0298347742

H	-9.3367569883	-33.8357299466	19.4374304890
H	-9.0931122079	-33.7588265304	21.1880244846
S	-4.2029581033	-28.4181372889	12.1252711241
C	-2.7488737747	-28.9975334452	13.0602274401
C	-4.4324827319	-26.7214009080	12.7596594541
H	-3.6922492534	-26.0844897237	12.2710404041
H	-5.4443309368	-26.4130112857	12.4863263644
H	-4.3167769008	-26.7529685666	13.8474691431
H	-2.5517822909	-30.0313210955	12.7709882839
H	-1.9184328503	-28.3587653229	12.7501811730
H	-2.9570795686	-28.8992748337	14.1280463876
H	-0.4305369351	-32.7106829877	21.7931728215
H	-0.8988024321	-33.9730964532	20.6439844120
Fe	-4.9863205254	-30.6179776426	17.5702308531

### React<sub>Mg(II),I</sub>

C	-5.8569950000	-37.2389910000	19.1709910000
C	-5.1437657503	-35.8947631817	19.3933304566
C	-5.4908263338	-34.8309163886	18.3996175955
N	-5.2340826086	-34.9454701707	17.0439565942
C	-5.9846663716	-33.5584546866	18.5499318823
C	-5.5514914304	-33.7614969390	16.4539547682
N	-6.0011178958	-32.8877593717	17.3390694009
C	-0.1150060000	-33.2509900000	20.8939940000
C	-0.6217446554	-33.2597594996	19.4359032869
C	-1.7310662784	-32.2950910036	19.1277809584
N	-1.7233179087	-30.9693299117	19.5410821211
C	-2.8721258081	-32.4091633201	18.3684497819
C	-2.8202059571	-30.3519916371	19.0231311782
N	-3.5383033045	-31.1985745652	18.3070346808
C	-3.1080190000	-25.0239970000	19.3379980000
C	-3.2932819515	-26.4231867796	18.7499358637
C	-3.5930982429	-26.3801778560	17.2513862320
C	-3.8047253026	-27.7459981241	16.5990954238
O	-3.4799780993	-27.8663294758	15.3908778832
O	-4.3300497296	-28.6507259930	17.3226481063
C	-8.1409660000	-23.1040170000	14.9750030000
C	-8.9562884136	-24.1306449809	15.8008158525
C	-8.3972514896	-25.5448368814	15.8978291656
C	-7.5280691983	-25.9310048765	16.9331687045
C	-8.7944248716	-26.5625316736	15.0161791905
C	-7.0682886302	-27.2396349147	17.0798977239
C	-8.3453269327	-27.8791330188	15.1476574027
C	-7.4433320699	-28.2711353919	16.1752739205

O	-7.0005380470	-29.5113834551	16.2631553207
C	-9.7309990000	-33.4130130000	20.3670160000
C	-9.7181526142	-31.8663229812	20.3795055485
C	-8.3855916506	-31.2672700120	20.0435707871
N	-7.3216339715	-31.2067817354	20.9391120686
C	-7.8770506402	-30.7651405078	18.8728818760
C	-6.2406129609	-30.6972568233	20.2822125714
N	-6.5439450839	-30.4318374768	19.0275790760
C	0.6729850000	-36.5289920000	17.1749980000
C	-0.8153625276	-36.7773150166	17.4760774732
C	-1.7388635368	-36.2436468472	16.3992826245
C	-1.7622801785	-34.8782119545	16.0753362684
C	-2.5839933280	-37.0918939465	15.6732449538
C	-2.5906106710	-34.3697511434	15.0799203262
C	-3.4207679782	-36.6053931011	14.6657308853
C	-3.4314286971	-35.2364762079	14.3566424211
O	-4.2864551487	-34.8033583146	13.4084490945
C	-5.6913215304	-29.0302607867	13.5569247401
C	-6.0864424517	-30.4994113736	13.5647812949
C	-4.9608691349	-31.3810307678	14.1174300211
O	-4.6196235542	-31.2144052753	15.3248953487
O	-4.4193462958	-32.1927705429	13.3145567968
H	-5.3803242966	-35.5085858257	20.3910617680
H	-4.0561386554	-36.0590805978	19.3788126017
H	-6.2960233853	-33.0834761150	19.4650653390
H	-5.4080025232	-33.5835357615	15.4032800038
H	-5.5610231338	-37.9683041919	19.9319327417
H	0.2294669023	-33.0680236735	18.7661376741
H	-0.9809349126	-34.2607542236	19.1794935568
H	-3.2384679350	-33.2759900165	17.8436684496
H	-3.0543368252	-29.3067086540	19.1480670549
H	0.6685034928	-34.0022173868	21.0286207330
H	-4.1093978107	-26.9488993342	19.2579396372
H	-2.3835979523	-27.0167357227	18.9219937345
H	-4.5224285525	-25.8190118444	17.0794298764
H	-2.7996655423	-25.8570072121	16.7069656046
H	-2.2799269976	-24.4955653163	18.8510198381
H	-9.0772128805	-23.7306021505	16.8164435609
H	-9.9689603479	-24.1808670596	15.3790858711
H	-7.2166619471	-25.1849793596	17.6649217896
H	-9.5011180548	-26.3273356875	14.2201537299
H	-6.3989298073	-27.5013450541	17.8914309723
H	-8.7077805409	-28.6482016409	14.4674036384
H	-8.0389767287	-23.4334802500	13.9347275168

H	-10.0600426522	-31.5026140889	21.3582172674
H	-10.4409921810	-31.4923864119	19.6473334859
H	-8.3468324085	-30.6312102511	17.9111737201
H	-5.2684925326	-30.5709758475	20.7341133147
H	-10.7355201498	-33.7927658164	20.5773870313
H	-1.0640805346	-36.3224811387	18.4460448675
H	-0.9864858322	-37.8533685690	17.6001907064
H	-2.5880442300	-38.1575356378	15.8937461984
H	-1.1286740206	-34.1856477680	16.6237838845
H	-4.0723473584	-37.2687401473	14.1051144789
H	-2.6327669506	-33.3040540737	14.8764122199
H	-4.2702770645	-33.8093900580	13.3499422640
H	0.8852479400	-35.4581877682	17.0902625389
H	-5.2416225903	-28.7261954756	14.5033392323
H	-6.5337844427	-28.3761683080	13.3213587535
H	-6.9224489944	-30.5450059695	14.2711729157
H	-6.3944030620	-30.8559101370	12.5781567562
H	-4.7837874769	-35.7195959809	16.5695941292
H	-7.3548334742	-31.4648149494	21.9136714659
H	-1.0125737569	-30.5281107063	20.1035764603
H	-8.6299556030	-22.1232782390	14.9778248190
H	-7.1321305736	-22.9860468436	15.3861898626
H	-4.0111952501	-24.4186644262	19.1974655342
H	-2.8948086084	-25.0578899067	20.4126775089
H	0.9587637338	-36.9978525825	16.2280538824
H	1.3105193656	-36.9364816841	17.9672927193
H	-5.6073687982	-37.6603268708	18.1908578757
H	-6.9436001426	-37.1158236057	19.2137787681
H	-9.4087297990	-33.7897317980	19.3920034431
H	-9.0490588017	-33.8204280370	21.1219607328
S	-4.4475752553	-28.6232190576	12.2548616407
C	-2.9037900711	-29.3851335422	12.8595361939
C	-4.1578765305	-26.8672852534	12.6492714979
H	-3.3939035817	-26.4959506873	11.9629609034
H	-5.1005846817	-26.3422843228	12.4812286716
H	-3.8432926812	-26.8084605016	13.6975641956
H	-2.8319464503	-29.1786690575	13.9313433493
H	-2.9714606924	-30.4529980640	12.6470431939
H	-2.0896434581	-28.9242506007	12.2956123614
H	0.3138431066	-32.2804357531	21.1692103042
H	-0.9273900283	-33.4699495342	21.5938430449
Mg	-5.3680995016	-30.4019965974	17.0801433874

**TS<sub>Mg(II),I</sub>**

C	-5.85699500	-37.23899100	19.17099100
C	-5.19212100	-35.87902000	19.44856600
C	-5.51373900	-34.79873900	18.46196400
N	-5.28462800	-34.92188100	17.10100300
C	-5.93557900	-33.50060800	18.62321000
C	-5.54885000	-33.72390900	16.51559300
N	-5.93664800	-32.82992100	17.41038900
C	-0.11500600	-33.25099000	20.89399400
C	-0.56842600	-33.23500000	19.42177700
C	-1.67318800	-32.27085000	19.11205300
N	-1.64089400	-30.93444000	19.48876700
C	-2.84578500	-32.40108100	18.40744900
C	-2.75529900	-30.32568200	19.00298200
N	-3.50918900	-31.18833000	18.34350100
C	-3.10801900	-25.02399700	19.33799800
C	-3.23866800	-26.44169400	18.78499500
C	-3.53456600	-26.45598000	17.28285000
C	-3.67824200	-27.86334200	16.70445000
O	-3.10138400	-28.13301200	15.62841000
O	-4.41591700	-28.66022900	17.38150700
C	-8.14096600	-23.10401700	14.97500300
C	-8.91602500	-24.17094900	15.78461700
C	-8.33122000	-25.57732500	15.80645900
C	-7.58654700	-26.05100800	16.89998400
C	-8.57999900	-26.49430800	14.77468900
C	-7.10995300	-27.36116200	16.97028000
C	-8.11988700	-27.81361600	14.83126200
C	-7.37150000	-28.28236400	15.93463400
O	-6.93563600	-29.56309400	15.97767500
C	-9.73099900	-33.41301300	20.36701600
C	-9.83719200	-31.88809800	20.13754200
C	-8.52665100	-31.23170700	19.82763000
N	-7.53084500	-31.02586000	20.77792000
C	-7.97261900	-30.79923000	18.65008000
C	-6.44162400	-30.50272600	20.14780500
N	-6.67626600	-30.36410100	18.85767200
C	0.67298500	-36.52899200	17.17499800
C	-0.81649000	-36.73294200	17.50123900
C	-1.75007600	-36.18435900	16.44084500
C	-1.76029300	-34.81991900	16.10934900
C	-2.62680000	-37.02249400	15.73921500
C	-2.60672500	-34.30135100	15.13229700
C	-3.48022700	-36.52685800	14.75070400
C	-3.48007800	-35.15707000	14.43296600

O	-4.35544400	-34.72432100	13.50882300
C	-5.21869900	-28.85772200	13.51650600
C	-5.85456600	-30.11731600	13.64707100
C	-4.98455300	-31.26142500	14.14716500
O	-4.57702800	-31.23270600	15.35096600
O	-4.70275100	-32.15965400	13.31135700
H	-5.48238100	-35.51835400	20.44147800
H	-4.10139700	-36.01820900	19.48066200
H	-6.19967500	-33.00410900	19.54319800
H	-5.42152300	-33.54501200	15.46281100
H	-5.57838000	-37.96954700	19.93657200
H	0.30031700	-33.02229100	18.78214500
H	-0.91522200	-34.23096800	19.13368400
H	-3.23564600	-33.28050700	17.92301000
H	-2.97736100	-29.27706300	19.11518400
H	0.67218100	-33.99545900	21.04446500
H	-4.03796100	-26.98329700	19.30314600
H	-2.30656400	-26.99390200	18.97591000
H	-4.48739400	-25.94068700	17.09768700
H	-2.75581600	-25.92430700	16.72741800
H	-2.29842400	-24.47810900	18.84009500
H	-9.01320100	-23.81733300	16.81886400
H	-9.93897500	-24.22409200	15.38904800
H	-7.38447500	-25.37861400	17.73259900
H	-9.17653200	-26.18396900	13.91832100
H	-6.52610100	-27.69612000	17.81788600
H	-8.36596200	-28.50770800	14.03233700
H	-8.05662800	-23.39674600	13.92284400
H	-10.29929400	-31.41462400	21.01444800
H	-10.50907600	-31.69273300	19.29594800
H	-8.38939800	-30.78984400	17.65489200
H	-5.51296400	-30.26943000	20.64633400
H	-10.71948000	-33.84722900	20.54449100
H	-1.03438600	-36.26731400	18.47328200
H	-1.01370600	-37.80318900	17.63565500
H	-2.64200600	-38.08691300	15.96485600
H	-1.10246900	-34.13422600	16.63704600
H	-4.15322600	-37.18241600	14.20652400
H	-2.63746500	-33.23420500	14.93389200
H	-4.38165200	-33.72431600	13.45218200
H	0.91227200	-35.46530900	17.07361600
H	-4.57138000	-28.52434100	14.32467800
H	-5.72564600	-28.07820600	12.95414600
H	-6.52004500	-29.84242200	14.73265800

H	-6.50331200	-30.41617200	12.82284400
H	-4.87362900	-35.71298900	16.61840400
H	-7.61249700	-31.20700400	21.76678000
H	-0.90221500	-30.48130600	20.00395400
H	-8.65084800	-22.13597700	15.02187000
H	-7.12548700	-22.97864900	15.36584600
H	-4.03233600	-24.45673800	19.17770600
H	-2.89861500	-25.02263500	20.41369700
H	0.93106600	-37.01551300	16.22921600
H	1.31164600	-36.94438300	17.96221600
H	-5.54486300	-37.64005500	18.20055400
H	-6.94747900	-37.14781300	19.15929500
H	-9.28233200	-33.90076100	19.49677800
H	-9.10177500	-33.64001000	21.23502600
S	-3.30326100	-28.88951100	12.09333900
C	-2.24681400	-29.96854400	13.12016900
C	-2.67593600	-27.25289000	12.60525200
H	-1.66048300	-27.11551100	12.22389700
H	-3.33126400	-26.49873400	12.16211500
H	-2.69437000	-27.18634800	13.69694400
H	-2.40453500	-29.72713000	14.17393400
H	-2.55207100	-30.99510900	12.91254800
H	-1.20361600	-29.81686800	12.83055600
H	0.29032500	-32.28110400	21.20457100
H	-0.95005600	-33.49233400	21.55895800
Mg	-5.30131100	-30.45798500	17.09021300

**The optimizations without any aotm constraints**

**React<sub>Ni(II),III,nofix</sub>**

C	-7.3695605555	-36.8552245474	17.3955954538
C	-5.9477761639	-36.3345432849	17.6711825292
C	-5.6867151161	-34.9855203784	17.0856325335
N	-5.5612042137	-34.7748007425	15.7225864364
C	-5.5418203676	-33.7413600558	17.6458068553
C	-5.3118985223	-33.4559976021	15.5163428839
N	-5.3046586402	-32.8023736461	16.6611139781
C	0.3518412081	-32.5997073424	21.0507156955
C	-0.6130023328	-33.4177330700	20.1735977021
C	-1.3478943739	-32.5922797506	19.1668808462
N	-0.7142569910	-31.9277692546	18.1241607218
C	-2.6791291533	-32.3004259296	19.0008835720
C	-1.6552123432	-31.2854484747	17.3826081749
N	-2.8524978902	-31.4984388511	17.8924574580
C	-3.4088227508	-25.3515231345	19.9638590031

C	-3.4796234964	-26.7206302407	19.2798760859
C	-2.7029937742	-26.7649292768	17.9627501376
C	-2.8066406936	-28.0781545615	17.1635166297
O	-1.9120486810	-28.2872330902	16.3014930488
O	-3.8250399611	-28.7997819737	17.3949869791
C	-10.5015143579	-25.3739725650	16.0155610161
C	-10.3167639166	-26.4689858473	17.0819481776
C	-9.2090690598	-27.4459563877	16.7461362568
C	-7.8836392182	-27.2168377566	17.1455890090
C	-9.4551254389	-28.6034587783	15.9916061118
C	-6.8516994262	-28.0960915230	16.8270145283
C	-8.4392377084	-29.4981171221	15.6649099828
C	-7.1007146828	-29.2819882054	16.0840538568
O	-6.1602469307	-30.1507878461	15.7777451724
C	-9.6536538465	-28.8435356671	20.1887968309
C	-8.9916621182	-30.2129807627	20.4349120097
C	-7.5964325295	-30.2855021918	19.9020914030
N	-6.5415551896	-29.5537631298	20.4351177330
C	-7.0564325363	-30.9310222715	18.8208712014
C	-5.4382361419	-29.7686112759	19.6716256317
N	-5.7212765261	-30.6043795356	18.6928390025
C	-0.9758847422	-37.2322145552	18.3170296101
C	-2.4298300685	-37.0204924365	17.8636282697
C	-2.5342451153	-36.3306447494	16.5194556950
C	-2.2822474225	-34.9546095988	16.4101721679
C	-2.8760566440	-37.0210837157	15.3515110086
C	-2.3757513135	-34.2826629813	15.1965598722
C	-2.9840948784	-36.3651043826	14.1216311360
C	-2.7470895619	-34.9849862863	14.0345442377
O	-2.9349027505	-34.3790328124	12.8431000896
C	-4.5090102879	-28.6469067910	13.9761125020
C	-4.6894029519	-30.0218285613	13.3404754116
C	-3.6369563496	-31.0352686954	13.8153446486
O	-3.4051781408	-31.1044158232	15.0588498256
O	-3.0724519706	-31.7332848711	12.9293170407
H	-5.7741143731	-36.2775655156	18.7513550917
H	-5.2093397063	-37.0428043825	17.2744382585
H	-5.6018080355	-33.4556880763	18.6844927504
H	-5.1177138454	-33.0315902325	14.5463018030
H	-7.5147825443	-37.8483713701	17.8333498759
H	-0.0586840652	-34.2193447448	19.6654104282
H	-1.3571286744	-33.9169943971	20.8027319834
H	-3.5199871500	-32.6241990319	19.5939018028
H	-1.4631812127	-30.6628603582	16.5223675451



H	0.8623306572	-33.2417062208	21.7756824913
H	-4.5220630905	-26.9934747239	19.0835941491
H	-3.0772033695	-27.4887762938	19.9555393987
H	-3.0765320313	-25.9698336714	17.2970141301
H	-1.6400872269	-26.5484477182	18.1202825323
H	-2.3727699936	-25.0678547296	20.1849719800
H	-10.1088588456	-25.9936827429	18.0504081700
H	-11.2641548121	-27.0110261043	17.2048245988
H	-7.6568005759	-26.3276034191	17.7354885470
H	-10.4731498839	-28.8138331831	15.6635311480
H	-5.8387643993	-27.9278091706	17.1756784780
H	-8.6532086107	-30.4028787603	15.1004357922
H	-10.7428886743	-25.8188324624	15.0437852973
H	-9.5763496357	-30.9968564189	19.9423390314
H	-9.0014234114	-30.4483550224	21.5089612552
H	-7.5378321208	-31.5650296433	18.0939695851
H	-4.4838900509	-29.2918855489	19.8151864831
H	-10.6789982574	-28.8327966979	20.5736625249
H	-2.9572631186	-36.4211878141	18.6187350415
H	-2.9422997240	-37.9902622836	17.8262825774
H	-3.0706628322	-38.0914268481	15.3998717239
H	-2.0452164951	-34.3857774418	17.3052098709
H	-3.2595074376	-36.9027471841	13.2186571732
H	-2.2470585410	-33.2055742148	15.1495013287
H	-2.8742204292	-33.3901654224	12.9291464547
H	-0.4476950602	-36.2737637390	18.3677518873
H	-4.1859118115	-28.7229511380	15.0151033234
H	-5.4082597634	-28.0290320006	13.9092033329
H	-5.6528857222	-30.3760816322	13.7225054970
H	-4.7148345714	-29.9899231002	12.2467214067
H	-5.3950823172	-35.4970702834	15.0340221314
H	-6.5979108522	-28.9292725750	21.2249385405
H	0.2750363471	-31.9388450148	17.9282175107
H	-11.3072696471	-24.6790632865	16.2829453624
H	-9.5789343719	-24.7955657318	15.8923872451
H	-3.8334219319	-24.5698703786	19.3221772819
H	-3.9645371352	-25.3421209479	20.9084541460
H	-0.4353108519	-37.8667446260	17.6065858363
H	-0.9256301346	-37.7027305303	19.3059565786
H	-7.5596493827	-36.9297088288	16.3195826020
H	-8.1197138275	-36.1791396884	17.8181339528
H	-9.1011569376	-28.0387426084	20.6882572992
H	-9.6707641445	-28.6146790632	19.1197139057
S	-3.2258642394	-27.6933288847	13.0401288426

C	-1.7194615160	-28.6933602499	13.2754853008
C	-2.8917104952	-26.2868475896	14.1468014528
H	-2.2350187517	-25.5941683988	13.6162950874
H	-3.8491512450	-25.8057482742	14.3584530189
H	-2.4252639912	-26.6791395610	15.0553204219
H	-1.6405174134	-28.9227420603	14.3423102329
H	-1.8254496369	-29.5932112114	12.6664331936
H	-0.8824549731	-28.0853747640	12.9249064998
H	1.1202083425	-32.1055614176	20.4451137277
H	-0.1883076946	-31.8209227160	21.5983698589
Ni	-4.5952756839	-30.7785157534	16.8867233408

**TS<sub>Ni(II),III,nofix</sub>**

C	-7.08200300	-37.09100800	17.35433700
C	-5.73386500	-36.41429900	17.65762800
C	-5.61942200	-35.03488300	17.09732100
N	-5.63331800	-34.77944200	15.73622900
C	-5.48947500	-33.80009300	17.68114000
C	-5.47229200	-33.44494000	15.54821700
N	-5.39343300	-32.82196300	16.70930400
C	0.28771000	-32.47366900	21.13283200
C	-0.72966700	-33.32883000	20.35677800
C	-1.44979800	-32.57631000	19.28445800
N	-0.80868300	-32.02912600	18.17913100
C	-2.77238700	-32.25588600	19.10655700
C	-1.73738600	-31.42371900	17.39289400
N	-2.93406300	-31.54925700	17.93277500
C	-3.24411100	-25.27680100	19.78371800
C	-3.43438100	-26.66740000	19.17021500
C	-2.60064100	-26.87560200	17.90512600
C	-2.79488800	-28.21797700	17.17791800
O	-1.89842800	-28.56422100	16.37286600
O	-3.89200500	-28.82871400	17.40985200
C	-10.46142000	-25.26045200	16.13548100
C	-10.29268700	-26.32941700	17.22975400
C	-9.23927900	-27.35792200	16.87978600
C	-7.88770800	-27.14497600	17.18639500
C	-9.57411800	-28.53654800	16.19577300
C	-6.90114000	-28.06325700	16.82803000
C	-8.60311500	-29.46975100	15.83763400
C	-7.24931100	-29.24902600	16.15105500
O	-6.32301000	-30.16074800	15.79571800
C	-9.93108000	-29.10904300	20.08026400
C	-9.15933700	-30.41233600	20.35721000

C	-7.75690500	-30.37787100	19.84134800
N	-6.79287700	-29.50481600	20.33097000
C	-7.13133100	-31.04827200	18.82293600
C	-5.65703200	-29.66368300	19.60400900
N	-5.83246600	-30.59747300	18.68959100
C	-0.53032100	-36.84626100	18.07417000
C	-2.03161000	-36.86920100	17.73950100
C	-2.35010300	-36.18812700	16.42618600
C	-2.27569300	-34.79051900	16.32360400
C	-2.70822100	-36.90310200	15.27756500
C	-2.53788100	-34.12364800	15.13289100
C	-2.99833300	-36.25182600	14.07434600
C	-2.92336300	-34.85230400	13.99157700
O	-3.27196800	-34.25870500	12.83109700
C	-4.34797400	-28.42460100	14.05711100
C	-4.91826400	-29.66825200	13.66829300
C	-4.06653100	-30.90036300	13.91241000
O	-3.60621100	-31.07164500	15.08962900
O	-3.86705400	-31.67736300	12.94258800
H	-5.57939600	-36.35539400	18.74024900
H	-4.91479000	-37.02630800	17.25863900
H	-5.46169600	-33.55086600	18.72992400
H	-5.38388800	-32.98706100	14.57690300
H	-7.11633600	-38.09990700	17.77762500
H	-0.22155200	-34.20090000	19.92278400
H	-1.48109500	-33.72830300	21.04581400
H	-3.61277100	-32.48927600	19.74124900
H	-1.53897700	-30.87904000	16.48407200
H	0.78366700	-33.06556400	21.90830000
H	-4.48996800	-26.83376900	18.92961400
H	-3.15918300	-27.43402600	19.90803800
H	-2.84651700	-26.09184900	17.17194800
H	-1.53113000	-26.76253700	18.11465800
H	-2.19514800	-25.09849900	20.04704900
H	-10.03030400	-25.83807400	18.17568200
H	-11.25566900	-26.82791000	17.39827400
H	-7.60185100	-26.23968900	17.72058400
H	-10.61628600	-28.72757000	15.94570300
H	-5.85944900	-27.91873800	17.09281200
H	-8.86773600	-30.38877100	15.32279100
H	-10.75185700	-25.72266100	15.18623000
H	-9.66946400	-31.25231600	19.87507800
H	-9.16182300	-30.62701500	21.43514300
H	-7.52827700	-31.79091900	18.14966800

H	-4.76208200	-29.07592200	19.71605300
H	-10.95715100	-29.17805200	20.45522900
H	-2.58449000	-36.37367100	18.54966900
H	-2.38257800	-37.90836100	17.71677500
H	-2.77017100	-37.98905500	15.32072300
H	-2.03612200	-34.20847700	17.20800100
H	-3.28659800	-36.80960900	13.18817800
H	-2.53145100	-33.03968400	15.09536000
H	-3.37362000	-33.27286100	12.93853900
H	-0.16023000	-35.81536300	18.10448600
H	-3.78369900	-28.41968400	14.98376300
H	-4.89467100	-27.51331600	13.82659500
H	-5.73379500	-29.81790500	14.66408700
H	-5.45779600	-29.68840700	12.72127000
H	-5.50527300	-35.47321100	15.01218700
H	-6.92993600	-28.82965800	21.06716600
H	0.17780200	-32.08577300	17.97808900
H	-11.22703700	-24.52506600	16.40743100
H	-9.51919500	-24.72806400	15.96776900
H	-3.54309300	-24.49268800	19.07825500
H	-3.84194900	-25.15083400	20.69311200
H	0.04651900	-37.37706400	17.30978300
H	-0.32572000	-37.31190100	19.04506900
H	-7.24662800	-37.17574000	16.27494100
H	-7.91232200	-36.51295800	17.77181800
H	-9.45461500	-28.25188500	20.56958100
H	-9.95618500	-28.90107400	19.00783900
S	-2.49976500	-27.85512600	12.80255400
C	-1.44942100	-29.28228300	13.23424900
C	-1.77960900	-26.58439400	13.89573200
H	-0.79860400	-26.29059900	13.51319000
H	-2.44720500	-25.71927100	13.87700600
H	-1.69473100	-26.99545400	14.90643400
H	-1.52777900	-29.45701300	14.30901900
H	-1.82808700	-30.14137200	12.67762100
H	-0.42110600	-29.06296700	12.93647600
H	1.06515300	-32.07743000	20.47027200
H	-0.20566300	-31.62159900	21.61020200
Ni	-4.65196400	-30.79532600	16.93722700

**Optimizations with the model built from the crystal structure of free *Pu*DddK  
(PDB code: 6A53)**

**React<sub>Ni(II),III,PDB</sub>**

C	13.4720000000	-15.1850000000	-7.5700000000
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C	12.3578569519	-14.2109818131	-7.1278221919
C	11.7744580082	-14.4270664723	-5.7528033403
N	10.4514689897	-14.1072605368	-5.4694607656
C	12.3030251412	-14.7777423559	-4.5313153837
C	10.2468429968	-14.2417824675	-4.1308722790
N	11.3477901662	-14.6491601093	-3.5360293090
C	18.1830000000	-16.1620000000	-2.3160000000
C	17.4270460994	-14.8153372318	-2.2614765632
C	15.9988430009	-14.9200328150	-1.8103432245
N	15.6141862379	-15.6811097016	-0.7144914319
C	14.8307242535	-14.3418882843	-2.2533129008
C	14.2737458312	-15.5379284827	-0.5377075514
N	13.7693297235	-14.7394377042	-1.4606291928
C	12.8120000000	-16.1570000000	4.5340000000
C	12.8605311582	-15.6176373600	3.1051686716
C	12.2708057441	-14.2091894351	2.9980413452
C	12.2638129100	-13.6473310730	1.5758005431
O	11.9794685655	-14.4965971605	0.6689386585
O	12.4919171843	-12.4259412426	1.4106528286
C	6.4940000000	-13.6480000000	5.0950000000
C	6.2738762533	-14.5109594355	3.8176048648
C	7.2046429068	-14.3459255965	2.6114739612
C	8.4000680103	-15.0785065893	2.4780374176
C	6.8338346425	-13.5913280892	1.4862689796
C	9.1745148643	-15.0647657675	1.3153431781
C	7.5978856646	-13.5618525212	0.3137825878
C	8.8126360095	-14.2925532609	0.1753705566
O	9.5049065582	-14.2643800337	-0.9596491345
C	9.2350000000	-17.9460000000	-5.2780000000
C	9.1541196791	-18.5621526074	-3.8641006177
C	10.1698829216	-17.9749834190	-2.9362792399
N	11.5314766024	-18.2183362778	-3.0699917385
C	10.0827767094	-17.0231802393	-1.9533702007
C	12.1938825602	-17.4129080888	-2.1985282726
N	11.3458122056	-16.6707266847	-1.5109014773
C	18.5200000000	-11.6570000000	-5.0030000000
C	17.3862365343	-11.7367458991	-6.0411820733
C	16.0884268037	-11.1667746965	-5.5099209250
C	15.9838699738	-9.7991111937	-5.2188038251
C	14.9778792452	-11.9739010853	-5.2346689708
C	14.8270421827	-9.2568376956	-4.6682936635
C	13.8090250293	-11.4542515145	-4.6765606349
C	13.7297598058	-10.0818456721	-4.3878009040
O	12.6238776311	-9.5123001576	-3.8477784672

H	12.7520629666	-13.1857551874	-7.1704568038
H	11.5416019503	-14.2524053933	-7.8614410720
H	13.3062981435	-15.0966030774	-4.2983549183
H	9.3204940936	-14.0300190322	-3.6181985717
H	13.8296237628	-14.9179310187	-8.5684147834
H	17.9747083441	-14.1260760184	-1.6026434686
H	17.4287501170	-14.3482781667	-3.2519852069
H	14.6941642420	-13.6358683449	-3.0580739359
H	13.6993370331	-15.9955400995	0.2520524684
H	19.2021324139	-16.0130015382	-2.6845708727
H	13.9019147184	-15.6022754900	2.7505541439
H	12.3089917203	-16.2784718318	2.4274907414
H	12.8016039035	-13.5085828470	3.6517322279
H	11.2198154476	-14.2320698699	3.3209012420
H	13.3722989873	-15.5130323549	5.2227124985
H	6.3053656171	-15.5653559192	4.1239982609
H	5.2451954782	-14.3374541248	3.4744023326
H	8.7231244842	-15.7141959866	3.3034774904
H	5.8957087299	-13.0360788192	1.5062862690
H	10.0850700868	-15.6482141412	1.2564638988
H	7.2329221620	-12.9978634970	-0.5425632213
H	6.4045654454	-12.5793663292	4.8689578711
H	9.2710166565	-19.6532611079	-3.9269361065
H	8.1616751966	-18.3826296867	-3.4381594475
H	9.2223326151	-16.4880611388	-1.5829084697
H	13.2694401794	-17.3748537362	-2.1256801919
H	8.4722983811	-18.3731327630	-5.9374160765
H	17.6941028966	-11.1966808548	-6.9472805680
H	17.2363157470	-12.7815740765	-6.3422220228
H	16.8267417885	-9.1435090036	-5.4302771394
H	15.0254537877	-13.0407896514	-5.4531980317
H	14.7473194887	-8.1946972180	-4.4556094462
H	12.9643347909	-12.0924428333	-4.4391026864
H	11.8877783372	-10.1833865529	-3.8281635477
H	18.2517469168	-12.2060504641	-4.0933644404
H	11.9548303755	-18.8783097585	-3.7044386969
H	9.7968169923	-13.6959477480	-6.1175528765
H	16.2278241480	-16.2202974705	-0.1232106498
H	5.7493770176	-13.9024482912	5.8571036797
H	7.4907904678	-13.8164267858	5.5180828354
H	11.7785706924	-16.2050881636	4.8976691025
H	13.2352587516	-17.1659107594	4.6037680171
H	10.2156210391	-18.1253114044	-5.7327278615
H	9.0912646033	-16.8622894435	-5.2293128294

H	14.3259083849	-15.1413419407	-6.8849933990
H	13.1100745957	-16.2181340580	-7.5929743590
H	18.7117818852	-10.6192745095	-4.7115647581
H	19.4544976225	-12.0765480924	-5.3942442621
H	17.6771043473	-16.8704524328	-2.9797231778
H	18.2606082474	-16.6250383576	-1.3253850594
C	10.0015136443	-11.1925275378	-0.0318498865
C	9.6212133891	-11.3049918198	-1.4961201589
C	10.7899704677	-11.6925354385	-2.4052955333
O	11.7300127032	-12.3868359243	-1.9124012834
O	10.7267545365	-11.2825518679	-3.5971810680
H	10.6401895255	-12.0172721566	0.2848492874
H	9.1277569220	-11.1112625588	0.6209351676
H	8.9246048542	-12.1457143256	-1.5572637787
H	9.1280341248	-10.4085929202	-1.8841722604
S	10.9576249802	-9.6432857252	0.2978511550
C	12.6219910968	-9.9601709216	-0.3881354429
C	11.2626048045	-9.8083857847	2.0864051628
H	11.8735950785	-8.9570922204	2.3952694806
H	10.2895599936	-9.7671013641	2.5812520877
H	11.7667735964	-10.7674871852	2.2538856006
H	12.8913493317	-10.9907228957	-0.1476280293
H	12.5847123119	-9.7817157857	-1.4648652499
H	13.2816608317	-9.2311508446	0.0902088115
Ni	11.5614004069	-14.4316254671	-1.3128537501

### **TS<sub>Ni(II),III,PDB</sub>**

C	13.47201800	-15.18498300	-7.56999300
C	12.53993500	-14.05987800	-7.08689400
C	11.91174300	-14.26009200	-5.73352000
N	10.66340300	-13.72858000	-5.43891700
C	12.34140600	-14.79356700	-4.53920800
C	10.40569000	-13.92613700	-4.12001000
N	11.40010200	-14.57084900	-3.54481800
C	18.18302000	-16.16162700	-2.31613900
C	17.43268300	-14.81591000	-2.22580900
C	16.00637800	-14.94318400	-1.78320200
N	15.63337000	-15.72257400	-0.69661300
C	14.82909600	-14.39461500	-2.23778400
C	14.28991000	-15.61889700	-0.53334000
N	13.77536400	-14.83141300	-1.45917400
C	12.81207800	-16.15697000	4.53382500
C	12.91130700	-15.67692800	3.08575600
C	12.66665100	-14.17065600	2.94586400

C	12.70277400	-13.68560300	1.49244700
O	12.00322700	-14.40339800	0.69295300
O	13.35279200	-12.66178000	1.20021300
C	6.49400100	-13.64800200	5.09500100
C	6.63079900	-14.77917500	4.04870500
C	7.45693800	-14.48627700	2.80046700
C	8.51852900	-15.32344000	2.41777900
C	7.13646200	-13.44059500	1.92195200
C	9.22938500	-15.14111100	1.22917500
C	7.83420400	-13.24372000	0.72635700
C	8.89917900	-14.09200900	0.35392500
O	9.56345800	-13.88187400	-0.81854000
C	9.23502000	-17.94597100	-5.27797300
C	8.88370900	-18.29696400	-3.81609300
C	9.89003900	-17.76139300	-2.84849700
N	11.20404600	-18.21158600	-2.81545700
C	9.86153300	-16.71125500	-1.96859400
C	11.90100200	-17.42583700	-1.95392600
N	11.11867500	-16.50185300	-1.42807000
C	18.51986300	-11.65744700	-5.00272100
C	17.40432500	-11.82642400	-6.04964900
C	16.10066800	-11.21886100	-5.58334200
C	15.96002400	-9.82620100	-5.49317000
C	15.02796100	-12.00734200	-5.15000200
C	14.80527700	-9.24350400	-4.98184800
C	13.86367400	-11.44659000	-4.62050000
C	13.74660500	-10.04858600	-4.53241200
O	12.65532100	-9.43117500	-4.02642200
H	13.10221800	-13.11645700	-7.06280800
H	11.73899100	-13.91966400	-7.82454100
H	13.26877100	-15.29930800	-4.32129100
H	9.52500000	-13.56190700	-3.61532000
H	13.88561900	-14.93873000	-8.55174500
H	17.97527700	-14.14700700	-1.54340800
H	17.43686300	-14.31941500	-3.20127600
H	14.67543900	-13.68525700	-3.03472600
H	13.72541300	-16.07905900	0.26188300
H	19.20445100	-16.00701400	-2.67524200
H	13.90793700	-15.91974800	2.68757000
H	12.18368100	-16.20174000	2.45768400
H	13.39586600	-13.59838800	3.52827500
H	11.66588900	-13.93913900	3.33642200
H	13.54058400	-15.64533600	5.17359000
H	7.05366800	-15.66238700	4.54299700



H	5.61889400	-15.07360600	3.73477200
H	8.79819600	-16.15161500	3.06713400
H	6.30798400	-12.77549800	2.15822600
H	10.06334900	-15.78092900	0.97369600
H	7.54528600	-12.43838800	0.05708500
H	6.03621400	-12.75450400	4.65742600
H	8.78508500	-19.38599200	-3.70956600
H	7.90882900	-17.87250500	-3.55699700
H	9.05170300	-16.04182900	-1.72595000
H	12.95846900	-17.53485600	-1.77251500
H	8.47051500	-18.32164000	-5.96514700
H	17.72559600	-11.36122000	-6.99118700
H	17.26207400	-12.89300400	-6.26567300
H	16.77394000	-9.18604500	-5.82835800
H	15.10451000	-13.09218600	-5.21824600
H	14.69631000	-8.16503200	-4.92085400
H	13.06134800	-12.06949000	-4.23974900
H	11.94117700	-10.09640800	-3.81513700
H	18.23659500	-12.13187100	-4.05653900
H	11.57488900	-18.98931300	-3.33952800
H	10.11550400	-13.14362200	-6.05181800
H	16.25868300	-16.23747400	-0.09642000
H	5.86715700	-13.97315600	5.93161100
H	7.47387700	-13.35837500	5.48905400
H	11.81540800	-15.95294700	4.94199300
H	12.99231400	-17.23455400	4.61813200
H	10.19537000	-18.38364600	-5.57178500
H	9.31634600	-16.86162200	-5.40071900
H	14.31080000	-15.32143600	-6.87885200
H	12.93886100	-16.13806100	-7.64483700
H	18.69763000	-10.59784800	-4.79349400
H	19.46356900	-12.10039400	-5.34177300
H	17.67738500	-16.84858700	-3.00200600
H	18.25442600	-16.65365800	-1.33930500
C	10.64194900	-11.15527500	0.24499400
C	10.06138300	-11.33216000	-1.04814900
C	11.01482400	-11.61212900	-2.16902200
O	11.99551500	-12.39937500	-1.92465700
O	10.78790500	-11.08936100	-3.29674600
H	11.43449500	-11.84692300	0.51405400
H	9.97752800	-10.87617200	1.06065400
H	9.66508300	-12.62828100	-0.91934000
H	9.23954600	-10.67145300	-1.32293000
S	11.98292600	-9.39047300	0.41183600

C	13.37657400	-9.94039100	-0.63286400
C	12.65403700	-9.73982400	2.07066700
H	13.46352600	-9.03742300	2.28532300
H	11.84388700	-9.58852700	2.78856200
H	13.01201700	-10.77385900	2.09625900
H	13.53759500	-11.00880800	-0.48019700
H	13.11118500	-9.72803400	-1.66984800
H	14.25456800	-9.35187300	-0.35350200
Ni	11.69278500	-14.36279100	-1.30175000