Mechanistic Insights into Metabolic Pathways of Vanillin: Unraveling Cytochrome P450 Interaction Mechanisms and Implications for Food Safety

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Relative energies (RE) (in kcal/mol) and atomic energies (in a.u.) at the B3LYP level of theory for the mechanism of vanillin deformylation by CYP450 (Path A)

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE +Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_{A}$	-2120.84996200	0.00	-2120.41187200	0.00	-2121.86456200	0.00	-2121.42647200	0.00	-2121.88321900	0.00	-2121.44512900	0.00
$^{4}RC_{A}$	-2120.85013900	-0.11	-2120.41202800	-0.10	-2121.86445600	0.07	-2121.42634500	0.08	-2121.88311370	0.07	-2121.44500270	0.08
$^{2}TS\text{-}O_{A}$	-2120.81193300	23.86	-2120.37531200	22.94	-2121.84314700	13.44	-2121.40652600	12.52	-2121.86464600	11.65	-2121.42802500	10.73
$^{4}TS\text{-}O_{A}$	-2120.81660200	20.93	-2120.37962300	20.24	-2121.84623200	11.50	-2121.40925300	10.81	-2121.86772900	9.72	-2121.43075000	9.02
$^{2}INT\text{-}O_{A}$	-2120.83276000	10.79	-2120.39394200	11.25	-2121.86811300	-2.23	-2121.42929500	-1.77	-2121.88583	-1.64	-2121.44701200	-1.18
$^{4}INT\text{-}O_{A}$	-2120.83043900	12.25	-2120.39267300	12.05	-2121.86374700	0.51	-2121.42598100	0.31	-2121.88182	0.88	-2121.44405200	0.68
$^{2}TS\text{-}def_{A}$	-2120.80015000	31.26	-2120.36531600	29.21	-2121.83875300	16.20	-2121.40391900	14.15	-2121.863245	12.53	-2121.42841100	10.49
$^{4}TS\text{-}def_{A}$	-2120.79986200	31.44	-2120.36416300	29.94	-2121.84650500	11.33	-2121.41080600	9.83	-2121.86659	10.43	-2121.43089100	8.93
$^{2}INT\text{-}def_{A}$	-2120.83431100	9.82	-2120.39794900	8.74	-2121.86527200	-0.45	-2121.42891000	-1.53	-2121.88193200	0.81	-2121.44557000	-0.28
$^{4}INT\text{-}def_{A}$	-2120.83437800	9.78	-2120.39798600	8.71	-2121.86804000	-2.18	-2121.43164800	-3.25	-2121.88322600	0.00	-2121.44683400	-1.07
$^{2}P\text{-}OH_{A}$	-2120.90218900	-32.77	-2120.45953400	-29.91	-2121.93680600	-45.33	-2121.49415100	-42.47	-2121.95956700	-47.91	-2121.51691200	-45.04
$^{4}P\text{-}OH_{A}$	-2120.88170300	-19.92	-2120.44335000	-19.75	-2121.91248800	-30.07	-2121.47413500	-29.91	-2121.93174200	-30.45	-2121.49338900	-30.28

Table S2. Relative energies (RE) (in kcal/mol) and atomic energies (in a.u.) at the B3LYP level of theory for the mechanism of methoxy dealkylation of vanillin by CYP450 (Path B)

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE +Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_{B}$	-2120.86782300	0.00	-2120.42988500	0.00	-2121.89414600	0.00	-2121.45620800	0.00	-2121.91111500	0.00	-2121.47317700	0.00
$^{4}RC_{B}$	-2120.86790300	-0.05	-2120.42980300	0.05	-2121.89404800	0.06	-2121.45594800	0.16	-2121.91095700	0.10	-2121.47285700	0.20
$^{2}TS\text{-}H_{B}$	-2120.84172500	16.38	-2120.40951500	12.78	-2121.86218500	20.06	-2121.42997500	16.46	-2121.87941200	19.89	-2121.44720200	16.30
$^{4}TS\text{-}H_{B}$	-2120.84063000	17.06	-2120.40929700	12.92	-2121.86819800	16.28	-2121.43686500	12.14	-2121.88397400	17.03	-2121.45264100	12.89
$^{2}INT_{B}$	-2120.83764900	18.93	-2120.40203900	17.47	-2121.88265700	7.21	-2121.44704700	5.75	-2121.89657	9.13	-2121.46096300	7.66
$^{4}INT_{B}$	-2120.83748400	19.04	-2120.40190200	17.56	-2121.88255600	7.27	-2121.44697400	5.79	-2121.89648	9.19	-2121.46089500	7.71
$^{4}TS\text{-}reb_{B}$	-2120.84942100	11.55	-2120.41667200	8.29	-2121.88940300	2.98	-2121.45665400	-0.28	-2121.905339	3.62	-2121.47259000	0.37
$^{2}P\text{-}OH_{B}$	-2120.93233200	-40.48	-2120.49082500	-38.24	-2121.97646200	-51.65	-2121.53495500	-49.41	-2121.99486700	-52.56	-2121.55336000	-50.32
$^{4}P\text{-}OH_{B}$	-2120.91394200	-28.94	-2120.47378900	-27.55	-2121.96098900	-41.94	-2121.52083600	-40.55	-2121.98052600	-43.56	-2121.54037300	-42.17

Table S3. Relative energies (RE) (in kcal/mol) and atomic energies (in a.u.) at the B3LYP level of theory for the mechanism of acetal formation from vanillin by CYP450 (Path C)

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE+ Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_{C}$	-2120.86743000	0.00	-2120.42950400	0.00	-2121.89356600	0.00	-2121.45564000	0.00	-2121.91119300	0.00	-2121.47326700	0.00
$^{4}RC_{C}$	-2120.86958500	-1.35	-2120.43096200	-0.91	-2121.89673700	-1.99	-2121.45811400	-1.55	-2121.91545600	-2.68	-2121.47683300	-2.24
$^{2}TS1\text{-}H_{C}$	-2120.84172500	16.13	-2120.40951500	12.54	-2121.86218500	19.69	-2121.42997500	16.11	-2121.87941200	19.94	-2121.44720200	16.36
$^{4}TS1\text{-}H_{C}$	-2120.84063000	16.82	-2120.40929700	12.68	-2121.86819800	15.92	-2121.43686500	11.78	-2121.88397400	17.08	-2121.45264100	12.94
$^{2}INT1\text{-}H_{C}$	-2120.83764900	18.69	-2120.40203900	17.23	-2121.88265700	6.85	-2121.44704700	5.39	-2121.89657	9.17	-2121.46096300	7.72
$^{4}INT1\text{-}H_{C}$	-2120.83748400	18.79	-2120.40190200	17.32	-2121.88255600	6.91	-2121.44697400	5.44	-2121.89648	9.23	-2121.46089500	7.76
$^{2}TS1\text{-}H_{C}$	-2120.85643200	6.90	-2120.42371400	3.63	-2121.88432400	5.80	-2121.45160600	2.53	-2121.901245	6.24	-2121.46852700	2.97
$^{4}TS1\text{-}H_{C}$	-2120.85709100	6.49	-2120.42670400	1.76	-2121.88551600	5.05	-2121.45512900	0.32	-2121.903285	4.96	-2121.47289800	0.23
$^{2}INT2\text{-}H_{C}$	-2120.85742500	6.28	-2120.42905500	0.28	-2121.87653240	10.69	-2121.44816240	4.69	-2121.89101400	12.66	-2121.46264400	6.67
$^{4}INT2\text{-}H_{C}$	-2120.85938600	5.05	-2120.42466500	3.04	-2121.87930600	8.95	-2121.44458500	6.94	-2121.89793600	8.32	-2121.46321500	6.31
$^{2}P\text{-}epo_{C}$	-2120.93547200	-42.70	-2120.49406700	-40.51	-2121.97463600	-50.87	-2121.53323100	-48.69	-2121.99255900	-51.06	-2121.55115400	-48.87
$^{4}P\text{-}epo_{C}$	-2120.91867600	-32.16	-2120.47943100	-31.33	-2121.96011000	-41.76	-2121.52086500	-40.93	-2121.97711900	-41.37	-2121.53787400	-40.54

Cartesian coordinates of all structures represented in this study.

Path A

^2RC_A

Fe	-1.49341	-0.09561	0.10746
O	-0.78157	-0.0002	-1.38072
S	-2.25787	-0.09451	2.51857
H	-1.77029	-1.34125	2.86119
N	-1.51213	-2.11	0.11895
C	-2.09066	-4.31394	-0.31754
C	-0.85237	-4.32855	0.26155
H	-2.68433	-5.15086	-0.65385
H	-0.23137	-5.18027	0.49635
N	0.25169	-0.12785	1.13176
C	1.03434	-1.24678	1.41971
C	2.27727	-0.83229	2.03107
C	2.25937	0.53013	2.10155
H	3.06417	-1.50559	2.33542
H	3.02776	1.18999	2.47366
N	-1.57106	1.9014	0.35488
C	-0.57452	2.72145	0.85501
C	-2.58351	2.75124	-0.07561
C	-0.96335	4.10925	0.72888
C	-2.20452	4.12784	0.16177
H	-0.34835	4.94264	1.03149
H	-2.81705	4.98176	-0.08559
N	-3.36227	-0.07953	-0.61696
C	-5.38926	0.62626	-1.4921
H	-6.16908	1.30699	-1.79917
C	-4.13487	1.03112	-0.89621
C	-2.49944	-2.93005	-0.40719
C	-0.49545	-2.95341	0.53214
C	1.00319	0.97406	1.5403
C	-3.77357	2.3476	-0.64663
H	-4.48107	3.12003	-0.9271
C	-3.70386	-2.497	-0.93337
H	-4.38866	-3.25301	-1.30156
C	0.68775	-2.55146	1.13702
H	1.39503	-3.32613	1.41245
C	0.62458	2.29224	1.40011
H	1.32462	3.05255	1.72433
C	-5.36982	-0.73765	-1.57394
H	-6.13064	-1.39841	-1.96177
C	-4.10357	-1.1748	-1.02828
C	1.8143	2.13248	-1.53915
H	0.81978	1.8507	-1.91701
O	2.09416	3.32662	-1.31061

C	2.73586	1.01388	-1.304
C	4.02671	1.24783	-0.7966
C	2.31481	-0.30003	-1.56205
C	4.88785	0.1921	-0.53063
H	4.35065	2.26154	-0.59441
C	3.17895	-1.36331	-1.3056
H	1.30276	-0.47854	-1.90892
C	4.45383	-1.1274	-0.78437
H	2.85066	-2.38468	-1.47999
O	6.11707	0.47558	0.06133
O	5.32863	-2.16281	-0.47282
H	4.94513	-3.02959	-0.70691
C	7.32521	-0.00137	-0.6209
H	8.15353	0.41525	-0.04848
H	7.36575	-1.09134	-0.62007
H	7.35429	0.37801	-1.64882

$^{4}RC_{A}$

Fe	-1.48016	-0.09445	0.1145
O	-0.80177	-0.01391	-1.39317
S	-2.26686	-0.09851	2.50319
H	-1.7748	-1.34115	2.85387
N	-1.50234	-2.11034	0.1224
C	-2.08766	-4.31314	-0.31119
C	-0.84623	-4.33038	0.26095
H	-2.68468	-5.14879	-0.64475
H	-0.22564	-5.18337	0.49223
N	0.26204	-0.13013	1.13156
C	1.04252	-1.25048	1.42137
C	2.28178	-0.83825	2.04125
C	2.26271	0.52372	2.1189
H	3.06698	-1.51291	2.34701
H	3.02836	1.18205	2.49931
N	-1.55588	1.9013	0.35725
C	-0.5641	2.72043	0.86826
C	-2.56688	2.75238	-0.07591
C	-0.95309	4.10822	0.74538
C	-2.19007	4.12812	0.16925
H	-0.34097	4.94088	1.0557
H	-2.80156	4.98259	-0.0788
N	-3.35169	-0.07588	-0.61515
C	-5.37197	0.63264	-1.50329
H	-6.14757	1.31471	-1.81796
C	-4.11864	1.03579	-0.90325
C	-2.49434	-2.92832	-0.3986
C	-0.48583	-2.95596	0.53068
C	1.00983	0.97002	1.55276

C	-3.75458	2.35146	-0.65363
H	-4.45875	3.12572	-0.93743
C	-3.69947	-2.49347	-0.92156
H	-4.38702	-3.24897	-1.28572
C	0.69783	-2.55479	1.13484
H	1.40536	-3.32941	1.40975
C	0.63203	2.28886	1.41776
H	1.32994	3.04745	1.7505
C	-5.35763	-0.73168	-1.57683
H	-6.11904	-1.39177	-1.96463
C	-4.09504	-1.17056	-1.02313
C	1.78815	2.12789	-1.54308
H	0.79355	1.84315	-1.91901
O	2.06506	3.32286	-1.31601
C	2.71302	1.01192	-1.30892
C	4.00388	1.24943	-0.80317
C	2.29539	-0.30306	-1.56675
C	4.86826	0.19608	-0.53846
H	4.32513	2.26398	-0.60097
C	3.16288	-1.36399	-1.31195
H	1.28363	-0.48455	-1.91327
C	4.43767	-1.12462	-0.79221
H	2.8372	-2.38621	-1.48613
O	6.0969	0.48297	0.05282
O	5.31567	-2.1576	-0.48191
H	4.93417	-3.02548	-0.71518
C	7.3063	0.00855	-0.629
H	8.13347	0.42801	-0.05701
H	7.34976	-1.08129	-0.62711
H	7.33431	0.387	-1.65728

^{2}TS-O$_{A}$

Fe	1.2362	0.36168	-0.11389
O	-0.25774	-0.36392	0.33317
S	3.31606	1.32013	-0.8523
H	4.11741	0.81064	0.15088
N	1.97401	0.31428	1.75235
C	2.46599	0.86587	3.95026
C	2.92124	-0.40521	3.7406
H	2.51497	1.45661	4.85269
H	3.4212	-1.0631	4.43551
N	2.07051	-1.43254	-0.47224
C	2.71173	-2.25967	0.44295
C	3.13336	-3.47759	-0.21049
C	2.75865	-3.38591	-1.51859
H	3.64549	-4.28836	0.28509
H	2.90224	-4.10621	-2.30974

N	0.68128	0.49997	-2.04382
C	0.89538	-0.43869	-3.03299
C	-0.07459	1.5097	-2.6251
C	0.27786	-0.00622	-4.26651
C	-0.32619	1.19374	-4.01272
H	0.30461	-0.56198	-5.19167
H	-0.88891	1.81845	-4.68997
N	0.50632	2.20901	0.2122
C	-0.61836	4.22079	-0.03046
H	-1.19859	4.99747	-0.50573
C	-0.22851	2.98247	-0.66819
C	1.86506	1.31082	2.71256
C	2.61291	-0.74537	2.36929
C	2.09647	-2.11159	-1.68653
C	-0.51262	2.65283	-1.98339
H	-1.10083	3.35727	-2.56061
C	1.23943	2.53064	2.539
H	1.23049	3.21186	3.38254
C	2.94812	-1.94813	1.76442
H	3.45317	-2.68969	2.37258
C	1.55489	-1.65168	-2.86795
H	1.63831	-2.29294	-3.73806
C	-0.10232	4.19775	1.23447
H	-0.17871	4.94958	2.00559
C	0.59581	2.93943	1.38267
C	-0.85714	-1.89794	-0.19693
H	-0.73651	-1.71724	-1.27615
O	-0.13641	-2.84635	0.31922
C	-2.27914	-1.7213	0.26048
C	-2.76577	-2.41916	1.36904
C	-3.11039	-0.8218	-0.41786
C	-4.08403	-2.22204	1.78494
H	-2.11085	-3.10862	1.88732
C	-4.42451	-0.6168	-0.00698
H	-2.74132	-0.2529	-1.26361
C	-4.91725	-1.33145	1.10181
H	-4.47324	-2.76849	2.64051
O	-5.2166	0.25286	-0.7574
O	-6.24494	-1.1179	1.47125
H	-6.49402	-1.68679	2.22413
C	-5.83246	1.37568	-0.04377
H	-6.32026	1.96855	-0.81754
H	-6.56197	1.01822	0.68433
H	-5.06181	1.97444	0.4563

^{4}TS-O$_A$

Fe	1.17005	0.25409	-0.36342

O	0.12715	-0.15612	0.9452
S	2.60526	0.66503	-2.20357
H	3.69182	-0.06139	-1.7581
N	1.22588	2.157	0.2189
C	0.68175	4.38133	0.57137
C	1.85123	4.14238	1.23543
H	0.12535	5.3041	0.50264
H	2.43931	4.82793	1.82701
N	2.77553	-0.15924	0.7655
C	3.51172	0.74226	1.51328
C	4.51732	0.03544	2.27889
C	4.35592	-1.29591	2.01769
H	5.2267	0.50824	2.94141
H	4.91116	-2.13077	2.41792
N	1.16727	-1.65609	-1.02869
C	1.9257	-2.70928	-0.53113
C	0.41249	-2.17986	-2.07746
C	1.62581	-3.91466	-1.26919
C	0.70873	-3.58546	-2.22951
H	2.07332	-4.8776	-1.07407
H	0.2559	-4.22798	-2.96964
N	-0.32986	0.68109	-1.62203
C	-2.01296	0.5047	-3.20634
H	-2.63363	0.06024	-3.96933
C	-0.90419	-0.164	-2.56081
C	0.30141	3.14374	-0.07644
C	2.18398	2.74935	1.02258
C	3.27207	-1.41354	1.06561
C	-0.53821	-1.48032	-2.79611
H	-1.07766	-2.01682	-3.56834
C	-0.78168	2.99744	-0.92623
H	-1.43027	3.85512	-1.06489
C	3.26582	2.10218	1.59658
H	3.93159	2.69407	2.21465
C	2.85461	-2.60446	0.48972
H	3.34145	-3.51521	0.81836
C	-2.11472	1.74692	-2.64635
H	-2.82476	2.5278	-2.87353
C	-1.05802	1.85948	-1.66485
C	-0.53303	-1.67738	1.4341
H	-0.32151	-2.15839	0.46008
O	0.16509	-2.1388	2.42271
C	-1.96571	-1.28956	1.60005
C	-2.54365	-1.18802	2.86936
C	-2.72558	-0.97587	0.46486
C	-3.87179	-0.77617	2.99522

H	-1.9479	-1.43089	3.74115
C	-4.04687	-0.56067	0.58107
H	-2.29401	-1.03162	-0.52596
C	-4.62697	-0.46271	1.86009
H	-4.32757	-0.69581	3.97901
O	-4.76454	-0.30698	-0.58999
O	-5.95487	-0.04846	1.9352
H	-6.27272	-0.05404	2.85804
C	-5.28032	1.05485	-0.75315
H	-5.74371	1.06735	-1.73976
H	-6.0171	1.28365	0.01885
H	-4.45477	1.77526	-0.72002

^{2}INT-O_A

Fe	-1.15936	0.12269	0.34761
O	-0.41452	0.00078	-1.30585
S	-2.19185	0.3196	2.4278
H	-3.44553	-0.08964	2.01943
N	-2.53963	1.3647	-0.41315
C	-3.652	3.27136	-1.10538
C	-4.41193	2.20165	-1.48553
H	-3.84671	4.32222	-1.25921
H	-5.35545	2.20052	-2.01064
N	-2.35325	-1.44837	-0.06001
C	-3.55744	-1.41582	-0.75017
C	-4.07662	-2.75763	-0.87937
C	-3.18761	-3.59757	-0.26748
H	-5.00188	-3.00767	-1.37668
H	-3.2402	-4.67127	-0.16553
N	0.18867	-1.12159	1.17992
C	0.06828	-2.49829	1.3297
C	1.40345	-0.77292	1.75383
C	1.23984	-3.01743	1.99559
C	2.06332	-1.95639	2.25085
H	1.3956	-4.06018	2.22922
H	3.02908	-1.95489	2.73334
N	-0.01218	1.68322	0.85916
C	1.77172	2.98622	1.5564
H	2.75087	3.22079	1.94363
C	1.2487	1.64454	1.43738
C	-2.47897	2.74721	-0.44048
C	-3.7184	1.00915	-1.04999
C	-2.10843	-2.78195	0.23916
C	1.91282	0.50764	1.85357
H	2.90008	0.63017	2.2812
C	-1.44515	3.52255	0.05118
H	-1.52955	4.59804	-0.05194

C	-4.19026	-0.2789	-1.22035
H	-5.13197	-0.40617	-1.74127
C	-0.99032	-3.27202	0.89161
H	-0.93748	-4.34071	1.06421
C	0.8175	3.835	1.07254
H	0.85202	4.91151	0.9973
C	-0.29668	3.0229	0.63437
C	0.31486	-1.06675	-1.88899
H	-0.11045	-2.03272	-1.57515
O	0.32004	-0.99533	-3.2872
C	1.79307	-0.98914	-1.51054
C	2.56065	-2.14763	-1.35894
C	2.3774	0.26795	-1.31649
C	3.89466	-2.04586	-0.96309
H	2.1142	-3.1224	-1.51923
C	3.70176	0.3752	-0.90231
H	1.78317	1.16562	-1.41615
C	4.46474	-0.79228	-0.71889
H	4.48895	-2.94355	-0.81435
O	4.17969	1.6422	-0.56976
O	5.77425	-0.6447	-0.26556
H	6.21514	-1.51066	-0.17427
C	5.38517	2.1129	-1.26124
H	5.51762	3.14177	-0.92742
H	6.2488	1.50424	-0.9895
H	5.23106	2.09001	-2.34588

^{4}INT-O$_{A}$

Fe	-1.15436	0.10177	0.33494
O	-0.46012	0.0894	-1.37321
S	-2.00052	0.30621	2.56911
H	-2.44363	1.61151	2.47897
N	-2.54891	1.37803	-0.36535
C	-3.65433	3.28133	-1.09714
C	-4.44441	2.21279	-1.41308
H	-3.83647	4.32945	-1.282
H	-5.4036	2.21026	-1.90898
N	-2.33739	-1.47362	-0.06405
C	-3.56558	-1.42455	-0.69869
C	-4.10085	-2.76074	-0.84296
C	-3.19338	-3.61744	-0.28245
H	-5.04615	-2.99644	-1.30854
H	-3.24834	-4.69252	-0.19864
N	0.19393	-1.15545	1.15959
C	0.09122	-2.5377	1.29962
C	1.40921	-0.80951	1.72719
C	1.26838	-3.05677	1.96023

C	2.08396	-1.99173	2.21738
H	1.43326	-4.09926	2.18849
H	3.05177	-1.9862	2.69564
N	-0.0099	1.67639	0.85418
C	1.80336	2.96418	1.52911
H	2.78769	3.18706	1.9098
C	1.25608	1.62841	1.42387
C	-2.47107	2.75114	-0.44947
C	-3.74723	1.02516	-0.96017
C	-2.09837	-2.80808	0.20317
C	1.91324	0.47831	1.81936
H	2.90813	0.5963	2.23271
C	-1.40358	3.51781	0.00405
H	-1.46645	4.59146	-0.13724
C	-4.21589	-0.26935	-1.11066
H	-5.17943	-0.39318	-1.59363
C	-0.96988	-3.30106	0.84977
H	-0.91711	-4.3727	1.00957
C	0.86674	3.82311	1.03202
H	0.92313	4.89756	0.94176
C	-0.26108	3.02258	0.60271
C	0.23955	-1.00517	-1.91474
H	-0.18499	-1.96622	-1.5787
O	0.23513	-0.99322	-3.32334
C	1.72721	-0.95492	-1.55062
C	2.47834	-2.12321	-1.39241
C	2.33044	0.29174	-1.35096
C	3.8103	-2.0435	-0.98197
H	2.0186	-3.09115	-1.55799
C	3.65116	0.37872	-0.92051
H	1.74698	1.19573	-1.45622
C	4.3954	-0.79957	-0.72792
H	4.38909	-2.95052	-0.82756
O	4.14848	1.63814	-0.57946
O	5.70174	-0.67083	-0.25554
H	6.13114	-1.54324	-0.17098
C	5.35888	2.09163	-1.27299
H	5.51469	3.11461	-0.93077
H	6.21177	1.46329	-1.0115
H	5.19864	2.08179	-2.35695

^{2}TS-def$_{A}$

Fe	1.18824	0.1024	-0.33462
O	0.45626	0.10537	1.40322
S	2.2767	0.2652	-2.43072
H	2.32116	1.64343	-2.50709
N	2.60308	1.36176	0.34599

C	3.74663	3.25858	1.04948
C	4.54422	2.18446	1.31977
H	3.94237	4.30368	1.23707
H	5.5244	2.1735	1.77234
N	2.37736	-1.47579	0.01362
C	3.63442	-1.43986	0.59668
C	4.18105	-2.77708	0.68085
C	3.25654	-3.62413	0.13911
H	5.1476	-3.01776	1.09731
H	3.31458	-4.69619	0.02525
N	-0.19365	-1.15146	-1.1008
C	-0.11633	-2.52712	-1.23408
C	-1.41741	-0.78868	-1.63229
C	-1.32417	-3.03872	-1.8402
C	-2.13153	-1.9618	-2.08372
H	-1.51466	-4.08141	-2.04568
H	-3.11794	-1.94483	-2.52155
N	0.02423	1.69578	-0.76661
C	-1.80862	2.98654	-1.37036
H	-2.80376	3.2094	-1.72033
C	-1.24427	1.65487	-1.31692
C	2.53121	2.74418	0.45373
C	3.82564	1.00254	0.88848
C	2.13239	-2.81446	-0.27396
C	-1.90496	0.50742	-1.72537
H	-2.90587	0.63407	-2.12125
C	1.44417	3.51262	0.07869
H	1.50989	4.58294	0.24206
C	4.29352	-0.29448	1.01513
H	5.27094	-0.42556	1.46672
C	0.9722	-3.29981	-0.85185
H	0.907	-4.36981	-1.0171
C	-0.86951	3.83546	-0.8553
H	-0.93079	4.90543	-0.72493
C	0.26999	3.0242	-0.48096
C	0.03786	-0.99465	2.06828
H	0.13007	-1.9392	1.51251
O	-0.07533	-1.01702	3.33786
C	-2.03809	-0.94627	1.66171
C	-2.75819	-2.12108	1.56347
C	-2.53003	0.30034	1.32262
C	-4.05967	-2.03717	1.03897
H	-2.34071	-3.07534	1.86286
C	-3.82123	0.37509	0.78755
H	-1.92108	1.19046	1.40413
C	-4.57992	-0.8029	0.63936

H	-4.65874	-2.93727	0.92165
O	-4.26881	1.60737	0.30543
O	-5.84693	-0.67749	0.06018
H	-6.30054	-1.54078	0.0249
C	-5.49285	2.15209	0.90502
H	-5.6161	3.13696	0.45464
H	-6.34777	1.51366	0.67691
H	-5.36846	2.25009	1.98898

^{4}TS-def$_{A}$

Fe	1.19238	0.11169	-0.31599
O	0.499	-0.02588	1.40104
S	2.09485	0.31916	-2.47778
H	2.51964	1.62386	-2.32775
N	2.68439	1.25185	0.3729
C	3.89971	3.04053	1.19537
C	4.71119	1.94153	1.2511
H	4.12127	4.0539	1.4951
H	5.72701	1.8753	1.61084
N	2.31134	-1.53618	-0.05748
C	3.63267	-1.5756	0.36895
C	4.08443	-2.94626	0.41745
C	3.03653	-3.73297	0.02717
H	5.07484	-3.25065	0.72095
H	3.00063	-4.8087	-0.05865
N	-0.24632	-1.01833	-1.12939
C	-0.28861	-2.40544	-1.19781
C	-1.41813	-0.56266	-1.72223
C	-1.52049	-2.82133	-1.82396
C	-2.2093	-1.68761	-2.15639
H	-1.803	-3.85061	-1.98711
H	-3.17364	-1.60148	-2.63354
N	0.10382	1.75827	-0.65028
C	-1.6218	3.17968	-1.25271
H	-2.57578	3.48427	-1.65294
C	-1.12688	1.82387	-1.29109
C	2.63547	2.61208	0.64336
C	3.94826	0.82089	0.75313
C	1.93492	-2.85302	-0.28494
C	-1.82133	0.75473	-1.81989
H	-2.79001	0.95555	-2.25896
C	1.56319	3.44827	0.39161
H	1.66059	4.49246	0.66389
C	4.40088	-0.4849	0.72931
H	5.41763	-0.67117	1.05445
C	0.7115	-3.26574	-0.78148
H	0.54553	-4.32986	-0.90003

C	-0.69128	3.93126	-0.59156
H	-0.71918	4.98635	-0.36386
C	0.39379	3.04773	-0.22701
C	0.04112	-1.0822	2.12226
H	0.09326	-2.04465	1.59734
O	-0.07003	-1.03332	3.38314
C	-2.0632	-0.98345	1.67337
C	-2.81985	-2.13809	1.63169
C	-2.50675	0.26315	1.27678
C	-4.11798	-2.031	1.10425
H	-2.43714	-3.09078	1.97855
C	-3.79565	0.35813	0.73924
H	-1.87066	1.13683	1.3192
C	-4.59464	-0.79849	0.64732
H	-4.75005	-2.91294	1.03107
O	-4.2004	1.58352	0.20761
O	-5.85899	-0.65634	0.06779
H	-6.3353	-1.50792	0.05649
C	-5.41101	2.19003	0.77428
H	-5.49845	3.1595	0.28399
H	-6.28422	1.57081	0.56413
H	-5.29206	2.32751	1.85462

^{2}INT-def$_{A}$

Fe	-1.04006	0.03712	-0.3678
O	-0.36694	-0.03377	1.43864
S	-1.76407	0.20625	-2.58729
H	-0.52573	0.16886	-3.197
N	0.38607	-1.29855	-0.8965
C	2.33824	-2.28701	-1.66561
C	1.4905	-3.29791	-1.29956
H	3.34569	-2.35251	-2.04706
H	1.65961	-4.36347	-1.3445
N	-2.34852	-1.44013	-0.01882
C	-2.06994	-2.79804	-0.04221
C	-3.26817	-3.55122	0.2625
C	-4.27537	-2.64338	0.43669
H	-3.31967	-4.62851	0.31411
H	-5.31312	-2.82889	0.66897
N	-2.46154	1.36278	0.08206
C	-3.80591	1.12056	0.33091
C	-2.29272	2.73134	0.20308
C	-4.48982	2.36566	0.60299
C	-3.5541	3.35746	0.54407
H	-5.54214	2.44915	0.8286
H	-3.6889	4.41717	0.70045
N	0.27309	1.51372	-0.75162

C	1.23348	3.61994	-0.91589
H	1.32494	4.69245	-0.83363
C	0.06558	2.86169	-0.5204
C	1.64635	-1.04576	-1.40424
C	0.2732	-2.6765	-0.82657
C	-3.69325	-1.33126	0.26355
C	-1.1135	3.41694	-0.04249
H	-1.13128	4.49295	0.09425
C	2.18643	0.22177	-1.59624
H	3.19392	0.2786	-1.98982
C	-0.8564	-3.3639	-0.40042
H	-0.79867	-4.44751	-0.39288
C	-4.38436	-0.13164	0.38441
H	-5.44666	-0.18571	0.59484
C	2.14645	2.72503	-1.39732
H	3.14033	2.91326	-1.77114
C	1.55333	1.41081	-1.28006
C	-1.06788	0.001	2.56662
H	-0.4056	-0.06801	3.4489
O	-2.29744	0.09661	2.71149
C	3.52969	1.9173	1.588
C	2.94788	0.68493	1.83614
C	3.57816	-0.4187	1.24818
C	4.70605	-0.24375	0.41819
C	5.2461	1.02055	0.20116
C	4.6494	2.14395	0.81043
H	2.02625	0.57828	2.39241
H	6.12114	1.11557	-0.43132
H	5.05982	3.13566	0.65984
O	5.25178	-1.35848	-0.20739
H	4.76831	-2.15101	0.11376
O	3.19856	-1.74771	1.37019
C	2.00863	-2.07442	2.15096
H	1.14816	-1.51257	1.7818
H	1.86379	-3.14399	2.00834
H	2.18661	-1.85547	3.21001

^{4}INT-def$_A$

Fe	-1.03501	-0.03688	0.36896
O	-0.3653	0.0317	-1.43945
S	-1.75767	-0.20023	2.58875
H	-0.51938	-0.15738	3.19821
N	0.38549	1.30627	0.89371
C	2.33001	2.30581	1.66749
C	1.47893	3.31188	1.29592
H	3.33497	2.37709	2.05442
H	1.64267	4.37834	1.33951

N	-2.34997	1.43336	0.01583
C	-2.077	2.79225	0.03382
C	-3.27843	3.53938	-0.27345
C	-4.28203	2.62682	-0.44357
H	-3.33434	4.61625	-0.32921
H	-5.32062	2.80726	-0.67613
N	-2.45075	-1.37007	-0.07706
C	-3.79613	-1.13482	-0.32507
C	-2.27546	-2.73818	-0.19472
C	-4.47464	-2.38376	-0.59322
C	-3.53424	-3.37108	-0.53283
H	-5.52679	-2.47271	-0.81754
H	-3.66428	-4.43181	-0.68637
N	0.28551	-1.50621	0.75566
C	1.25476	-3.60778	0.92597
H	1.35097	-4.68007	0.84628
C	0.08406	-2.85544	0.52756
C	1.64516	1.06062	1.40622
C	0.26613	2.68364	0.82035
C	-3.69456	1.31771	-0.26561
C	-1.09278	-3.41739	0.05151
H	-1.10554	-4.49384	-0.0824
C	2.19112	-0.20393	1.60201
H	3.19716	-0.25506	1.99998
C	-0.86582	3.36459	0.39047
H	-0.81288	4.44842	0.37942
C	-4.38036	0.11484	-0.38186
H	-5.44306	0.16344	-0.59163
C	2.1632	-2.7078	1.40668
H	3.15724	-2.89102	1.78255
C	1.56448	-1.39646	1.28588
C	-1.06739	-0.00911	-2.56644
H	-0.4064	0.0602	-3.44977
O	-2.29669	-0.11003	-2.70999
C	3.5167	-1.91422	-1.60591
C	2.93484	-0.68099	-1.84953
C	3.56195	0.41971	-1.25307
C	4.68654	0.24072	-0.41923
C	5.22743	-1.02442	-0.20779
C	4.6344	-2.1444	-0.8261
H	2.01518	-0.57192	-2.4084
H	6.10027	-1.12216	0.4273
H	5.04512	-3.13664	-0.68009
O	5.22938	1.35214	0.21387
H	4.74515	2.14593	-0.10323
O	3.18323	1.74929	-1.36959

C	1.99766	2.08103	-2.15499
H	1.13493	1.51936	-1.79104
H	1.85441	3.15041	-2.00948
H	2.18034	1.86514	-3.21387

^{2}P-def$_A$

Fe	1.44137	-0.01349	-0.45411
O	0.20032	-0.01439	1.25114
S	2.74839	-0.03996	-2.30555
H	2.21381	1.07979	-2.91422
N	3.02836	-0.33817	0.73764
C	4.98549	-0.00277	1.94029
C	4.75676	-1.34942	1.91259
H	5.80016	0.52913	2.40909
H	5.34899	-2.1392	2.35051
N	1.1571	-1.99799	-0.56633
C	1.89892	-2.9979	0.04059
C	1.38902	-4.2976	-0.34829
C	0.3502	-4.07884	-1.20602
H	1.79285	-5.23979	-0.00859
H	-0.2709	-4.80647	-1.7072
N	-0.21657	0.31331	-1.54491
C	-0.95747	-0.65631	-2.20413
C	-0.79145	1.53448	-1.86764
C	-2.01725	-0.02831	-2.96211
C	-1.92037	1.3265	-2.74647
H	-2.72316	-0.55745	-3.58586
H	-2.53066	2.11545	-3.16145
N	1.64394	1.97128	-0.219
C	1.3452	4.27141	-0.34034
H	0.88257	5.21453	-0.591
C	0.80833	2.97437	-0.69551
C	3.90721	0.62955	1.20832
C	3.54309	-1.56	1.15219
C	0.20422	-2.64263	-1.34147
C	-0.33469	2.77451	-1.4478
H	-0.88933	3.64991	-1.76638
C	3.75546	1.9971	1.05747
H	4.51347	2.63535	1.49767
C	3.00089	-2.79825	0.85596
H	3.49947	-3.67512	1.25332
C	-0.76337	-2.02605	-2.11262
H	-1.43734	-2.66381	-2.67375
C	2.51195	4.0513	0.33455
H	3.1935	4.77864	0.75032
C	2.69648	2.61623	0.41255
C	0.53828	0.10634	2.44408

H	1.57376	0.20883	2.76026
O	-0.32478	0.12312	3.45917
H	-1.29787	0.03177	3.15953
C	-5.3873	0.14314	1.22506
C	-5.32943	-0.05767	2.6248
C	-4.012	-0.19863	2.99641
C	-2.91232	-0.13192	2.37773
C	-2.91512	0.02816	0.97155
C	-4.20146	0.18944	0.42438
H	-6.22708	-0.114	3.22143
H	-2.01029	0.07346	0.37858
O	-6.64722	0.33198	0.67982
O	-4.40034	0.42035	-0.9242
H	-3.55614	0.48351	-1.42643
C	-7.08516	-0.6006	-0.37143
H	-8.10364	-0.29396	-0.60587
H	-6.44064	-0.51544	-1.24569
H	-7.07981	-1.62624	0.01395

^{4}P-def$_A$

Fe	1.4869	0.20853	-0.44496
O	0.19143	-0.50748	1.54163
S	2.73718	0.79419	-2.46591
H	2.62638	2.16178	-2.29993
N	2.95233	-0.94186	0.32327
C	4.94256	-1.60945	1.31132
C	4.38848	-2.71738	0.73347
H	5.8679	-1.53313	1.86259
H	4.77202	-3.72666	0.71564
N	0.65602	-1.42691	-1.27024
C	1.15444	-2.72218	-1.2501
C	0.3024	-3.58836	-2.03406
C	-0.70275	-2.81334	-2.54092
H	0.46945	-4.6459	-2.17435
H	-1.52353	-3.11139	-3.17603
N	-0.13549	1.28489	-0.96888
C	-1.14379	0.88254	-1.83516
C	-0.38923	2.61569	-0.66373
C	-2.04563	1.98501	-2.07825
C	-1.5857	3.05262	-1.34518
H	-2.90475	1.94219	-2.73128
H	-1.99456	4.05088	-1.28975
N	2.16709	1.7727	0.6167
C	2.44372	3.89811	1.50457
H	2.22274	4.92998	1.7339
C	1.59124	3.03322	0.7196
C	4.04676	-0.5024	1.05817

C	3.15247	-2.29987	0.10857
C	-0.48477	-1.46642	-2.06357
C	0.40041	3.42561	0.13624
H	0.07485	4.44743	0.29406
C	4.24416	0.78784	1.51447
H	5.14492	0.98788	2.08327
C	2.3087	-3.13334	-0.60424
H	2.58296	-4.17896	-0.68308
C	-1.30953	-0.39368	-2.34511
H	-2.15994	-0.56898	-2.99379
C	3.53706	3.16345	1.86924
H	4.3868	3.47382	2.45879
C	3.36121	1.83669	1.32188
C	0.451	-1.53122	2.19064
H	1.46473	-1.86904	2.40211
O	-0.46563	-2.36834	2.70562
H	-1.41466	-2.09778	2.47834
C	-5.3877	-0.29522	1.08331
C	-5.43951	-1.50588	1.81346
C	-4.15432	-1.94742	2.04156
C	-3.01757	-1.46702	1.77867
C	-2.90001	-0.27824	1.02707
C	-4.14236	0.29934	0.70433
H	-6.38236	-1.95698	2.08345
H	-1.95025	0.17336	0.77088
O	-6.60419	0.30515	0.79392
O	-4.23675	1.5	0.02032
H	-3.36279	1.82656	-0.28707
C	-6.93008	0.54289	-0.62043
H	-7.94312	0.94291	-0.60794
H	-6.2339	1.25976	-1.05483
H	-6.90578	-0.40244	-1.17425

Path B

$^{2}RC_{B}$

Fe	-1.31642	0.02881	-0.18858
O	-0.68951	0.07213	1.34922
S	-2.14255	-0.36556	-2.52252
H	-1.0489	0.15119	-3.19038
N	-0.19252	1.57062	-0.81475
C	0.6587	3.7156	-1.05229
C	1.59774	2.85144	-1.54111
H	0.70185	4.79291	-0.99691
H	2.5694	3.07556	-1.95378
N	0.07101	-1.24577	-0.90232
C	1.29722	-0.92397	-1.48118
C	2.05911	-2.12841	-1.72349

C	1.31559	-3.17409	-1.26238
H	3.04629	-2.14667	-2.15988
H	1.56646	-4.22404	-1.25921
N	-2.53037	-1.53006	0.17883
C	-2.17918	-2.86824	0.18067
C	-3.85809	-1.47939	0.58453
C	-3.30567	-3.67291	0.59933
C	-4.34516	-2.81762	0.83399
H	-3.29098	-4.74936	0.68107
H	-5.34918	-3.05352	1.15341
N	-2.81371	1.29293	0.23265
C	-4.84501	2.16733	0.92401
H	-5.87387	2.1834	1.25096
C	-4.09623	0.96555	0.63034
C	-0.45946	2.91751	-0.60413
C	1.06795	1.5168	-1.38303
C	0.07821	-2.6292	-0.74848
C	-4.59105	-0.32297	0.76957
H	-5.62267	-0.42952	1.08606
C	-1.63496	3.42849	-0.08691
H	-1.71069	4.50545	0.01298
C	1.75303	0.35586	-1.71428
H	2.74636	0.46469	-2.13328
C	-0.95176	-3.37634	-0.2168
H	-0.81063	-4.44936	-0.15286
C	-4.0015	3.2231	0.71769
H	-4.20301	4.27712	0.83642
C	-2.73827	2.67346	0.27858
C	6.37939	-0.20025	-0.18053
H	7.09684	0.6229	-0.35989
O	6.68046	-1.36768	-0.49706
C	5.11204	0.20467	0.42191
C	4.13486	-0.75657	0.74177
C	4.85045	1.56381	0.68181
C	2.91789	-0.37109	1.28056
H	4.33005	-1.80573	0.55607
C	3.62632	1.95603	1.2106
H	5.6075	2.30782	0.45053
C	2.63254	1.00286	1.48905
H	3.38569	2.99709	1.38576
O	1.94263	-1.34638	1.49751
O	1.43213	1.4504	1.95168
H	0.63906	0.84521	1.76792
C	1.50742	-1.56451	2.88326
H	0.63349	-2.20811	2.80678
H	2.30647	-2.05632	3.44802

H	1.22903	-0.62411	3.36358

^4RC_B

Fe	-1.31031	0.02119	-0.19628
O	-0.69423	0.09957	1.34673
S	-2.13793	-0.35196	-2.51246
H	-1.05841	0.19171	-3.1818
N	-0.18762	1.5676	-0.82155
C	0.65655	3.71476	-1.06552
C	1.60074	2.85198	-1.54658
H	0.69565	4.79244	-1.01434
H	2.57324	3.0778	-1.95636
N	0.08023	-1.24771	-0.90051
C	1.30539	-0.92431	-1.48155
C	2.06746	-2.12804	-1.72678
C	1.32429	-3.17519	-1.26848
H	3.05441	-2.14494	-2.16378
H	1.57511	-4.22516	-1.26876
N	-2.51992	-1.5364	0.17958
C	-2.16933	-2.87454	0.17756
C	-3.84767	-1.48655	0.58626
C	-3.29509	-3.68021	0.59542
C	-4.33425	-2.82527	0.83337
H	-3.28037	-4.75685	0.67459
H	-5.33795	-3.06187	1.15331
N	-2.81026	1.287	0.23045
C	-4.83965	2.15934	0.92994
H	-5.86656	2.17411	1.26303
C	-4.08969	0.95815	0.63519
C	-0.46054	2.91455	-0.61773
C	1.07452	1.51615	-1.38547
C	0.08712	-2.63205	-0.75253
C	-4.58162	-0.3313	0.77536
H	-5.61213	-0.44008	1.09474
C	-1.63823	3.42399	-0.10412
H	-1.71771	4.50129	-0.01078
C	1.76169	0.35547	-1.71319
H	2.75577	0.46437	-2.13038
C	-0.9417	-3.38112	-0.22186
H	-0.79982	-4.4542	-0.16058
C	-3.99994	3.21616	0.71467
H	-4.20299	4.27016	0.83096
C	-2.7377	2.66759	0.27009
C	6.3615	-0.2204	-0.17502
H	7.08596	0.59615	-0.3563
O	6.65161	-1.3908	-0.4909
C	5.09852	0.19629	0.42867

C	4.11344	-0.7561	0.75046
C	4.84866	1.55804	0.68673
C	2.90013	-0.35928	1.28922
H	4.2993	-1.80711	0.56577
C	3.62813	1.96161	1.21529
H	5.61186	2.29523	0.45383
C	2.62635	1.01731	1.49515
H	3.39647	3.00499	1.38872
O	1.91626	-1.32555	1.50806
O	1.42923	1.47538	1.95615
H	0.63268	0.87525	1.77337
C	1.48308	-1.54057	2.89495
H	0.60438	-2.17789	2.82068
H	2.27999	-2.03812	3.45767
H	1.21307	-0.59799	3.37594

^{2}TS-H_B

Fe	1.27439	-0.01992	0.28721
O	0.63834	0.14601	-1.37355
S	2.2381	0.02866	2.418
H	1.24902	0.76486	3.03918
N	-0.52397	0.32095	1.11974
C	-2.434	1.36294	1.91262
C	-2.60222	0.01848	2.09615
H	-3.1218	2.16142	2.14473
H	-3.45743	-0.5011	2.50076
N	0.94516	-1.98365	0.37355
C	-0.16235	-2.62273	0.91986
C	-0.01864	-4.05212	0.77427
C	1.17863	-4.27908	0.15467
H	-0.74782	-4.77389	1.11047
H	1.6286	-5.22458	-0.10908
N	3.13354	-0.3569	-0.36478
C	3.69528	-1.5811	-0.68682
C	4.09979	0.60279	-0.6362
C	5.04956	-1.38709	-1.15177
C	5.30137	-0.04408	-1.11146
H	5.70784	-2.18439	-1.46301
H	6.20505	0.47763	-1.38889
N	1.58673	1.9749	0.19171
C	2.56567	4.03948	-0.17307
H	3.32588	4.76023	-0.43451
C	2.75782	2.60506	-0.19415
C	-1.13728	1.55585	1.30746
C	-1.41686	-0.63272	1.59009
C	1.79343	-2.99164	-0.07375
C	3.93363	1.97271	-0.55168

H	4.77943	2.59689	-0.81572
C	-0.59888	2.7863	0.97889
H	-1.20658	3.66454	1.16171
C	-1.24801	-2.00201	1.50598
H	-2.0421	-2.63107	1.89016
C	3.06512	-2.80874	-0.58164
H	3.62152	-3.68961	-0.87981
C	1.27954	4.26837	0.22558
H	0.77634	5.21409	0.36025
C	0.67213	2.97736	0.46911
C	-6.29299	-0.19224	0.09932
H	-7.0237	0.62749	0.22988
O	-6.56801	-1.34156	0.49241
C	-5.03402	0.19424	-0.53622
C	-4.04762	-0.76424	-0.79381
C	-4.78472	1.5388	-0.87538
C	-2.83341	-0.40703	-1.37143
H	-4.22846	-1.80402	-0.54983
C	-3.56217	1.90352	-1.4161
H	-5.54675	2.29019	-0.69054
C	-2.54301	0.95741	-1.65468
H	-3.32866	2.93329	-1.65651
O	-1.98051	-1.50126	-1.57451
O	-1.37805	1.43821	-2.16087
C	-0.87939	-1.50282	-2.43941
H	0.07192	-0.85451	-1.88088
H	-0.53957	-2.5293	-2.551
H	-1.02811	-0.94499	-3.36615
H	-0.5012	0.99398	-1.83449

^{4}TS-H$_B$

Fe	1.30264	0.04551	0.26683
O	0.61255	0.06957	-1.38644
S	2.30842	-0.26077	2.40007
H	1.20024	-0.76052	3.05517
N	-0.50744	0.24688	1.13319
C	-2.4552	1.17642	1.97781
C	-2.58486	-0.18204	2.07225
H	-3.16908	1.93727	2.25293
H	-3.42762	-0.75059	2.43486
N	1.06203	-1.98459	0.3387
C	-0.03372	-2.69061	0.81413
C	0.17444	-4.10888	0.61949
C	1.39881	-4.25764	0.02937
H	-0.53147	-4.87522	0.90267
H	1.89687	-5.17093	-0.26009
N	3.16839	-0.19652	-0.38655

C	3.78709	-1.39781	-0.71981
C	4.09183	0.80112	-0.6579
C	5.12998	-1.13808	-1.18725
C	5.32093	0.21429	-1.14099
H	5.8234	-1.90203	-1.50574
H	6.19963	0.77724	-1.41797
N	1.52541	2.01795	0.22744
C	2.39014	4.14847	-0.09399
H	3.10636	4.91386	-0.35275
C	2.64924	2.72475	-0.16683
C	-1.16245	1.43967	1.39109
C	-1.37571	-0.76204	1.53541
C	1.95561	-2.93127	-0.13343
C	3.85196	2.161	-0.5538
H	4.66004	2.83378	-0.81796
C	-0.66749	2.7048	1.11003
H	-1.30422	3.55058	1.34297
C	-1.15882	-2.12154	1.38407
H	-1.94691	-2.78946	1.71203
C	3.21767	-2.65475	-0.63464
H	3.82132	-3.49608	-0.95668
C	1.11045	4.29984	0.35335
H	0.567	5.21432	0.53789
C	0.5756	2.97112	0.57102
C	-6.38644	-0.1386	0.06957
H	-7.09726	0.69825	0.20402
O	-6.70214	-1.28827	0.4321
C	-5.10655	0.2275	-0.5322
C	-4.13795	-0.75074	-0.79079
C	-4.81596	1.57045	-0.84001
C	-2.90191	-0.41736	-1.33304
H	-4.3514	-1.78969	-0.57008
C	-3.57531	1.91045	-1.35559
H	-5.56104	2.33882	-0.65523
C	-2.57461	0.94364	-1.59374
H	-3.31231	2.93738	-1.57773
O	-2.06211	-1.52923	-1.50641
O	-1.39491	1.41217	-2.07515
C	-0.96891	-1.57223	-2.38714
H	0.04944	-0.88269	-1.8254
H	-0.63902	-2.60468	-2.4685
H	-1.1174	-1.03699	-3.32701
H	-0.5227	0.92704	-1.78702

$^{2}INT_{B}$

Fe	-1.69815	0.00183	-0.14549
O	-0.95741	-0.26239	1.49105

S	-2.79559	0.29489	-2.16896
H	-2.5714	1.65118	-2.29856
N	-0.93849	1.85026	-0.29861
C	-0.5562	4.11426	0.00202
C	0.47963	3.62495	-0.74398
H	-0.72083	5.12698	0.33879
H	1.33629	4.15213	-1.13611
N	-0.08083	-0.74292	-1.03539
C	0.97774	-0.02649	-1.57948
C	1.94163	-0.94171	-2.15173
C	1.46164	-2.20576	-1.95494
H	2.85474	-0.62439	-2.63001
H	1.90454	-3.14487	-2.25157
N	-2.55289	-1.80979	-0.15164
C	-1.9517	-3.00046	-0.52467
C	-3.83597	-2.13014	0.27256
C	-2.88406	-4.09028	-0.34465
C	-4.04676	-3.55351	0.13353
H	-2.66318	-5.12402	-0.56485
H	-4.96483	-4.06127	0.38904
N	-3.32822	0.75822	0.79359
C	-5.44544	0.99396	1.69694
H	-6.43849	0.71972	2.02043
C	-4.50887	0.08468	1.0775
C	-1.44409	3.00799	0.28116
C	0.25058	2.20873	-0.91677
C	0.18661	-2.08246	-1.28147
C	-4.75289	-1.25322	0.82366
H	-5.72126	-1.65037	1.10496
C	-2.62949	3.11395	0.98638
H	-2.90326	4.09248	1.36356
C	1.13211	1.3468	-1.54584
H	2.0327	1.75634	-1.98854
C	-0.66682	-3.13724	-1.02077
H	-0.32731	-4.13522	-1.27214
C	-4.83351	2.21461	1.77737
H	-5.22885	3.13779	2.17428
C	-3.51964	2.07394	1.19173
C	5.3075	1.10275	-1.8474
H	6.27277	1.19564	-2.37595
O	4.26819	1.53799	-2.38728
C	5.37385	0.45078	-0.54514
C	4.21545	0.31695	0.25287
C	6.60602	-0.05117	-0.08785
C	4.31508	-0.32716	1.47192
H	3.27773	0.7286	-0.09287

C	6.6998	-0.69015	1.14782
H	7.49015	0.06049	-0.70774
C	5.5541	-0.82938	1.93054
H	7.63576	-1.08486	1.52154
O	3.27437	-0.53849	2.37384
O	5.62498	-1.45589	3.14926
H	4.73425	-1.46128	3.56333
C	1.94281	-0.29986	2.02021
H	1.25605	-0.44601	2.83531
H	1.64585	-0.38533	0.98583
H	-1.61284	-0.12191	2.20762

$^4INT_B$

Fe	1.70276	0.00418	0.14326
O	0.96285	-0.27801	-1.49058
S	2.79688	0.3121	2.16707
H	2.56309	1.66724	2.29144
N	0.96125	1.86208	0.27048
C	0.60276	4.12577	-0.06035
C	-0.44202	3.65584	0.68565
H	0.77914	5.13255	-0.40878
H	-1.29575	4.1961	1.0662
N	0.07549	-0.71286	1.03856
C	-0.97935	0.02074	1.56652
C	-1.95338	-0.8774	2.14852
C	-1.48315	-2.14834	1.97356
H	-2.86586	-0.54515	2.61767
H	-1.93517	-3.07901	2.28273
N	2.54111	-1.81528	0.178
C	1.9282	-2.99452	0.56804
C	3.82126	-2.15408	-0.24024
C	2.8504	-4.0956	0.40548
C	4.01848	-3.57708	-0.07976
H	2.61955	-5.12377	0.64096
H	4.9319	-4.09725	-0.32682
N	3.34233	0.7319	-0.80181
C	5.46352	0.93424	-1.70422
H	6.45406	0.64551	-2.02275
C	4.51636	0.0425	-1.07541
C	1.48108	3.00754	-0.32105
C	-0.22794	2.23978	0.8773
C	-0.20416	-2.04614	1.30417
C	4.74701	-1.29402	-0.80313
H	5.71176	-1.70436	-1.0778
C	2.66981	3.09272	-1.02354
H	2.95497	4.06377	-1.41142
C	-1.12141	1.39471	1.51213

H	-2.0208	1.81849	1.9437
C	0.64102	-3.11211	1.063
H	0.29194	-4.10308	1.32858
C	4.86503	2.16035	-1.79987
H	5.27087	3.07455	-2.20683
C	3.54885	2.04078	-1.21473
C	-5.30405	1.17759	1.81528
H	-6.26707	1.2936	2.34341
O	-4.26012	1.62199	2.33855
C	-5.37879	0.48591	0.53416
C	-4.22415	0.32155	-0.26362
C	-6.61508	-0.02425	0.09752
C	-4.3313	-0.36071	-1.46109
H	-3.28321	0.73997	0.06496
C	-6.71651	-0.70167	-1.11694
H	-7.49634	0.11122	0.71677
C	-5.57438	-0.87151	-1.89879
H	-7.65572	-1.10358	-1.47449
O	-3.29494	-0.6058	-2.35934
O	-5.65244	-1.5367	-3.09644
H	-4.76303	-1.55954	-3.51283
C	-1.96121	-0.36051	-2.01612
H	-1.27787	-0.52443	-2.83088
H	-1.66071	-0.42678	-0.98123
H	1.61694	-0.14365	-2.20947

^{4}TS-reb$_{B}$

Fe	1.30386	-0.00853	0.31288
O	0.57047	-0.02741	-1.41998
S	2.28566	-0.08634	2.45012
H	2.90674	1.1449	2.37486
N	1.36617	1.98429	0.33491
C	1.97829	4.1773	-0.08208
C	0.80269	4.21047	0.61542
H	2.56325	5.00718	-0.44953
H	0.23172	5.07263	0.92574
N	-0.52813	0.04073	1.11046
C	-1.20772	1.1583	1.57493
C	-2.48698	0.75807	2.11571
C	-2.58197	-0.59664	1.97203
H	-3.21765	1.44118	2.52022
H	-3.40276	-1.24345	2.24152
N	1.28749	-2.01426	0.37932
C	0.2063	-2.81763	0.70705
C	2.33767	-2.87067	0.07157
C	0.58607	-4.20637	0.59735
C	1.90138	-4.23917	0.22164

H	-0.07533	-5.03623	0.79651
H	2.52671	-5.10162	0.04525
N	3.1466	-0.06392	-0.50492
C	5.21749	-0.78659	-1.24012
H	6.02333	-1.46726	-1.47103
C	3.95172	-1.18471	-0.67048
C	2.33612	2.78885	-0.25503
C	0.41085	2.84313	0.86167
C	-1.35068	-1.05008	1.36373
C	3.5859	-2.48826	-0.38695
H	4.31298	-3.2688	-0.57823
C	3.49587	2.34889	-0.86568
H	4.17026	3.09832	-1.26311
C	-0.76812	2.46358	1.47613
H	-1.4163	3.24533	1.85343
C	-1.03146	-2.37351	1.13913
H	-1.78477	-3.11881	1.36384
C	5.17333	0.56911	-1.42151
H	5.93864	1.21643	-1.82311
C	3.88785	1.02319	-0.94452
C	-6.39609	-0.24254	0.08153
H	-7.06876	0.58037	0.38884
O	-6.75414	-1.42743	0.22878
C	-5.11426	0.18195	-0.47267
C	-4.18914	-0.76939	-0.93536
C	-4.77958	1.54759	-0.53837
C	-2.96055	-0.36886	-1.43035
H	-4.44153	-1.82263	-0.90848
C	-3.53708	1.94409	-1.01364
H	-5.49416	2.29054	-0.19549
C	-2.5834	1.00018	-1.44301
H	-3.24137	2.98559	-1.04144
O	-2.10497	-1.40611	-1.86012
O	-1.37683	1.46175	-1.84644
C	-1.35656	-1.28309	-3.00392
H	1.11231	-0.47866	-2.09281
H	-0.77259	-2.15874	-3.23318
H	-1.52253	-0.45347	-3.67562
H	-0.56792	0.81304	-1.73665

^{2}P-OH$_{B}$

Fe	-0.73909	-0.09968	0.80602
S	-1.45904	-0.41247	2.93371
H	-1.17532	0.8602	3.39244
N	-1.64067	1.64849	0.56604
C	-2.10858	3.92134	0.47411
C	-3.29146	3.25909	0.29919

H	-1.93459	4.98697	0.49595
H	-4.27422	3.67582	0.13601
N	-2.31856	-1.01698	-0.0139
C	-3.61429	-0.4919	-0.07211
C	-4.53491	-1.51603	-0.49658
C	-3.80733	-2.65649	-0.71425
H	-5.59639	-1.36763	-0.6284
H	-4.16227	-3.62118	-1.04509
N	0.25623	-1.81141	0.72692
C	-0.15172	-3.02433	0.1779
C	1.47746	-2.06137	1.34054
C	0.85987	-4.03196	0.4089
C	1.84964	-3.44614	1.14897
H	0.79276	-5.05521	0.07073
H	2.75713	-3.89289	1.52728
N	0.91355	0.84661	1.33582
C	2.99667	1.26904	2.27413
H	3.96888	1.06188	2.69373
C	2.04129	0.253	1.89256
C	-1.08401	2.9192	0.66416
C	-2.99977	1.84352	0.34249
C	-2.43524	-2.35836	-0.38948
C	2.27798	-1.10823	1.94508
H	3.20925	-1.4379	2.38951
C	0.23131	3.18608	1.00514
H	0.53659	4.22449	1.07063
C	-3.92816	0.8428	0.11113
H	-4.9638	1.13783	-0.01397
C	-1.39666	-3.27302	-0.37276
H	-1.60048	-4.27672	-0.72798
C	2.45647	2.47726	1.93132
H	2.8876	3.46028	2.04952
C	1.14904	2.21782	1.37034
C	-0.92111	-0.27473	-3.48662
H	-0.80911	0.44097	-4.29381
H	-1.50427	-1.15037	-3.78153
O	0.38335	-0.87499	-3.16851
C	1.37502	-0.12599	-2.54366
C	2.29097	-0.84555	-1.77968
C	1.5363	1.26906	-2.65961
C	3.3422	-0.20091	-1.11149
H	2.15515	-1.91808	-1.6992
C	2.55428	1.92101	-1.948
C	3.45541	1.1986	-1.17783
H	2.64671	2.99998	-2.03441
H	4.25122	1.68784	-0.6312

C	4.29024	-0.98944	-0.32628
O	5.19453	-0.51384	0.38831
H	4.15544	-2.08378	-0.39326
O	0.70182	1.95946	-3.5247
H	0.66754	2.91153	-3.31528
O	-1.48379	0.43031	-2.40038
H	-1.7534	-0.1679	-1.66512

^{4}P-OH$_{B}$

Fe	-0.87876	-0.08392	0.80344
S	-1.63836	-0.4463	2.98203
H	-2.70017	0.43815	2.97227
N	-2.29189	1.22318	0.32963
C	-3.46227	3.19055	0.00309
C	-4.33672	2.16253	-0.20785
H	-3.65035	4.25191	-0.0615
H	-5.37716	2.21657	-0.49128
N	-1.97054	-1.559	-0.18436
C	-3.33693	-1.48645	-0.4557
C	-3.81517	-2.78998	-0.84904
C	-2.751	-3.65294	-0.78578
H	-4.83495	-3.01168	-1.12685
H	-2.74146	-4.7127	-0.99318
N	0.60225	-1.37954	1.06241
C	0.60711	-2.73186	0.73836
C	1.79341	-1.1221	1.73232
C	1.82587	-3.33433	1.23704
C	2.54222	-2.35356	1.86458
H	2.08275	-4.37616	1.11649
H	3.51148	-2.42498	2.33366
N	0.44545	1.45211	1.10952
C	2.24132	2.64951	1.93613
H	3.20101	2.83988	2.39317
C	1.68191	1.33233	1.72282
C	-2.17797	2.60857	0.33261
C	-3.59918	0.92814	-0.04125
C	-1.61036	-2.89533	-0.32692
C	2.28567	0.1314	2.06067
H	3.26273	0.17134	2.52705
C	-1.02918	3.34106	0.5945
H	-1.11391	4.42147	0.55319
C	-4.09346	-0.32816	-0.36447
H	-5.14314	-0.394	-0.62726
C	-0.39059	-3.42427	0.06655
H	-0.22862	-4.48351	-0.09842
C	1.33402	3.55808	1.45907
H	1.40257	4.63607	1.46762

C	0.19342	2.80647	0.97612
C	-0.53319	-0.19169	-3.53872
H	-0.45705	0.69486	-4.15831
H	-1.03432	-1.01728	-4.04937
O	0.80269	-0.74991	-3.29434
C	1.71913	-0.06653	-2.50111
C	2.63579	-0.85731	-1.81221
C	1.80186	1.33414	-2.37482
C	3.61808	-0.28253	-0.99286
H	2.54828	-1.93399	-1.90508
C	2.76696	1.90986	-1.53676
C	3.67084	1.11462	-0.84743
H	2.79842	2.99019	-1.43438
H	4.41689	1.54721	-0.19274
C	4.53525	-1.1441	-0.24872
O	5.32492	-0.74685	0.631
H	4.48153	-2.21747	-0.5001
O	0.93551	2.11885	-3.12065
H	0.84523	3.01421	-2.74356
O	-1.18587	0.20712	-2.35025
H	-1.42404	-0.55491	-1.77117

Path C

^2RC_C

Fe	-1.31642	0.02881	-0.18858
O	-0.68951	0.07213	1.34922
S	-2.14255	-0.36556	-2.52252
H	-1.0489	0.15119	-3.19038
N	-0.19252	1.57062	-0.81475
C	0.6587	3.7156	-1.05229
C	1.59774	2.85144	-1.54111
H	0.70185	4.79291	-0.99691
H	2.5694	3.07556	-1.95378
N	0.07101	-1.24577	-0.90232
C	1.29722	-0.92397	-1.48118
C	2.05911	-2.12841	-1.72349
C	1.31559	-3.17409	-1.26238
H	3.04629	-2.14667	-2.15988
H	1.56646	-4.22404	-1.25921
N	-2.53037	-1.53006	0.17883
C	-2.17918	-2.86824	0.18067
C	-3.85809	-1.47939	0.58453
C	-3.30567	-3.67291	0.59933
C	-4.34516	-2.81762	0.83399
H	-3.29098	-4.74936	0.68107
H	-5.34918	-3.05352	1.15341
N	-2.81371	1.29293	0.23265

C	-4.84501	2.16733	0.92401
H	-5.87387	2.1834	1.25096
C	-4.09623	0.96555	0.63034
C	-0.45946	2.91751	-0.60413
C	1.06795	1.5168	-1.38303
C	0.07821	-2.6292	-0.74848
C	-4.59105	-0.32297	0.76957
H	-5.62267	-0.42952	1.08606
C	-1.63496	3.42849	-0.08691
H	-1.71069	4.50545	0.01298
C	1.75303	0.35586	-1.71428
H	2.74636	0.46469	-2.13328
C	-0.95176	-3.37634	-0.2168
H	-0.81063	-4.44936	-0.15286
C	-4.0015	3.2231	0.71769
H	-4.20301	4.27712	0.83642
C	-2.73827	2.67346	0.27858
C	6.37939	-0.20025	-0.18053
H	7.09684	0.6229	-0.35989
O	6.68046	-1.36768	-0.49706
C	5.11204	0.20467	0.42191
C	4.13486	-0.75657	0.74177
C	4.85045	1.56381	0.68181
C	2.91789	-0.37109	1.28056
H	4.33005	-1.80573	0.55607
C	3.62632	1.95603	1.2106
H	5.6075	2.30782	0.45053
C	2.63254	1.00286	1.48905
H	3.38569	2.99709	1.38576
O	1.94263	-1.34638	1.49751
O	1.43213	1.4504	1.95168
H	0.63906	0.84521	1.76792
C	1.50742	-1.56451	2.88326
H	0.63349	-2.20811	2.80678
H	2.30647	-2.05632	3.44802
H	1.22903	-0.62411	3.36358

^{4}RC$_{C}$

Fe	-1.31031	0.02119	-0.19628
O	-0.69423	0.09957	1.34673
S	-2.13793	-0.35196	-2.51246
H	-1.05841	0.19171	-3.1818
N	-0.18762	1.5676	-0.82155
C	0.65655	3.71476	-1.06552
C	1.60074	2.85198	-1.54658
H	0.69565	4.79244	-1.01434
H	2.57324	3.0778	-1.95636

N	0.08023	-1.24771	-0.90051
C	1.30539	-0.92431	-1.48155
C	2.06746	-2.12804	-1.72678
C	1.32429	-3.17519	-1.26848
H	3.05441	-2.14494	-2.16378
H	1.57511	-4.22516	-1.26876
N	-2.51992	-1.5364	0.17958
C	-2.16933	-2.87454	0.17756
C	-3.84767	-1.48655	0.58626
C	-3.29509	-3.68021	0.59542
C	-4.33425	-2.82527	0.83337
H	-3.28037	-4.75685	0.67459
H	-5.33795	-3.06187	1.15331
N	-2.81026	1.287	0.23045
C	-4.83965	2.15934	0.92994
H	-5.86656	2.17411	1.26303
C	-4.08969	0.95815	0.63519
C	-0.46054	2.91455	-0.61773
C	1.07452	1.51615	-1.38547
C	0.08712	-2.63205	-0.75253
C	-4.58162	-0.3313	0.77536
H	-5.61213	-0.44008	1.09474
C	-1.63823	3.42399	-0.10412
H	-1.71771	4.50129	-0.01078
C	1.76169	0.35547	-1.71319
H	2.75577	0.46437	-2.13038
C	-0.9417	-3.38112	-0.22186
H	-0.79982	-4.4542	-0.16058
C	-3.99994	3.21616	0.71467
H	-4.20299	4.27016	0.83096
C	-2.7377	2.66759	0.27009
C	6.3615	-0.2204	-0.17502
H	7.08596	0.59615	-0.3563
O	6.65161	-1.3908	-0.4909
C	5.09852	0.19629	0.42867
C	4.11344	-0.7561	0.75046
C	4.84866	1.55804	0.68673
C	2.90013	-0.35928	1.28922
H	4.2993	-1.80711	0.56577
C	3.62813	1.96161	1.21529
H	5.61186	2.29523	0.45383
C	2.62635	1.01731	1.49515
H	3.39647	3.00499	1.38872
O	1.91626	-1.32555	1.50806
O	1.42923	1.47538	1.95615
H	0.63268	0.87525	1.77337

C	1.48308	-1.54057	2.89495
H	0.60438	-2.17789	2.82068
H	2.27999	-2.03812	3.45767
H	1.21307	-0.59799	3.37594

^{2}TS1-H$_{C}$

Fe	1.27439	-0.01992	0.28721
O	0.63834	0.14601	-1.37355
S	2.2381	0.02866	2.418
H	1.24902	0.76486	3.03918
N	-0.52397	0.32095	1.11974
C	-2.434	1.36294	1.91262
C	-2.60222	0.01848	2.09615
H	-3.1218	2.16142	2.14473
H	-3.45743	-0.5011	2.50076
N	0.94516	-1.98365	0.37355
C	-0.16235	-2.62273	0.91986
C	-0.01864	-4.05212	0.77427
C	1.17863	-4.27908	0.15467
H	-0.74782	-4.77389	1.11047
H	1.6286	-5.22458	-0.10908
N	3.13354	-0.3569	-0.36478
C	3.69528	-1.5811	-0.68682
C	4.09979	0.60279	-0.6362
C	5.04956	-1.38709	-1.15177
C	5.30137	-0.04408	-1.11146
H	5.70784	-2.18439	-1.46301
H	6.20505	0.47763	-1.38889
N	1.58673	1.9749	0.19171
C	2.56567	4.03948	-0.17307
H	3.32588	4.76023	-0.43451
C	2.75782	2.60506	-0.19415
C	-1.13728	1.55585	1.30746
C	-1.41686	-0.63272	1.59009
C	1.79343	-2.99164	-0.07375
C	3.93363	1.97271	-0.55168
H	4.77943	2.59689	-0.81572
C	-0.59888	2.7863	0.97889
H	-1.20658	3.66454	1.16171
C	-1.24801	-2.00201	1.50598
H	-2.0421	-2.63107	1.89016
C	3.06512	-2.80874	-0.58164
H	3.62152	-3.68961	-0.87981
C	1.27954	4.26837	0.22558
H	0.77634	5.21409	0.36025
C	0.67213	2.97736	0.46911
C	-6.29299	-0.19224	0.09932

H	-7.0237	0.62749	0.22988
O	-6.56801	-1.34156	0.49241
C	-5.03402	0.19424	-0.53622
C	-4.04762	-0.76424	-0.79381
C	-4.78472	1.5388	-0.87538
C	-2.83341	-0.40703	-1.37143
H	-4.22846	-1.80402	-0.54983
C	-3.56217	1.90352	-1.4161
H	-5.54675	2.29019	-0.69054
C	-2.54301	0.95741	-1.65468
H	-3.32866	2.93329	-1.65651
O	-1.98051	-1.50126	-1.57451
O	-1.37805	1.43821	-2.16087
C	-0.87939	-1.50282	-2.43941
H	0.07192	-0.85451	-1.88088
H	-0.53957	-2.5293	-2.551
H	-1.02811	-0.94499	-3.36615
H	-0.5012	0.99398	-1.83449

^{4}TS1-H$_C$

Fe	1.30264	0.04551	0.26683
O	0.61255	0.06957	-1.38644
S	2.30842	-0.26077	2.40007
H	1.20024	-0.76052	3.05517
N	-0.50744	0.24688	1.13319
C	-2.4552	1.17642	1.97781
C	-2.58486	-0.18204	2.07225
H	-3.16908	1.93727	2.25293
H	-3.42762	-0.75059	2.43486
N	1.06203	-1.98459	0.3387
C	-0.03372	-2.69061	0.81413
C	0.17444	-4.10888	0.61949
C	1.39881	-4.25764	0.02937
H	-0.53147	-4.87522	0.90267
H	1.89687	-5.17093	-0.26009
N	3.16839	-0.19652	-0.38655
C	3.78709	-1.39781	-0.71981
C	4.09183	0.80112	-0.6579
C	5.12998	-1.13808	-1.18725
C	5.32093	0.21429	-1.14099
H	5.8234	-1.90203	-1.50574
H	6.19963	0.77724	-1.41797
N	1.52541	2.01795	0.22744
C	2.39014	4.14847	-0.09399
H	3.10636	4.91386	-0.35275
C	2.64924	2.72475	-0.16683
C	-1.16245	1.43967	1.39109

C	-1.37571	-0.76204	1.53541
C	1.95561	-2.93127	-0.13343
C	3.85196	2.161	-0.5538
H	4.66004	2.83378	-0.81796
C	-0.66749	2.7048	1.11003
H	-1.30422	3.55058	1.34297
C	-1.15882	-2.12154	1.38407
H	-1.94691	-2.78946	1.71203
C	3.21767	-2.65475	-0.63464
H	3.82132	-3.49608	-0.95668
C	1.11045	4.29984	0.35335
H	0.567	5.21432	0.53789
C	0.5756	2.97112	0.57102
C	-6.38644	-0.1386	0.06957
H	-7.09726	0.69825	0.20402
O	-6.70214	-1.28827	0.4321
C	-5.10655	0.2275	-0.5322
C	-4.13795	-0.75074	-0.79079
C	-4.81596	1.57045	-0.84001
C	-2.90191	-0.41736	-1.33304
H	-4.3514	-1.78969	-0.57008
C	-3.57531	1.91045	-1.35559
H	-5.56104	2.33882	-0.65523
C	-2.57461	0.94364	-1.59374
H	-3.31231	2.93738	-1.57773
O	-2.06211	-1.52923	-1.50641
O	-1.39491	1.41217	-2.07515
C	-0.96891	-1.57223	-2.38714
H	0.04944	-0.88269	-1.8254
H	-0.63902	-2.60468	-2.4685
H	-1.1174	-1.03699	-3.32701
H	-0.5227	0.92704	-1.78702

^{2}INT1-H$_{C}$

Fe	-1.69815	0.00183	-0.14549
O	-0.95741	-0.26239	1.49105
S	-2.79559	0.29489	-2.16896
H	-2.5714	1.65118	-2.29856
N	-0.93849	1.85026	-0.29861
C	-0.5562	4.11426	0.00202
C	0.47963	3.62495	-0.74398
H	-0.72083	5.12698	0.33879
H	1.33629	4.15213	-1.13611
N	-0.08083	-0.74292	-1.03539
C	0.97774	-0.02649	-1.57948
C	1.94163	-0.94171	-2.15173
C	1.46164	-2.20576	-1.95494

H	2.85474	-0.62439	-2.63001
H	1.90454	-3.14487	-2.25157
N	-2.55289	-1.80979	-0.15164
C	-1.9517	-3.00046	-0.52467
C	-3.83597	-2.13014	0.27256
C	-2.88406	-4.09028	-0.34465
C	-4.04676	-3.55351	0.13353
H	-2.66318	-5.12402	-0.56485
H	-4.96483	-4.06127	0.38904
N	-3.32822	0.75822	0.79359
C	-5.44544	0.99396	1.69694
H	-6.43849	0.71972	2.02043
C	-4.50887	0.08468	1.0775
C	-1.44409	3.00799	0.28116
C	0.25058	2.20873	-0.91677
C	0.18661	-2.08246	-1.28147
C	-4.75289	-1.25322	0.82366
H	-5.72126	-1.65037	1.10496
C	-2.62949	3.11395	0.98638
H	-2.90326	4.09248	1.36356
C	1.13211	1.3468	-1.54584
H	2.0327	1.75634	-1.98854
C	-0.66682	-3.13724	-1.02077
H	-0.32731	-4.13522	-1.27214
C	-4.83351	2.21461	1.77737
H	-5.22885	3.13779	2.17428
C	-3.51964	2.07394	1.19173
C	5.3075	1.10275	-1.8474
H	6.27277	1.19564	-2.37595
O	4.26819	1.53799	-2.38728
C	5.37385	0.45078	-0.54514
C	4.21545	0.31695	0.25287
C	6.60602	-0.05117	-0.08785
C	4.31508	-0.32716	1.47192
H	3.27773	0.7286	-0.09287
C	6.6998	-0.69015	1.14782
H	7.49015	0.06049	-0.70774
C	5.5541	-0.82938	1.93054
H	7.63576	-1.08486	1.52154
O	3.27437	-0.53849	2.37384
O	5.62498	-1.45589	3.14926
H	4.73425	-1.46128	3.56333
C	1.94281	-0.29986	2.02021
H	1.25605	-0.44601	2.83531
H	1.64585	-0.38533	0.98583
H	-1.61284	-0.12191	2.20762

^{4}INT1-H$_C$

Fe	1.70276	0.00418	0.14326
O	0.96285	-0.27801	-1.49058
S	2.79688	0.3121	2.16707
H	2.56309	1.66724	2.29144
N	0.96125	1.86208	0.27048
C	0.60276	4.12577	-0.06035
C	-0.44202	3.65584	0.68565
H	0.77914	5.13255	-0.40878
H	-1.29575	4.1961	1.0662
N	0.07549	-0.71286	1.03856
C	-0.97935	0.02074	1.56652
C	-1.95338	-0.8774	2.14852
C	-1.48315	-2.14834	1.97356
H	-2.86586	-0.54515	2.61767
H	-1.93517	-3.07901	2.28273
N	2.54111	-1.81528	0.178
C	1.9282	-2.99452	0.56804
C	3.82126	-2.15408	-0.24024
C	2.8504	-4.0956	0.40548
C	4.01848	-3.57708	-0.07976
H	2.61955	-5.12377	0.64096
H	4.9319	-4.09725	-0.32682
N	3.34233	0.7319	-0.80181
C	5.46352	0.93424	-1.70422
H	6.45406	0.64551	-2.02275
C	4.51636	0.0425	-1.07541
C	1.48108	3.00754	-0.32105
C	-0.22794	2.23978	0.8773
C	-0.20416	-2.04614	1.30417
C	4.74701	-1.29402	-0.80313
H	5.71176	-1.70436	-1.0778
C	2.66981	3.09272	-1.02354
H	2.95497	4.06377	-1.41142
C	-1.12141	1.39471	1.51213
H	-2.0208	1.81849	1.9437
C	0.64102	-3.11211	1.063
H	0.29194	-4.10308	1.32858
C	4.86503	2.16035	-1.79987
H	5.27087	3.07455	-2.20683
C	3.54885	2.04078	-1.21473
C	-5.30405	1.17759	1.81528
H	-6.26707	1.2936	2.34341
O	-4.26012	1.62199	2.33855
C	-5.37879	0.48591	0.53416
C	-4.22415	0.32155	-0.26362

C	-6.61508	-0.02425	0.09752
C	-4.3313	-0.36071	-1.46109
H	-3.28321	0.73997	0.06496
C	-6.71651	-0.70167	-1.11694
H	-7.49634	0.11122	0.71677
C	-5.57438	-0.87151	-1.89879
H	-7.65572	-1.10358	-1.47449
O	-3.29494	-0.6058	-2.35934
O	-5.65244	-1.5367	-3.09644
H	-4.76303	-1.55954	-3.51283
C	-1.96121	-0.36051	-2.01612
H	-1.27787	-0.52443	-2.83088
H	-1.66071	-0.42678	-0.98123
H	1.61694	-0.14365	-2.20947

^{2}TS2-H$_{C}$

Fe	1.35513	-0.00276	0.28334
O	0.56717	-0.03696	-1.45335
S	2.40068	-0.00352	2.3671
H	1.88921	-1.19603	2.84132
N	-0.44139	-0.34504	1.13686
C	-2.53411	-0.01595	2.08851
C	-2.34572	-1.36546	1.98184
H	-3.39957	0.51278	2.45685
H	-3.02516	-2.15963	2.24862
N	1.63931	-1.98624	0.15831
C	0.76148	-2.99708	0.51771
C	1.33989	-4.28875	0.21521
C	2.5685	-4.05617	-0.33328
H	0.8554	-5.23567	0.39951
H	3.29232	-4.77498	-0.6868
N	3.17099	0.35099	-0.50871
C	4.07823	-0.61008	-0.92079
C	3.77754	1.57433	-0.74965
C	5.28021	0.02399	-1.41975
C	5.09546	1.37316	-1.31138
H	6.14102	-0.5066	-1.79807
H	5.77438	2.16734	-1.58344
N	1.06098	1.99414	0.40115
C	1.33216	4.29711	0.28518
H	1.80219	5.24653	0.07687
C	1.92834	3.0075	0.02116
C	-1.34611	0.61834	1.55726
C	-1.04146	-1.56209	1.38849
C	2.75023	-2.61941	-0.3716
C	3.19505	2.80846	-0.50992
H	3.777	3.69059	-0.75438

C	-1.16705	1.98593	1.45352
H	-1.9726	2.61723	1.8117
C	-0.48549	-2.7984	1.08482
H	-1.07958	-3.67799	1.30599
C	3.87499	-1.98052	-0.86962
H	4.67295	-2.61096	-1.24728
C	0.10399	4.06036	0.84108
H	-0.63125	4.77706	1.17456
C	-0.05375	2.62554	0.91969
C	-6.47009	0.09494	-0.10834
H	-7.18208	-0.73648	0.05386
O	-6.82133	1.2704	0.13022
C	-4.17447	0.67255	-0.85515
C	-4.8397	-1.66267	-0.78369
C	-2.91665	0.29565	-1.28319
H	-4.42801	1.71303	-0.69045
C	-3.5694	-2.03916	-1.18873
H	-5.599	-2.41739	-0.59653
C	-2.54754	-1.08176	-1.42227
H	-3.2993	-3.07967	-1.32383
O	-1.9089	1.23541	-1.56546
O	-1.32812	-1.49223	-1.73206
H	-0.37524	-0.73637	-1.62626
C	-2.23154	2.57008	-1.76454
H	-1.35873	3.19699	-1.86738
H	0.37401	0.85595	-1.78787
H	-3.18487	2.80751	-2.22212

^{4}TS2-H$_{C}$

Fe	1.35513	-0.00276	0.28334
O	0.56717	-0.03696	-1.45335
S	2.40068	-0.00352	2.3671
H	1.88921	-1.19603	2.84132
N	-0.44139	-0.34504	1.13686
C	-2.53411	-0.01595	2.08851
C	-2.34572	-1.36546	1.98184
H	-3.39957	0.51278	2.45685
H	-3.02516	-2.15963	2.24862
N	1.63931	-1.98624	0.15831
C	0.76148	-2.99708	0.51771
C	1.33989	-4.28875	0.21521
C	2.5685	-4.05617	-0.33328
H	0.8554	-5.23567	0.39951
H	3.29232	-4.77498	-0.6868
N	3.17099	0.35099	-0.50871
C	4.07823	-0.61008	-0.92079
C	3.77754	1.57433	-0.74965

C	5.28021	0.02399	-1.41975
C	5.09546	1.37316	-1.31138
H	6.14102	-0.5066	-1.79807
H	5.77438	2.16734	-1.58344
N	1.06098	1.99414	0.40115
C	1.33216	4.29711	0.28518
H	1.80219	5.24653	0.07687
C	1.92834	3.0075	0.02116
C	-1.34611	0.61834	1.55726
C	-1.04146	-1.56209	1.38849
C	2.75023	-2.61941	-0.3716
C	3.19505	2.80846	-0.50992
H	3.777	3.69059	-0.75438
C	-1.16705	1.98593	1.45352
H	-1.9726	2.61723	1.8117
C	-0.48549	-2.7984	1.08482
H	-1.07958	-3.67799	1.30599
C	3.87499	-1.98052	-0.86962
H	4.67295	-2.61096	-1.24728
C	0.10399	4.06036	0.84108
H	-0.63125	4.77706	1.17456
C	-0.05375	2.62554	0.91969
C	-6.47009	0.09494	-0.10834
H	-7.18208	-0.73648	0.05386
O	-6.82133	1.2704	0.13022
C	-5.15749	-0.30294	-0.59146
C	-4.17447	0.67255	-0.85515
C	-4.8397	-1.66267	-0.78369
C	-2.91665	0.29565	-1.28319
H	-4.42801	1.71303	-0.69045
C	-3.5694	-2.03916	-1.18873
H	-5.599	-2.41739	-0.59653
C	-2.54754	-1.08176	-1.42227
H	-3.2993	-3.07967	-1.32383
O	-1.9089	1.23541	-1.56546
O	-1.32812	-1.49223	-1.73206
H	-0.37524	-0.73637	-1.62626
C	-2.23154	2.57008	-1.76454
H	-1.35873	3.19699	-1.86738
H	0.37401	0.85595	-1.78787
H	-3.18487	2.80751	-2.22212

^{4}INT2-H$_{C}$

Fe	1.40428	-0.00195	0.30409
O	0.57396	-0.05543	-1.49677
S	2.42586	0.0487	2.35563

H	1.87656	-1.11242	2.86464
N	-0.39493	-0.36471	1.13247
C	-2.47893	-0.06366	2.10789
C	-2.30059	-1.4101	1.93842
H	-3.3361	0.45287	2.51238
H	-2.98082	-2.2116	2.18154
N	1.70296	-1.9808	0.1525
C	0.81893	-3.00107	0.46724
C	1.42503	-4.28482	0.18647
C	2.67984	-4.03626	-0.29333
H	0.94275	-5.23806	0.34274
H	3.42927	-4.74591	-0.61062
N	3.19083	0.3757	-0.54297
C	4.13345	-0.57437	-0.90125
C	3.74974	1.60317	-0.8476
C	5.31159	0.07724	-1.43654
C	5.07312	1.4217	-1.40717
H	6.19195	-0.44052	-1.78705
H	5.71996	2.2255	-1.72567
N	1.06312	1.98892	0.37964
C	1.2968	4.29499	0.23792
H	1.74046	5.25001	-0.00119
C	1.89737	3.01292	-0.05533
C	-1.2904	0.58816	1.59849
C	-0.99942	-1.5887	1.33474
C	2.84583	-2.59739	-0.32291
C	3.14078	2.83227	-0.63716
H	3.69277	3.72013	-0.92554
C	-1.11687	1.95734	1.53247
H	-1.90823	2.57899	1.93589
C	-0.44741	-2.81842	0.99438
H	-1.0468	-3.70255	1.17923
C	3.9752	-1.94585	-0.79699
H	4.79944	-2.5662	-1.13208
C	0.11051	4.04436	0.87271
H	-0.6108	4.75352	1.25051
C	-0.02662	2.6074	0.96335
C	-6.57667	0.17565	-0.14163
H	-7.32153	-0.62575	0.01349
O	-6.88558	1.36661	0.07068
C	-5.26347	-0.27145	-0.58984
C	-4.24375	0.67281	-0.82846
C	-4.99793	-1.64848	-0.77308
C	-2.99177	0.25459	-1.23043
H	-4.46736	1.71943	-0.66234
C	-3.74283	-2.07336	-1.15795

H	-5.79203	-2.36866	-0.59703
C	-2.66961	-1.14942	-1.37731
H	-3.50727	-3.12279	-1.28775
O	-1.95209	1.14569	-1.49912
O	-1.47759	-1.58253	-1.66175
H	-0.21976	-0.69827	-1.5963
C	-2.20778	2.50923	-1.63231
H	-1.30621	3.1013	-1.65372
H	0.2817	0.83094	-1.77062
H	-3.1313	2.81201	-2.11157

^2P_C

Fe	-1.33741	0.1431	0.30606
O	-0.65678	-0.05987	-1.61908
S	-2.2053	0.38651	2.39275
H	-1.04973	0.13135	3.10595
N	-0.33984	-1.5341	0.81783
C	0.12405	-3.75299	1.31255
C	1.2088	-3.01658	1.70882
H	-0.02655	-4.8196	1.39461
H	2.12632	-3.36289	2.1602
N	0.29718	1.2063	0.79993
C	1.46071	0.75615	1.40874
C	2.32915	1.87701	1.7001
C	1.69012	3.00272	1.26169
H	3.29701	1.7931	2.1714
H	2.02683	4.02782	1.31308
N	-2.28816	1.79633	-0.32922
C	-1.7812	3.08512	-0.28057
C	-3.58215	1.90794	-0.81557
C	-2.7761	4.0221	-0.76534
C	-3.88635	3.29736	-1.09127
H	-2.62945	5.09019	-0.83032
H	-4.83007	3.65201	-1.47864
N	-2.93648	-0.94077	-0.28503
C	-5.06482	-1.58434	-0.95196
H	-6.07833	-1.4899	-1.31297
C	-4.15684	-0.47439	-0.75665
C	-0.84685	-2.82594	0.76775
C	0.91641	-1.63343	1.40651
C	0.41956	2.5836	0.70494
C	-4.45869	0.85335	-1.01098
H	-5.45004	1.08326	-1.38482
C	-2.10024	-3.18963	0.29877
H	-2.35478	-4.2435	0.33157
C	1.75687	-0.56735	1.68449
H	2.7104	-0.78528	2.15103

C	-0.52958	3.44909	0.18506
H	-0.28366	4.50542	0.17269
C	-4.39497	-2.71952	-0.59187
H	-4.75258	-3.73872	-0.59742
C	-3.06953	-2.31797	-0.16691
C	5.83938	1.57165	-0.15459
H	5.77325	2.66292	-0.31423
O	6.81504	1.08275	0.44079
C	4.71085	0.79493	-0.68039
C	4.70081	-0.61301	-0.52312
C	3.64288	1.46683	-1.29778
C	3.60142	-1.2791	-1.01069
H	5.52428	-1.11276	-0.03052
C	2.52461	0.77229	-1.78373
H	3.67146	2.54792	-1.37459
C	2.54788	-0.59909	-1.6257
H	1.66892	1.27553	-2.21107
H	0.03355	-0.75599	-1.75896
H	-1.42189	-0.1577	-2.21222
C	2.04582	-2.86579	-1.62939
H	2.21007	-3.42393	-2.55189
H	1.34053	-3.33473	-0.94787
O	1.54248	-1.51291	-1.98654
O	3.32315	-2.65366	-0.94499

^4P_C

Fe	-1.32562	0.13132	0.32767
O	-0.64285	-0.07427	-1.74045
S	-2.22361	0.31092	2.48175
H	-1.2139	1.0644	3.04859
N	-0.23617	-1.63533	0.76111
C	0.24315	-3.82919	1.28945
C	1.31387	-3.06904	1.69161
H	0.11377	-4.89705	1.39152
H	2.22481	-3.40343	2.16535
N	0.28189	1.22609	0.83057
C	1.43986	0.7626	1.44268
C	2.28861	1.89762	1.75059
C	1.64519	3.02312	1.3121
H	3.25573	1.82418	2.22538
H	1.98222	4.04774	1.3717
N	-2.30306	1.85199	-0.39843
C	-1.80597	3.13527	-0.3441
C	-3.59759	1.92157	-0.86352
C	-2.82153	4.05721	-0.83126
C	-3.92513	3.31052	-1.14805
H	-2.70338	5.12881	-0.90052

H	-4.87536	3.65799	-1.52669
N	-2.90833	-0.98744	-0.25043
C	-5.03587	-1.62748	-0.87646
H	-6.05585	-1.54217	-1.22147
C	-4.13155	-0.50645	-0.70365
C	-0.74038	-2.91886	0.72438
C	1.00014	-1.68707	1.37457
C	0.38243	2.60722	0.73041
C	-4.4424	0.82143	-0.99654
H	-5.44716	1.01203	-1.35898
C	-2.02377	-3.24927	0.28941
H	-2.29604	-4.29938	0.32068
C	1.77291	-0.56881	1.68168
H	2.72908	-0.74805	2.16087
C	-0.55818	3.47413	0.17312
H	-0.29858	4.52791	0.17659
C	-4.35614	-2.76303	-0.53011
H	-4.71616	-3.78142	-0.53633
C	-3.01793	-2.36826	-0.13161
C	5.70026	1.699	-0.11977
H	5.58402	2.78803	-0.26632
O	6.69076	1.2497	0.48293
C	4.61619	0.87773	-0.66903
C	4.67026	-0.53126	-0.53165
C	3.52184	1.50818	-1.28437
C	3.60605	-1.24024	-1.03653
H	5.51237	-0.9996	-0.03971
C	2.43901	0.77059	-1.78612
H	3.50072	2.59049	-1.34463
C	2.52571	-0.60112	-1.64933
H	1.55971	1.23729	-2.20698
H	0.01521	-0.8045	-1.85105
H	-1.4531	-0.23331	-2.25706
C	2.1203	-2.88572	-1.67429
H	2.30198	-3.44277	-2.594
H	1.43386	-3.37714	-0.98904
O	1.56883	-1.55439	-2.03534
O	3.39246	-2.62711	-0.99421