

Supporting Information

The quasi-irreversible inactivation of Cytochrome P450 enzymes by paroxetine: A computational approach

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Table S1. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the methylenedioxy hydroxylation of paroxetine by P450 (Cpd I).

	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 _m	-2702.053927	0.00	-2701.402891	0.00	-2702.695408	0.00	-2702.044372	0.00	-2702.714922	0.00	-2702.063886	0.00
⁴ RC _m	-2702.053878	0.03	-2701.402811	0.05	-2702.695258	0.09	-2702.044191	0.11	-2702.714820	0.06	-2702.063753	0.08
² TS-H _m	-2702.031204	14.26	-2701.386160	10.50	-2702.676048	12.15	-2702.031004	8.39	-2702.700337	9.15	-2702.055293	5.39
⁴ TS-H _m	-2702.031459	14.10	-2701.385734	10.77	-2702.678572	10.57	-2702.032847	7.23	-2702.698250	10.46	-2702.052525	7.13
² INT _m	-2702.044057	6.19	-2701.394465	5.29	-2702.694524	0.55	-2702.044932	-0.35	-2702.714213	0.44	-2702.064621	-0.46
⁴ INT _m	-2702.043395	6.61	-2701.393803	5.70	-2702.694141	0.80	-2702.044549	-0.11	-2702.713534	0.87	-2702.063942	-0.04
⁴ TS-reb _m	-2702.035909	11.31	-2701.390865	7.55	-2702.681256	8.88	-2702.036226	5.11	-2702.704014	6.84	-2702.056984	4.33
² P-OH _m	-2702.149604	-60.04	-2701.495695	-58.24	-2702.799961	-65.61	-2702.146052	-63.81	-2702.818709	-65.13	-2702.164800	-63.32
⁴ P-OH _m	-2702.148072	-59.08	-2701.495317	-58.00	-2702.799943	-65.60	-2702.147188	-64.52	-2702.821751	-67.04	-2702.168996	-65.96

Table S2. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the secondary amine hydroxylation of paroxetine by P450 (Cpd I) by HAT mechanism.

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE+Bu lk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
² RC	-2702.057005	0.00	-2701.405768	0.00	-2702.698107	0.00	-2702.046870	-0.11	-2702.716480	0.02	-2702.065243	0.08
⁴ RC	-2702.056554	0.28	-2701.405402	0.23	-2702.697845	0.16	-2702.046693	0.00	-2702.716516	0.00	-2702.065364	0.00
² TS _H	-2702.037043	12.53	-2701.392800	8.14	-2702.681918	10.16	-2702.037675	5.66	-2702.704990	7.23	-2702.060747	2.90
⁴ TS _H	-2702.036797	12.68	-2701.392420	8.38	-2702.682472	9.81	-2702.038095	5.40	-2702.705669	6.81	-2702.061292	2.56
² INT _H	-2702.050805	3.89	-2701.402430	2.09	-2702.698198	-0.06	-2702.049823	-1.96	-2702.718408	-1.19	-2702.070033	-2.93
⁴ INT _H	-2702.053540	2.17	-2701.404657	0.70	-2702.701113	-1.89	-2702.052230	-3.47	-2702.719993	-2.18	-2702.071110	-3.61
² TS-reb _H	-2702.036672	12.76	-2701.388336	10.94	-2702.684986	8.23	-2702.036650	6.30	-2702.702574	8.75	-2702.054238	6.98
⁴ TS-reb _H	-2702.037573	12.19	-2701.389252	10.36	-2702.685314	8.03	-2702.037665	5.67	-2702.703014	8.47	-2702.054693	6.70
² P-OH	-2702.088946	-20.04	-2701.436230	-19.12	-2702.735781	-23.64	-2702.083065	-22.82	-2702.753607	-23.28	-2702.100891	-22.29
⁴ P-OH	-2702.083788	-16.81	-2701.432803	-16.96	-2702.712972	-9.33	-2702.061987	-9.60	-2702.734468	-11.27	-2702.083483	-11.37

Table S3. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the secondary amine hydroxylation of paroxetine by P450 (Cpd I) by OAR mechanism.

	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 TS _O	-2702.038069	11.88	-2701.388454	10.86	-2702.680964	10.76	-2702.031349	9.63	-2702.703778	7.99	-2702.054163	7.03
⁴ TS _O	-2702.04384	8.26	-2701.394634	6.99	-2702.686465	7.31	-2702.037259	5.92	-2702.705561	6.87	-2702.056355	5.65
² INT _O	-2702.093278	-22.76	-2701.437895	-20.16	-2702.737628	-24.80	-2702.082245	-22.31	-2702.761985	-28.53	-2702.106602	-25.88
⁴ INT _O	-2702.071242	-8.93	-2701.418825	-8.19	-2702.717036	-11.88	-2702.064619	-11.25	-2702.739841	-14.64	-2702.087424	-13.84
² TS-reb _O	-2702.024399	20.46	-2701.376651	18.27	-2702.67124	16.86	-2702.023492	14.56	-2702.691235	15.86	-2702.043487	13.73
⁴ TS-reb _O	-2702.003709	33.44	-2701.358247	29.82	-2702.651859	29.02	-2702.006397	25.29	-2702.67117	28.45	-2702.025708	24.88

Table S4. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the dehydration of hydroxylated paroxetine and coordination to the heme iron.

	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 TS-D _m	-2702.040988	8.12	-2701.394067	5.54	-2702.701781	-4.00	-2702.054860	-6.58	-2702.724136	-5.78	-2702.077215	-8.36
⁴ TS-D _m	-2702.023598	19.03	-2701.379765	14.51	-2702.685701	6.09	-2702.041868	1.57	-2702.709157	3.62	-2702.065324	-0.90
² P-C _m	-2702.107394	-33.55	-2701.457409	-34.21	-2702.768517	-45.88	-2702.118536	-46.54	-2702.788882	-46.41	-2702.138900	-47.07
⁴ P-C _m	-2702.082272	-17.79	-2701.434563	-19.87	-2702.734384	-24.46	-2702.086675	-26.55	-2702.754421	-24.79	-2702.106712	-26.87
² TS-D _N	-2702.002797	34.02	-2701.357845	30.07	-2702.656618	26.03	-2702.011666	22.09	-2702.674818	26.14	-2702.029866	22.20
⁴ TS-D _N	-2701.994945	38.94	-2701.352128	33.66	-2702.630323	42.53	-2701.987506	37.25	-2702.652463	40.17	-2702.009646	34.89
² P-C _N	-2702.146289	-56.03	-2701.495535	-56.33	-2702.806991	-68.33	-2702.156237	-68.63	-2702.828308	-70.17	-2702.177554	-70.48
⁴ P-C _N	-2702.124591	-42.41	-2701.476451	-44.35	-2702.784326	-54.10	-2702.136186	-56.05	-2702.807135	-56.89	-2702.158995	-58.83

Cartesian coordinates of all structures discussed in this work.

Methylenedioxo inactivation

²RCm

Fe	-4.23493	0.31347	0.14522
O	-3.45149	0.48284	-1.2717
S	-5.35131	-0.30342	2.37686
H	-6.56094	-0.65781	1.8865
N	-4.49631	-1.68136	-0.08126
C	-5.28564	-3.73163	-0.808
C	-4.08818	-3.95443	-0.20327
H	-5.95311	-4.44889	-1.26817
H	-3.56754	-4.89281	-0.06269
N	-2.55547	-0.05	1.20517
C	-1.9151	-1.25357	1.35011
C	-0.67505	-1.08114	2.06798
C	-0.57458	0.24317	2.36084
H	0.01571	-1.88029	2.3026
H	0.21515	0.7595	2.8911
N	-4.12024	2.26012	0.6382
C	-3.10935	2.8798	1.31974
C	-4.99132	3.25241	0.27503
C	-3.34626	4.3012	1.39239
C	-4.51762	4.53363	0.73961
H	-2.6931	5.01129	1.88307
H	-5.0291	5.47458	0.58246
N	-6.05568	0.62747	-0.66516
C	-7.90334	1.66758	-1.58404
H	-8.57428	2.47145	-1.85853
C	-6.66684	1.83966	-0.86184
C	-5.52816	-2.31124	-0.74291
C	-3.59768	-2.67285	0.24055
C	-1.74632	0.88013	1.81077
C	-6.17636	3.06278	-0.42519
H	-6.76998	3.94467	-0.64633
C	-6.62879	-1.67319	-1.29014
H	-7.36425	-2.29338	-1.79366
C	-2.38897	-2.47491	0.88767
H	-1.76517	-3.3463	1.05756
C	-2.00454	2.24082	1.8739
H	-1.27814	2.86185	2.38924
C	-8.03004	0.33434	-1.82792
H	-8.82645	-0.18552	-2.3449
C	-6.87007	-0.30256	-1.25354
C	1.45377	-1.03754	-1.16679
C	0.87715	-2.294	-1.32528
C	1.55826	-3.44402	-0.97141
C	2.85409	-3.295	-0.45252
C	3.43265	-2.02857	-0.29808
C	2.72912	-0.85959	-0.65751
C	-0.51023	-0.77755	-2.19517
H	1.1115	-4.42532	-1.09312

H	3.4381	-4.1634	-0.16684
H	3.14654	0.13327	-0.55166
H	-0.38343	-0.69738	-3.28542
H	-1.46788	-0.37092	-1.86715
O	0.56529	-0.06902	-1.55119
O	-0.40516	-2.15631	-1.80949
O	4.703	-2.01769	0.21698
C	5.36591	-0.76775	0.38311
H	5.43232	-0.24251	-0.57921
H	4.79851	-0.12997	1.07827
C	6.75705	-1.05303	0.94137
C	7.58293	-1.92374	-0.02963
C	7.49945	0.24579	1.37013
N	9.02509	-1.81914	0.25396
H	7.21155	-2.95731	0.04156
C	8.87017	-0.14082	2.02038
C	9.31927	-1.56891	1.66421
H	9.63467	0.56927	1.69048
H	10.40037	-1.6645	1.81413
H	9.50283	-2.65604	-0.06882
H	6.60569	-1.63004	1.86378
H	7.4077	-1.59384	-1.06284
H	8.84152	-2.3006	2.3435
H	8.8008	-0.04992	3.11131
H	6.8788	0.70095	2.15243
C	7.61355	1.29288	0.26481
C	6.79818	2.434	0.3038
C	8.51421	1.16377	-0.80683
C	6.8619	3.41652	-0.68635
H	6.10119	2.56557	1.12877
C	8.59218	2.13519	-1.80485
H	9.15781	0.28882	-0.84833
C	7.76259	3.24839	-1.72976
H	6.23385	4.30097	-0.65377
H	9.28572	2.04057	-2.63454
F	7.83769	4.19267	-2.69351
⁴RCm			
Fe	-4.22618	0.30101	0.14764
O	-3.45787	0.51585	-1.27352
S	-5.32354	-0.29355	2.37943
H	-6.53563	-0.65415	1.89983
N	-4.48352	-1.68719	-0.08432
C	-5.28318	-3.74004	-0.79294
C	-4.08323	-3.96252	-0.19317
H	-5.95533	-4.45822	-1.24479
H	-3.56459	-4.90151	-0.04931
N	-2.53733	-0.05762	1.19123
C	-1.89593	-1.26044	1.33601
C	-0.65243	-1.08652	2.04725
C	-0.55093	0.23842	2.33687
H	0.03992	-1.88493	2.27964

H	0.24128	0.75596	2.86223
N	-4.11088	2.2528	0.64316
C	-3.09344	2.87391	1.31201
C	-4.98661	3.24304	0.28781
C	-3.33002	4.29571	1.3845
C	-4.50894	4.52594	0.74479
H	-2.67161	5.00722	1.86604
H	-5.02268	5.46624	0.59114
N	-6.05302	0.61599	-0.65218
C	-7.90907	1.65623	-1.55394
H	-8.58364	2.45981	-1.82029
C	-6.6684	1.82797	-0.83857
C	-5.52204	-2.3189	-0.73486
C	-3.58667	-2.67988	0.2401
C	-1.72579	0.87422	1.79221
C	-6.17828	3.05076	-0.40066
H	-6.77655	3.93141	-0.61424
C	-6.62562	-1.68293	-1.27813
H	-7.36326	-2.3048	-1.77634
C	-2.37365	-2.48229	0.87892
H	-1.75102	-3.35455	1.04891
C	-1.98382	2.23479	1.85686
H	-1.25314	2.85576	2.36622
C	-8.03401	0.32397	-1.80398
H	-8.83235	-0.19529	-2.31859
C	-6.86919	-0.31268	-1.23918
C	1.43769	-0.98926	-1.18223
C	0.85232	-2.23987	-1.35428
C	1.52239	-3.39797	-1.00571
C	2.81634	-3.26317	-0.47835
C	3.40392	-2.00251	-0.31058
C	2.71148	-0.82528	-0.66442
C	-0.51881	-0.70584	-2.21875
H	1.06881	-4.37475	-1.13807
H	3.39214	-4.13833	-0.19667
H	3.13585	0.16345	-0.5481
H	-0.386	-0.61723	-3.30763
H	-1.47525	-0.29487	-1.8921
O	0.55875	-0.01085	-1.56348
O	-0.426	-2.08838	-1.84455
O	4.67136	-2.00577	0.21152
C	5.34599	-0.76307	0.38484
H	5.42003	-0.23432	-0.57499
H	4.78319	-0.12278	1.08145
C	6.73291	-1.06427	0.94525
C	7.55118	-1.94189	-0.02602
C	7.48823	0.22601	1.37763
N	8.99386	-1.85308	0.26013
H	7.16872	-2.97159	0.04264
C	8.8542	-0.17579	2.02863
C	9.28821	-1.60817	1.67128
H	9.62652	0.52634	1.69993

H	10.36792	-1.7158	1.823
H	9.4632	-2.69454	-0.06313
H	6.57393	-1.64131	1.86634
H	7.38105	-1.60833	-1.05894
H	8.80121	-2.33556	2.34863
H	8.78502	-0.08521	3.11959
H	6.87129	0.68589	2.16011
C	7.61412	1.27401	0.27451
C	6.81114	2.4238	0.31552
C	8.51362	1.13723	-0.79715
C	6.88566	3.40746	-0.67274
H	6.11543	2.56127	1.14062
C	8.60224	2.10962	-1.79334
H	9.14786	0.25554	-0.84016
C	7.78469	3.23156	-1.71631
H	6.26724	4.2986	-0.6386
H	9.29488	2.00908	-2.6231
F	7.87015	4.17675	-2.67829
²TS-Hm			
Fe	-3.97183	0.2975	0.1852
O	-2.34933	-0.2602	0.40061
S	-6.19196	1.26454	0.21722
H	-6.62418	0.7366	1.38433
N	-4.30902	-0.63144	-1.56545
C	-4.55252	-1.11161	-3.81476
C	-4.91728	-2.22631	-3.12529
H	-4.53721	-0.95401	-4.88575
H	-5.26527	-3.1755	-3.51256
N	-4.64369	-1.3128	1.21025
C	-5.02809	-2.50767	0.6683
C	-5.36647	-3.44769	1.71227
C	-5.17259	-2.80212	2.89442
H	-5.70451	-4.46234	1.54406
H	-5.31738	-3.17595	3.90009
N	-3.73432	1.27304	1.95242
C	-3.92511	0.77702	3.2162
C	-3.25088	2.54342	2.1117
C	-3.56575	1.77058	4.20334
C	-3.14425	2.86633	3.51765
H	-3.63202	1.62816	5.27453
H	-2.79342	3.81331	3.90786
N	-3.4483	1.95405	-0.83152
C	-2.71749	4.09006	-1.32255
H	-2.36594	5.09935	-1.15008
C	-3.02659	3.13933	-0.28084
C	-4.18134	-0.12167	-2.83135
C	-4.77176	-1.91408	-1.72278
C	-4.71551	-1.47106	2.56816
C	-2.91623	3.40831	1.07748
H	-2.55333	4.39354	1.35532
C	-3.75706	1.16965	-3.13073

H	-3.70019	1.44782	-4.17896
C	-5.09162	-2.7886	-0.69256
H	-5.4357	-3.779	-0.9761
C	-4.3898	-0.49788	3.50764
H	-4.49604	-0.76285	4.55548
C	-2.96318	3.46964	-2.50847
H	-2.85471	3.86248	-3.51144
C	-3.4164	2.13657	-2.19124
C	1.20378	-0.94895	-1.05121
C	0.58206	-2.14119	-1.40491
C	1.22609	-3.36094	-1.27235
C	2.52998	-3.33141	-0.77178
C	3.15833	-2.12193	-0.41463
C	2.49354	-0.88858	-0.54855
C	-0.88703	-0.49975	-1.6337
H	0.74235	-4.29237	-1.5441
H	3.09171	-4.25	-0.64171
H	2.94235	0.05823	-0.28003
H	-1.3682	0.00649	-2.47578
H	-1.67405	-0.37439	-0.63303
O	0.34503	0.08661	-1.29797
O	-0.67524	-1.86091	-1.88001
O	4.42876	-2.24739	0.06313
C	5.13757	-1.06995	0.45535
H	5.19601	-0.36975	-0.388
H	4.60143	-0.57243	1.27689
C	6.53224	-1.49522	0.90382
C	7.30545	-2.17486	-0.24765
C	7.31883	-0.32163	1.55762
N	8.75755	-2.1452	-0.00705
H	6.91556	-3.19832	-0.36021
C	8.7037	-0.84959	2.06087
C	9.10678	-2.18546	1.41238
H	9.47074	-0.10004	1.84371
H	10.18984	-2.32581	1.4981
H	9.20724	-2.90569	-0.50931
H	6.38704	-2.24005	1.698
H	7.09893	-1.65135	-1.1912
H	8.63598	-3.03012	1.95086
H	8.67869	-0.97394	3.15027
H	6.73717	-0.02703	2.44013
C	7.41312	0.92661	0.68365
C	6.64438	2.05567	1.00436
C	8.24982	0.99778	-0.44399
C	6.69096	3.21906	0.2336
H	5.9999	2.03349	1.88062
C	8.30893	2.15136	-1.22593
H	8.86041	0.13543	-0.69956
C	7.52621	3.24591	-0.87544
H	6.1001	4.0939	0.48497
H	8.95328	2.2126	-2.09737
F	7.58378	4.36536	-1.62956

⁴TS-Hm

Fe	-3.9846	0.29706	0.28765
O	-2.38891	-0.33874	0.18214
S	-6.17836	1.17106	0.16226
H	-5.87827	2.47153	0.37782
N	-4.80105	-1.3037	-0.63134
C	-5.52894	-2.79027	-2.23815
C	-5.68472	-3.3951	-1.02902
H	-5.76136	-3.17769	-3.22199
H	-6.07274	-4.38231	-0.81241
N	-4.26351	-0.56181	2.06181
C	-4.74955	-1.82346	2.29915
C	-4.77895	-2.08437	3.72002
C	-4.32285	-0.96165	4.3354
H	-5.11903	-3.00976	4.16736
H	-4.20732	-0.77085	5.39481
N	-3.35189	1.98585	1.1843
C	-3.2168	2.19115	2.53076
C	-2.86774	3.11723	0.57149
C	-2.65967	3.49863	2.78165
C	-2.43982	4.07116	1.5667
H	-2.46086	3.90417	3.76558
H	-2.02423	5.04599	1.34478
N	-3.73315	1.19798	-1.54063
C	-3.14987	2.68931	-3.19884
H	-2.77118	3.59737	-3.65087
C	-3.1972	2.43532	-1.77807
C	-4.9673	-1.48538	-1.98341
C	-5.2202	-2.4595	-0.03297
C	-4.00775	-0.01236	3.29252
C	-2.78556	3.33095	-0.79726
H	-2.37772	4.2811	-1.12841
C	-4.61896	-0.58072	-2.97603
H	-4.80859	-0.87423	-4.00396
C	-5.19396	-2.71249	1.33399
H	-5.56039	-3.67695	1.67148
C	-3.53143	1.26863	3.52133
H	-3.37687	1.56934	4.55287
C	-3.67803	1.5922	-3.81123
H	-3.82212	1.41441	-4.86953
C	-4.04412	0.66711	-2.76431
C	1.20244	-0.84023	-1.186
C	0.58638	-2.00434	-1.63749
C	1.21217	-3.23851	-1.54265
C	2.49079	-3.25286	-0.98326
C	3.11548	-2.0715	-0.53201
C	2.46968	-0.82545	-0.62342
C	-0.85361	-0.33112	-1.85008
H	0.73213	-4.14689	-1.88873
H	3.0382	-4.18354	-0.88097
H	2.91545	0.09887	-0.28151

H	-1.25685	0.21949	-2.70238
H	-1.72055	-0.27396	-0.84376
O	0.37024	0.21691	-1.41057
O	-0.63816	-1.68557	-2.15907
O	4.36274	-2.24008	-0.01086
C	5.08907	-1.08931	0.42717
H	5.17121	-0.36568	-0.39403
H	4.55207	-0.60671	1.25695
C	6.46951	-1.55482	0.87901
C	7.23608	-2.23175	-0.27846
C	7.27781	-0.41039	1.55797
N	8.68617	-2.2431	-0.02462
H	6.82209	-3.24281	-0.41376
C	8.64575	-0.97929	2.06323
C	9.02171	-2.31427	1.39696
H	9.43217	-0.24516	1.86345
H	10.1002	-2.48264	1.4896
H	9.12107	-3.00671	-0.53508
H	6.30196	-2.30972	1.65915
H	7.05111	-1.68564	-1.21366
H	8.52558	-3.15536	1.91803
H	8.60927	-1.11986	3.15032
H	6.69623	-0.11576	2.44057
C	7.4094	0.84844	0.70404
C	6.66257	1.98971	1.03321
C	8.25955	0.91711	-0.41365
C	6.74334	3.16267	0.27998
H	6.00823	1.96952	1.90218
C	8.35276	2.08015	-1.17806
H	8.85315	0.04482	-0.67552
C	7.59082	3.18676	-0.81983
H	6.16956	4.0469	0.53799
H	9.00756	2.13934	-2.04182
F	7.68125	4.31533	-1.55688
²INTm			
Fe	4.07342	0.22675	-0.29685
O	3.54192	0.15934	1.39539
S	4.83952	0.40188	-2.48619
H	4.93535	-0.91838	-2.75882
N	3.92556	-1.77338	-0.50743
C	4.3655	-4.03187	-0.38378
C	3.09607	-3.89472	-0.85713
H	4.92028	-4.94152	-0.19189
H	2.39112	-4.66831	-1.13408
N	2.16138	0.42737	-0.92559
C	1.30953	-0.58009	-1.30849
C	0.05573	-0.02179	-1.75011
C	0.16761	1.33131	-1.64662
H	-0.7871	-0.60676	-2.09508
H	-0.56271	2.09113	-1.89445
N	4.27387	2.22993	-0.26793

C	3.30709	3.15834	-0.55911
C	5.38129	2.93369	0.13268
C	3.82749	4.48822	-0.35935
C	5.11251	4.3489	0.06778
H	3.26505	5.3985	-0.52366
H	5.82512	5.12105	0.32835
N	5.96537	0.02124	0.37155
C	8.08847	0.4738	1.14413
H	8.9425	1.06063	1.45755
C	6.83602	1.02923	0.68753
C	4.87399	-2.70208	-0.15696
C	2.82268	-2.48058	-0.91745
C	1.49098	1.60562	-1.14581
C	6.57721	2.38676	0.57442
H	7.36685	3.07436	0.85981
C	6.13334	-2.42491	0.35576
H	6.77808	-3.26822	0.58166
C	1.60576	-1.93513	-1.30281
H	0.82542	-2.62078	-1.61677
C	2.01048	2.87885	-0.96648
H	1.35781	3.72079	-1.17372
C	7.96149	-0.87936	1.08901
H	8.68957	-1.63802	1.34661
C	6.63204	-1.15333	0.59564
C	-1.23692	-0.68235	1.71528
C	-0.62414	-1.8674	2.09646
C	-1.21947	-3.09793	1.86926
C	-2.46771	-3.0844	1.24098
C	-3.08859	-1.88048	0.85575
C	-2.47332	-0.63632	1.08954
C	0.75243	-0.2034	2.54372
H	-0.74217	-4.02496	2.16653
H	-2.99118	-4.01154	1.03403
H	-2.91907	0.30726	0.80505
H	1.18234	0.30109	3.40772
H	2.55876	0.09707	1.45067
O	-0.42395	0.36544	2.06547
O	0.57957	-1.56984	2.69477
O	-4.30067	-2.02255	0.24609
C	-5.00518	-0.85367	-0.17597
H	-5.19319	-0.19748	0.68397
H	-4.39758	-0.2966	-0.90474
C	-6.31524	-1.3087	-0.81104
C	-7.19275	-2.07401	0.20317
C	-7.07017	-0.13805	-1.50493
N	-8.60047	-2.10583	-0.22786
H	-6.76601	-3.08072	0.33053
C	-8.34859	-0.7029	-2.21057
C	-8.76013	-2.08834	-1.68129
H	-9.17602	-0.00224	-2.06305
H	-9.8138	-2.27522	-1.91556
H	-9.06859	-2.91265	0.1754

H	-6.04142	-2.00708	-1.61336
H	-7.14035	-1.58027	1.1833
H	-8.17881	-2.88061	-2.19042
H	-8.1758	-0.76998	-3.29153
H	-6.39604	0.23133	-2.2881
C	-7.34482	1.05521	-0.59276
C	-6.60162	2.23445	-0.75258
C	-8.32675	1.02648	0.413
C	-6.81266	3.35116	0.05873
H	-5.84686	2.28994	-1.53422
C	-8.55122	2.13215	1.23327
H	-8.91915	0.12416	0.54148
C	-7.78843	3.27929	1.0442
H	-6.24185	4.26527	-0.06888
H	-9.30833	2.11618	2.01096
F	-8.00537	4.35252	1.83516
⁴INTm			
Fe	-4.11435	0.22754	0.29496
O	-3.55524	0.16089	-1.39283
S	-4.83587	0.39704	2.49456
H	-4.89121	-0.9229	2.77936
N	-3.96556	-1.77415	0.50067
C	-4.40723	-4.03181	0.37171
C	-3.13587	-3.89707	0.84051
H	-4.96331	-4.94038	0.17861
H	-2.43031	-4.67206	1.11185
N	-2.19076	0.42243	0.92151
C	-1.3397	-0.58782	1.29473
C	-0.08116	-0.03409	1.73007
C	-0.19125	1.31957	1.63281
H	0.76318	-0.62205	2.06605
H	0.54244	2.07703	1.87774
N	-4.30683	2.22981	0.27287
C	-3.33525	3.15438	0.56601
C	-5.4115	2.93901	-0.12408
C	-3.85224	4.48637	0.37193
C	-5.13827	4.35297	-0.05392
H	-3.28648	5.39419	0.53836
H	-5.8485	5.1284	-0.31114
N	-5.99649	0.02829	-0.37444
C	-8.11995	0.48654	-1.14345
H	-8.9733	1.07545	-1.45478
C	-6.86709	1.03922	-0.68695
C	-4.91483	-2.70084	0.15038
C	-2.86061	-2.48339	0.90398
C	-1.51775	1.59772	1.14141
C	-6.60837	2.39584	-0.56822
H	-7.39754	3.08501	-0.85089
C	-6.17405	-2.41898	-0.36077
H	-6.82213	-3.25942	-0.58765
C	-1.64069	-1.94208	1.28512

H	-0.86048	-2.63137	1.59135
C	-2.03798	2.87201	0.96783
H	-1.38391	3.71308	1.17421
C	-7.99559	-0.86711	-1.09096
H	-8.72568	-1.6236	-1.34916
C	-6.66726	-1.14566	-0.5993
C	1.27957	-0.69143	-1.72548
C	0.66745	-1.8798	-2.09875
C	1.26012	-3.10834	-1.85515
C	2.50486	-3.09087	-1.2191
C	3.12479	-1.88439	-0.84249
C	2.51214	-0.64182	-1.09209
C	-0.70556	-0.21737	-2.57181
H	0.78371	-4.03769	-2.14672
H	3.0256	-4.0168	-1.00011
H	2.95803	0.30395	-0.815
H	-1.11828	0.27596	-3.45077
H	-2.5751	0.10033	-1.43435
O	0.47222	0.35427	-2.0914
O	-0.53142	-1.58807	-2.70836
O	4.33404	-2.02144	-0.22462
C	5.03799	-0.84913	0.18734
H	5.22703	-0.20036	-0.67802
H	4.43005	-0.28522	0.91066
C	6.34762	-1.29892	0.82723
C	7.22648	-2.07073	-0.18079
C	7.10149	-0.12354	1.51422
N	8.63382	-2.09954	0.25199
H	6.80006	-3.07829	-0.30206
C	8.37961	-0.68318	2.22466
C	8.79173	-2.07218	1.70542
H	9.20706	0.01652	2.07272
H	9.84511	-2.25747	1.94229
H	9.10227	-2.90921	-0.14513
H	6.07302	-1.99202	1.63388
H	7.17512	-1.58338	-1.16415
H	8.20974	-2.86092	2.21928
H	8.20615	-0.74265	3.30597
H	6.42648	0.2506	2.29434
C	7.37647	1.06391	0.59463
C	6.63258	2.24379	0.74605
C	8.35933	1.02912	-0.41004
C	6.84381	3.35531	-0.07232
H	5.87697	2.30388	1.52653
C	8.58399	2.12952	-1.23731
H	8.95234	0.12631	-0.53219
C	7.82049	3.27749	-1.05642
H	6.27235	4.26991	0.04872
H	9.34174	2.10881	-2.01428
F	8.03765	4.3457	-1.85419

⁴TS-reb m

Fe	4.11594	0.26919	0.14875
O	2.16474	0.32045	0.01175
S	6.39455	0.16852	0.3585
H	6.65881	1.49331	0.28472
N	3.92267	-1.04846	1.66474
C	3.72662	-1.92441	3.79083
C	3.78597	-2.97531	2.92916
H	3.63767	-1.94004	4.87012
H	3.75857	-4.03474	3.15292
N	4.15733	-1.29949	-1.14639
C	4.13378	-2.63734	-0.84526
C	4.26362	-3.41944	-2.05282
C	4.37552	-2.53505	-3.08342
H	4.27796	-4.50191	-2.08944
H	4.49904	-2.74307	-4.13918
N	4.2375	1.58695	-1.38754
C	4.36747	1.25969	-2.71328
C	4.26838	2.95687	-1.32483
C	4.47391	2.46054	-3.51176
C	4.41287	3.51316	-2.65046
H	4.58706	2.47662	-4.58881
H	4.46345	4.57165	-2.87383
N	4.0014	1.83461	1.4182
C	3.96195	3.95371	2.33577
H	3.98065	5.03578	2.37592
C	4.05411	3.17211	1.12282
C	3.816	-0.72265	2.98831
C	3.91035	-2.41483	1.6009
C	4.31485	-1.21161	-2.50558
C	4.17928	3.70538	-0.1555
H	4.2145	4.78685	-0.2478
C	3.79192	0.56566	3.51039
H	3.70172	0.65975	4.58877
C	4.00878	-3.16561	0.43502
H	4.00311	-4.24744	0.53251
C	4.39475	-0.02919	-3.23604
H	4.51382	-0.12161	-4.3119
C	3.85382	3.06784	3.36316
H	3.76681	3.27239	4.42306
C	3.88009	1.74457	2.77918
C	-1.36676	-1.36553	-0.89734
C	-0.71906	-2.46361	-0.37549
C	-1.39921	-3.49438	0.25508
C	-2.78022	-3.34148	0.32711
C	-3.44727	-2.21047	-0.20681
C	-2.73748	-1.17779	-0.84701
C	0.77564	-1.14557	-1.25024
H	-0.89092	-4.35703	0.66918
H	-3.39131	-4.0972	0.8081
H	-3.20898	-0.29795	-1.26271
H	1.94583	1.24349	-0.20354
O	-0.38655	-0.55176	-1.46089

O	0.64102	-2.29215	-0.62995
O	-4.79069	-2.21679	-0.05232
C	-5.55397	-1.09547	-0.52435
H	-5.19586	-0.17934	-0.03886
H	-5.41431	-0.99194	-1.6097
C	-7.01898	-1.35638	-0.19468
C	-7.23957	-1.48124	1.32962
C	-7.95597	-0.30726	-0.86281
N	-8.64469	-1.23293	1.68374
H	-6.89293	-2.47887	1.64269
C	-9.44384	-0.68581	-0.5575
C	-9.58499	-1.64111	0.6412
H	-10.00957	0.22913	-0.35808
H	-10.59993	-1.57706	1.04758
H	-8.86583	-1.68291	2.56758
H	-7.27146	-2.32198	-0.653
H	-6.61382	-0.74715	1.85584
H	-9.442	-2.68909	0.31504
H	-9.8943	-1.15284	-1.44154
H	-7.8037	-0.4149	-1.94427
C	-7.60162	1.14103	-0.53208
C	-6.98468	1.9422	-1.50499
C	-7.86874	1.71586	0.72278
C	-6.63296	3.26879	-1.24758
H	-6.7836	1.52936	-2.49145
C	-7.52474	3.03933	0.9977
H	-8.35553	1.11039	1.48306
C	-6.90929	3.79677	0.00698
H	-6.16211	3.89108	-2.00171
H	-7.72945	3.48861	1.96432
F	-6.57615	5.07792	0.26884
H	1.58865	-1.0999	-2.02113
²P-OHm			
Fe	-4.38385	0.38487	0.09935
O	-1.52255	-1.00397	0.27279
S	-6.57244	0.74879	-0.05831
H	-6.52015	1.80979	-0.8965
N	-4.49758	-1.61224	-0.19568
C	-4.90594	-3.64222	-1.23604
C	-4.98403	-3.85825	0.10698
H	-5.02965	-4.3553	-2.04102
H	-5.18737	-4.78395	0.62989
N	-4.42862	0.04472	2.07436
C	-4.64208	-1.14801	2.72952
C	-4.72962	-0.93567	4.15291
C	-4.58339	0.40051	4.35804
H	-4.88356	-1.71938	4.88353
H	-4.589	0.94498	5.29367
N	-3.87707	2.28792	0.42195
C	-3.92327	2.94698	1.62969
C	-3.55516	3.2512	-0.50992

C	-3.62056	4.34527	1.45305
C	-3.38577	4.53284	0.12601
H	-3.58513	5.07247	2.25419
H	-3.12036	5.44617	-0.39088
N	-3.97585	0.63945	-1.8482
C	-3.56229	1.59786	-3.91737
H	-3.30546	2.36121	-4.64068
C	-3.64052	1.81049	-2.49537
C	-4.61175	-2.24678	-1.41977
C	-4.74671	-2.5936	0.74749
C	-4.39661	1.00291	3.06071
C	-3.43292	3.03179	-1.87271
H	-3.17494	3.87984	-2.49932
C	-4.43814	-1.63783	-2.65249
H	-4.53315	-2.26206	-3.5355
C	-4.78715	-2.38291	2.11675
H	-4.97309	-3.24237	2.75309
C	-4.1792	2.35632	2.85732
H	-4.17841	2.99999	3.73151
C	-3.86951	0.28976	-4.13635
H	-3.91356	-0.24467	-5.07674
C	-4.12549	-0.30037	-2.84711
C	1.3928	-1.24287	-0.55845
C	0.87489	-2.45757	-0.98459
C	1.6583	-3.59585	-1.02446
C	2.99616	-3.46831	-0.62502
C	3.51545	-2.23787	-0.19837
C	2.7069	-1.0835	-0.15596
C	-0.79441	-0.96574	-0.90371
H	1.25768	-4.54786	-1.35584
H	3.66002	-4.32613	-0.63713
H	3.07274	-0.11909	0.17115
H	-1.33345	-0.46447	-1.71132
H	-2.39942	-1.39519	0.08603
O	0.4147	-0.27883	-0.63072
O	-0.44441	-2.28393	-1.3493
O	4.83445	-2.25119	0.17196
C	5.45101	-1.02768	0.56299
H	5.36537	-0.28592	-0.24253
H	4.94874	-0.62045	1.45374
C	6.91543	-1.32755	0.87009
C	7.63994	-1.89874	-0.36811
C	7.65166	-0.10664	1.4932
N	9.10121	-1.75237	-0.2478
H	7.32879	-2.94735	-0.48928
C	9.11285	-0.52737	1.86533
C	9.57314	-1.8021	1.13552
H	9.79404	0.29315	1.61962
H	10.66778	-1.84795	1.12614
H	9.56692	-2.45894	-0.81064
H	6.91428	-2.10513	1.6459
H	7.31025	-1.36395	-1.26931

H	9.22493	-2.70067	1.67974
H	9.18698	-0.68951	2.94763
H	7.12324	0.11722	2.42854
C	7.57212	1.16579	0.65283
C	6.73089	2.21282	1.05831
C	8.31901	1.33991	-0.5253
C	6.62222	3.39447	0.32232
H	6.15111	2.11064	1.97315
C	8.22365	2.51349	-1.27333
H	8.9809	0.54011	-0.84782
C	7.37412	3.52424	-0.83781
H	5.97427	4.20564	0.63844
H	8.79838	2.6534	-2.18356
F	7.28123	4.66379	-1.5588
⁴P-OHm			
Fe	-4.49522	0.38284	0.06955
O	-1.4584	-1.06851	0.35863
S	-6.87208	0.73368	-0.11386
H	-6.81252	1.38559	-1.29738
N	-4.45931	-1.63202	-0.21831
C	-4.7275	-3.68861	-1.24786
C	-4.89414	-3.88487	0.09033
H	-4.77244	-4.41769	-2.04654
H	-5.10524	-4.80809	0.61444
N	-4.5311	0.05338	2.05084
C	-4.77001	-1.14062	2.69528
C	-4.88253	-0.93005	4.11421
C	-4.70704	0.40311	4.32993
H	-5.06535	-1.71294	4.83898
H	-4.71532	0.9418	5.26872
N	-3.94873	2.29065	0.4156
C	-3.97705	2.94592	1.62556
C	-3.66093	3.25626	-0.52178
C	-3.69227	4.34638	1.44527
C	-3.49449	4.53891	0.11275
H	-3.65001	5.073	2.24642
H	-3.2566	5.45685	-0.40928
N	-3.99885	0.62452	-1.86553
C	-3.57608	1.59681	-3.9211
H	-3.3454	2.37114	-4.64148
C	-3.70975	1.81202	-2.50617
C	-4.47217	-2.28739	-1.43672
C	-4.7426	-2.60404	0.72376
C	-4.48582	1.0076	3.04331
C	-3.55386	3.04263	-1.88642
H	-3.32459	3.89704	-2.51498
C	-4.27343	-1.68643	-2.66866
H	-4.29111	-2.32251	-3.5476
C	-4.87833	-2.38071	2.08393
H	-5.08535	-3.23739	2.71694
C	-4.23655	2.35735	2.85223

H	-4.22956	2.99648	3.7292
C	-3.78472	0.26779	-4.14125
H	-3.75905	-0.27263	-5.07878
C	-4.04366	-0.33189	-2.86074
C	1.46585	-1.27539	-0.48739
C	0.95898	-2.49236	-0.92035
C	1.75712	-3.61974	-0.97866
C	3.09753	-3.47844	-0.59209
C	3.60523	-2.24546	-0.15915
C	2.78191	-1.10255	-0.09704
C	-0.72987	-1.01971	-0.81321
H	1.36572	-4.57394	-1.31478
H	3.77233	-4.32733	-0.61973
H	3.13827	-0.13656	0.23577
H	-1.27123	-0.52017	-1.62092
H	-2.36354	-1.37475	0.15378
O	0.47483	-0.32407	-0.53741
O	-0.36572	-2.33286	-1.26849
O	4.92836	-2.24416	0.19708
C	5.53329	-1.01471	0.58754
H	5.42658	-0.26929	-0.21208
H	5.03749	-0.61982	1.48747
C	7.00573	-1.29569	0.87332
C	7.72046	-1.85352	-0.3765
C	7.73424	-0.06648	1.48927
N	9.18132	-1.68969	-0.27521
H	7.42049	-2.90536	-0.49752
C	9.20604	-0.46847	1.83989
C	9.67231	-1.73603	1.10158
H	9.87288	0.36121	1.58574
H	10.76722	-1.76825	1.07749
H	9.64813	-2.38944	-0.8456
H	7.02609	-2.07528	1.64684
H	7.37205	-1.31944	-1.27107
H	9.34261	-2.63976	1.64885
H	9.29777	-0.6311	2.92077
H	7.21614	0.14819	2.4325
C	7.62613	1.20667	0.65317
C	6.77719	2.24175	1.07307
C	8.35359	1.39307	-0.53524
C	6.64224	3.42327	0.34128
H	6.21208	2.13026	1.99595
C	8.23178	2.5667	-1.27935
H	9.02149	0.60289	-0.86889
C	7.37528	3.5652	-0.82946
H	5.98839	4.22525	0.66854
H	8.79142	2.71601	-2.19745
F	7.25671	4.70473	-1.54671
Secondary amine hydroxylation by HAT mechanism			
² RC			
Fe	3.10556	-0.37376	-0.29726

O	2.37028	0.36343	0.95536
S	4.36472	-1.81074	-2.00804
H	5.57568	-1.22035	-1.88866
N	4.42715	-1.35139	0.88562
C	6.21776	-1.80844	2.2777
C	5.34343	-2.8434	2.39648
H	7.17051	-1.67024	2.77254
H	5.43012	-3.73243	3.0078
N	1.89685	-1.99147	-0.24598
C	2.03067	-3.09699	0.55349
C	0.89616	-3.97453	0.39157
C	0.07214	-3.38675	-0.51732
H	0.76827	-4.91585	0.91042
H	-0.87987	-3.73606	-0.89535
N	1.93478	0.44927	-1.71074
C	0.74247	-0.03304	-2.1783
C	2.12143	1.65502	-2.33388
C	0.15946	0.8899	-3.12164
C	1.01814	1.94134	-3.21791
H	-0.78161	0.73641	-3.63371
H	0.93037	2.83204	-3.82655
N	4.45439	1.10238	-0.5568
C	5.42968	3.10943	-1.15735
H	5.54973	4.06033	-1.66036
C	4.30087	2.22767	-1.32606
C	5.63508	-0.87422	1.34601
C	4.22522	-2.54882	1.53451
C	0.70165	-2.14718	-0.90432
C	3.21953	2.48747	-2.15691
H	3.23319	3.4186	-2.7152
C	6.20063	0.3376	0.98584
H	7.15656	0.59325	1.43279
C	3.1068	-3.35414	1.39392
H	3.07605	-4.27026	1.97566
C	0.16449	-1.24336	-1.80825
H	-0.79189	-1.49595	-2.25531
C	6.26693	2.50558	-0.27014
H	7.21841	2.85693	0.10796
C	5.64675	1.25636	0.09866
C	-6.2184	-2.45954	-0.37662
C	-5.81991	-3.78678	-0.46701
C	-4.59728	-4.20308	0.02617
C	-3.77599	-3.23001	0.61495
C	-4.18045	-1.88924	0.70215
C	-5.43304	-1.47649	0.20035
C	-7.77224	-3.5766	-1.52548
H	-4.28846	-5.24134	-0.03317
H	-2.80584	-3.49518	1.02148
H	-5.77842	-0.4525	0.25521
H	-7.6855	-3.47328	-2.61769
H	-8.78049	-3.89138	-1.24264
O	-7.47856	-2.31653	-0.90774

O	-6.82312	-4.53421	-1.05493
O	-3.28726	-1.04322	1.29441
C	-3.62389	0.33759	1.43399
H	-3.85398	0.77021	0.45122
H	-4.5173	0.43952	2.06881
C	-2.42716	1.04204	2.06572
C	-1.17872	0.93952	1.16349
C	-2.75317	2.50674	2.47725
N	-0.18127	1.96978	1.493
H	-0.76942	-0.07732	1.25636
C	-1.50538	3.11929	3.19757
C	-0.20696	2.34508	2.90399
H	-1.38579	4.1599	2.87943
H	0.65907	2.98434	3.10767
H	0.74347	1.62289	1.23753
H	-2.21465	0.50785	3.00161
H	-1.4761	1.06581	0.1127
H	-0.12024	1.4764	3.58521
H	-1.6778	3.13598	4.28109
H	-3.56448	2.44265	3.21397
C	-3.2921	3.36628	1.33619
C	-4.65415	3.70094	1.30212
C	-2.46946	3.84668	0.30179
C	-5.19435	4.481	0.27722
H	-5.31051	3.3535	2.09721
C	-2.99175	4.62737	-0.72959
H	-1.41058	3.59863	0.32059
C	-4.34829	4.93223	-0.72688
H	-6.24706	4.74411	0.25435
H	-2.36174	5.00252	-1.53027
F	-4.85593	5.69101	-1.72538
⁴RC			
Fe	-3.13009	-0.37194	0.29091
O	-2.37171	0.41306	-0.92037
S	-4.37173	-1.8195	1.98865
H	-5.59426	-1.25672	1.85495
N	-4.41725	-1.35533	-0.91363
C	-6.192	-1.83849	-2.31752
C	-5.30245	-2.86105	-2.42989
H	-7.14313	-1.71377	-2.81901
H	-5.37223	-3.75126	-3.04164
N	-1.89369	-1.96615	0.24268
C	-2.00231	-3.07132	-0.56068
C	-0.85759	-3.9332	-0.38824
C	-0.05283	-3.33666	0.53214
H	-0.71034	-4.87102	-0.90829
H	0.89966	-3.67371	0.91996
N	-1.98697	0.4617	1.72873
C	-0.79087	-0.00203	2.20285
C	-2.20107	1.65909	2.35777
C	-0.23211	0.9248	3.15748

C	-1.11083	1.95945	3.25388
H	0.70748	0.78502	3.67614
H	-1.04432	2.84761	3.86889
N	-4.50366	1.0849	0.54408
C	-5.51614	3.07216	1.14936
H	-5.65697	4.01643	1.65941
C	-4.37732	2.20477	1.32651
C	-5.62998	-0.89631	-1.38151
C	-4.19482	-2.55098	-1.56016
C	-0.70433	-2.10756	0.91604
C	-3.31207	2.47325	2.17519
H	-3.34868	3.39885	2.74163
C	-6.21739	0.30605	-1.02513
H	-7.17204	0.54854	-1.48204
C	-3.06633	-3.34063	-1.41276
H	-3.0181	-4.25489	-1.9962
C	-0.19066	-1.20121	1.83085
H	0.7645	-1.44266	2.28669
C	-6.3316	2.46537	0.24411
H	-7.28238	2.80679	-0.14469
C	-5.68855	1.2282	-0.12621
C	6.23246	-2.46879	0.38988
C	5.83052	-3.79476	0.48376
C	4.60618	-4.20887	-0.00698
C	3.78682	-3.23488	-0.597
C	4.19468	-1.89539	-0.68757
C	5.44903	-1.48492	-0.18829
C	7.78505	-3.58755	1.53892
H	4.29458	-5.24612	0.05512
H	2.81555	-3.49833	-1.00194
H	5.79708	-0.46197	-0.2457
H	7.70083	-3.48179	2.63108
H	8.79186	-3.90566	1.25466
O	7.49357	-2.32793	0.91922
O	6.83236	-4.54353	1.07224
O	3.30287	-1.04818	-1.28027
C	3.64448	0.33078	-1.42581
H	3.87805	0.76637	-0.44519
H	4.53712	0.42673	-2.06263
C	2.44943	1.03763	-2.05802
C	1.20219	0.94422	-1.15289
C	2.78151	2.49894	-2.47674
N	0.21067	1.98001	-1.48234
H	0.78693	-0.07055	-1.24313
C	1.535	3.11486	-3.19639
C	0.23327	2.34931	-2.89496
H	1.42215	4.15764	-2.88295
H	-0.62987	2.99259	-3.0982
H	-0.71546	1.6417	-1.22129
H	2.23263	0.50043	-2.99121
H	1.5025	1.07038	-0.10287
H	0.13926	1.47827	-3.57232

H	1.70428	3.12537	-4.28048
H	3.59038	2.42729	-3.21546
C	3.32825	3.36082	-1.34119
C	4.69212	3.68849	-1.31254
C	2.51107	3.85034	-0.30674
C	5.23929	4.47045	-0.2928
H	5.34437	3.33394	-2.1079
C	3.04033	4.63305	0.71955
H	1.45086	3.60771	-0.32156
C	4.39845	4.93074	0.71158
H	6.29341	4.72817	-0.2741
H	2.41455	5.01524	1.5202
F	4.91292	5.69147	1.70507
²TS_H			
Fe	3.22086	-0.43723	-0.30346
O	2.01858	-0.68187	0.87511
S	4.9158	-0.14731	-1.97097
H	5.81301	0.50177	-1.19551
N	4.6779	-0.95305	0.99313
C	6.24961	-0.89928	2.68059
C	6.14782	-2.19113	2.26719
H	6.88596	-0.48442	3.45206
H	6.68175	-3.06061	2.62907
N	3.08383	-2.35057	-0.93324
C	3.78985	-3.41764	-0.44692
C	3.37668	-4.63133	-1.11442
C	2.41146	-4.27939	-2.0048
H	3.78507	-5.61343	-0.91268
H	1.86106	-4.91081	-2.6907
N	1.86864	0.10465	-1.70975
C	1.19117	-0.72539	-2.56495
C	1.43103	1.37358	-1.97387
C	0.29432	0.04381	-3.39343
C	0.44562	1.34783	-3.02944
H	-0.34905	-0.37384	-4.15748
H	-0.044	2.22316	-3.43791
N	3.4576	1.50438	0.22398
C	3.20239	3.79066	0.37171
H	2.83265	4.78111	0.13747
C	2.79363	2.58013	-0.30085
C	5.32471	-0.13209	1.8786
C	5.15821	-2.21542	1.21476
C	2.23681	-2.84959	-1.88465
C	1.84425	2.52751	-1.31586
H	1.40797	3.46827	-1.63836
C	5.14131	1.23991	1.98919
H	5.73168	1.76489	2.73393
C	4.7558	-3.36423	0.54731
H	5.23128	-4.29788	0.83137
C	1.34783	-2.10252	-2.64595
H	0.74106	-2.63349	-3.37282

C	4.12061	3.42716	1.31068
H	4.65979	4.05731	2.00678
C	4.27519	1.99576	1.2095
C	-6.93132	-2.09945	0.3004
C	-6.82684	-3.47463	0.46448
C	-5.67514	-4.05267	0.9648
C	-4.61641	-3.19448	1.29626
C	-4.72636	-1.80821	1.12887
C	-5.90606	-1.22625	0.62063
C	-8.78719	-3.0399	-0.50844
H	-5.59261	-5.12587	1.09778
H	-3.68622	-3.59164	1.68796
H	-6.0244	-0.15979	0.47974
H	-8.79115	-3.16765	-1.60113
H	-9.8047	-3.0625	-0.10886
O	-8.17816	-1.78252	-0.1826
O	-8.01333	-4.07715	0.09576
O	-3.62097	-1.08048	1.49047
C	-3.64745	0.33295	1.33222
H	-3.85284	0.59646	0.28596
H	-4.44407	0.77047	1.95241
C	-2.28208	0.8602	1.76817
C	-1.16643	0.32137	0.86343
C	-2.24737	2.41679	1.89689
N	0.13854	0.86928	1.16349
H	-1.10893	-0.77393	0.94559
C	-0.7887	2.89805	2.19399
C	0.23269	1.74803	2.30252
H	-0.44897	3.56959	1.40032
H	1.25395	2.13611	2.35471
H	1.09652	0.17883	0.91477
H	-2.10794	0.46031	2.7759
H	-1.38314	0.51668	-0.19979
H	0.05611	1.17472	3.23046
H	-0.76304	3.47537	3.12459
H	-2.86631	2.65228	2.77079
C	-2.88043	3.1441	0.71473
C	-4.14736	3.73001	0.85313
C	-2.24378	3.2441	-0.53439
C	-4.77263	4.38635	-0.20833
H	-4.65684	3.68108	1.81274
C	-2.85332	3.89285	-1.60811
H	-1.25382	2.82005	-0.67831
C	-4.11263	4.45449	-1.42846
H	-5.75008	4.84452	-0.09849
H	-2.36609	3.97041	-2.57471
F	-4.70339	5.08652	-2.46313
⁴TS_H			
Fe	3.08177	-0.54453	-0.33606
O	2.24425	-0.16561	1.10042
S	4.14374	-1.1263	-2.37663

H	4.6159	0.09507	-2.71256
N	4.72139	-1.03718	0.70987
C	6.72325	-0.9293	1.85277
C	6.28612	-2.21418	1.92994
H	7.62541	-0.49582	2.26547
H	6.75354	-3.0593	2.41922
N	2.48178	-2.46812	-0.32157
C	3.10116	-3.51028	0.31486
C	2.33047	-4.7196	0.15023
C	1.23538	-4.3897	-0.58727
H	2.60735	-5.68502	0.55436
H	0.42514	-5.02782	-0.91649
N	1.44746	-0.05306	-1.46034
C	0.45619	-0.90234	-1.87556
C	1.13773	1.17992	-1.96459
C	-0.51888	-0.17974	-2.65865
C	-0.09654	1.11448	-2.71305
H	-1.39814	-0.62278	-3.10902
H	-0.55771	1.95333	-3.21893
N	3.76398	1.34611	-0.53178
C	3.90115	3.60242	-0.99109
H	3.61948	4.56947	-1.38839
C	3.12292	2.39615	-1.14069
C	5.7401	-0.20087	1.08344
C	5.03599	-2.27323	1.20664
C	1.33566	-2.9785	-0.8745
C	1.90345	2.3296	-1.80289
H	1.5321	3.2453	-2.2533
C	5.83852	1.14458	0.76294
H	6.70667	1.68411	1.12868
C	4.28931	-3.42868	1.02917
H	4.66549	-4.34204	1.47934
C	0.38989	-2.26069	-1.5959
H	-0.46387	-2.80915	-1.98158
C	5.01093	3.26886	-0.27646
H	5.82876	3.90527	0.03701
C	4.91069	1.85914	0.01492
C	-6.74826	-1.84635	-0.10832
C	-6.62653	-3.22807	-0.17842
C	-5.48309	-3.87086	0.25774
C	-4.45319	-3.07133	0.77506
C	-4.57974	-1.6778	0.8427
C	-5.74958	-1.03015	0.3942
C	-8.68312	-2.67898	-0.84895
H	-5.38408	-4.94941	0.20073
H	-3.53497	-3.52067	1.1377
H	-5.8798	0.04354	0.43058
H	-9.1256	-2.65984	-1.84868
H	-9.46025	-2.78427	-0.07743
O	-7.96028	-1.45964	-0.62742
O	-7.76026	-3.76508	-0.7554
O	-3.50538	-1.01226	1.37439

C	-3.54549	0.40832	1.44912
H	-3.70985	0.83864	0.45209
H	-4.37489	0.7302	2.09715
C	-2.21004	0.86845	2.02755
C	-1.04446	0.48155	1.10176
C	-2.19358	2.38802	2.37484
N	0.2089	1.11489	1.45634
H	-0.90514	-0.61141	1.11399
C	-0.80312	2.76389	2.98292
C	0.2707	1.66734	2.78934
H	-0.44336	3.69188	2.52953
H	1.27488	2.0682	2.9526
H	1.23596	0.55811	1.10562
H	-2.08452	0.33115	2.97723
H	-1.26524	0.72959	0.05333
H	0.11889	0.8658	3.53369
H	-0.90103	2.95526	4.05726
H	-2.95117	2.52926	3.15506
C	-2.60455	3.28659	1.21129
C	-3.88728	3.8545	1.19119
C	-1.74119	3.57622	0.14088
C	-4.31105	4.6745	0.1441
H	-4.57042	3.66082	2.01514
C	-2.14647	4.39294	-0.9147
H	-0.73582	3.16459	0.12612
C	-3.42888	4.92956	-0.89792
H	-5.30138	5.11786	0.13227
H	-1.48185	4.6207	-1.74186
F	-3.82278	5.72353	-1.91531
²INT_H			
Fe	3.39154	-0.50984	-0.36172
O	2.53942	-0.14027	1.1411
S	4.4502	-1.08284	-2.3579
H	5.25216	0.00036	-2.45901
N	4.60336	-1.74778	0.66883
C	6.34687	-2.58827	1.91983
C	5.47459	-3.6103	1.7105
H	7.28266	-2.59841	2.46411
H	5.54371	-4.6377	2.0447
N	2.16728	-2.05166	-0.79082
C	2.29276	-3.34124	-0.34122
C	1.18888	-4.13607	-0.81835
C	0.39565	-3.3099	-1.55535
H	1.05447	-5.18921	-0.60663
H	-0.52605	-3.54356	-2.07298
N	2.17089	0.73856	-1.39598
C	1.02409	0.39658	-2.06599
C	2.36919	2.07617	-1.61989
C	0.46819	1.55985	-2.71371
C	1.30132	2.60155	-2.43574
H	-0.43454	1.55814	-3.31137

H	1.2298	3.63079	-2.76474
N	4.6973	0.9982	-0.08715
C	5.65152	3.09559	-0.01443
H	5.76528	4.15788	-0.1897
C	4.53192	2.30766	-0.46734
C	5.79448	-1.427	1.26124
C	4.38997	-3.07745	0.9192
C	1.00933	-2.00556	-1.52695
C	3.45586	2.81832	-1.17837
H	3.47465	3.87538	-1.42407
C	6.39977	-0.17979	1.23634
H	7.34716	-0.06992	1.7542
C	3.31756	-3.82617	0.46012
H	3.28321	-4.87542	0.73541
C	0.47465	-0.87611	-2.1314
H	-0.44404	-0.99816	-2.69632
C	6.48409	2.25081	0.65376
H	7.42314	2.47534	1.14345
C	5.87419	0.94447	0.61557
C	-7.43062	-1.44251	-0.30051
C	-7.51225	-2.82642	-0.38417
C	-6.49373	-3.63501	0.08446
C	-5.3751	-3.00074	0.64442
C	-5.29665	-1.60436	0.72702
C	-6.34182	-0.78719	0.2483
C	-9.30134	-1.96439	-1.40098
H	-6.55729	-4.71612	0.02529
H	-4.54383	-3.5837	1.02605
H	-6.3138	0.29354	0.2963
H	-9.21472	-1.90084	-2.4959
H	-10.34788	-1.91438	-1.08833
O	-8.57693	-0.87816	-0.80673
O	-8.72327	-3.18694	-0.94162
O	-4.15118	-1.11009	1.29461
C	-4.00384	0.29962	1.43203
H	-4.06068	0.78619	0.44881
H	-4.81389	0.70517	2.05714
C	-2.6487	0.55051	2.08647
C	-1.49303	0.05937	1.19189
C	-2.44092	2.03705	2.50476
N	-0.17115	0.49596	1.58825
H	-1.48409	-1.04322	1.17056
C	-1.04197	2.18312	3.18419
C	-0.11357	0.9607	2.95428
H	-0.54189	3.0801	2.80769
H	0.92185	1.21364	3.19935
H	1.59144	0.11886	1.00835
H	-2.64219	-0.0379	3.0136
H	-1.64558	0.36092	0.14629
H	-0.41888	0.14176	3.62906
H	-1.15926	2.31926	4.26516
H	-3.20781	2.25558	3.25782

C	-2.6635	3.02692	1.36494
C	-3.85515	3.76522	1.30713
C	-1.71488	3.23125	0.34812
C	-4.10899	4.67065	0.27544
H	-4.60062	3.63861	2.08909
C	-1.9511	4.12935	-0.69244
H	-0.77272	2.69012	0.36044
C	-3.14788	4.836	-0.71365
H	-5.02848	5.24547	0.23501
H	-1.21907	4.28118	-1.47839
F	-3.37917	5.70873	-1.71746
⁴INT_H			
Fe	3.01895	-0.43907	-0.59739
O	2.1602	0.19923	0.81517
S	4.2163	-1.33401	-2.37989
H	3.53423	-0.74342	-3.38645
N	4.40924	0.99494	-0.33567
C	5.57673	2.97878	-0.44914
C	6.2715	2.15093	0.37666
H	5.81287	3.993	-0.7451
H	7.19922	2.34166	0.90101
N	4.1108	-1.71136	0.51927
C	5.28556	-1.4272	1.16671
C	5.72789	-2.58189	1.90863
C	4.8013	-3.55918	1.70845
H	6.63124	-2.61961	2.50402
H	4.78489	-4.56609	2.10579
N	1.60493	-1.86999	-0.84256
C	1.63084	-3.14285	-0.33191
C	0.46154	-1.77578	-1.59406
C	0.45378	-3.86405	-0.75029
C	-0.27253	-3.01658	-1.53029
H	0.23402	-4.88933	-0.48086
H	-1.21195	-3.20107	-2.03583
N	2.01403	0.76177	-1.86868
C	0.38571	1.64051	-3.24328
H	-0.53101	1.68907	-3.81704
C	0.80601	0.50024	-2.46781
C	4.41586	2.24444	-0.89537
C	5.53896	0.90773	0.43402
C	3.78703	-3.00398	0.84676
C	0.07583	-0.67412	-2.34517
H	-0.8603	-0.74104	-2.89031
C	3.46813	2.74136	-1.77741
H	3.60469	3.75376	-2.14395
C	5.9542	-0.2113	1.13921
H	6.87781	-0.13497	1.70394
C	2.64081	-3.67956	0.45281
H	2.52413	-4.70519	0.78799
C	1.34372	2.5967	-3.09157
H	1.37636	3.59252	-3.51506

C	2.35094	2.04533	-2.21857
C	-7.26274	-0.32199	-0.65542
C	-7.69129	-1.59285	-1.01614
C	-6.99793	-2.72221	-0.62285
C	-5.84372	-2.53123	0.15087
C	-5.41412	-1.24733	0.51212
C	-6.13021	-0.10085	0.10903
C	-9.02763	-0.10458	-2.00468
H	-7.33332	-3.71618	-0.89838
H	-5.25738	-3.38022	0.48548
H	-5.82749	0.90455	0.37079
H	-8.77169	0.10967	-3.05305
H	-10.05813	0.18871	-1.7866
O	-8.13687	0.61906	-1.14431
O	-8.86195	-1.4989	-1.7431
O	-4.27174	-1.19761	1.26696
C	-3.76845	0.07342	1.67012
H	-3.57518	0.70204	0.79074
H	-4.50967	0.58988	2.2987
C	-2.48351	-0.17624	2.45356
C	-1.40835	-0.83212	1.565
C	-1.9279	1.10734	3.14264
N	-0.07528	-0.869	2.12729
H	-1.69973	-1.86943	1.33048
C	-0.63121	0.73691	3.929
C	-0.05552	-0.65755	3.55451
H	0.13961	1.49075	3.74752
H	0.97284	-0.7475	3.9171
H	1.43948	-0.40084	1.1453
H	-2.74522	-0.87661	3.25813
H	-1.3422	-0.33021	0.58959
H	-0.65304	-1.4414	4.05183
H	-0.82863	0.73942	5.00697
H	-2.68729	1.41934	3.87001
C	-1.74415	2.28138	2.183
C	-2.71651	3.29222	2.13515
C	-0.63436	2.39433	1.32769
C	-2.60694	4.37483	1.26105
H	-3.57543	3.24042	2.80096
C	-0.50848	3.46825	0.44576
H	0.15865	1.65192	1.33854
C	-1.49993	4.44163	0.42436
H	-3.35576	5.15967	1.22882
H	0.34704	3.5499	-0.21636
F	-1.38174	5.48565	-0.42538
²TS-reb_H			
Fe	-3.21724	-0.62417	0.04709
O	-1.48259	-0.08085	0.42025
S	-5.34	-1.40852	-0.19275
H	-5.34205	-2.33581	0.79011
N	-3.82248	0.52629	1.61346

C	-4.44369	1.24841	3.71543
C	-4.72769	2.25497	2.84296
H	-4.59611	1.2214	4.78694
H	-5.16278	3.22437	3.05043
N	-3.70284	0.8252	-1.23408
C	-4.2455	2.04989	-0.92021
C	-4.45962	2.81683	-2.12393
C	-4.04155	2.045	-3.16457
H	-4.87822	3.81496	-2.15007
H	-4.04419	2.27864	-4.22172
N	-2.51501	-1.73142	-1.46003
C	-2.51385	-1.40978	-2.79307
C	-1.99518	-2.99972	-1.37037
C	-1.9523	-2.49198	-3.56503
C	-1.62917	-3.47639	-2.68296
H	-1.8374	-2.48531	-4.64155
H	-1.19276	-4.44649	-2.88444
N	-2.82011	-2.13335	1.3652
C	-2.08304	-4.12773	2.26072
H	-1.65778	-5.12295	2.28942
C	-2.2493	-3.33867	1.0611
C	-3.88935	0.16672	2.9392
C	-4.35013	1.78943	1.53124
C	-3.56495	0.80605	-2.59996
C	-1.86417	-3.74809	-0.20968
H	-1.4309	-4.73911	-0.30394
C	-3.50371	-1.06049	3.46306
H	-3.60169	-1.19806	4.53547
C	-4.53609	2.50792	0.35672
H	-4.96385	3.50196	0.44306
C	-3.00541	-0.23004	-3.33509
H	-2.95308	-0.1112	-4.41286
C	-2.54873	-3.37407	3.29308
H	-2.58438	-3.61965	4.3469
C	-2.99707	-2.12299	2.72517
C	6.96198	-1.83395	0.1503
C	6.8099	-3.20591	0.30131
C	5.57873	-3.81334	0.13902
C	4.49255	-2.9886	-0.18795
C	4.65007	-1.60444	-0.3402
C	5.90984	-0.99323	-0.16911
C	8.97875	-2.72376	0.49737
H	5.45601	-4.88398	0.2619
H	3.50325	-3.40934	-0.33189
H	6.06676	0.07217	-0.2753
H	9.63284	-2.69268	1.37298
H	9.56086	-2.88693	-0.42216
O	8.26897	-1.4822	0.39196
O	8.02073	-3.77103	0.65335
O	3.51408	-0.91331	-0.66855
C	3.59296	0.49914	-0.82977
H	3.96722	0.96664	0.09111

H	4.29257	0.74673	-1.6431
C	2.19256	1.00217	-1.16406
C	1.20991	0.73749	0.0024
C	2.17309	2.50147	-1.58305
N	-0.02205	1.51	-0.06401
H	0.94674	-0.32818	0.02195
C	0.70634	2.89582	-1.94202
C	-0.35224	1.88287	-1.42077
H	0.48225	3.88772	-1.53907
H	-1.34236	2.34217	-1.43826
H	-1.51575	0.44594	1.23835
H	1.85724	0.42907	-2.03784
H	1.69064	0.95533	0.96565
H	-0.37899	1.00436	-2.08243
H	0.58909	2.96204	-3.03
H	2.77876	2.5796	-2.49442
C	2.81596	3.43389	-0.55941
C	4.10447	3.93844	-0.79008
C	2.16255	3.81776	0.62449
C	4.73409	4.78853	0.12076
H	4.62735	3.67021	-1.70544
C	2.77513	4.6657	1.54732
H	1.15955	3.45188	0.82946
C	4.05521	5.13819	1.28091
H	5.72855	5.18296	-0.06108
H	2.27337	4.96405	2.46222
F	4.65079	5.9626	2.16907
⁴TS-reb_H			
Fe	-2.94563	-0.45278	0.01012
O	-1.5737	0.36574	-0.41903
S	-4.91804	-1.81728	0.39004
H	-5.79986	-1.07112	-0.3125
N	-3.12845	-0.9895	-1.92707
C	-3.57151	-0.95138	-4.19019
C	-2.87841	-2.09308	-3.93586
H	-3.95886	-0.59225	-5.13528
H	-2.5742	-2.86739	-4.62859
N	-1.93325	-2.15194	0.39814
C	-1.58323	-3.11464	-0.51105
C	-0.80959	-4.14875	0.13673
C	-0.68762	-3.78776	1.44343
H	-0.42244	-5.02918	-0.36033
H	-0.18142	-4.31062	2.24501
N	-2.88499	0.02277	1.98104
C	-2.24812	-0.67911	2.97671
C	-3.54435	1.05765	2.60359
C	-2.48184	-0.0496	4.25282
C	-3.28992	1.02272	4.02262
H	-2.08809	-0.40633	5.1962
H	-3.69215	1.7293	4.73759
N	-4.14574	1.14123	-0.32406

C	-5.36957	3.0779	-0.04774
H	-5.84132	3.90776	0.46326
C	-4.59203	2.0487	0.60146
C	-3.7248	-0.26665	-2.92583
C	-2.6001	-2.10546	-2.51704
C	-1.39467	-2.53671	1.59607
C	-4.3279	2.01034	1.96537
H	-4.77139	2.78627	2.58191
C	-4.40743	0.92921	-2.75584
H	-4.83966	1.38792	-3.6399
C	-1.8913	-3.10365	-1.86443
H	-1.53709	-3.93735	-2.46266
C	-1.52315	-1.85043	2.79781
H	-1.05848	-2.28921	3.67543
C	-5.37624	2.78448	-1.37693
H	-5.85633	3.32246	-2.18464
C	-4.61062	1.57104	-1.53947
C	5.85976	-2.42524	-0.0593
C	5.46809	-3.74384	0.12846
C	4.13418	-4.08493	0.25492
C	3.19346	-3.04728	0.18257
C	3.59406	-1.71771	-0.00719
C	4.95748	-1.37792	-0.13279
C	7.67722	-3.7146	-0.1784
H	3.82658	-5.11408	0.4062
H	2.13213	-3.25462	0.27019
H	5.30098	-0.36228	-0.27966
H	8.50372	-3.85264	0.52408
H	7.99195	-3.95187	-1.20592
O	7.23168	-2.35277	-0.12391
O	6.58534	-4.55449	0.19766
O	2.57895	-0.79935	-0.066
C	2.90723	0.57274	-0.24461
H	3.56268	0.91244	0.56939
H	3.45208	0.71408	-1.18882
C	1.59812	1.36051	-0.2715
C	0.83299	1.23509	1.05663
C	1.78797	2.86002	-0.71674
N	-0.4537	1.88791	0.95246
H	0.66801	0.18274	1.29657
C	0.72454	3.77073	-0.04542
C	-0.62325	3.06727	0.12371
H	1.07681	4.09521	0.94077
H	-1.3552	3.73109	0.59846
H	0.95407	0.88054	-1.01636
H	1.42229	1.67356	1.88349
H	-1.03634	2.77667	-0.85313
H	0.59373	4.67976	-0.6426
H	1.58884	2.87473	-1.79498
C	3.18827	3.43645	-0.53353
C	3.96963	3.74787	-1.6556
C	3.7382	3.68758	0.73525

C	5.25145	4.28696	-1.53185
H	3.56807	3.56959	-2.65032
C	5.01796	4.22163	0.88261
H	3.16421	3.4638	1.63069
C	5.75688	4.5148	-0.25859
H	5.85322	4.53027	-2.40137
H	5.4448	4.41343	1.86167
F	6.99394	5.03563	-0.1236
H	-1.57533	0.17793	-1.37067
²P-OH			
Fe	2.70718	-0.69664	-0.60474
O	1.75615	0.06322	1.37997
S	3.7713	-1.56716	-2.36524
H	4.99787	-1.66986	-1.80375
N	3.50289	-2.00134	0.71385
C	4.95151	-3.07162	2.16459
C	3.94564	-3.94646	1.88344
H	5.81132	-3.21661	2.80653
H	3.80909	-4.95647	2.24901
N	1.11868	-1.91577	-0.86479
C	0.98635	-3.19444	-0.3779
C	-0.24015	-3.78758	-0.85547
C	-0.84731	-2.85738	-1.6416
H	-0.57668	-4.7871	-0.6103
H	-1.78849	-2.93178	-2.17106
N	1.79027	0.6843	-1.73732
C	0.60202	0.56403	-2.41718
C	2.31592	1.89704	-2.11053
C	0.3633	1.73737	-3.22245
C	1.43015	2.56264	-3.03657
H	-0.5068	1.88821	-3.84874
H	1.61971	3.5316	-3.48145
N	4.19188	0.58623	-0.18912
C	5.59237	2.42386	-0.26359
H	5.96009	3.39891	-0.55743
C	4.37695	1.82112	-0.75863
C	4.67424	-1.86617	1.42522
C	3.04846	-3.27477	0.97638
C	0.01219	-1.69844	-1.65054
C	3.51594	2.43003	-1.66119
H	3.79827	3.4087	-2.03714
C	5.49005	-0.74308	1.41301
H	6.38596	-0.76621	2.02598
C	1.88106	-3.83241	0.4711
H	1.64408	-4.84833	0.77224
C	-0.24147	-0.538	-2.36928
H	-1.15235	-0.50051	-2.95882
C	6.13872	1.54071	0.61553
H	7.05004	1.63747	1.19209
C	5.26104	0.39524	0.65199
C	-6.44887	-1.27293	-0.1701

C	-6.46135	-2.65095	-0.34213
C	-5.41711	-3.43929	0.10419
C	-4.34505	-2.7907	0.73481
C	-4.33798	-1.40034	0.90933
C	-5.40842	-0.60409	0.45127
C	-8.26177	-1.80993	-1.35667
H	-5.42608	-4.51601	-0.02646
H	-3.49198	-3.35511	1.09516
H	-5.43481	0.47128	0.56967
H	-8.1489	-1.67267	-2.44248
H	-9.31767	-1.82874	-1.07332
O	-7.60731	-0.7315	-0.67426
O	-7.63802	-3.03129	-0.95763
O	-3.23901	-0.89047	1.54879
C	-3.10656	0.52252	1.6645
H	-3.15924	0.99038	0.67264
H	-3.9221	0.93283	2.27895
C	-1.75728	0.80356	2.32035
C	-0.60616	0.20327	1.47659
C	-1.57137	2.30995	2.66203
N	0.6576	0.91482	1.7085
H	-0.50035	-0.86115	1.74492
C	-0.17515	2.52042	3.33574
C	0.80628	1.36032	3.09121
H	0.26852	3.44564	2.95692
H	1.8373	1.69802	3.21903
H	1.66074	-0.7797	1.87667
H	-1.76522	0.27841	3.28462
H	-0.82721	0.24129	0.40637
H	0.63707	0.53032	3.80585
H	-0.29832	2.64553	4.41755
H	-2.33566	2.53458	3.41609
C	-1.8421	3.26221	1.50015
C	-2.99377	4.06337	1.52305
C	-0.98094	3.37704	0.39514
C	-3.29307	4.94886	0.486
H	-3.67114	4.00315	2.37224
C	-1.26509	4.25452	-0.65124
H	-0.07603	2.77749	0.35571
C	-2.41871	5.02766	-0.59
H	-4.18152	5.57168	0.50642
H	-0.6054	4.33415	-1.50867
F	-2.69561	5.87968	-1.60154
⁴P-OH			
Fe	2.79552	-0.75494	-0.65508
O	1.68981	0.44368	1.63158
S	3.87326	-1.99034	-2.4522
H	4.91961	-1.1441	-2.58451
N	3.53077	-1.86109	0.87977
C	4.99144	-2.76833	2.42553
C	3.94319	-3.63005	2.31129

H	5.8696	-2.85399	3.05283
H	3.78303	-4.56948	2.82497
N	1.16419	-1.93051	-0.67949
C	0.99082	-3.12473	-0.01505
C	-0.25143	-3.73617	-0.40685
C	-0.8364	-2.90065	-1.31089
H	-0.61844	-4.68113	-0.02685
H	-1.78685	-3.01456	-1.81571
N	1.82884	0.58408	-1.81929
C	0.62209	0.40446	-2.45217
C	2.32027	1.78138	-2.28121
C	0.33864	1.52309	-3.31685
C	1.39353	2.37742	-3.21189
H	-0.55306	1.62244	-3.92246
H	1.55	3.32206	-3.71729
N	4.26825	0.58021	-0.37431
C	5.67371	2.39569	-0.63056
H	6.03596	3.3454	-1.00315
C	4.43575	1.77888	-1.02936
C	4.73295	-1.67504	1.52329
C	3.04263	-3.06352	1.33949
C	0.05055	-1.7795	-1.47588
C	3.53717	2.34169	-1.92445
H	3.80254	3.29538	-2.36952
C	5.59251	-0.60568	1.32521
H	6.51022	-0.58413	1.90446
C	1.86149	-3.66004	0.92411
H	1.59653	-4.61472	1.36729
C	-0.20951	-0.69519	-2.30196
H	-1.13381	-0.70915	-2.87066
C	6.2506	1.56682	0.2843
H	7.18398	1.69581	0.81737
C	5.36586	0.44275	0.44483
C	-6.32444	-1.43725	-0.3395
C	-6.27176	-2.81994	-0.45739
C	-5.22849	-3.54671	0.08531
C	-4.22607	-2.83083	0.75691
C	-4.28392	-1.43544	0.87557
C	-5.35324	-0.70279	0.31877
C	-8.04076	-2.09363	-1.60858
H	-5.18768	-4.62718	-0.00121
H	-3.37857	-3.34566	1.19588
H	-5.42987	0.37412	0.39215
H	-7.87659	-1.99221	-2.69166
H	-9.10873	-2.14696	-1.37957
O	-7.46811	-0.96341	-0.93625
O	-7.38998	-3.27186	-1.13028
O	-3.24994	-0.85641	1.56177
C	-3.19726	0.56447	1.64893
H	-3.20511	1.00536	0.64351
H	-4.07484	0.94351	2.19402
C	-1.91416	0.93504	2.38724

C	-0.6712	0.39012	1.64195
C	-1.83448	2.4576	2.69758
N	0.51959	1.19319	1.93385
H	-0.51222	-0.65799	1.95122
C	-0.51353	2.75336	3.48233
C	0.55609	1.65686	3.31598
H	-0.10199	3.70725	3.13988
H	1.55361	2.06248	3.50107
H	1.63668	-0.40872	2.11839
H	-1.95943	0.43346	3.36306
H	-0.82199	0.38342	0.55801
H	0.39833	0.8248	4.03179
H	-0.73407	2.86589	4.55012
H	-2.66998	2.66393	3.37784
C	-2.05484	3.36018	1.48501
C	-3.24753	4.09254	1.38322
C	-1.11278	3.48979	0.44951
C	-3.50939	4.92248	0.29139
H	-3.98951	4.0212	2.17568
C	-1.35875	4.31099	-0.65075
H	-0.17709	2.94209	0.51122
C	-2.55565	5.01529	-0.7138
H	-4.43011	5.49191	0.21576
H	-0.63666	4.40118	-1.45579
F	-2.79636	5.81252	-1.77809

Secondary amine hydroxylation by OAR mechanism

²TS_o

Fe	-2.94563	-0.45278	0.01012
O	-1.5737	0.36574	-0.41903
S	-4.91804	-1.81728	0.39004
H	-5.79986	-1.07112	-0.3125
N	-3.12845	-0.9895	-1.92707
C	-3.57151	-0.95138	-4.19019
C	-2.87841	-2.09308	-3.93586
H	-3.95886	-0.59225	-5.13528
H	-2.5742	-2.86739	-4.62859
N	-1.93325	-2.15194	0.39814
C	-1.58323	-3.11464	-0.51105
C	-0.80959	-4.14875	0.13673
C	-0.68762	-3.78776	1.44343
H	-0.42244	-5.02918	-0.36033
H	-0.18142	-4.31062	2.24501
N	-2.88499	0.02277	1.98104
C	-2.24812	-0.67911	2.97671
C	-3.54435	1.05765	2.60359
C	-2.48184	-0.0496	4.25282
C	-3.28992	1.02272	4.02262
H	-2.08809	-0.40633	5.1962
H	-3.69215	1.7293	4.73759
N	-4.14574	1.14123	-0.32406
C	-5.36957	3.0779	-0.04774

H	-5.84132	3.90776	0.46326
C	-4.59203	2.0487	0.60146
C	-3.7248	-0.26665	-2.92583
C	-2.6001	-2.10546	-2.51704
C	-1.39467	-2.53671	1.59607
C	-4.3279	2.01034	1.96537
H	-4.77139	2.78627	2.58191
C	-4.40743	0.92921	-2.75584
H	-4.83966	1.38792	-3.6399
C	-1.8913	-3.10365	-1.86443
H	-1.53709	-3.93735	-2.46266
C	-1.52315	-1.85043	2.79781
H	-1.05848	-2.28921	3.67543
C	-5.37624	2.78448	-1.37693
H	-5.85633	3.32246	-2.18464
C	-4.61062	1.57104	-1.53947
C	5.85976	-2.42524	-0.0593
C	5.46809	-3.74384	0.12846
C	4.13418	-4.08493	0.25492
C	3.19346	-3.04728	0.18257
C	3.59406	-1.71771	-0.00719
C	4.95748	-1.37792	-0.13279
C	7.67722	-3.7146	-0.1784
H	3.82658	-5.11408	0.4062
H	2.13213	-3.25462	0.27019
H	5.30098	-0.36228	-0.27966
H	8.50372	-3.85264	0.52408
H	7.99195	-3.95187	-1.20592
O	7.23168	-2.35277	-0.12391
O	6.58534	-4.55449	0.19766
O	2.57895	-0.79935	-0.066
C	2.90723	0.57274	-0.24461
H	3.56268	0.91244	0.56939
H	3.45208	0.71408	-1.18882
C	1.59812	1.36051	-0.2715
C	0.83299	1.23509	1.05663
C	1.78797	2.86002	-0.71674
N	-0.4537	1.88791	0.95246
H	0.66801	0.18274	1.29657
C	0.72454	3.77073	-0.04542
C	-0.62325	3.06727	0.12371
H	1.07681	4.09521	0.94077
H	-1.3552	3.73109	0.59846
H	0.95407	0.88054	-1.01636
H	1.42229	1.67356	1.88349
H	-1.03634	2.77667	-0.85313
H	0.59373	4.67976	-0.6426
H	1.58884	2.87473	-1.79498
C	3.18827	3.43645	-0.53353
C	3.96963	3.74787	-1.6556
C	3.7382	3.68758	0.73525
C	5.25145	4.28696	-1.53185

H	3.56807	3.56959	-2.65032
C	5.01796	4.22163	0.88261
H	3.16421	3.4638	1.63069
C	5.75688	4.5148	-0.25859
H	5.85322	4.53027	-2.40137
H	5.4448	4.41343	1.86167
F	6.99394	5.03563	-0.1236
H	-1.248	1.49949	1.44633
⁴TS₀			
Fe	-2.8885	-0.48012	-0.18581
O	-1.53077	0.3653	-0.49699
S	-4.91945	-1.84238	0.54484
H	-5.7413	-0.81107	0.84536
N	-3.03857	-1.13611	-2.08487
C	-3.45499	-1.23376	-4.35495
C	-2.71593	-2.33024	-4.03509
H	-3.84272	-0.93779	-5.32128
H	-2.36883	-3.12463	-4.68327
N	-1.91083	-2.17402	0.31888
C	-1.49551	-3.167	-0.5331
C	-0.75394	-4.17184	0.1909
C	-0.71947	-3.77048	1.49029
H	-0.32586	-5.06104	-0.2536
H	-0.26204	-4.26363	2.33848
N	-2.98045	0.02473	1.77174
C	-2.3678	-0.6199	2.82233
C	-3.56146	1.15153	2.30817
C	-2.58804	0.10609	4.04954
C	-3.32856	1.20395	3.73112
H	-2.22476	-0.20398	5.0212
H	-3.6966	1.98274	4.38707
N	-4.09649	1.07449	-0.62784
C	-5.2651	3.06352	-0.50081
H	-5.70561	3.94602	-0.05469
C	-4.51038	2.06653	0.22014
C	-3.64919	-0.49578	-3.12893
C	-2.46306	-2.25678	-2.61514
C	-1.44219	-2.52222	1.55801
C	-4.26285	2.10691	1.58901
H	-4.65974	2.95359	2.14102
C	-4.3646	0.6914	-3.03379
H	-4.7989	1.08515	-3.94782
C	-1.74758	-3.20897	-1.89633
H	-1.35267	-4.05584	-2.4492
C	-1.64045	-1.79527	2.72513
H	-1.20695	-2.19117	3.63841
C	-5.30041	2.6606	-1.80026
H	-5.77529	3.14357	-2.64468
C	-4.56465	1.42092	-1.86911
C	5.8126	-2.35991	-0.1013
C	5.49594	-3.67172	0.22417

C	4.23537	-4.0125	0.67835
C	3.29259	-2.9811	0.796
C	3.61687	-1.65556	0.47105
C	4.90653	-1.31908	0.00608
C	7.562	-3.64638	-0.61371
H	3.98542	-5.03672	0.93422
H	2.28238	-3.1899	1.13143
H	5.19036	-0.30902	-0.25828
H	8.539	-3.75628	-0.13505
H	7.61416	-3.921	-1.67848
O	7.12833	-2.28553	-0.49805
O	6.60856	-4.47527	0.05144
O	2.61153	-0.74531	0.63449
C	2.85138	0.61532	0.27332
H	3.70751	1.00435	0.84151
H	3.10508	0.67618	-0.79413
C	1.57986	1.40601	0.57155
C	1.26493	1.4455	2.07822
C	1.58318	2.8479	-0.06657
N	-0.0107	2.08024	2.29406
H	1.22373	0.41879	2.45734
C	0.79983	3.84678	0.82638
C	-0.42604	3.20586	1.48334
H	1.45516	4.2317	1.61722
H	-0.9321	3.95557	2.10946
H	0.74782	0.86367	0.10908
H	2.10251	1.94277	2.61477
H	-1.14566	2.90537	0.70179
H	0.49721	4.7099	0.22153
H	1.02628	2.75488	-1.00679
C	2.95214	3.41184	-0.43146
C	3.29646	3.61029	-1.77652
C	3.90197	3.76564	0.54275
C	4.53462	4.1373	-2.14974
H	2.57979	3.3499	-2.55184
C	5.14645	4.28937	0.19296
H	3.67234	3.63033	1.59637
C	5.44327	4.46887	-1.15366
H	4.79735	4.29226	-3.19123
H	5.88127	4.56004	0.94441
F	6.64519	4.98017	-1.4995
H	-0.568	1.8143	3.08832
²INTo			
Fe	2.949	-0.51757	-0.27115
O	1.44778	0.24144	0.78667
S	4.70023	-1.42819	-1.40291
H	4.95815	-2.45564	-0.56228
N	2.05168	-2.3095	-0.08857
C	1.3681	-4.38041	0.67117
C	0.75039	-4.16649	-0.52222
H	1.29592	-5.24091	1.32441

H	0.07008	-4.81747	-1.05717
N	1.99289	-0.16482	-2.03707
C	1.1623	-1.05201	-2.67726
C	0.74829	-0.51261	-3.95109
C	1.34854	0.70365	-4.08086
H	0.09228	-1.01679	-4.64977
H	1.28755	1.40082	-4.90732
N	3.77609	1.33211	-0.43905
C	3.67578	2.22565	-1.47802
C	4.64766	1.88924	0.46299
C	4.48671	3.39066	-1.21272
C	5.0897	3.18124	-0.00898
H	4.58273	4.24128	-1.876
H	5.78221	3.82613	0.51765
N	3.84622	-0.81951	1.50105
C	5.15535	-0.51132	3.37738
H	5.83734	-0.021	4.06081
C	4.69433	0.05327	2.12656
C	2.17915	-3.21205	0.9328
C	1.18593	-2.86716	-0.98959
C	2.13144	0.90972	-2.8859
C	5.06572	1.30736	1.65439
H	5.75839	1.87906	2.26527
C	2.97519	-3.03885	2.05863
H	2.98967	-3.83908	2.79237
C	0.77019	-2.29254	-2.18634
H	0.09045	-2.87398	-2.80231
C	2.9028	2.03903	-2.62206
H	2.91746	2.82408	-3.37209
C	4.5701	-1.73329	3.49475
H	4.66947	-2.4561	4.29483
C	3.75069	-1.91465	2.31653
C	-5.98426	-2.30382	0.12153
C	-5.65081	-3.64472	-0.01752
C	-4.34086	-4.07413	0.08867
C	-3.36178	-3.10133	0.33818
C	-3.70472	-1.75036	0.47757
C	-5.04313	-1.31984	0.37203
C	-7.83328	-3.4272	-0.42576
H	-4.07976	-5.12177	-0.01466
H	-2.31559	-3.37654	0.42409
H	-5.34035	-0.28452	0.47841
H	-8.09045	-3.37728	-1.49442
H	-8.7063	-3.69912	0.17367
O	-7.34464	-2.14808	0.00204
O	-6.79652	-4.38818	-0.22372
O	-2.65568	-0.90027	0.71963
C	-2.90565	0.49232	0.83116
H	-3.39985	0.86848	-0.0752
H	-3.57042	0.69963	1.68203
C	-1.55127	1.16926	1.04845
C	-0.6286	0.95747	-0.14843

C	-1.65533	2.68894	1.43565
N	0.79109	1.32752	0.21975
H	-0.58252	-0.08677	-0.4504
C	-0.34531	3.41618	1.02623
C	0.86879	2.50428	1.16819
H	-0.41042	3.78664	-0.00388
H	1.81585	3.00711	0.96532
H	-1.0815	0.64174	1.88706
H	-0.92248	1.56937	-1.00874
H	0.92758	2.05106	2.15931
H	-0.20145	4.30279	1.65317
H	-1.70957	2.71664	2.53068
C	-2.89528	3.41429	0.92515
C	-3.90385	3.78577	1.82675
C	-3.08136	3.73363	-0.4306
C	-5.05882	4.44636	1.40582
H	-3.78456	3.55857	2.88344
C	-4.2291	4.39029	-0.87378
H	-2.32406	3.47255	-1.16482
C	-5.20364	4.73763	0.05543
H	-5.83572	4.73632	2.1055
H	-4.37428	4.63617	-1.92057
F	-6.31321	5.37623	-0.36557
H	1.28151	1.56961	-0.65071
⁴INTo			
Fe	-2.98045	-0.52618	0.24539
O	-1.42203	0.14414	-0.84159
S	-4.78683	-1.36868	1.43228
H	-5.12131	-2.35748	0.57317
N	-1.64664	-1.79659	1.2766
C	-0.44087	-3.65728	1.86777
C	-0.31694	-2.75399	2.88317
H	-0.01356	-4.65068	1.80541
H	0.23626	-2.86355	3.80793
N	-2.70966	0.90724	1.74419
C	-2.0568	0.69387	2.94497
C	-2.31815	1.81044	3.82243
C	-3.15508	2.66435	3.15931
H	-1.92667	1.91207	4.82729
H	-3.57524	3.59533	3.5199
N	-4.2262	0.84036	-0.77393
C	-4.6555	2.0529	-0.32789
C	-4.84712	0.58281	-1.96053
C	-5.58287	2.6169	-1.29386
C	-5.69957	1.70776	-2.30458
H	-6.08099	3.57403	-1.19803
H	-6.31357	1.77683	-3.19427
N	-3.19474	-1.88903	-1.23816
C	-3.81577	-2.92217	-3.18787
H	-4.30198	-3.07357	-4.14369
C	-3.94358	-1.7299	-2.37087

C	-1.29324	-3.04677	0.86188
C	-1.09089	-1.58546	2.50136
C	-3.42143	2.0871	1.86299
C	-4.703	-0.59795	-2.69995
H	-5.25427	-0.65094	-3.63518
C	-1.72	-3.64461	-0.33063
H	-1.34375	-4.64463	-0.53004
C	-1.27874	-0.42558	3.2677
H	-0.8066	-0.41003	4.24657
C	-4.27346	2.63041	0.89221
H	-4.72654	3.58711	1.13882
C	-2.98189	-3.77371	-2.5254
H	-2.65167	-4.75816	-2.83316
C	-2.58884	-3.11332	-1.29462
C	6.15566	-2.20145	-0.18186
C	5.86648	-3.54686	0.00423
C	4.56871	-4.0188	-0.06302
C	3.55634	-3.08393	-0.32411
C	3.85421	-1.72861	-0.51345
C	5.18046	-1.25473	-0.44475
C	8.0492	-3.2511	0.36176
H	4.34145	-5.06955	0.08036
H	2.51742	-3.39158	-0.37588
H	5.44383	-0.21481	-0.58798
H	8.32924	-3.16151	1.42197
H	8.91621	-3.51489	-0.25005
O	7.51234	-2.00049	-0.09171
O	7.03783	-4.24831	0.21286
O	2.77632	-0.91892	-0.76843
C	2.98024	0.4818	-0.87303
H	3.45721	0.86718	0.03846
H	3.64337	0.71495	-1.71856
C	1.6098	1.12247	-1.09756
C	0.67228	0.85797	0.07786
C	1.68511	2.65412	-1.4467
N	-0.7478	1.22657	-0.28404
H	0.63429	-0.19665	0.34352
C	0.35139	3.3433	-1.04823
C	-0.83682	2.40446	-1.22417
H	0.3905	3.69695	-0.01081
H	-1.79952	2.88213	-1.03396
H	1.16927	0.60559	-1.95864
H	0.95264	1.44185	0.96198
H	-0.86699	1.96162	-2.22171
H	0.19784	4.23718	-1.66236
H	1.76125	2.70828	-2.53943
C	2.89611	3.39768	-0.89405
C	3.91054	3.82087	-1.76573
C	3.04715	3.68697	0.47283
C	5.03759	4.50324	-1.30538
H	3.81797	3.61802	-2.83004
C	4.16661	4.36429	0.95518

H	2.28378	3.38525	1.18478
C	5.14804	4.76364	0.0545
H	5.81884	4.83347	-1.98199
H	4.28458	4.58699	2.01056
F	6.2302	5.423	0.51345
H	-1.25679	1.44776	0.59413
²TS-reb₀			
Fe	-2.71531	-0.67545	0.52989
O	-1.86507	-0.07509	-1.35398
S	-3.82985	-1.23922	2.39507
H	-4.75328	-2.04746	1.8268
N	-2.48019	-2.57767	-0.04523
C	-2.80776	-4.67818	-0.95091
C	-1.64341	-4.72102	-0.24861
H	-3.28661	-5.46921	-1.51419
H	-0.96735	-5.55578	-0.11276
N	-0.9709	-0.71358	1.54389
C	-0.16111	-1.8104	1.69742
C	0.95724	-1.49072	2.55327
C	0.80434	-0.19195	2.93109
H	1.74475	-2.18316	2.82233
H	1.43946	0.40286	3.57542
N	-2.83875	1.31596	0.94588
C	-2.04617	2.05107	1.80171
C	-3.89239	2.13803	0.6045
C	-2.58919	3.37411	1.96636
C	-3.73038	3.42914	1.22115
H	-2.15451	4.14728	2.58771
H	-4.41835	4.25733	1.10608
N	-4.40865	-0.58764	-0.55831
C	-6.34905	0.18508	-1.54614
H	-7.13064	0.88173	-1.82235
C	-5.20769	0.51429	-0.72117
C	-3.3242	-3.3363	-0.81654
C	-1.45003	-3.40647	0.31941
C	-0.40282	0.28494	2.29839
C	-4.97423	1.77662	-0.1886
H	-5.71679	2.54311	-0.38988
C	-4.50937	-2.88964	-1.38534
H	-5.08416	-3.59871	-1.9732
C	-0.37037	-3.05626	1.12003
H	0.36571	-3.82751	1.32595
C	-0.89993	1.57639	2.42713
H	-0.35944	2.25982	3.07491
C	-6.22539	-1.12724	-1.88142
H	-6.88231	-1.73367	-2.4922
C	-5.00693	-1.5988	-1.26421
C	6.40637	-1.50616	0.02942
C	6.37737	-2.89083	0.13153
C	5.27819	-3.61843	-0.28497
C	4.19564	-2.90167	-0.81587

C	4.22915	-1.50477	-0.91659
C	5.35439	-0.77038	-0.48824
C	8.39406	-2.19037	0.78174
H	5.25165	-4.69956	-0.20227
H	3.30717	-3.41849	-1.16224
H	5.41246	0.30846	-0.55005
H	8.83702	-2.11867	1.77888
H	9.17449	-2.26142	0.00958
O	7.59095	-1.02743	0.53537
O	7.54559	-3.33751	0.71704
O	3.11283	-0.92523	-1.46183
C	3.04635	0.49327	-1.54105
H	3.19042	0.93824	-0.54759
H	3.84012	0.87419	-2.20161
C	1.67361	0.85524	-2.10516
C	0.5627	0.37138	-1.15171
C	1.55883	2.36418	-2.4708
N	-0.75158	0.95423	-1.50367
H	0.46717	-0.71519	-1.20993
C	0.12922	2.6519	-3.03975
C	-0.85298	1.48331	-2.86569
H	-0.28526	3.54151	-2.55629
H	-1.88355	1.81191	-3.01251
H	-1.73936	1.0181	-0.80161
H	1.5739	0.30081	-3.04711
H	0.78766	0.63634	-0.11647
H	-0.66366	0.66591	-3.57473
H	0.19112	2.87919	-4.10967
H	2.28033	2.52938	-3.27977
C	1.96164	3.30751	-1.34103
C	3.20948	3.94782	-1.38172
C	1.12707	3.56521	-0.24091
C	3.62628	4.80804	-0.36467
H	3.86961	3.77944	-2.22962
C	1.52524	4.42166	0.78522
H	0.14859	3.09941	-0.17663
C	2.77276	5.02998	0.70854
H	4.58911	5.30727	-0.39928
H	0.87987	4.62243	1.63396
F	3.16076	5.86208	1.69735
⁴TS-reb_o			
Fe	2.66993	-0.7113	-0.54679
O	1.9118	0.01064	1.41576
S	3.71653	-1.31062	-2.51269
H	4.96762	-1.45091	-2.01883
N	2.30489	-2.66198	0.12334
C	2.59179	-4.74765	1.04126
C	1.39552	-4.75453	0.38546
H	3.05604	-5.55733	1.59064
H	0.69084	-5.57158	0.29172
N	0.88702	-0.69762	-1.5186

C	0.02932	-1.76598	-1.62467
C	-1.0816	-1.39939	-2.47566
C	-0.87038	-0.11592	-2.8834
H	-1.91119	-2.05087	-2.7196
H	-1.49375	0.49256	-3.52661
N	2.81821	1.40189	-0.91443
C	2.05425	2.11285	-1.80137
C	3.92392	2.15936	-0.62689
C	2.66234	3.40439	-2.03064
C	3.81781	3.43472	-1.29971
H	2.27126	4.17242	-2.6868
H	4.54871	4.23209	-1.24455
N	4.3966	-0.66079	0.48608
C	6.37064	0.0358	1.43022
H	7.18377	0.69682	1.70314
C	5.22527	0.42424	0.63391
C	3.15957	-3.42463	0.86266
C	1.23188	-3.43714	-0.19971
C	0.36718	0.32567	-2.27768
C	5.01398	1.71069	0.12627
H	5.80668	2.43083	0.31033
C	4.39439	-2.98017	1.34246
H	4.97974	-3.68871	1.92182
C	0.17288	-3.01328	-1.00718
H	-0.6179	-3.73337	-1.19804
C	0.90045	1.6122	-2.41291
H	0.36731	2.28312	-3.0808
C	6.20465	-1.27554	1.76074
H	6.85406	-1.90216	2.35923
C	4.9537	-1.70892	1.17434
C	-6.28406	-1.52251	-0.05778
C	-6.20411	-2.90018	-0.21447
C	-5.08862	-3.60586	0.19635
C	-4.04257	-2.87426	0.77801
C	-4.12746	-1.48443	0.93367
C	-5.2694	-0.7726	0.51143
C	-8.23123	-2.24417	-0.87758
H	-5.02243	-4.68119	0.07106
H	-3.14272	-3.37318	1.12135
H	-5.36708	0.29999	0.61716
H	-8.65913	-2.14746	-1.87914
H	-9.02181	-2.37385	-0.12354
O	-7.47447	-1.06493	-0.56974
O	-7.34356	-3.36252	-0.8431
O	-3.04454	-0.88966	1.52661
C	-3.00087	0.52983	1.61102
H	-3.15119	0.97447	0.61848
H	-3.80079	0.89657	2.2723
C	-1.63293	0.91041	2.17505
C	-0.51836	0.42306	1.22857
C	-1.52959	2.42492	2.51989
N	0.79249	1.02147	1.56615

H	-0.4113	-0.66136	1.30251
C	-0.1031	2.73104	3.08752
C	0.89347	1.57377	2.91891
H	0.29963	3.62425	2.60075
H	1.92091	1.91683	3.05451
H	1.75423	1.10304	0.8423
H	-1.52968	0.36938	3.12451
H	-0.74888	0.66996	0.19009
H	0.72032	0.7622	3.6389
H	-0.16814	2.96203	4.15651
H	-2.25399	2.59762	3.32474
C	-1.93507	3.34984	1.37582
C	-3.18569	3.98527	1.40534
C	-1.09944	3.59621	0.27385
C	-3.60388	4.83024	0.37609
H	-3.847	3.82498	2.25388
C	-1.49889	4.43731	-0.76437
H	-0.1192	3.1331	0.21766
C	-2.74895	5.0416	-0.69811
H	-4.56889	5.32577	0.40201
H	-0.8524	4.62885	-1.6144
F	-3.13839	5.85915	-1.69864

Dehydration mechanisms

²TS-D_m

Fe	3.54821	0.45516	0.47453
S	4.83333	1.50383	1.9654
H	4.73036	0.59722	2.96464
N	4.82284	0.71212	-1.05502
C	6.67073	0.49245	-2.43289
C	6.03639	1.63973	-2.79595
H	7.56657	0.05375	-2.85381
H	6.30179	2.34146	-3.57621
N	2.59218	2.12529	-0.09239
C	2.94524	3.00714	-1.08802
C	2.06239	4.1467	-1.09085
C	1.17569	3.95665	-0.07693
H	2.12907	4.97458	-1.78512
H	0.35936	4.59567	0.23528
N	2.07099	0.03426	1.76521
C	1.06001	0.88813	2.14747
C	1.93741	-1.07877	2.56799
C	0.27241	0.29548	3.19842
C	0.81322	-0.92759	3.45536
H	-0.58394	0.76603	3.66484
H	0.49541	-1.66846	4.17808
N	4.31953	-1.365	0.82248
C	4.80273	-3.42485	1.76486
H	4.68808	-4.29389	2.40036
C	3.90083	-2.3016	1.74197
C	5.91005	-0.0792	-1.34951
C	4.89447	1.77454	-1.92786

C	1.51027	2.69528	0.53759
C	2.78256	-2.1782	2.55253
H	2.5667	-2.98938	3.24123
C	6.22329	-1.27737	-0.72679
H	7.11247	-1.79962	-1.06637
C	4.01279	2.84335	-1.9569
H	4.18184	3.61636	-2.69989
C	0.80359	2.13126	1.58822
H	-0.03273	2.69614	1.98861
C	5.78184	-3.15928	0.85725
H	6.63714	-3.76684	0.58973
C	5.4732	-1.87762	0.27399
C	-0.48724	-1.26202	-1.16427
C	0.16014	-2.46597	-0.98105
C	-0.53113	-3.6404	-0.73801
C	-1.92275	-3.53618	-0.69558
C	-2.58359	-2.30429	-0.88437
C	-1.86329	-1.11973	-1.12584
C	1.66756	-0.9187	-1.3651
H	-0.02514	-4.58786	-0.59128
H	-2.5351	-4.41298	-0.5152
H	-2.33345	-0.15746	-1.27593
H	2.5566	-0.51177	-1.98623
O	0.48033	-0.2907	-1.35051
O	1.52764	-2.21934	-1.05691
O	-3.9427	-2.3609	-0.81812
C	-4.6922	-1.15605	-0.99552
H	-4.38442	-0.41145	-0.25005
H	-4.49426	-0.74229	-1.99522
C	-6.16994	-1.49971	-0.84097
C	-6.47066	-2.05954	0.56692
C	-7.0898	-0.30533	-1.22906
N	-7.90165	-1.94281	0.89343
H	-6.11182	-3.09984	0.6028
C	-8.5853	-0.75563	-1.12625
C	-8.76993	-2.02747	-0.28013
H	-9.17253	0.05612	-0.68618
H	-9.80822	-2.09586	0.06229
H	-8.15837	-2.64484	1.58191
H	-6.38092	-2.29244	-1.57128
H	-5.89677	-1.49946	1.31807
H	-8.58069	-2.92794	-0.895
H	-8.98819	-0.93228	-2.13085
H	-6.87978	-0.09719	-2.28581
C	-6.777	0.9867	-0.47827
C	-6.11463	2.03044	-1.14209
C	-7.12656	1.18006	0.86957
C	-5.7975	3.22708	-0.49622
H	-5.84567	1.91379	-2.1898
C	-6.81826	2.36889	1.53108
H	-7.64898	0.38507	1.39542
C	-6.15567	3.37541	0.83724

H	-5.28986	4.03604	-1.01155
H	-7.08666	2.52439	2.57132
F	-5.85677	4.52829	1.47494
O	2.2305	-0.83376	-3.32624
H	2.6947	-1.6869	-3.42107
⁴TS-D_m			
Fe	3.83028	0.53887	0.4806
S	5.45476	1.65904	1.67843
H	5.44221	0.88162	2.78585
N	5.00198	-0.84124	-0.57217
C	6.39598	-2.61761	-1.02483
C	6.55129	-1.71328	-2.03517
H	6.8909	-3.57286	-0.90173
H	7.19697	-1.78369	-2.90149
N	3.89114	1.77539	-1.15557
C	4.75592	1.67252	-2.21802
C	4.63785	2.84717	-3.05461
C	3.69025	3.64489	-2.48898
H	5.19836	3.01564	-3.96535
H	3.31977	4.59858	-2.84314
N	2.12477	1.56987	1.13771
C	1.67544	2.76945	0.65405
C	1.42157	1.31456	2.28578
C	0.62465	3.27754	1.50809
C	0.46707	2.37558	2.51967
H	0.09049	4.20652	1.35253
H	-0.22084	2.42158	3.35468
N	3.42431	-0.91954	1.86252
C	2.71836	-1.96407	3.79111
H	2.15536	-2.13628	4.69993
C	2.56372	-0.8129	2.93037
C	5.4312	-2.05631	-0.10576
C	5.68228	-0.59732	-1.73577
C	3.21958	2.96497	-1.30129
C	1.63576	0.21362	3.11829
H	1.01266	0.14504	4.00585
C	5.01953	-2.6327	1.0982
H	5.45475	-3.59563	1.35116
C	5.57378	0.57506	-2.48819
H	6.1823	0.6354	-3.38599
C	2.19364	3.41715	-0.47055
H	1.7472	4.37297	-0.73031
C	3.66697	-2.76246	3.22374
H	4.03515	-3.71769	3.57669
C	4.10183	-2.10772	2.01039
C	-0.72791	-1.35321	-1.04136
C	-0.07859	-2.52943	-0.73035
C	-0.76816	-3.67289	-0.3647
C	-2.16004	-3.56781	-0.33591
C	-2.82301	-2.36428	-0.65505
C	-2.10449	-1.21019	-1.01907

C	1.4296	-1.0261	-1.26798
H	-0.26065	-4.59809	-0.11638
H	-2.77097	-4.42173	-0.06405
H	-2.57631	-0.26976	-1.26924
H	2.32145	-0.68564	-1.92329
O	0.23982	-0.40547	-1.32617
O	1.28828	-2.28762	-0.8269
O	-4.1822	-2.41626	-0.58472
C	-4.93196	-1.23421	-0.87721
H	-4.62305	-0.42118	-0.20756
H	-4.73521	-0.91903	-1.91241
C	-6.41	-1.55935	-0.68846
C	-6.70697	-1.99241	0.764
C	-7.32631	-0.39902	-1.17696
N	-8.13554	-1.83948	1.08574
H	-6.35351	-3.02763	0.88857
C	-8.82373	-0.82922	-1.02698
C	-9.01104	-2.02053	-0.0718
H	-9.40302	0.02183	-0.65612
H	-10.04767	-2.05181	0.28094
H	-8.39248	-2.47757	1.8338
H	-6.62619	-2.4122	-1.34594
H	-6.12561	-1.3727	1.46059
H	-8.83153	-2.97258	-0.60672
H	-9.23426	-1.09043	-2.00984
H	-7.12046	-0.28558	-2.2488
C	-7.00445	0.9525	-0.54352
C	-6.34908	1.9343	-1.3019
C	-7.33901	1.26149	0.78647
C	-6.02336	3.18111	-0.76433
H	-6.09268	1.72807	-2.33891
C	-7.02138	2.50159	1.34051
H	-7.85778	0.51591	1.38351
C	-6.3653	3.44353	0.5558
H	-5.52075	3.94201	-1.35262
H	-7.27774	2.74604	2.36659
F	-6.05742	4.64588	1.0892
O	2.04595	-1.1346	-3.2347
H	2.5063	-1.99477	-3.22827
²P-C_m			
Fe	-3.52761	0.38194	0.23658
S	-5.5153	1.27231	0.85074
H	-5.96533	1.64534	-0.36921
N	-4.42533	-0.87737	-1.06105
C	-5.39513	-1.79607	-2.94376
C	-5.56632	-2.68556	-1.92786
H	-5.71993	-1.87626	-3.9736
H	-6.06022	-3.64891	-1.95125
N	-3.70736	-0.97898	1.72926
C	-4.34477	-2.18818	1.64145
C	-4.31574	-2.85671	2.92309

C	-3.64889	-2.03599	3.77989
H	-4.75558	-3.82585	3.12254
H	-3.428	-2.19054	4.82856
N	-2.53239	1.59693	1.5042
C	-2.25143	1.37247	2.82729
C	-2.06435	2.85279	1.22001
C	-1.57807	2.51782	3.39395
C	-1.46388	3.43734	2.39747
H	-1.25224	2.59376	4.42378
H	-1.02337	4.42572	2.43778
N	-3.29454	1.72013	-1.26608
C	-2.75655	3.63295	-2.44036
H	-2.36637	4.6257	-2.62689
C	-2.70991	2.95627	-1.16406
C	-4.68594	-0.66592	-2.38985
C	-4.95756	-2.10268	-0.75399
C	-3.2732	-0.86352	3.02358
C	-2.138	3.48806	-0.01351
H	-1.71579	4.48596	-0.08431
C	-4.34658	0.47927	-3.10422
H	-4.62568	0.51702	-4.15305
C	-4.92447	-2.71537	0.49318
H	-5.3949	-3.69036	0.57803
C	-2.5807	0.22549	3.53995
H	-2.29676	0.18843	4.58727
C	-3.37802	2.78905	-3.31157
H	-3.60013	2.94566	-4.35976
C	-3.71129	1.59655	-2.56727
C	0.39456	-1.04337	-0.15922
C	-0.29313	-2.11213	-0.68303
C	0.34653	-3.27178	-1.09349
C	1.73035	-3.28475	-0.93835
C	2.43673	-2.18494	-0.3963
C	1.76919	-1.0176	0.01149
C	-1.75738	-0.53573	-0.18298
H	-0.19212	-4.11537	-1.50942
H	2.30937	-4.1531	-1.2334
H	2.2737	-0.15534	0.42585
O	-0.54847	-0.07841	0.15278
O	-1.63657	-1.7637	-0.67767
O	3.78161	-2.35895	-0.30121
C	4.57533	-1.30476	0.25323
H	4.45652	-0.39437	-0.34808
H	4.23456	-1.08847	1.27621
C	6.02803	-1.76811	0.26056
C	6.5362	-2.04698	-1.17071
C	6.94559	-0.78971	1.05102
N	8.00696	-2.02148	-1.22784
H	6.11607	-3.01028	-1.49931
C	8.39764	-1.37227	1.09304
C	8.64293	-2.4462	0.01846
H	9.11264	-0.55572	0.95421

H	9.71851	-2.55031	-0.1609
H	8.33382	-2.58361	-2.00873
H	6.0471	-2.71537	0.8161
H	6.14867	-1.28091	-1.85634
H	8.28664	-3.43202	0.37386
H	8.59474	-1.80394	2.08177
H	6.56139	-0.78325	2.07891
C	6.87163	0.65722	0.56839
C	6.17732	1.60698	1.33304
C	7.47649	1.08667	-0.62574
C	6.07427	2.94003	0.93058
H	5.71291	1.30489	2.2694
C	7.38422	2.41432	-1.04348
H	8.02441	0.3641	-1.22505
C	6.68217	3.32211	-0.25818
H	5.54205	3.67593	1.52458
H	7.84935	2.7521	-1.96425
F	6.59299	4.60877	-0.65884
O	-0.84201	0.16179	-2.89577
H	-0.8702	1.10774	-2.68383
H	-1.76508	-0.02759	-3.12967
⁴P-C_m			
Fe	-3.55767	0.39831	0.2193
S	-5.55616	1.33912	0.79761
H	-5.67221	2.2001	-0.23876
N	-4.46901	-1.11517	-0.93922
C	-5.53726	-2.2109	-2.64844
C	-5.65263	-2.98791	-1.53241
H	-5.92528	-2.40715	-3.64047
H	-6.15257	-3.94383	-1.43523
N	-3.69988	-0.78553	1.88178
C	-4.31307	-2.0084	1.94817
C	-4.24949	-2.48973	3.31354
C	-3.59219	-1.54367	4.04307
H	-4.65917	-3.43184	3.65616
H	-3.35801	-1.55927	5.1003
N	-2.44619	1.81893	1.32116
C	-2.18565	1.75769	2.65716
C	-2.00343	3.02198	0.85992
C	-1.51553	2.97787	3.06762
C	-1.40221	3.76039	1.95519
H	-1.19105	3.20265	4.0763
H	-0.96774	4.74952	1.87737
N	-3.38505	1.56975	-1.45326
C	-2.88004	3.29972	-2.87335
H	-2.49258	4.25294	-3.21137
C	-2.7787	2.79877	-1.51772
C	-4.79935	-1.02366	-2.25803
C	-4.98377	-2.28095	-0.45592
C	-3.24432	-0.46943	3.13475
C	-2.14377	3.46543	-0.46003

H	-1.73051	4.44334	-0.69192
C	-4.49629	0.07084	-3.07831
H	-4.8144	0.00511	-4.1154
C	-4.89718	-2.69781	0.87746
H	-5.34872	-3.65673	1.11679
C	-2.54322	0.69029	3.48998
H	-2.26456	0.77689	4.53669
C	-3.54336	2.35529	-3.60345
H	-3.80017	2.38453	-4.65517
C	-3.85484	1.26272	-2.70471
C	0.42521	-1.06973	-0.1077
C	-0.25946	-2.15263	-0.60559
C	0.382	-3.32274	-0.98274
C	1.76495	-3.33019	-0.8226
C	2.4689	-2.21521	-0.30816
C	1.7994	-1.03838	0.06747
C	-1.72561	-0.56249	-0.16071
H	-0.15488	-4.17736	-1.37789
H	2.34597	-4.20524	-1.09292
H	2.30213	-0.16493	0.46
O	-0.52062	-0.09672	0.17164
O	-1.60318	-1.80442	-0.61537
O	3.81351	-2.38555	-0.20743
C	4.60856	-1.31383	0.31075
H	4.48137	-0.4209	-0.31451
H	4.27624	-1.07045	1.3304
C	6.0625	-1.77354	0.31651
C	6.55705	-2.0882	-1.11232
C	6.98558	-0.7741	1.07343
N	8.02701	-2.06038	-1.1851
H	6.13624	-3.0608	-1.41123
C	8.43951	-1.35229	1.11463
C	8.67611	-2.45264	0.06514
H	9.15077	-0.53779	0.94722
H	9.75004	-2.55964	-0.12216
H	8.3474	-2.64126	-1.95489
H	6.0887	-2.70638	0.89571
H	6.16047	-1.3412	-1.81369
H	8.32476	-3.42965	0.44856
H	8.64842	-1.75813	2.11185
H	6.61169	-0.74339	2.10467
C	6.90343	0.66032	0.55632
C	6.21926	1.62865	1.3066
C	7.49105	1.05967	-0.6567
C	6.1096	2.95109	0.87205
H	5.76855	1.35012	2.25684
C	7.39181	2.37622	-1.1066
H	8.03135	0.32223	-1.24469
C	6.70021	3.3032	-0.33456
H	5.58522	3.70153	1.45472
H	7.84356	2.69086	-2.0421
F	6.6044	4.57931	-0.76624

O	-0.83933	0.06321	-2.88767
H	-0.90643	1.01547	-2.71557
H	-1.75019	-0.1707	-3.12834
²TS-D_N			
Fe	2.87151	-0.60095	0.25833
S	4.52689	-1.93401	0.97808
H	4.34081	-2.95312	0.10859
N	3.42937	-0.80827	-1.6669
C	3.73061	-1.62658	-3.80824
C	4.59864	-0.58948	-3.65015
H	3.5809	-2.25375	-4.67782
H	5.30697	-0.18842	-4.36396
N	4.07199	1.00792	0.45885
C	4.96311	1.47365	-0.47651
C	5.72928	2.57078	0.06597
C	5.3013	2.75546	1.34461
H	6.49442	3.11396	-0.47411
H	5.64176	3.48093	2.07254
N	2.20967	-0.30049	2.13856
C	2.63285	0.64821	3.03836
C	1.32118	-1.09666	2.81858
C	1.96921	0.46538	4.30685
C	1.1565	-0.61779	4.17124
H	2.12672	1.08608	5.17984
H	0.50677	-1.07036	4.90972
N	1.61478	-2.15484	0.03154
C	0.11935	-3.85538	0.4947
H	-0.57294	-4.46025	1.06632
C	0.82037	-2.70267	1.00889
C	3.0148	-1.76436	-2.56419
C	4.41202	-0.08875	-2.30936
C	4.27394	1.77079	1.58412
C	0.67224	-2.21015	2.29945
H	-0.002	-2.74568	2.96089
C	2.075	-2.75269	-2.30293
H	1.8415	-3.44775	-3.10349
C	5.11916	0.97545	-1.76346
H	5.86386	1.45151	-2.39398
C	3.5909	1.62093	2.7853
H	3.84426	2.29891	3.59457
C	0.50042	-4.00081	-0.8043
H	0.19176	-4.75372	-1.51852
C	1.43715	-2.93897	-1.08394
O	1.31836	1.3761	-2.21717
C	-1.37872	1.12289	-1.02417
C	-0.2708	0.27245	-0.35883
C	-1.20182	2.66576	-0.76805
N	1.06636	0.84239	-0.29176
H	-0.52066	0.09545	0.70187
C	-0.17383	2.89993	0.35847
C	1.12764	2.18519	0.03642

H	0.01894	3.97217	0.47241
H	1.43848	2.34241	-1.20717
H	2.20835	1.02918	-2.41868
H	-0.21378	-0.70284	-0.833
H	-0.56573	2.54586	1.32484
H	-1.28188	0.95525	-2.10104
H	-0.73501	3.0556	-1.67883
H	2.00692	2.43908	0.62543
C	-2.49667	3.44735	-0.58313
C	-3.09497	4.06342	-1.69367
C	-3.12888	3.59025	0.66235
C	-4.28177	4.78759	-1.58032
H	-2.61994	3.97862	-2.66826
C	-4.31593	4.3118	0.79873
H	-2.69243	3.14017	1.54926
C	-4.87614	4.89946	-0.32909
H	-4.74171	5.26576	-2.43901
H	-4.80387	4.4259	1.76132
F	-6.0222	5.6013	-0.20449
C	-2.74515	0.57798	-0.59956
H	-2.92469	0.73895	0.47418
H	-3.54591	1.08453	-1.15192
O	-2.75629	-0.81734	-0.88554
C	-3.87119	-1.54739	-0.57077
C	-5.0573	-0.97566	-0.0646
C	-3.76835	-2.92823	-0.78721
C	-6.09668	-1.85166	0.19732
H	-5.17053	0.08617	0.1113
C	-4.84203	-3.78858	-0.51477
H	-2.82837	-3.31647	-1.1643
C	-6.00068	-3.21985	-0.01947
H	-4.76625	-4.85681	-0.68723
O	-7.35167	-1.5424	0.66554
O	-7.2006	-3.8262	0.29838
C	-7.9849	-2.80448	0.91558
H	-8.98744	-2.79847	0.4785
H	-8.03204	-2.97734	2.00116
⁴TS-D_N			
Fe	3.19414	-0.63365	0.1804
S	5.14812	-2.05677	0.4872
H	5.1342	-2.0182	1.83913
N	3.68742	-0.20126	-1.72458
C	4.06769	-0.41138	-3.99347
C	4.80774	0.64813	-3.55908
H	3.98644	-0.80926	-4.99686
H	5.45652	1.29699	-4.13335
N	4.08331	1.07878	0.78004
C	4.88235	1.9001	0.01881
C	5.45699	2.9373	0.83811
C	5.00685	2.7319	2.10648
H	6.11959	3.71234	0.47459

H	5.22423	3.30271	3.00034
N	2.43877	-0.86765	2.02909
C	2.73586	-0.12247	3.14792
C	1.60634	-1.87672	2.45845
C	2.08552	-0.68106	4.30439
C	1.38624	-1.77019	3.87703
H	2.16101	-0.27952	5.30698
H	0.76891	-2.44501	4.45627
N	1.96656	-2.09098	-0.4902
C	0.57264	-3.93467	-0.55441
H	-0.08588	-4.71278	-0.19008
C	1.19501	-2.93309	0.27546
C	3.37625	-0.93771	-2.84741
C	4.56833	0.77407	-2.1463
C	4.15933	1.56647	2.06391
C	1.02783	-2.84472	1.64903
H	0.38874	-3.58096	2.12596
C	2.51545	-2.02534	-2.88239
H	2.35017	-2.50333	-3.84259
C	5.12115	1.75921	-1.34031
H	5.78888	2.47443	-1.80988
C	3.53463	1.01257	3.17206
H	3.68474	1.50026	4.1301
C	0.98263	-3.69697	-1.83065
H	0.73173	-4.24019	-2.73277
C	1.85895	-2.55273	-1.78053
O	1.08009	1.73769	-1.91314
C	-1.66964	1.2167	-0.84186
C	-0.50818	0.38971	-0.23639
C	-1.57096	2.74576	-0.479
N	0.77588	1.0403	-0.07156
H	-0.76385	0.09951	0.79932
C	-0.60885	2.95705	0.71085
C	0.74349	2.33951	0.3916
H	-0.49107	4.0282	0.90886
H	1.10075	2.61042	-0.83428
H	2.00126	1.4423	-2.04547
H	-0.36684	-0.53472	-0.79366
H	-1.02305	2.5119	1.62974
H	-1.57204	1.13114	-1.92863
H	-1.07925	3.21053	-1.34015
H	1.58788	2.57581	1.04344
C	-2.91042	3.45394	-0.31825
C	-3.50003	4.07363	-1.43163
C	-3.59494	3.5221	0.90542
C	-4.72768	4.72954	-1.34192
H	-2.98524	4.04581	-2.3892
C	-4.82339	4.17554	1.01834
H	-3.16721	3.06736	1.79412
C	-5.37273	4.76927	-0.11147
H	-5.18093	5.21071	-2.20252
H	-5.35157	4.23263	1.96465

F	-6.55887	5.40558	-0.00972
C	-3.00223	0.57256	-0.45197
H	-3.18684	0.66071	0.62961
H	-3.83393	1.06065	-0.97409
O	-2.93171	-0.80296	-0.81767
C	-4.00122	-1.61425	-0.54977
C	-5.21167	-1.14737	0.00418
C	-3.8247	-2.96855	-0.86461
C	-6.19742	-2.09672	0.21175
H	-5.38179	-0.10836	0.25469
C	-4.84526	-3.90526	-0.64462
H	-2.87125	-3.2751	-1.28171
C	-6.02764	-3.43893	-0.10079
H	-4.71261	-4.95265	-0.89354
O	-7.46186	-1.89176	0.71016
O	-7.18757	-4.13308	0.1837
C	-8.02518	-3.20098	0.86931
H	-9.02733	-3.21855	0.4313
H	-8.06176	-3.45204	1.93981
²P-C_N			
Fe	-2.56324	-0.70379	0.5556
S	-4.02627	-1.59417	2.01636
H	-4.26993	-2.75353	1.3633
N	-1.54313	-2.43339	0.40062
C	-0.82447	-4.52601	-0.25768
C	-0.1282	-4.19556	0.86913
H	-0.76357	-5.43312	-0.84583
H	0.62151	-4.77665	1.39151
N	-1.3806	-0.11591	2.08235
C	-0.45283	-0.89369	2.72947
C	0.13435	-0.15725	3.82544
C	-0.44752	1.07318	3.82888
H	0.89389	-0.54576	4.49214
H	-0.26963	1.90151	4.50306
N	-3.51528	1.07407	0.64335
C	-3.25676	2.12048	1.49221
C	-4.62873	1.43078	-0.07509
C	-4.21872	3.17907	1.28613
C	-5.07532	2.74722	0.32105
H	-4.2328	4.11482	1.83076
H	-5.93467	3.2578	-0.09518
N	-3.69048	-1.25005	-1.02131
C	-5.37693	-1.31692	-2.59852
H	-6.25048	-1.0001	-3.15442
C	-4.78249	-0.57639	-1.50951
C	-1.71396	-3.42279	-0.534
C	-0.58559	-2.88678	1.27386
C	-1.40316	1.08389	2.74527
C	-5.22981	0.66453	-1.06704
H	-6.10786	1.07898	-1.55313
C	-2.64558	-3.40148	-1.56609

H	-2.67336	-4.25704	-2.23373
C	-0.08602	-2.183	2.36538
H	0.67242	-2.6738	2.96766
C	-2.25321	2.1455	2.45381
H	-2.1684	3.03769	3.067
C	-4.62809	-2.44154	-2.76517
H	-4.76221	-3.24131	-3.48259
C	-3.58454	-2.39819	-1.76788
C	6.56967	-0.45116	0.17408
C	6.94987	-1.78735	0.20915
C	6.06816	-2.79548	-0.1319
C	4.77069	-2.41696	-0.50931
C	4.39414	-1.06956	-0.5321
C	5.29892	-0.04437	-0.19256
C	8.65316	-0.56082	0.96896
H	6.3683	-3.83753	-0.12099
H	4.04129	-3.16173	-0.81075
H	5.03428	1.00496	-0.20588
H	8.72778	-0.50809	2.06507
H	9.60414	-0.29534	0.49919
O	7.6342	0.34452	0.52108
O	8.2773	-1.88124	0.57407
O	3.08424	-0.82288	-0.88728
C	2.70221	0.50123	-1.26439
H	2.82653	1.18507	-0.41519
H	3.34998	0.84999	-2.08168
C	1.24097	0.45856	-1.71033
C	0.31493	0.13456	-0.53049
C	0.81096	1.76336	-2.43475
N	-1.11989	0.20949	-0.83272
H	0.51359	-0.87584	-0.17104
C	-0.66013	1.58259	-2.86254
C	-1.51645	0.8498	-1.86324
H	-1.13107	2.55062	-3.07589
H	-2.58972	0.86443	-2.04462
H	1.14756	-0.35797	-2.43956
H	0.50517	0.80861	0.31347
H	-0.71013	1.01496	-3.80387
H	1.41356	1.83833	-3.34836
C	1.06628	3.03905	-1.63897
C	2.17593	3.83746	-1.95847
C	0.23731	3.46081	-0.58546
C	2.46682	5.00658	-1.25496
H	2.82562	3.54484	-2.78017
C	0.51104	4.62752	0.12914
H	-0.64096	2.88601	-0.3077
C	1.6253	5.38293	-0.2154
H	3.32296	5.62433	-1.50559
H	-0.12923	4.95178	0.94281
F	1.89286	6.51267	0.47159
O	1.67153	-3.09062	-2.06723
H	1.11628	-3.44259	-1.35262

H	2.13193	-2.33363	-1.66676
⁴ P-C _N			
Fe	-2.57478	-0.73076	0.54405
S	-4.03963	-1.69997	2.04676
H	-4.97483	-2.10174	1.15668
N	-1.46867	-2.5148	0.28629
C	-0.84824	-4.61168	-0.40823
C	-0.09287	-4.30638	0.69161
H	-0.83082	-5.52156	-0.99539
H	0.65664	-4.92092	1.17509
N	-1.38525	-0.23169	2.11476
C	-0.43763	-1.03455	2.70134
C	0.11388	-0.34815	3.85103
C	-0.51362	0.85882	3.93762
H	0.88492	-0.74841	4.49742
H	-0.35992	1.64035	4.67127
N	-3.52818	1.15732	0.64978
C	-3.29237	2.10996	1.59713
C	-4.61797	1.54933	-0.07152
C	-4.25113	3.18847	1.44154
C	-5.07439	2.83946	0.41059
H	-4.29626	4.07828	2.05744
H	-5.92109	3.38934	0.01843
N	-3.74397	-1.21022	-1.04759
C	-5.41461	-1.20747	-2.62496
H	-6.26814	-0.86183	-3.19484
C	-4.80089	-0.4789	-1.53473
C	-1.72501	-3.47998	-0.64091
C	-0.50639	-2.98734	1.13031
C	-1.46379	0.92623	2.84613
C	-5.20237	0.78828	-1.09046
H	-6.06482	1.21984	-1.59098
C	-2.72961	-3.39714	-1.6125
H	-2.82075	-4.24081	-2.29084
C	-0.02824	-2.29424	2.24934
H	0.74156	-2.7868	2.83678
C	-2.3178	2.00848	2.59678
H	-2.24354	2.84212	3.28985
C	-4.71316	-2.36639	-2.77983
H	-4.88081	-3.1572	-3.50036
C	-3.66329	-2.36892	-1.78283
C	6.60356	-0.41909	0.20417
C	6.98719	-1.75474	0.21406
C	6.10792	-2.75861	-0.14532
C	4.80933	-2.37649	-0.5154
C	4.42919	-1.02991	-0.51265
C	5.33154	-0.00898	-0.15404
C	8.68745	-0.53837	0.99638
H	6.41091	-3.79986	-0.15432
H	4.08235	-3.11727	-0.83211
H	5.06343	1.03955	-0.14696

H	8.76152	-0.50633	2.09336
H	9.63797	-0.26156	0.53222
O	7.66643	0.37271	0.56537
O	8.31524	-1.85194	0.57623
O	3.1186	-0.77908	-0.86148
C	2.74035	0.54648	-1.23915
H	2.85653	1.22867	-0.38736
H	3.3961	0.89657	-2.04946
C	1.28393	0.50162	-1.69917
C	0.34433	0.17838	-0.53029
C	0.85337	1.80222	-2.43119
N	-1.08381	0.23183	-0.859
H	0.54803	-0.8254	-0.15548
C	-0.60857	1.60552	-2.88438
C	-1.47169	0.86091	-1.89897
H	-1.08712	2.56837	-3.10452
H	-2.54243	0.8577	-2.0985
H	1.20026	-0.31742	-2.42687
H	0.5117	0.86403	0.30999
H	-0.63647	1.03852	-3.82696
H	1.47087	1.8846	-3.33417
C	1.07984	3.07978	-1.62952
C	2.19736	3.88063	-1.91345
C	0.21487	3.50168	-0.60543
C	2.46126	5.052	-1.20315
H	2.87485	3.58861	-2.71259
C	0.46083	4.67093	0.11527
H	-0.67064	2.92429	-0.35752
C	1.58409	5.42848	-0.19349
H	3.32356	5.67169	-1.42639
H	-0.20789	4.99584	0.90547
F	1.82525	6.5608	0.49911
O	1.72409	-3.03893	-2.10093
H	1.14919	-3.42745	-1.42162
H	2.16023	-2.29259	-1.65602