Supporting Information

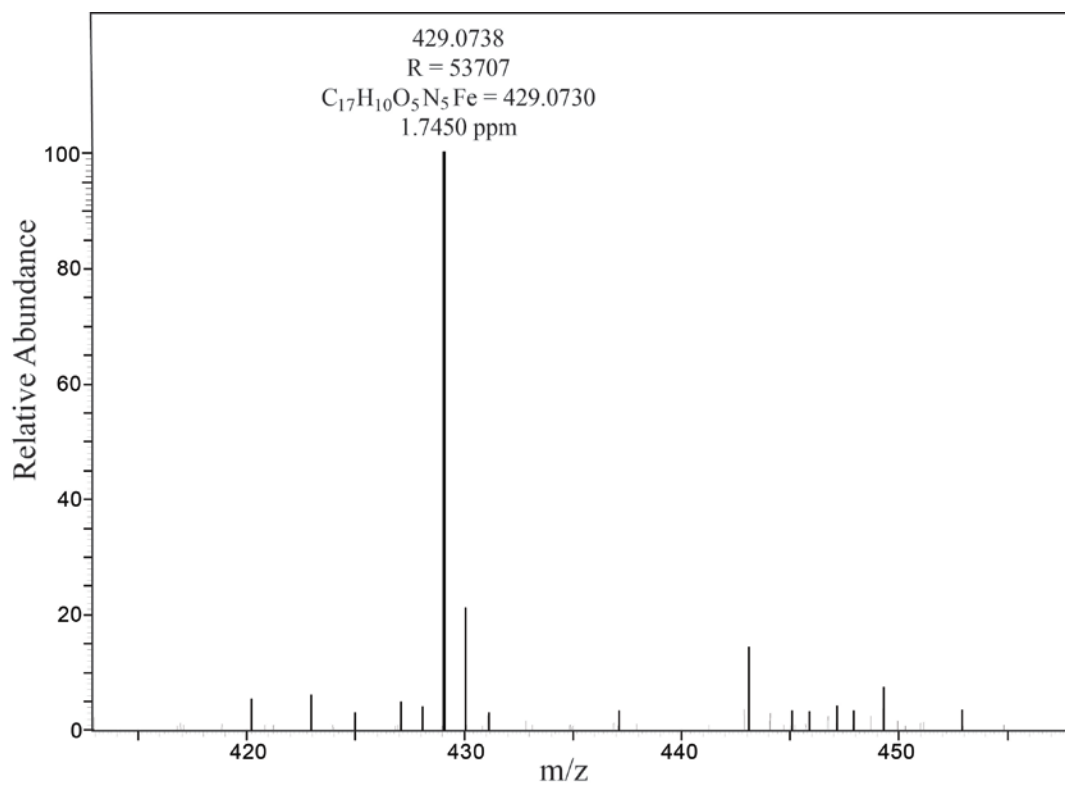# Tuning the Reactivity of Fe$^\text{V}$(O) Towards C-H bonds at Room Temperature: Effect of Water

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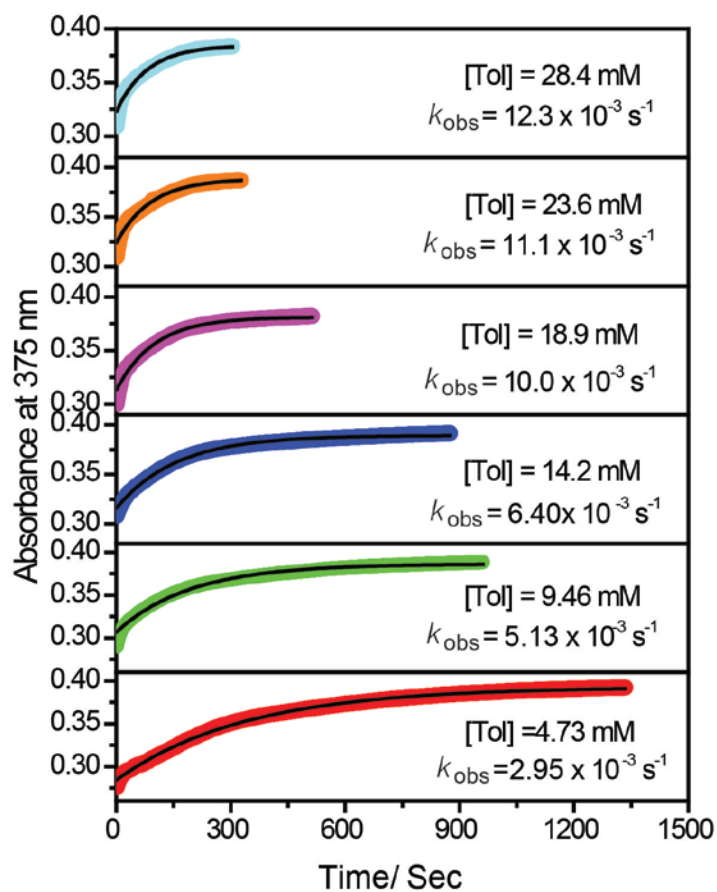[a]Chemical Engineering Division, CSIR-National Chemical Laboratory, Pune 411008, India; [b]Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune 411008, India; [c]Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, PA, USA

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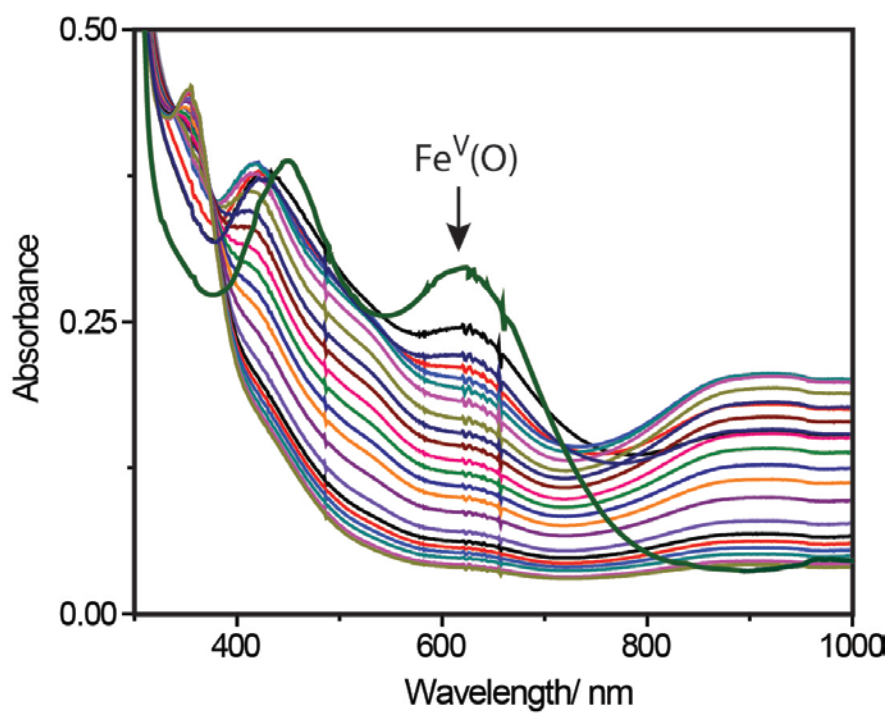
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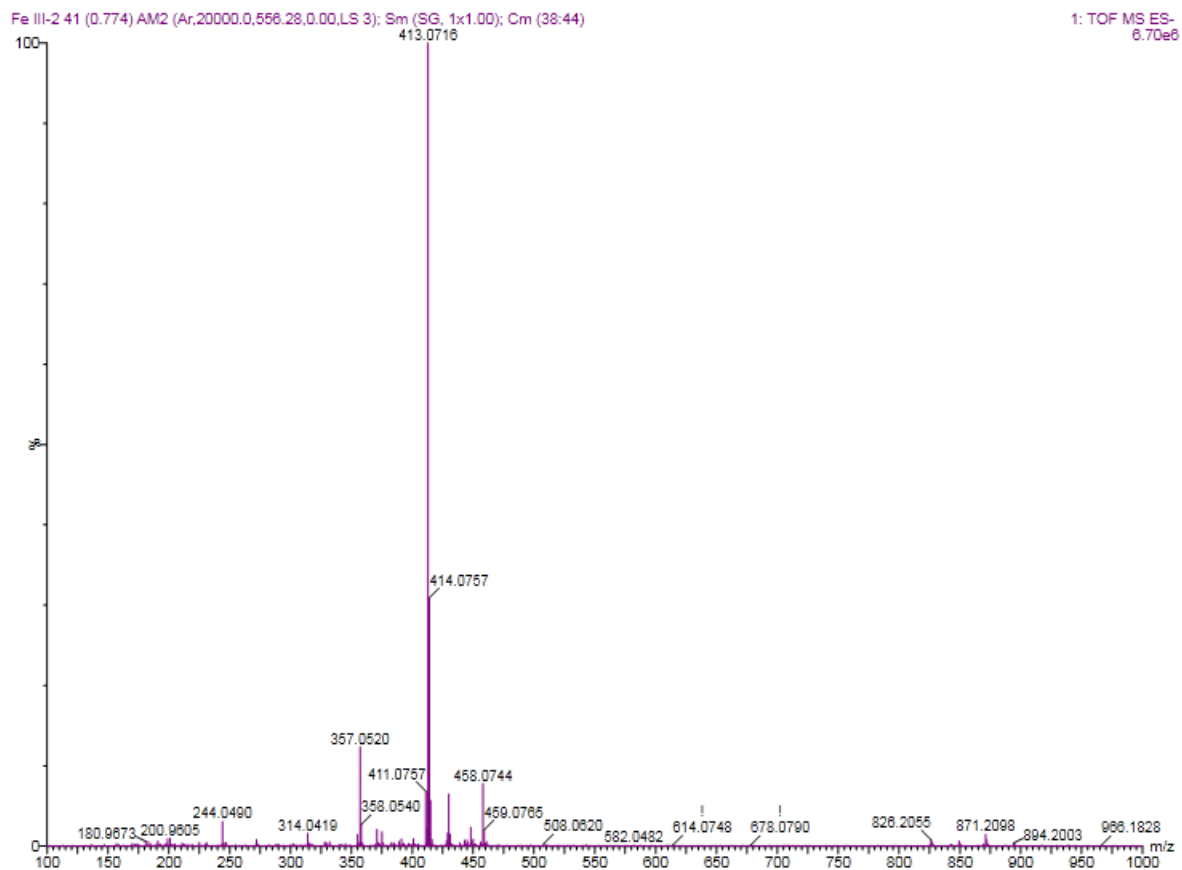
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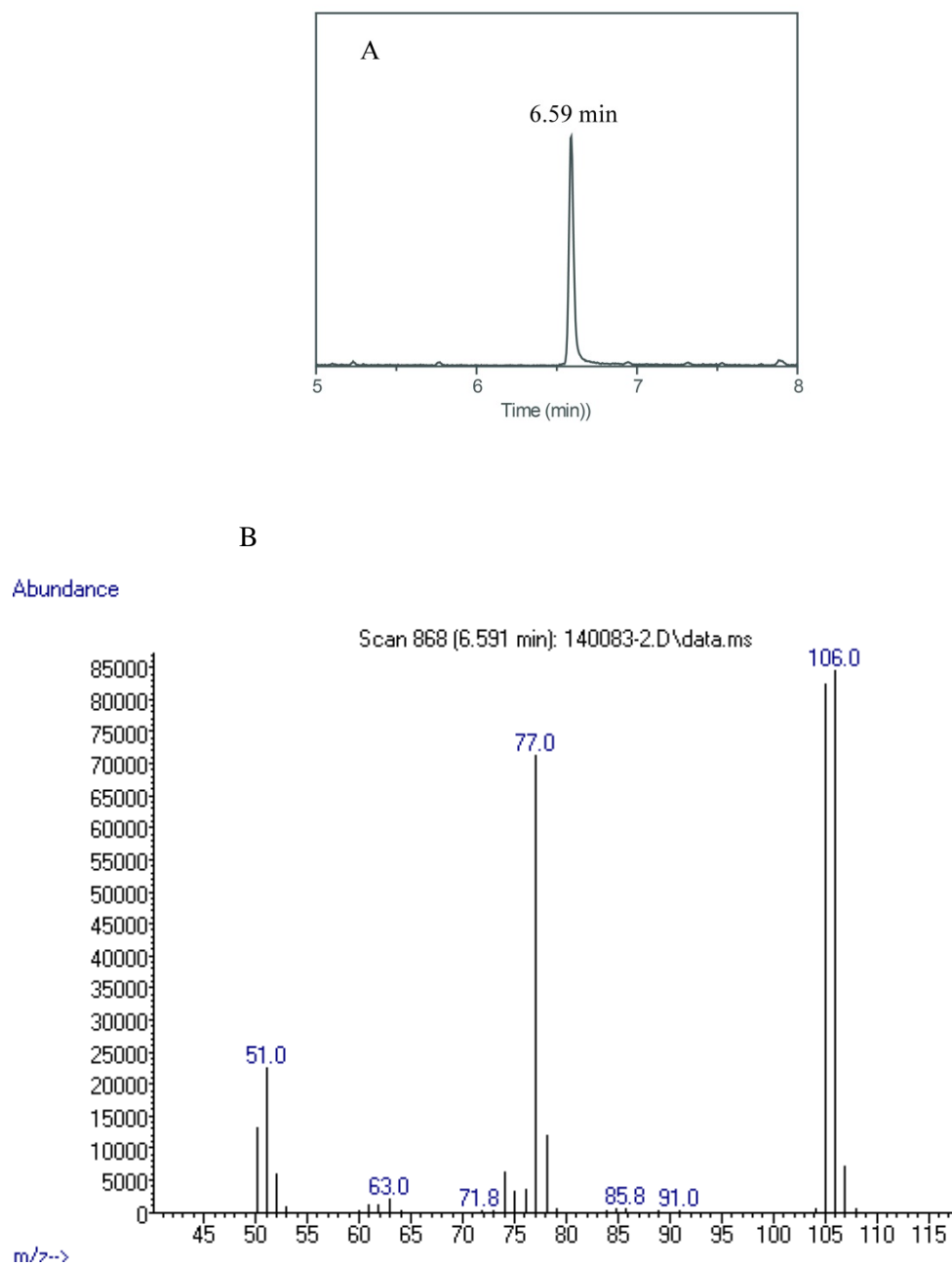
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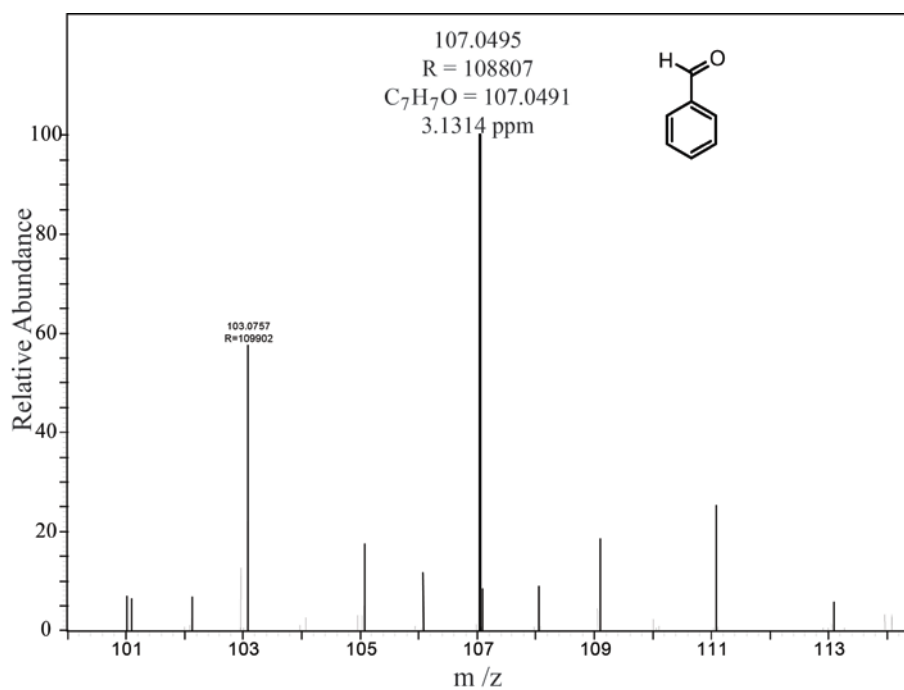
Figure SI 6. The HR-MS spectra of benzaldehyde obtained after reaction with Toluene (1000 equiv) and **2** (10^{-4} M) in 30 % H_2O-CH_3CN mixture.

A

$k_{2(\text{Toluene})} = 1.39 \text{ M}^{-1}\text{s}^{-1}$

$k_{\text{H}} / k_{\text{D}} = 13$

$k_{2(\text{Toluene-d}_8)} = 0.12 \text{ M}^{-1}\text{s}^{-1}$

$k_{\text{obs}} / \text{s}^{-1}$

[Toluene]/ M

B

$k_{2(\text{Toluene})} = 19.6 \text{ M}^{-1}\text{s}^{-1}$

$k_{\text{H}} / k_{\text{D}} = 9$

$k_{2(\text{Toluene-d}_8)} = 2.2 \text{ M}^{-1}\text{s}^{-1}$

$k_{\text{obs}} / \text{s}^{-1}$
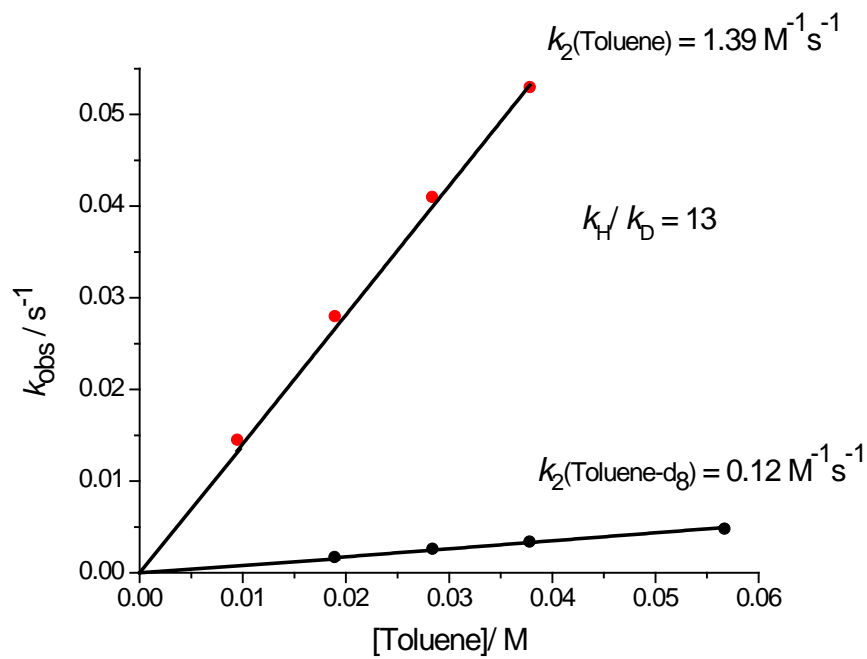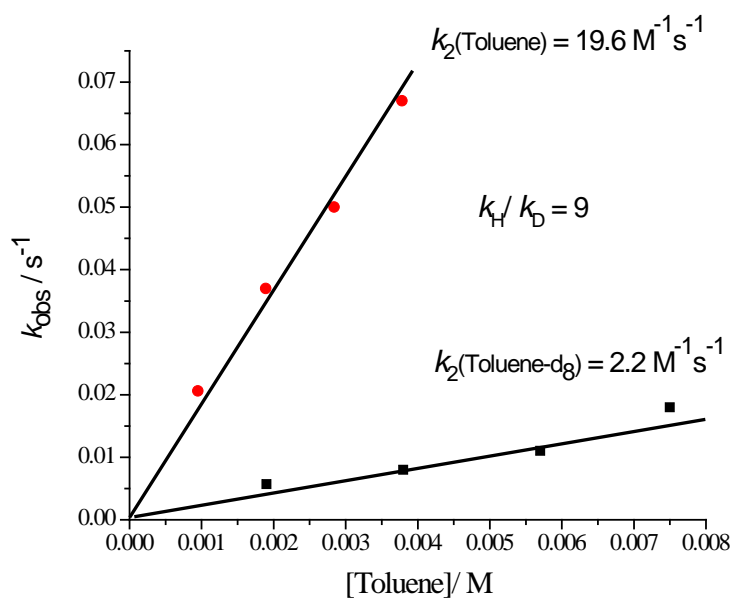
[Toluene]/ M

Figure SI 7. Plot of k_{obs} vs. [toluene] (red dots) and [d_8-toluene-] (black dots) showing pronounce KIE at 25 ^{o}C (A) in 50% H_2O-CH_3CN mixture; (B) in 70% H_2O-CH_3CN mixture.
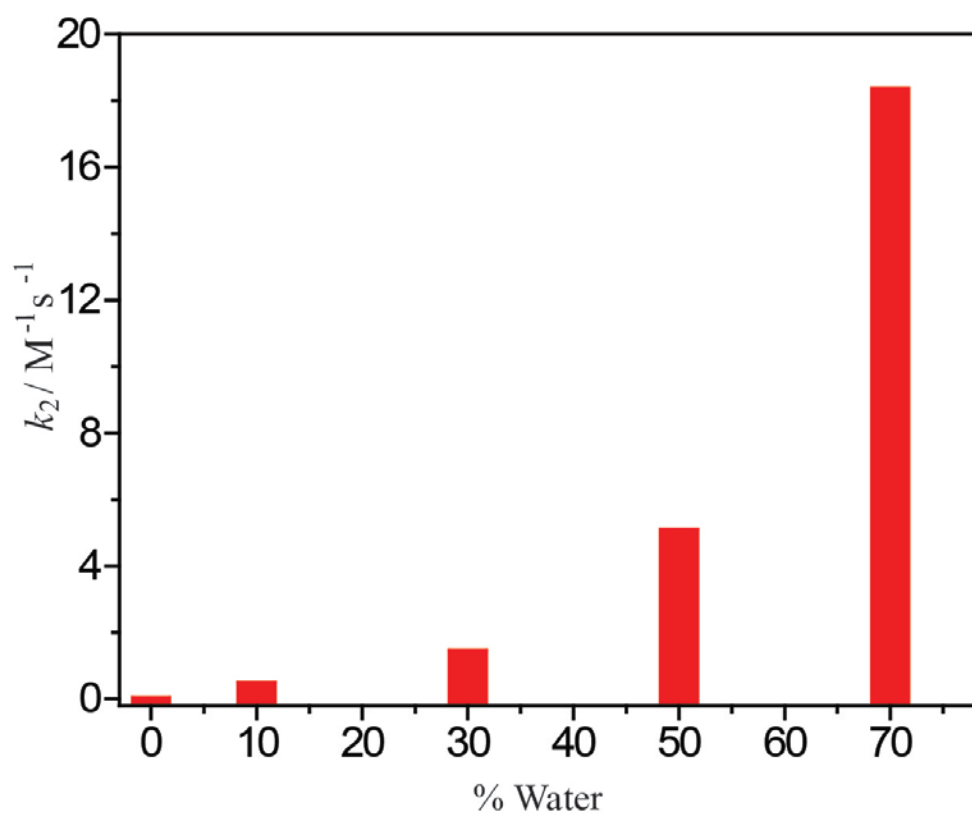
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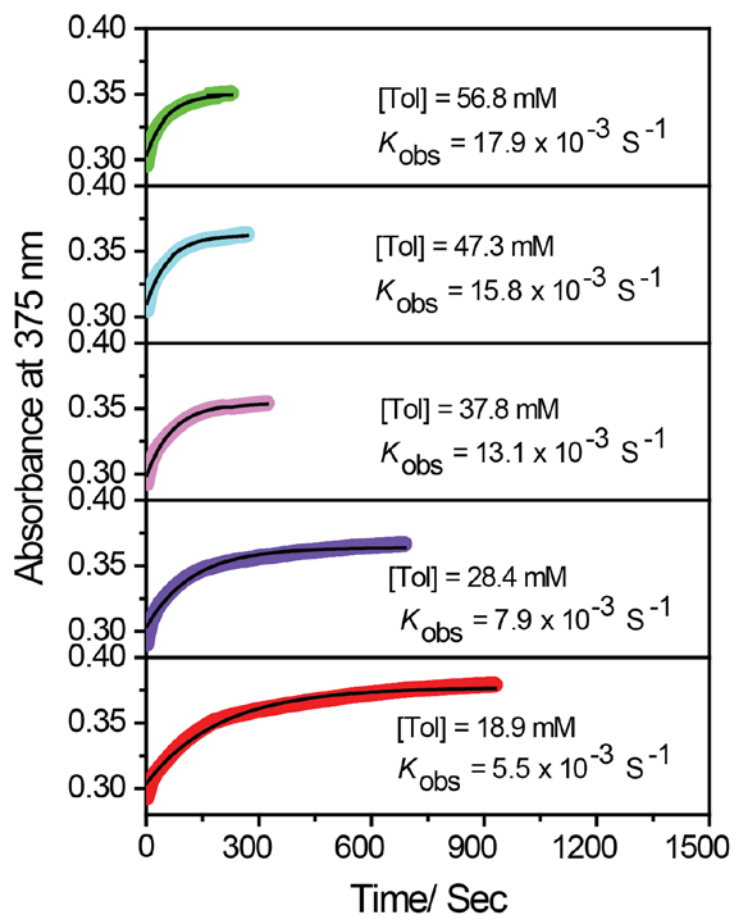
Figure SI 9. Kinetic traces for reaction of **2** with toluene at various toluene concentrations in 30% D_2O-CH_3CN. The kinetic traces were fitted to the equation, $[(A_t = A_\alpha - (A_\alpha - A_o)e^{(-k_{obs}t)}]$ for obtaining k_{obs} values (black line).
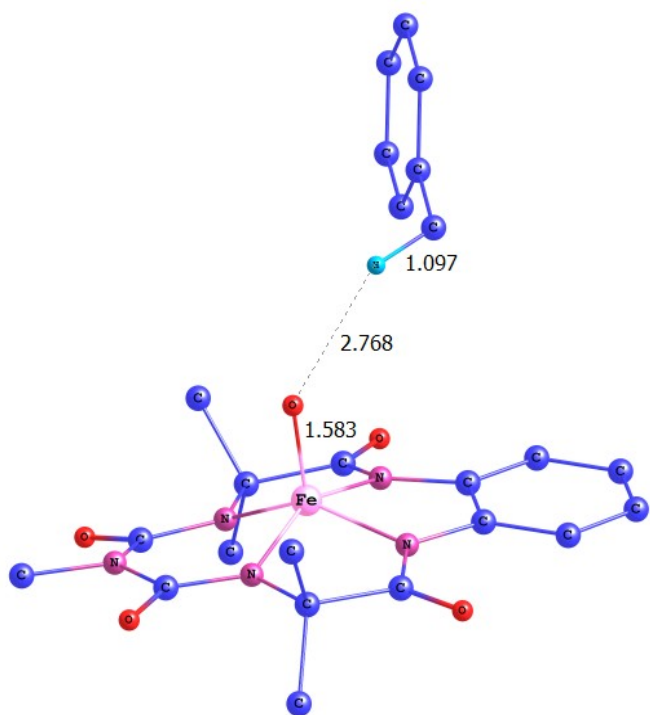
(i)
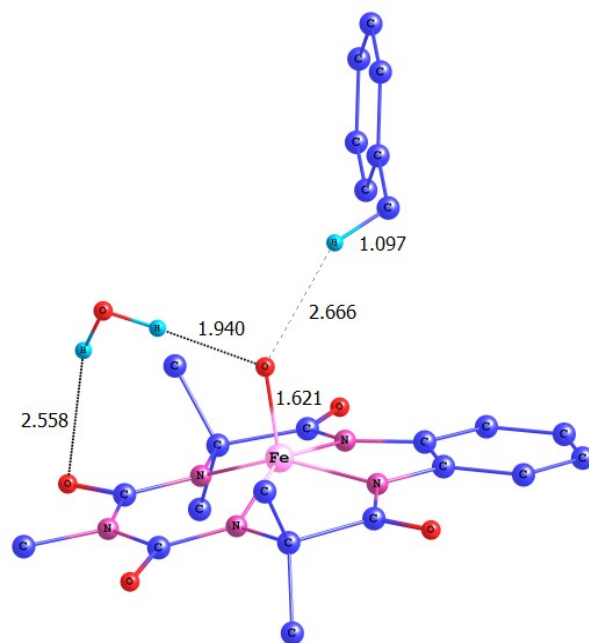
(ii)
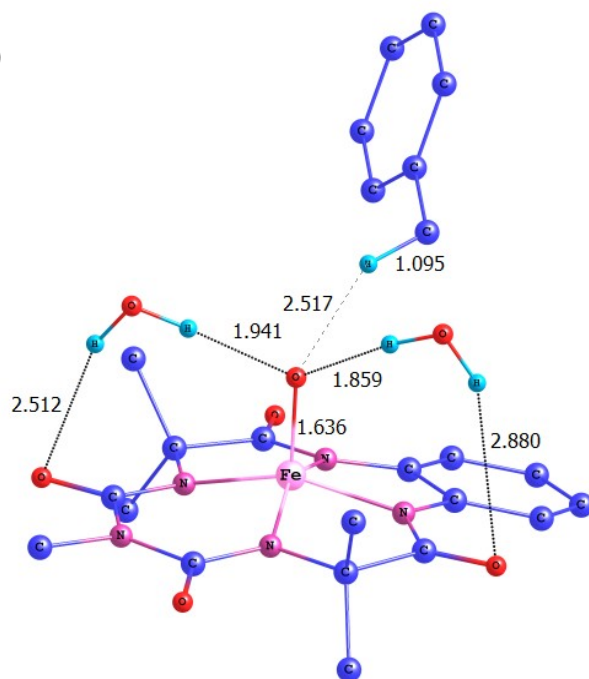
(iii)

Figure SI 10. (i), (ii), and (iii) are UB3LYP optimized reactant structures with none, one and two explicitly added water molecules respectively; all the atom-atom distances are in Å.

Table SI 1. Rate constant (k_2) values for toluene oxidation in CH_3CN and in 70 % of H_2O-CH_3CN mixture at different temperature.

Temperature/ Kelvin	$k_2(CH_3CN)/ M^{-1}s^{-1}$	$k_2(70\% H_2O)/ M^{-1}s^{-1}$
283	0.04	5.40
288	0.08	9.40
293	0.13	14.3
300	0.25	19.6

Table SI 2. The relative gas phase energies of the $Fe^V(O)$ (**2**) catalyst in doublet ($S = 1/2$) and quartet ($S = 3/2$) electronic states in kcal/mol at the UB3LYP/6-31G*, LANL2DZ (Fe) and ROM062X/6-31G*, LANL2DZ (Fe) level of theories.

	ΔE (UB3LYP)	$\Delta(E+ZPE)$ (UB3LYP)	ΔG (UB3LYP)	ΔE (ROM062X)
$S = 1/2$	0.0	0.0	0.0	0.0
$S = 3/2$	12.4	11.2	9.4	6.0

The energy values indicate that the $Fe^V(O)$ (**2**) complex is significantly more stable in the doublet electronic state than the quartet.

Table SI 3. The relative gas phase reaction energies in kcal/mol at the UB3LYP/6-31G*, LANL2DZ (Fe) level of theory for toluene hydroxylation catalyzed by $Fe^V(O)$ (**2**).

	R	TS1	I	TS2	P
ΔE^a	0.0	17.2	4.1	11.2	-15.1
$\Delta(E+ZPE)^a$	0.0	13.1	1.9	9.5	-14.0
ΔG^a	0.0	15.2	1.9	11.8	-12.8
ΔE^b	0.0	32.8	1.3	4.1	-41.9
$\Delta(E+ZPE)^b$	0.0	28.8	-0.2	2.2	-39.7
ΔG^b	0.0	30.6	-1.4	2.0	-38.2
ΔE^c	0.0	17.2	4.3	7.1	-38.8
$\Delta(E+ZPE)^c$	0.0	13.1	2.0	4.3	-37.5
ΔG^c	0.0	15.2	0.1	3.5	-36.8

a. $S = 1/2$ spin state; b. $S = 3/2$ spin state; c. most favorable energy profile when the spin flip occurs at an intermediate state.

These energy values clearly indicate that the intermediate in quartet state is more stable than the doublet state. This result is further confirmed by the separate optimization of the intermediate complex $Fe^{IV}(OH)$ radical in singlet and triplet spin states. The energy values are summarized in Table SI 4.

Table SI 4. The relative gas phase energies of the intermediate complex $Fe^{IV}(OH)$ in singlet and triplet electronic states in kcal/mol at the UB3LYP/6-31G*, LANL2DZ (Fe) and ROM062X/6-31G*, LANL2DZ (Fe) level of theories. Values outside the parenthesis are in gas phase and inside the parenthesis are in solvent phase.

	ΔE (UB3LYP)	Δ(E+ZPE) (UB3LYP)	ΔG (UB3LYP)	ΔE (ROM062X)
$S = 0$	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
$S = 1$	-15.5 (-15.6)	-16.2 (-16.3)	-17.8 (-17.3)	-18.7 (-18.5)

Table SI 5 The relative reaction energies in kcal/mol for the rate determining step of toluene hydroxylation catalyzed by $Fe^V(O)$ (**2**) in dielectric continuum of acetonitrile and water at the CPCM/UB3LYP/6-31G*, LANL2DZ (Fe) and CPCM/ROM062X/6-31G*, LANL2DZ (Fe) level of theories.

	ΔE (UB3LYP)	Δ(E+ZPE) (UB3LYP)	ΔG (UB3LYP)	ΔE (ROM062X)
$^2R^a$	0.0	0.0	0.0	0.0
$^2TS1^a$	17.2	13.1	15.2	23.3
$^4I^a$	4.3	2.0	3.4	-5.3
$^2R^b$	0.0	0.0	0.0	0.0
$^2TS1^b$	13.8	9.9	11.7	18.7
$^4I^b$	1.1	-0.8	-0.9	-17.9
$^2R^c$	0.0	0.0	0.0	0.0
$^2TS1^c$	13.7	10.0	12.3	17.5
$^4I^c$	1.0	-0.9	-0.9	-18.0

a. gas phase; b. in dielectric continuum of acetonitrile; c. in dielectric continuum of water

A marginal effect of solvent dielectric changing from pure acetonitrile to water on the rate determining barrier (RDB) at both UB3LYP and ROM062X level of theories are suggestive of a diminutive role of bulk solvation (macrosolvation) in the rate enhancement of the hydroxylation reaction with rising water concentration.

Table SI 6. The relative gas phase reaction energies in kcal/mol for the rate determining step of toluene hydroxylation catalyzed by $Fe^V(O)$ (**2**) with explicitly added water molecules at the UB3LYP/6-31G*, LANL2DZ (Fe) and ROM062X/6-31G*, LANL2DZ (Fe) level of theories.

	ΔE (UB3LYP)	$\Delta(E+ZPE)$ (UB3LYP)	ΔG (UB3LYP)	ΔE (ROM062X)
$^2R^a$	0.0	0.0	0.0	0.0
$^2TS1^a$	17.2	13.1	15.2	23.3
$^4I^a$	4.3	2.0	3.4	-5.3
$^2R^b$	0.0	0.0	0.0	0.0
$^2TS1^b$	16.1	13.0	16.3	14.0
$^4I^b$	2.5	1.2	2.7	-21.9
$^2R^c$	0.0	0.0	0.0	0.0
$^2TS1^c$	15.4	12.6	15.1	11.2
$^4I^c$	0.9	0.1	0.2	-24.6

a. With no explicit water; b. with one explicit water; c. with two explicit water molecules

A clear decrease (by 9.3 kcal/mol) in the rate determining barrier (RDB) at the ROM062X level, which is known to provide a better treatment of the hydrogen bond, on inclusion of one explicit water and a further decrease of 2.8 kcal/mol on inclusion of the second explicit water are indicative that solute-solvent interactions through hydrogen bonding (microsolvation) is the main reason for the rate enhancement of the hydroxylation reaction with increase in the relative water concentration.

Table SI 7. Fe-O distances (in Å) in water bound reactant, transition state and intermediate structures obtained by geometry optimization at the UB3LYP/6-31G*, LANL2DZ (Fe) level of theory.

	Gas phase	CH$_3$CN dielectric	Water dielectric	1 H$_2$O explicit	2H$_2$O explicit	3H$_2$O explicit
^{2}R	1.583	1.590	1.590	1.621	1.636	1.645
^{2}TS1	1.703	1.696	1.695	1.713	1.723	-
^{4}I	1.776	1.778	1.778	1.792	1.815	-

The increase in Fe-O distance on increasing the explicit water molecules from 0 to 3 at the reactant structure is indicative of the reactivity of the Fe^V(O) (**2**) complex with increase in the concentration of water.

Table SI 8. Mulliken population analysis of reactant, TS1 and intermediate with and without explicit water at UB3LYP/6-31gG*, LANL2DZ(Fe) level of theory.

		^2R	$^2TS1$	^4I
Without water	O_1	-0.42286	-0.54984	-0.71367
	Fe	0.767298	0.749967	0.766455
One explicit water	O_1	-0.50248	-0.67346	-0.74256
	Fe	0.724989	0.728948	0.771006
	H_1	0.463241	0.511496	0.45797
	O	-0.87027	-0.87519	-0.87547
	H	0.411398	0.41589	0.414554
Two explicit water	O_1	-0.559	-0.6607	-0.77745
	Fe	0.720593	0.760374	0.771028
	H_1	0.47157	0.464143	0.461174
	O	-0.85732	-0.87523	-0.86243
	H	0.400214	0.409659	0.416611
	H_1	0.478431	0.457258	0.459801
	O	-0.85603	-0.87664	-0.87335
	H	0.422106	0.414891	0.415717

O_1 : oxygen atom of Fe-O ; H_1 : Hydrogen atom of water molecule bonded with O_1 of Fe-O

The greater value of the negative Mulliken charge in TS1 at the oxo atom (first oxygen in each case) explains the key reason for the greater (electrostatic) stabilization of the transition state over the reactant through hydrogen bonding.

XYZ coordinates of all the stationary points obtained by full optimization at UB3LYP/6-31G*, LANL2DZ (Fe) level of theory

Doublet Reactant, gas

C	1.843327	3.824391	1.768575
C	0.792962	4.590627	1.253422
C	-0.321119	3.981495	0.671598
C	-0.367923	2.582455	0.598324
C	0.700621	1.805653	1.114309
C	1.806660	2.429763	1.707882
N	-1.401465	1.785519	0.082106
Fe	-1.012675	-0.009849	-0.136211
N	-0.947947	-1.615742	0.757325
C	-1.775348	-2.687895	0.494310
N	-2.889976	-2.519778	-0.337485
C	-3.610522	-3.764698	-0.620823
N	0.448114	0.443327	0.990212
C	1.084352	-0.568662	1.627342
O	2.134775	-0.485523	2.272530
C	-2.599627	2.237500	-0.422382
O	-2.918192	3.420156	-0.516880
C	-3.520993	1.101406	-0.886628
C	-4.866175	1.292376	-0.151686
N	-2.859720	-0.165784	-0.526846
C	-3.523474	-1.320352	-0.764439
O	-4.634751	-1.403778	-1.305972
C	-3.698797	1.250295	-2.415145
C	0.317541	-1.898062	1.493386
C	1.226656	-2.877337	0.719743
C	0.047976	-2.392695	2.930572
O	-0.311168	-0.181609	-1.544283
O	-1.555082	-3.819867	0.941609
H	2.410711	0.269946	-1.759079
H	-2.738162	1.106384	-2.922181
H	-4.070448	2.254533	-2.644469
H	-4.404585	0.499153	-2.773859
H	-5.598235	0.570984	-0.514637
H	-5.221883	2.313176	-0.320835
H	-4.729688	1.147030	0.926610
H	-1.144581	4.559742	0.276990
H	0.837578	5.676159	1.302521
H	-4.359844	-3.543716	-1.376424
H	1.375761	-2.524849	-0.307218
H	2.201743	-2.918316	1.215406
H	0.780058	-3.871994	0.693475
H	-0.395406	-3.387886	2.912803
H	0.995368	-2.406359	3.477810

H	-0.636455	-1.706126	3.442710
H	2.600574	1.817536	2.114710
H	2.702370	4.314722	2.220878
H	-4.099194	-4.150730	0.280956
H	-2.905258	-4.520405	-0.971503
C	3.301845	0.909357	-1.736209
H	3.119818	1.663024	-0.961250
C	4.557489	0.118239	-1.450550
H	3.367479	1.424427	-2.701041
C	5.571888	-0.004063	-2.409399
C	6.731507	-0.738817	-2.148076
C	6.896718	-1.367352	-0.913621
C	5.892878	-1.252923	0.052565
C	4.736259	-0.518430	-0.210719
H	5.450185	0.483436	-3.374959
H	7.504058	-0.818060	-2.910188
H	7.797230	-1.940680	-0.705172
H	6.008931	-1.737893	1.019074
H	3.965503	-0.438636	0.553044

Quartet Reactant, gas

C	2.049807	3.494912	2.187521
C	1.145550	4.390652	1.567554
C	0.053897	3.928347	0.854627
C	-0.159462	2.533191	0.746581
C	0.769347	1.613568	1.382203
C	1.874863	2.124409	2.102735
N	-1.182214	1.895186	0.110446
Fe	-1.034922	-0.005376	0.012156
N	-1.043747	-1.725752	0.714591
C	-1.936311	-2.701427	0.383267
N	-3.089416	-2.335559	-0.362246
C	-3.940418	-3.485071	-0.689528
N	0.418888	0.306404	1.209932
C	1.016892	-0.825880	1.717233
O	2.074134	-0.853301	2.347065
C	-2.293844	2.438401	-0.502255
O	-2.505818	3.638521	-0.655262
C	-3.298131	1.356893	-0.983385
C	-4.668728	1.738222	-0.381534
N	-2.824450	0.030780	-0.505817
C	-3.585136	-1.065902	-0.781600
O	-4.680878	-1.024236	-1.360880
C	-3.330807	1.424993	-2.527320

C	0.201650	-2.113734	1.425742	O	0.512782	3.975081	-0.264855
C	1.087683	-3.034037	0.557158	N	-0.445823	-0.529084	-1.475605
C	-0.092045	-2.761455	2.797862	C	-0.373869	-1.830010	-1.881341
O	-0.194430	-0.130486	-1.394214	O	-1.145209	-2.391103	-2.661277
O	-1.818233	-3.896711	0.690758	Fe	0.741385	0.017576	-0.119345
H	2.215053	0.388785	-1.617031	N	1.617071	-1.582227	-0.477108
H	-2.352724	1.143111	-2.931808	C	2.762018	-2.008382	0.136289
H	-3.569256	2.444460	-2.849416	N	3.491220	-1.085590	0.921591
H	-4.085370	0.732272	-2.904853	C	4.652485	-1.679759	1.591193
H	-5.439314	1.068590	-0.762268	O	-0.136142	-0.281188	1.309760
H	-4.902327	2.775038	-0.641934	N	2.278428	0.911622	0.470704
H	-4.636800	1.653801	0.711696	C	2.128011	2.379801	0.603298
H	-0.648200	4.597753	0.375349	C	3.288059	3.144404	-0.071361
H	1.314388	5.461439	1.652451	C	3.372862	0.326187	1.030716
H	-4.745175	-3.127918	-1.325860	O	4.265472	0.945456	1.627542
H	1.278398	-2.561334	-0.412196	C	1.963515	2.811780	2.077733
H	2.044899	-3.210746	1.058716	C	0.833073	-2.570116	-1.259087
H	0.573842	-3.983366	0.395242	C	0.267469	-3.690821	-0.358997
H	-0.599966	-3.714631	2.652139	C	1.644255	-3.157585	-2.433940
H	0.847895	-2.910119	3.338434	O	3.201832	-3.163724	0.060893
H	-0.737576	-2.105363	3.394540	C	-2.237264	1.075070	1.759560
H	2.556893	1.426858	2.570772	C	-3.337554	0.133134	1.977329
H	2.899102	3.891508	2.738580	C	-3.624535	-0.368635	3.264336
H	-4.350497	-3.933671	0.221780	C	-4.659539	-1.277373	3.465445
H	-3.348692	-4.250576	-1.197355	C	-5.430308	-1.714244	2.383169
C	3.134966	0.983640	-1.681767	C	-5.152983	-1.235230	1.098391
H	3.071838	1.744845	-0.893902	C	-4.120031	-0.324825	0.894804
C	4.376317	0.137561	-1.519260	H	-1.174024	0.377588	1.479283
H	3.131216	1.501105	-2.647449	H	1.155860	2.238389	2.547038
C	5.342916	0.063066	-2.531024	H	1.709442	3.876275	2.118195
C	6.493760	-0.714975	-2.379346	H	2.889968	2.627386	2.624133
C	6.699203	-1.437094	-1.203569	H	4.217568	2.971013	0.470932
C	5.742905	-1.373532	-0.185906	H	3.048922	4.212063	-0.087475
C	4.595182	-0.595907	-0.341006	H	3.411474	2.801994	-1.105752
H	5.189692	0.622806	-3.451780	H	-1.477093	3.834704	-1.439955
H	7.227646	-0.755733	-3.181622	H	-3.468456	3.537452	-2.924771
H	7.592465	-2.045377	-1.080919	H	5.045368	-0.944158	2.288077
H	5.888069	-1.934555	0.734378	H	-0.286346	-3.255576	0.480513
H	3.860507	-0.559938	0.460280	H	-0.418148	-4.311249	-0.945755
				H	1.082980	-4.302216	0.031210

Doublet TS1, gas

				H	2.448284	-3.790880	-2.059055
C	-1.761687	2.857357	-1.806679	H	0.969626	-3.734881	-3.073399
C	-0.989492	1.744625	-1.446193	H	2.079426	-2.348556	-3.032899
C	-1.332745	0.449480	-1.926660	H	-2.681831	-0.706833	-3.129296
C	-2.445727	0.283658	-2.762863	H	-4.069642	1.277649	-3.764054
C	-3.206751	1.403631	-3.113624	H	5.429325	-1.951028	0.866819
C	-2.868654	2.675260	-2.641812	H	4.344745	-2.590672	2.107574
N	0.147670	1.718974	-0.629361	H	-2.323479	1.705880	0.874363
C	0.839039	2.793839	-0.141568	H	-1.905197	1.624717	2.643056
				H	-3.023735	-0.033204	4.106593

H	-4.866763	-1.648147	4.466497
H	-6.237290	-2.425959	2.539033
H	-5.743389	-1.575977	0.251603
H	-3.901322	0.037727	-0.106415

Quartet TS1, gas

C	1.380694	3.334801	1.507970
C	0.737723	2.110311	1.265090
C	1.094890	0.952118	2.021306
C	2.087889	1.039926	3.010631
C	2.718353	2.267498	3.237832
C	2.368604	3.401766	2.495944
N	-0.279127	1.845130	0.343045
C	-0.969367	2.761986	-0.411814
O	-0.709564	3.967166	-0.492429
N	0.336685	-0.162953	1.664802
C	0.290779	-1.369946	2.308562
O	1.006309	-1.713271	3.256864
Fe	-0.725124	0.031812	0.109856
N	-1.553643	-1.533423	0.697847
C	-2.623641	-2.149147	0.100513
N	-3.344859	-1.416042	-0.881565
C	-4.438663	-2.140409	-1.536115
O	0.367051	-0.430583	-1.146549
N	-2.240103	0.699190	-0.766810
C	-2.154542	2.122607	-1.175986
C	-3.410759	2.926295	-0.781945
C	-3.267149	-0.048819	-1.265988
O	-4.139930	0.377821	-2.043141
C	-1.859198	2.261756	-2.683608
C	-0.795767	-2.304813	1.719957
C	-0.062824	-3.503747	1.084545
C	-1.677147	-2.751124	2.902945
O	-2.983735	-3.310451	0.361111
C	2.621585	0.870346	-1.518121
C	3.588282	-0.145903	-1.811888
C	3.835773	-0.573163	-3.145167
C	4.754789	-1.579461	-3.421690
C	5.458531	-2.204288	-2.382135
C	5.224889	-1.805714	-1.057725
C	4.309144	-0.799160	-0.773921
H	1.432782	0.169052	-1.279036
H	-0.981877	1.655405	-2.952911
H	-1.648796	3.316206	-2.914108
H	-2.724246	1.916727	-3.263163
H	-4.270011	2.595585	-1.375054
H	-3.214338	3.993810	-0.953612
H	-3.634516	2.780753	0.285533
H	1.092271	4.205842	0.923040
H	2.872116	4.353284	2.682550

H	-4.384902	-1.982951	-2.620389
H	0.538850	-3.167672	0.227010
H	0.606816	-3.950912	1.833446
H	-0.792575	-4.247877	0.743288
H	-2.385558	-3.521271	2.580868
H	-1.023924	-3.138272	3.697087
H	-2.238517	-1.893233	3.303307
H	2.338082	0.148952	3.583671
H	3.493994	2.334876	4.004425
H	-5.416552	-1.770952	-1.192319
H	-4.333427	-3.198208	-1.281496
H	2.782273	1.508963	-0.645768
H	2.438269	1.643370	-2.269044
H	3.286191	-0.095039	-3.959745
H	4.926672	-1.885748	-4.456465
H	6.176968	-2.996720	-2.601201
H	5.762130	-2.291672	-0.240041
H	4.124146	-0.500460	0.260643

Doublet Intermediate, gas

C	3.173106	1.501703	-2.969441
C	3.287726	0.120305	-3.159555
C	2.349555	-0.757330	-2.606575
C	1.286428	-0.234100	-1.857129
C	1.162561	1.173700	-1.674980
C	2.115327	2.038554	-2.231353
N	0.244639	-0.936347	-1.239833
Fe	-0.847037	0.074749	-0.102257
N	-2.169098	1.309412	0.311893
C	-3.344978	1.038470	0.952411
N	-3.722628	-0.322621	1.091853
C	-4.969081	-0.556132	1.828345
N	0.027560	1.511217	-0.936041
C	-0.445609	2.763457	-0.659247
O	0.070839	3.826332	-1.005283
C	-0.025050	-2.273830	-1.324889
O	0.691915	-3.121892	-1.860974
C	-1.378377	-2.645205	-0.672782
C	-2.243520	-3.264850	-1.793849
N	-1.984277	-1.403477	-0.135976
C	-3.188627	-1.493665	0.496852
O	-3.849798	-2.536670	0.599621
C	-1.092200	-3.680031	0.436895
C	-1.762578	2.729154	0.155114
C	-1.470590	3.392346	1.519615
C	-2.798251	3.544638	-0.648701
O	0.038893	-0.073712	1.425722
O	-4.095076	1.906405	1.418637
H	0.924619	-0.429389	1.217921

H	-0.512810	-3.216063	1.243450
H	-0.509961	-4.506674	0.016882
H	-2.030770	-4.053513	0.849150
H	-3.190011	-3.614985	-1.380932
H	-1.697509	-4.095605	-2.251755
H	-2.448880	-2.515557	-2.567575
H	2.414183	-1.827971	-2.751613
H	4.111429	-0.281223	-3.745772
H	-4.857044	-1.448170	2.445455
H	-0.749560	2.789566	2.082626
H	-1.043124	4.386740	1.353053
H	-2.393081	3.475538	2.097125
H	-3.719391	3.654892	-0.076589
H	-2.372379	4.525897	-0.878683
H	-3.026186	3.037184	-1.593940
H	2.001535	3.104694	-2.085852
H	3.911073	2.171640	-3.405364
H	-5.809547	-0.722915	1.143704
H	-5.169096	0.323468	2.434717
C	2.759740	-2.117669	1.231872
H	2.530994	-2.274554	0.183017
C	3.708676	-1.163888	1.651627
H	2.260103	-2.757402	1.953107
C	4.043303	-1.007560	3.030760
C	4.982215	-0.073190	3.438931
C	5.624375	0.746138	2.498206
C	5.308542	0.616554	1.137507
C	4.373479	-0.315668	0.714374
H	3.543077	-1.636585	3.763372
H	5.218120	0.027760	4.495801
H	6.355500	1.481852	2.822917
H	5.793091	1.257090	0.404916
H	4.123985	-0.401576	-0.339570

Quartet Intermediate, gas

C	2.722007	2.278252	3.231280
C	2.372461	3.410703	2.486288
C	1.384984	3.341358	1.497642
C	0.742461	2.116150	1.257472
C	1.098544	0.960082	2.018238
C	2.092197	1.049505	3.006862
N	-0.274329	1.848848	0.335204
Fe	-0.732538	0.035795	0.118170
N	-1.554155	-1.533963	0.702471
C	-2.622260	-2.150671	0.106802
N	-3.343759	-1.417479	-0.877180
C	-4.438221	-2.143117	-1.529289
N	0.339602	-0.156461	1.664636
C	0.294103	-1.362436	2.311726

O	1.009097	-1.703966	3.261145
C	-0.965902	2.763707	-0.419220
O	-0.709159	3.969902	-0.503209
C	-2.153167	2.121784	-1.180439
C	-3.409057	2.926477	-0.788460
N	-2.241720	0.699351	-0.766895
C	-3.267434	-0.051116	-1.265170
O	-4.140062	0.373702	-2.043670
C	-1.858651	2.256335	-2.688684
C	-0.793484	-2.300114	1.725530
C	-0.060491	-3.501208	1.093686
C	-1.674380	-2.742620	2.910639
O	0.354703	-0.464537	-1.167408
O	-2.984451	-3.311087	0.369620
H	1.243691	0.032771	-1.212973
H	-0.981365	1.648909	-2.956487
H	-1.648746	3.310023	-2.922907
H	-2.723865	1.908376	-3.266505
H	-4.268242	2.594665	-1.380977
H	-3.211859	3.993518	-0.961367
H	-3.633527	2.782503	0.279189
H	1.095070	4.211136	0.911665
H	2.874230	4.363108	2.672858
H	-4.386009	-1.987241	-2.613954
H	0.540357	-3.166634	0.235329
H	0.609180	-3.946490	1.843629
H	-0.791253	-4.245388	0.755312
H	-2.382644	-3.513647	2.591153
H	-1.020532	-3.126545	3.705917
H	-2.235308	-1.883146	3.307747
H	2.341114	0.160494	3.583267
H	3.496286	2.348830	3.999025
H	-5.415979	-1.773986	-1.184876
H	-4.332189	-3.200388	-1.272902
C	2.683720	0.905124	-1.530960
H	2.643285	1.345357	-0.532915
C	3.598628	-0.140027	-1.814526
H	2.249295	1.485075	-2.346885
C	3.836938	-0.580275	-3.149364
C	4.752827	-1.587957	-3.420786
C	5.457991	-2.208598	-2.378104
C	5.224563	-1.807400	-1.053272
C	4.313192	-0.799037	-0.770960
H	3.286906	-0.103559	-3.964195
H	4.922388	-1.901207	-4.453720
H	6.175851	-3.002028	-2.594912
H	5.760387	-2.293937	-0.235114
H	4.129559	-0.494812	0.262117

Doublet TS2, gas

C	0.539152	2.245535	1.166426
C	-0.506994	2.765943	0.345993
C	-0.602355	4.146412	0.124221
C	0.338909	4.998400	0.708728
C	1.368649	4.488377	1.505680
C	1.478665	3.114606	1.739591
N	-1.346747	1.761403	-0.143724
C	-2.518352	1.911226	-0.830355
O	-3.014087	2.976555	-1.202797
N	0.461169	0.857562	1.307470
C	1.279362	0.038355	2.021915
O	2.298874	0.371547	2.637350
Fe	-0.735530	0.013403	0.119144
N	-0.350634	-1.543281	1.071064
C	-1.004740	-2.736370	0.967856
N	-2.075759	-2.827093	0.037462
C	-2.608735	-4.182427	-0.134662
O	0.390860	-0.117085	-1.317394
C	2.171142	0.986474	-1.887405
C	3.295241	0.114513	-1.849710
C	4.045432	-0.064138	-0.653767
C	5.145307	-0.911630	-0.627222
C	5.537214	-1.609578	-1.777998
C	4.806598	-1.453874	-2.963986
C	3.704382	-0.610547	-3.002474
N	-2.421431	-0.520195	-0.465908
C	-3.219951	0.555156	-1.106334
C	-4.635771	0.661642	-0.499754
C	-2.871645	-1.803752	-0.551939
O	-3.920652	-2.145807	-1.115531
C	-3.287974	0.380371	-2.639330
C	0.772141	-1.429175	2.038546
C	1.949345	-2.354937	1.677034
C	0.301832	-1.691244	3.489504
O	-0.703156	-3.758408	1.600427
H	0.765802	-1.015322	-1.276027
H	-2.276105	0.289513	-3.051173
H	-3.767750	1.258799	-3.083368
H	-3.853767	-0.519816	-2.886597
H	-5.220287	-0.224212	-0.749630
H	-5.121987	1.561758	-0.888066
H	-4.570651	0.747187	0.591653
H	-1.409738	4.521963	-0.490965
H	0.265797	6.070191	0.536967
H	-3.096561	-4.238371	-1.105839
H	2.280635	-2.174608	0.647534
H	2.792177	-2.142437	2.341914
H	1.646038	-3.398507	1.773631
H	-0.013474	-2.729737	3.598474

H	1.123865	-1.473215	4.179058
H	-0.541462	-1.035115	3.735066
H	2.264323	2.701374	2.359082
H	2.094975	5.163973	1.952542
H	-3.346388	-4.429197	0.639596
H	-1.785453	-4.890989	-0.060245
H	1.981426	1.667701	-1.068986
H	1.694067	1.214585	-2.832868
H	3.139783	-0.491240	-3.924569
H	5.103124	-1.995680	-3.859250
H	6.398450	-2.272103	-1.749614
H	5.699916	-1.037406	0.299166
H	3.734999	0.453222	0.250425

Quartet TS2, gas

C	2.125551	-2.090559	0.451534
C	2.610356	-1.495015	-0.751446
C	3.518481	-2.190135	-1.562591
C	3.933420	-3.466871	-1.178477
C	3.455524	-4.052316	-0.000025
C	2.553025	-3.373847	0.821425
N	2.089600	-0.214449	-0.952945
C	2.463944	0.700673	-1.898778
O	3.281126	0.519532	-2.802327
N	1.253472	-1.247664	1.142501
C	0.686528	-1.452425	2.368910
O	0.816894	-2.453263	3.075726
Fe	0.679508	0.263142	0.183950
N	-0.102023	0.807107	1.791420
C	-0.734306	1.993415	2.011651
N	-0.692726	2.969364	0.977287
C	-1.487590	4.169608	1.257112
O	-0.795129	-0.360677	-0.720364
C	-2.063530	-1.857969	-2.079905
C	-3.433796	-1.679907	-1.784230
C	-4.065906	-2.411660	-0.737369
C	-5.411819	-2.234163	-0.452296
C	-6.182251	-1.325512	-1.192557
C	-5.582426	-0.591578	-2.226094
C	-4.237147	-0.760724	-2.519302
N	0.897424	1.990214	-0.507945
C	1.750572	2.065978	-1.718783
C	2.863506	3.126087	-1.569008
C	0.180017	3.087281	-0.144825
O	0.214768	4.177897	-0.733136
C	0.918247	2.317856	-2.995196
C	-0.165721	-0.243311	2.837978
C	-1.608722	-0.749139	3.050750
C	0.451479	0.231283	4.172331

O	-1.370522	2.270416	3.038627
H	-1.550462	0.165403	-0.402600
H	0.124753	1.566020	-3.078268
H	1.567245	2.238536	-3.873490
H	0.464768	3.309841	-2.953425
H	2.426899	4.124680	-1.534028
H	3.554662	3.041121	-2.413324
H	3.424497	2.951897	-0.643001
H	3.882773	-1.717253	-2.465239
H	4.637192	-4.009356	-1.806232
H	-1.700094	4.667022	0.313083
H	-2.036826	-1.079560	2.096660
H	-1.598849	-1.601371	3.737869
H	-2.226801	0.053125	3.458429
H	-0.159397	1.021397	4.609776
H	0.518228	-0.621346	4.855168
H	1.463068	0.618606	4.001795
H	2.179718	-3.805630	1.740957
H	3.789428	-5.048007	0.284300
H	-0.947848	4.870288	1.906952
H	-2.402737	3.870085	1.765738
H	-1.473072	-2.607557	-1.569976
H	-1.601456	-1.346991	-2.915025
H	-3.774965	-0.185634	-3.318061
H	-6.173721	0.117708	-2.800350
H	-7.235437	-1.187168	-0.963198
H	-5.870142	-2.801436	0.354143
H	-3.470565	-3.111651	-0.156646

Doublet Product, gas

C	0.878762	2.723188	-0.452310
C	0.221637	2.667069	0.817159
C	-0.254406	3.845130	1.407464
C	-0.077455	5.065445	0.747479
C	0.570893	5.120706	-0.489291
C	1.054128	3.956039	-1.093500
N	0.151739	1.365639	1.343274
C	-0.225192	0.980054	2.595656
O	-0.681558	1.707166	3.482990
N	1.297839	1.463768	-0.908919
C	2.168276	1.179153	-1.922775
O	2.660574	1.984458	-2.716183
Fe	0.734611	0.026506	0.152083
N	1.865263	-1.032031	-0.860563
C	2.006242	-2.384214	-0.720615
N	1.328275	-3.022885	0.360078
C	1.486420	-4.481362	0.359275
O	-1.160175	-0.525706	-0.491858
C	-2.165617	0.472824	-0.768151

C	-3.488160	-0.158387	-1.136619
C	-3.541922	-1.221683	-2.049532
C	-4.766830	-1.782746	-2.408116
C	-5.954767	-1.285400	-1.863948
C	-5.909336	-0.228809	-0.953674
C	-4.680821	0.326842	-0.588439
N	0.413944	-1.192576	1.586187
C	0.011392	-0.541545	2.861039
C	1.127132	-0.620472	3.927984
C	0.801076	-2.491208	1.588674
O	0.688631	-3.269589	2.548874
C	-1.296857	-1.138054	3.417908
C	2.522029	-0.339279	-1.999693
C	2.007848	-0.854967	-3.361749
C	4.058482	-0.450806	-1.924834
O	2.673553	-3.101190	-1.480297
H	-1.382755	-1.039463	0.312913
H	-2.098564	-1.080641	2.667550
H	-1.618849	-0.567152	4.294133
H	-1.141989	-2.186215	3.679719
H	1.306251	-1.661654	4.202600
H	0.831847	-0.044980	4.811140
H	2.056401	-0.194125	3.531334
H	-0.735959	3.784819	2.375331
H	-0.446754	5.978862	1.209383
H	0.737213	-4.904720	1.025016
H	0.913898	-0.785458	-3.406706
H	2.425355	-0.236273	-4.162811
H	2.299288	-1.897338	-3.500710
H	4.363966	-1.489849	-2.059161
H	4.505136	0.179442	-2.699938
H	4.413942	-0.101256	-0.948066
H	1.572230	3.978840	-2.044008
H	0.704746	6.076691	-0.991407
H	2.479806	-4.785011	0.712438
H	1.364119	-4.848309	-0.659859
H	-1.749744	1.047802	-1.600187
H	-2.269651	1.148561	0.086425
H	-4.646502	1.143745	0.128945
H	-6.827528	0.158288	-0.519052
H	-6.909213	-1.723646	-2.144931
H	-4.795252	-2.609128	-3.113867
H	-2.616662	-1.610619	-2.465355

Quartet Product, gas

C	0.450993	2.828488	-0.329818
C	-0.126348	2.618153	0.959689
C	-0.753687	3.675951	1.625706
C	-0.809469	4.935433	1.016253

C	-0.243669	5.141798	-0.242854
C	0.390141	4.094238	-0.922156
N	0.033241	1.295614	1.419668
C	-0.281356	0.779494	2.642181
O	-0.872597	1.359125	3.557242
N	1.047573	1.667687	-0.859034
C	1.823227	1.547756	-1.976689
O	2.058150	2.431837	-2.803345
Fe	0.815838	0.133516	0.176288
N	2.012693	-0.707882	-0.974097
C	2.461305	-1.988515	-0.873136
N	2.042475	-2.758503	0.262329
C	2.520829	-4.145855	0.277665
O	-1.179487	-0.705713	-0.682215
C	-2.339559	0.142891	-0.707980
C	-3.602182	-0.618842	-1.048448
C	-3.593778	-1.607350	-2.042804
C	-4.764461	-2.290797	-2.370466
C	-5.961139	-1.992421	-1.712539
C	-5.977685	-1.010783	-0.720541
C	-4.802661	-0.332920	-0.387812
N	0.808921	-1.150406	1.535320
C	0.211228	-0.692105	2.818988
C	1.250296	-0.662581	3.962029
C	1.405321	-2.376832	1.478304
O	1.398028	-3.205953	2.399924
C	-1.004625	-1.550158	3.222960
C	2.433908	0.120211	-2.136786
C	1.904561	-0.454656	-3.467821
C	3.965783	0.300393	-2.195718
O	3.191866	-2.542603	-1.707048
H	-1.281679	-1.368268	0.024808
H	-1.747559	-1.572550	2.412913
H	-1.485475	-1.113766	4.103915
H	-0.686218	-2.573083	3.431357
H	1.584792	-1.675329	4.191948
H	0.802496	-0.202120	4.848281
H	2.118557	-0.063305	3.662149
H	-1.177546	3.497323	2.606019
H	-1.298647	5.757152	1.535304
H	1.731612	-4.795993	0.658663
H	0.817845	-0.592586	-3.413134
H	2.124982	0.245440	-4.280246
H	2.371892	-1.420608	-3.668143
H	4.448435	-0.656124	-2.401137
H	4.213517	1.024921	-2.977594
H	4.337473	0.685114	-1.238045
H	0.842651	4.236589	-1.895389
H	-0.291369	6.124817	-0.706910
H	3.393307	-4.261620	0.932262

H	2.797080	-4.414779	-0.738480
H	-2.110215	0.890055	-1.473880
H	-2.447839	0.673200	0.245014
H	-4.815402	0.423357	0.394049
H	-6.901792	-0.778571	-0.196935
H	-6.873061	-2.526347	-1.968346
H	-4.743431	-3.057753	-3.140834
H	-2.660060	-1.841652	-2.546120

Doublet Reactant, CPCM CH$_3$CN

C	1.747627	3.902365	1.707446
C	0.683850	4.642140	1.177207
C	-0.416692	4.003685	0.603416
C	-0.438619	2.601446	0.550472
C	0.640817	1.851539	1.086733
C	1.734537	2.507061	1.671187
N	-1.452531	1.777646	0.038908
Fe	-1.027573	-0.014585	-0.143214
N	-0.924475	-1.618648	0.753992
C	-1.720210	-2.711341	0.483212
N	-2.815735	-2.574013	-0.379258
C	-3.493717	-3.838100	-0.700003
N	0.409964	0.481575	0.990431
C	1.046136	-0.504144	1.670112
O	2.069113	-0.376707	2.351879
C	-2.671277	2.192695	-0.446732
O	-3.016430	3.368305	-0.549077
C	-3.576831	1.033864	-0.879551
C	-4.900400	1.189576	-0.097400
N	-2.868894	-0.216237	-0.539378
C	-3.499731	-1.391116	-0.765133
O	-4.623044	-1.508256	-1.278265
C	-3.809375	1.178740	-2.400969
C	0.323827	-1.856449	1.536416
C	1.286186	-2.819844	0.808174
C	0.019590	-2.335614	2.972073
O	-0.309881	-0.169012	-1.553324
O	-1.480355	-3.835011	0.943345
H	2.571765	0.360315	-1.931872
H	-2.863632	1.074357	-2.944522
H	-4.226972	2.166884	-2.617401
H	-4.500566	0.407141	-2.742497
H	-5.625605	0.448143	-0.431711
H	-5.298716	2.195070	-0.260633
H	-4.725611	1.055856	0.976541
H	-1.243803	4.566856	0.195857
H	0.710549	5.727857	1.206781
H	-4.149650	-3.660988	-1.547830
H	1.473112	-2.473918	-0.214805

H	2.240164	-2.839485	1.343675
H	0.867793	-3.825834	0.772110
H	-0.399104	-3.341067	2.958318
H	0.947835	-2.328115	3.550475
H	-0.694001	-1.658870	3.456165
H	2.543117	1.922564	2.088331
H	2.596571	4.415501	2.150803
H	-4.088994	-4.198722	0.146334
H	-2.745399	-4.591865	-0.943059
C	3.455975	0.992161	-1.774768
H	3.210075	1.680510	-0.957732
C	4.678521	0.163632	-1.449216
H	3.605624	1.583283	-2.684225
C	5.711316	0.000985	-2.382967
C	6.835626	-0.775906	-2.087704
C	6.946101	-1.405313	-0.846240
C	5.924029	-1.249545	0.095510
C	4.802878	-0.472559	-0.202950
H	5.635140	0.489586	-3.351970
H	7.624534	-0.885785	-2.827610
H	7.819527	-2.008390	-0.612623
H	6.001675	-1.732020	1.066769
H	4.016957	-0.356210	0.540625

Doublet TS1, CPCM CH$_3$CN

C	-1.831926	2.783506	-1.848234
C	-1.024962	1.695249	-1.489663
C	-1.328223	0.392096	-1.971843
C	-2.435161	0.194050	-2.808308
C	-3.230874	1.289471	-3.159249
C	-2.932172	2.570329	-2.684901
N	0.113641	1.703849	-0.668009
C	0.788199	2.794522	-0.200436
O	0.457020	3.971234	-0.370586
N	-0.411472	-0.563036	-1.515601
C	-0.275486	-1.848825	-1.938563
O	-1.003442	-2.426696	-2.752740
Fe	0.726352	0.019796	-0.130003
N	1.655665	-1.567128	-0.457477
C	2.787138	-1.963348	0.192533
N	3.426472	-1.033984	1.049011
C	4.559660	-1.578095	1.809919
O	-0.174588	-0.293540	1.272876
N	2.231851	0.948775	0.493643
C	2.066498	2.419841	0.580489
C	3.234185	3.172678	-0.094104
C	3.308478	0.379524	1.096862
O	4.193118	1.009704	1.698125
C	1.867579	2.896422	2.036901

C	0.942793	-2.557873	-1.304097
C	0.401152	-3.741822	-0.473492
C	1.820529	-3.054704	-2.473718
O	3.281743	-3.097577	0.098941
C	-2.264405	1.096497	1.795996
C	-3.340733	0.129924	2.025757
C	-3.553467	-0.429884	3.305393
C	-4.562225	-1.365472	3.515317
C	-5.377248	-1.770088	2.450860
C	-5.175621	-1.231450	1.173851
C	-4.167678	-0.295680	0.961254
H	-1.228104	0.437128	1.482755
H	1.043311	2.348414	2.507262
H	1.622960	3.963316	2.042613
H	2.778131	2.728161	2.613829
H	4.155268	3.021448	0.468470
H	2.997482	4.239609	-0.137815
H	3.380372	2.809097	-1.118167
H	-1.586748	3.770509	-1.480198
H	-3.558165	3.413207	-2.965375
H	4.687237	-0.985539	2.713420
H	-0.209342	-3.375913	0.360048
H	-0.226086	-4.374373	-1.109426
H	1.227389	-4.331488	-0.074100
H	2.649843	-3.653606	-2.098201
H	1.206761	-3.654552	-3.151715
H	2.223526	-2.203344	-3.035114
H	-2.651017	-0.800315	-3.175620
H	-4.089304	1.137501	-3.808165
H	5.491496	-1.539854	1.232768
H	4.345489	-2.615621	2.056597
H	-2.396152	1.744210	0.927553
H	-1.924590	1.638654	2.681643
H	-2.922929	-0.114681	4.132987
H	-4.718176	-1.780034	4.507291
H	-6.164633	-2.500177	2.615385
H	-5.808411	-1.542213	0.347237
H	-4.010829	0.120207	-0.030926

Quartet Intermediate, CPCM CH$_3$CN

C	3.367530	0.394816	-3.147479
C	3.310412	-1.001450	-3.065866
C	2.265448	-1.635060	-2.387359
C	1.268399	-0.853473	-1.787134
C	1.323465	0.566854	-1.874565
C	2.380508	1.186870	-2.555875
N	0.145226	-1.293124	-1.071113
Fe	-0.776297	0.037548	-0.136256
N	-1.931401	1.487151	0.039800

C	-3.110035	1.480254	0.725367
N	-3.603334	0.235340	1.189452
C	-4.813189	0.332151	2.018163
N	0.239636	1.175515	-1.231886
C	-0.093356	2.498679	-1.228953
O	0.531418	3.403583	-1.789022
C	-0.332526	-2.570804	-0.976749
O	0.213303	-3.578009	-1.433391
C	-1.688885	-2.648998	-0.239407
C	-2.684218	-3.303624	-1.224116
N	-2.096357	-1.265723	0.113138
C	-3.268400	-1.082587	0.780870
O	-4.057832	-1.994323	1.072492
C	-1.482316	-3.534493	1.009075
C	-1.397993	2.784371	-0.448380
C	-1.037366	3.738247	0.711647
C	-2.365871	3.462886	-1.443398
O	0.108366	0.075796	1.405699
O	-3.771195	2.496555	0.986955
H	0.868008	-0.537684	1.333870
H	-0.779007	-3.060665	1.703250
H	-1.067863	-4.500419	0.704297
H	-2.432578	-3.689890	1.521384
H	-3.643745	-3.468349	-0.734151
H	-2.275952	-4.258096	-1.568807
H	-2.837503	-2.657199	-2.096194
H	2.206964	-2.713311	-2.323656
H	4.083828	-1.604180	-3.534196
H	-4.885820	-0.564773	2.628896
H	-0.353396	3.247709	1.413243
H	-0.540353	4.626492	0.309598
H	-1.939132	4.036537	1.247858
H	-3.275503	3.776820	-0.931636
H	-1.872989	4.332206	-1.887994
H	-2.633258	2.768123	-2.248400
H	2.409778	2.266312	-2.618993
H	4.186506	0.873114	-3.677974
H	-5.718902	0.414598	1.405381
H	-4.736892	1.218882	2.644246
C	2.652930	-1.973885	1.730910
H	2.535004	-2.376815	0.729874
C	3.516652	-0.887815	1.982158
H	2.146092	-2.484092	2.544457
C	3.716075	-0.390838	3.306554
C	4.564395	0.679401	3.547765
C	5.246842	1.298721	2.488302
C	5.068704	0.828450	1.177414
C	4.223695	-0.241532	0.921784
H	3.189712	-0.867763	4.129572
H	4.701584	1.040223	4.563643

H	5.909616	2.137035	2.682194
H	5.596433	1.305156	0.355620
H	4.088825	-0.601979	-0.094698

Doublet Reactant, CPCM water

C	1.747963	3.900236	1.712322
C	0.685564	4.640937	1.180290
C	-0.414245	4.003431	0.604320
C	-0.436932	2.601119	0.550594
C	0.641045	1.850224	1.088951
C	1.734049	2.505033	1.675750
N	-1.450317	1.778364	0.037079
Fe	-1.026977	-0.014705	-0.142846
N	-0.924465	-1.619864	0.753053
C	-1.720773	-2.711842	0.481862
N	-2.816239	-2.573148	-0.380621
C	-3.495127	-3.836570	-0.702433
N	0.409204	0.480529	0.992654
C	1.044882	-0.505911	1.672135
O	2.067506	-0.378882	2.354433
C	-2.668777	2.193991	-0.448898
O	-3.012852	3.369810	-0.552455
C	-3.575377	1.035497	-0.880499
C	-4.898277	1.192697	-0.097460
N	-2.868093	-0.215028	-0.539967
C	-3.499760	-1.389619	-0.765285
O	-4.623569	-1.505933	-1.277601
C	-3.808920	1.179712	-2.401812
C	0.322563	-1.858066	1.537290
C	1.285795	-2.821695	0.810499
C	0.016140	-2.337211	2.972516
O	-0.307733	-0.168447	-1.552737
O	-1.481726	-3.836030	0.941270
H	2.572529	0.365626	-1.936083
H	-2.863665	1.074620	-2.946081
H	-4.226180	2.167934	-2.618478
H	-4.500812	0.408407	-2.742541
H	-5.624200	0.451446	-0.430582
H	-5.296244	2.198219	-0.261326
H	-4.722824	1.059853	0.976477
H	-1.240105	4.567354	0.195274
H	0.713066	5.726604	1.210128
H	-4.149493	-3.658973	-1.551363
H	1.474621	-2.475741	-0.212124
H	2.238870	-2.841943	1.347569
H	0.867081	-3.827509	0.773569
H	-0.403410	-3.342296	2.958041
H	0.943591	-2.330888	3.552197
H	-0.697452	-1.659970	3.455906

H	2.541533	1.920070	2.094320
H	2.596401	4.412751	2.157308
H	-4.092209	-4.196572	0.142892
H	-2.747206	-4.591047	-0.944360
C	3.457238	0.996178	-1.776419
H	3.211072	1.683369	-0.958481
C	4.678249	0.165413	-1.450681
H	3.608928	1.588759	-2.684574
C	5.710816	0.000897	-2.384380
C	6.833584	-0.778209	-2.089059
C	6.942727	-1.407976	-0.847634
C	5.920895	-1.250337	0.094073
C	4.801278	-0.471128	-0.204470
H	5.635742	0.489789	-3.353311
H	7.622373	-0.889500	-2.828858
H	7.814985	-2.012710	-0.614001
H	5.997613	-1.733010	1.065303
H	4.015567	-0.353217	0.539097

Doublet TS1, CPCM water

C	4.159640	-0.122754	0.965429
C	3.296885	-0.537443	2.005681
C	3.539169	-0.054956	3.311651
C	4.609474	0.796033	3.569777
C	5.458620	1.191533	2.528559
C	5.229367	0.728363	1.226914
C	2.157120	-1.414423	1.728806
O	0.130490	0.111816	1.342388
Fe	-0.738080	0.022581	-0.110943
N	-2.129157	-1.191242	0.241156
C	-3.284523	-0.899611	0.892889
O	-4.111903	-1.744085	1.272334
N	0.078168	-1.417292	-0.979116
C	-0.459050	-2.655849	-0.780157
C	-1.803629	-2.613592	-0.022233
C	-1.626989	-3.427253	1.278470
C	1.220906	-1.093190	-1.728961
C	2.163975	-1.972484	-2.277757
C	3.239017	-1.451686	-3.005760
C	3.376848	-0.072041	-3.187066
C	2.444228	0.816667	-2.643134
C	1.362755	0.310176	-1.910356
N	0.327546	1.026360	-1.297074
C	0.039077	2.348229	-1.434215
C	-1.256615	2.753255	-0.694885
C	-2.186787	3.390194	-1.750201
O	0.031289	-3.720976	-1.166169
O	0.694297	3.172335	-2.081209
N	-1.846903	1.523290	-0.106676

C	-3.021437	1.630847	0.579272
O	-3.642010	2.694238	0.733858
N	-3.558294	0.465013	1.175517
C	-4.756416	0.697811	1.993480
C	-2.847380	-3.276169	-0.950067
C	-0.861482	3.780691	0.388563
H	1.161434	-0.671304	1.470417
H	-0.903495	-2.938641	1.940797
H	-1.252239	-4.425991	1.034320
H	-2.580029	-3.513106	1.801860
H	-3.809534	-3.345890	-0.442544
H	-2.502404	-4.276494	-1.227517
H	-2.971407	-2.686215	-1.865860
H	2.042024	-3.037975	-2.137846
H	3.970624	-2.131806	-3.433696
H	-4.869083	-0.135132	2.683486
H	-0.210911	3.317264	1.139236
H	-0.314880	4.606314	-0.077859
H	-1.752430	4.166951	0.885305
H	-3.080451	3.793609	-1.274618
H	-1.648564	4.190488	-2.266149
H	-2.487440	2.641977	-2.493201
H	2.536512	1.885549	-2.782033
H	4.216411	0.319298	-3.755457
H	-5.661169	0.769627	1.377846
H	-4.632163	1.632966	2.536149
H	2.242332	-2.020382	0.825692
H	1.785623	-1.982144	2.585377
H	2.881975	-0.363746	4.120742
H	4.787226	1.151393	4.580842
H	6.294323	1.855489	2.730604
H	5.889322	1.031203	0.418807
H	3.984993	-0.484051	-0.044624

Quartet Intermediate, CPCM water

C	3.368440	0.390539	-3.148562
C	3.310962	-1.005646	-3.065454
C	2.265728	-1.638272	-2.386498
C	1.268711	-0.855817	-1.787342
C	1.324186	0.564394	-1.876210
C	2.381524	1.183446	-2.557963
N	0.145334	-1.294421	-1.070898
Fe	-0.775094	0.037349	-0.136730
N	-1.929844	1.487590	0.038485
C	-3.108026	1.481629	0.724751
N	-3.600775	0.237393	1.191254
C	-4.809732	0.335271	2.021260
N	0.240453	1.173982	-1.234093
C	-0.092530	2.497120	-1.232808

O	0.532074	3.401235	-1.794437					
C	-0.333656	-2.571659	-0.976517	C	0.742349	1.874595	1.163979
O	0.210819	-3.579207	-1.434014	C	-0.222621	2.699236	0.475260
C	-1.689567	-2.648855	-0.238336	C	-0.085034	4.106017	0.495207
C	-2.686115	-3.302457	-1.222511	C	0.987577	4.668772	1.166316
N	-2.095658	-1.265241	0.114565	C	1.928635	3.862668	1.844823
C	-3.267098	-1.080957	0.782922	C	1.811786	2.482126	1.860212
O	-4.057054	-1.991953	1.075536	N	-1.239662	1.967746	-0.074368
C	-1.482908	-3.534768	1.009845	C	-2.401723	2.438762	-0.648910
C	-1.396811	2.784056	-0.452138	O	-2.632617	3.613667	-0.919145
C	-1.035716	3.740071	0.705994	N	0.431968	0.541602	1.104315
C	-2.365240	3.460739	-1.447864	C	1.045677	-0.496204	1.768502
O	0.110470	0.076840	1.404860	O	2.095248	-0.408318	2.404299
O	-3.769158	2.498279	0.985241	Fe	-1.023034	0.086594	-0.021609
H	0.867834	-0.539745	1.334751	N	-0.982419	-1.534494	0.894918
H	-0.778482	-3.061986	1.703595	C	-1.838331	-2.566098	0.649654
H	-1.069798	-4.501109	0.704601	N	-3.074613	-2.291433	0.025992
H	-2.432888	-3.689363	1.522905	C	-3.898661	-3.490104	-0.175323
H	-3.645480	-3.466449	-0.731991	O	-0.266424	-0.201265	-1.426412
H	-2.279041	-4.257308	-1.567528	N	-2.853951	0.049865	-0.377610
H	-2.839407	-2.655860	-2.094458	C	-3.418958	1.311375	-0.923441
H	2.207224	-2.716441	-2.321605	C	-4.725026	1.733842	-0.212718
H	4.084370	-1.609020	-3.532916	C	-3.629976	-1.071625	-0.444490
H	-4.881494	-0.560648	2.633574	O	-4.781892	-1.083712	-0.898576
H	-0.351118	3.251145	1.408113	C	-3.616575	1.226403	-2.453148
H	-0.539264	4.627797	0.302144	C	0.273742	-1.825390	1.633443
H	-1.937166	4.039146	1.242275	C	1.203526	-2.825797	0.907050
H	-3.274625	3.775545	-0.936212	C	-0.026379	-2.309767	3.069630
H	-1.872792	4.329395	-1.894213	O	-1.598610	-3.749804	0.939764
H	-2.633023	2.764593	-2.251534	C	3.239105	0.800078	-1.725228
H	2.411282	2.262802	-2.622232	C	4.527459	0.077924	-1.405742
H	4.187657	0.868039	-3.679359	C	4.750149	-0.458095	-0.126387
H	-5.716228	0.416586	1.409509	C	5.937621	-1.126722	0.171514
H	-4.732808	1.222893	2.645982	C	6.931060	-1.273792	-0.800833
C	2.651087	-1.973651	1.735285	C	6.722955	-0.745717	-2.075151
H	2.535620	-2.378978	0.734915	C	5.531972	-0.076988	-2.370114
C	3.513839	-0.886606	1.985786	O	-0.295283	-3.010881	-2.205614
H	2.143502	-2.482796	2.549036	H	2.366695	0.137461	-1.668545
C	3.710501	-0.386639	3.309489	H	-2.682638	0.914194	-2.932830
C	4.557812	0.684589	3.549934	H	-3.903798	2.209013	-2.842233
C	5.241925	1.301953	2.490378	H	-4.394736	0.496122	-2.681543
C	5.066578	0.828684	1.180167	H	-5.525591	1.035623	-0.452978
C	4.222574	-0.242299	0.925318	H	-4.993462	2.745483	-0.531947
H	3.183025	-0.862164	4.132599	H	-4.577972	1.741093	0.874306
H	4.693046	1.047612	4.565276	H	-0.816787	4.706381	-0.028159
H	5.904007	2.140929	2.683700	H	1.111127	5.748976	1.164640
H	5.595871	1.303706	0.358409	H	-4.840661	-3.170350	-0.611392
H	4.090034	-0.605265	-0.090586	H	1.292740	-2.573988	-0.153864
				H	2.196483	-2.791037	1.366652
Doublet Reactant, 1 explicit H₂O, gas				H	0.797823	-3.835035	0.987775

Doublet Reactant, 1 explicit H_2O, gas

H -0.532592 -3.275427   3.031127
H   0.910805 -2.402122   3.627116
H -0.671100 -1.590377   3.588540
H   2.522138   1.851566   2.377271
H   2.764677   4.332279   2.357180
H -4.065072 -3.995679   0.779442
H -3.386774 -4.189574 -0.842773
H   3.056109   1.615870 -1.015347
H   3.263322   1.229876 -2.732539
H   5.376343   0.330237 -3.367268
H   7.486139 -0.853402 -2.843068
H   7.855857 -1.796156 -0.566711
H   6.085889 -1.535612   1.168334
H   3.986447 -0.353242   0.641060
H -0.292231 -2.055632 -1.993240
H -0.544899 -3.431475 -1.369044

Doublet TS1, 1 explicit H₂O, gas

C   4.131772   0.119869 -0.399913
C   3.454154   0.212809 -1.635798
C   3.962824 -0.516504 -2.731614
C   5.112254 -1.290060 -2.605698
C   5.778773 -1.360687 -1.378048
C   5.281057 -0.655373 -0.277354
C   2.241349   1.024272 -1.770560
O   0.104979 -0.291589 -1.328810
Fe -0.793778   0.085899   0.079127
N -2.554053 -0.347974 -0.343381
C -3.094707 -1.604223 -0.338615
O -4.208970 -1.872723 -0.804592
N -1.345307   1.863025 -0.191671
C -2.543252   2.056928 -0.817873
C -3.333510   0.739699 -0.988550
C -3.503096   0.495657 -2.503786
C -0.458761   2.844803   0.254877
C -0.511011   4.224756   0.016175
C   0.464917   5.049752   0.581186
C   1.483517   4.514305   1.374882
C   1.551239   3.139617   1.620405
C   0.579277   2.299202   1.060078
N   0.464751   0.908799   1.195026
C   1.202273   0.095052   2.008893
C   0.692867 -1.363594   2.015160
C   0.326206 -1.703184   3.477030
O -2.996302   3.136568 -1.199272
O   2.170928   0.446763   2.686885
N -0.512906 -1.416750   1.153056
C -1.118869 -2.618664   0.954791
O -0.679266 -3.701316   1.378544

N -2.319411 -2.656432   0.213785
C -2.851880 -4.012309   0.033564
C -4.699412   0.964351 -0.302891
C   1.856623 -2.258911   1.531586
H   1.207799   0.319482 -1.474912
H -2.526836   0.312429 -2.966878
H -3.946940   1.385185 -2.962818
H -4.144284 -0.371028 -2.673050
H -5.360211   0.117140 -0.484463
H -5.141442   1.884488 -0.696666
H -4.562246   1.082282   0.778785
H -1.313556   4.620809 -0.591863
H   0.425978   6.121319   0.398299
H -3.765786 -3.930912 -0.548094
H   2.021351 -2.143195   0.456269
H   2.767852 -1.964181   2.061543
H   1.633542 -3.306953   1.733091
H   0.005285 -2.744750   3.542370
H   1.198979 -1.541357   4.117164
H -0.486910 -1.056093   3.826024
H   2.324125   2.709479   2.243310
H   2.234660   5.169175   1.810722
H -3.058194 -4.474958   1.002919
H -2.115317 -4.629787 -0.487655
H   2.143227   1.850091 -1.064297
H   1.988703   1.316829 -2.792634
H   3.441486 -0.468175 -3.684550
H   5.488037 -1.843739 -3.462473
H   6.674753 -1.968260 -1.277831
H   5.787045 -0.715516   0.682695
H   3.739024   0.645775   0.466115
H   0.517868 -2.225239 -1.532898
O   0.711352 -3.179385 -1.607449
H   0.479313 -3.530312 -0.733246

Quartet Intermediate, 1 explicit H₂O, gas

C   0.567119   2.221682   1.048268
C -0.492466   2.826588   0.312778
C -0.505132   4.214507   0.112419
C   0.525920   4.987012   0.650274
C   1.561037   4.394454   1.381835
C   1.591993   3.012919   1.587068
N -1.436343   1.891269 -0.112030
C -2.633325   2.139432 -0.728662
O -3.058017   3.243770 -1.065920
N   0.412377   0.832771   1.144265
C   1.140471 -0.030827   1.916654
O   2.132543   0.264598   2.586908

Fe	-0.936364	0.093947	0.074275
N	-0.665930	-1.454191	1.078181
C	-1.303489	-2.634223	0.837066
N	-2.515988	-2.615575	0.113359
C	-3.079756	-3.952560	-0.110986
O	-0.061263	-0.285059	-1.443042
N	-2.696519	-0.287992	-0.374322
C	-3.458626	0.849726	-0.949487
C	-4.806065	1.072185	-0.226126
C	-3.269850	-1.528650	-0.405139
O	-4.392869	-1.755949	-0.870622
C	-3.664339	0.686861	-2.471185
C	0.582098	-1.473530	1.882409
C	1.693407	-2.378343	1.299316
C	0.276944	-1.872559	3.342997
O	-0.883106	-3.741817	1.210454
C	3.002214	1.243198	-1.722613
C	4.058453	0.337291	-1.498283
C	4.489862	0.015150	-0.175508
C	5.540562	-0.865552	0.033323
C	6.202599	-1.459549	-1.051292
C	5.791023	-1.165303	-2.359767
C	4.741196	-0.288569	-2.583877
O	0.397288	-3.146686	-1.837160
H	0.836612	0.092920	-1.372880
H	-2.702277	0.508308	-2.964023
H	-4.100637	1.606198	-2.875192
H	-4.326268	-0.158040	-2.668525
H	-5.489147	0.249137	-0.434801
H	-5.235092	2.018935	-0.567804
H	-4.646354	1.135348	0.857030
H	-1.320417	4.656118	-0.445155
H	0.518209	6.063947	0.498094
H	-4.007750	-3.828225	-0.661810
H	1.799155	-2.228412	0.220433
H	2.641411	-2.129015	1.785898
H	1.453631	-3.427648	1.473384
H	-0.067627	-2.907919	3.375394
H	1.184003	-1.761215	3.944901
H	-0.501074	-1.223484	3.761222
H	2.375963	2.539492	2.163115
H	2.353386	5.011627	1.799013
H	-3.266855	-4.453215	0.842908
H	-2.371012	-4.559556	-0.681251
H	2.533396	1.776671	-0.901943
H	2.683223	1.488734	-2.731336
H	4.421319	-0.066540	-3.599201
H	6.294205	-1.631121	-3.203800
H	7.022842	-2.151580	-0.879361
H	5.845422	-1.101455	1.049775

H	3.966892	0.448923	0.672657
H	0.187377	-2.196015	-1.742470
H	0.192025	-3.518408	-0.965436

Doublet Reactant, 2 explicit H₂O, gas

C	5.882754	-1.451515	-0.020572
C	4.668877	-0.791201	-0.211361
C	4.443896	-0.008726	-1.356420
C	5.474022	0.084062	-2.302000
C	6.691451	-0.575856	-2.115511
C	6.901723	-1.346611	-0.971707
C	3.133338	0.715451	-1.550419
O	-0.228558	-0.204643	-1.312872
Fe	-1.003841	0.028878	0.109339
N	-1.280263	-1.681580	0.780425
C	-2.285734	-2.502320	0.359106
O	-2.257607	-3.739164	0.461542
N	-0.885133	1.911959	0.320932
C	-1.913486	2.654651	-0.229903
C	-3.111679	1.780808	-0.649749
C	-3.307051	1.966110	-2.171781
C	0.200381	2.368824	1.011478
C	0.976886	1.295542	1.598532
C	2.092091	1.603236	2.414775
C	2.431052	2.928442	2.617242
C	1.673464	3.976871	2.041307
C	0.566040	3.714079	1.255685
N	0.458549	0.064205	1.325642
C	0.865667	-1.157470	1.824186
O	1.891101	-1.347595	2.472770
O	-1.893124	3.872258	-0.382989
N	-2.789405	0.371147	-0.296570
C	-3.754565	-0.571540	-0.512688
O	-4.883120	-0.312105	-0.948148
N	-3.431892	-1.926185	-0.227848
C	-4.440022	-2.919173	-0.621887
C	-0.115850	-2.295579	1.472343
C	-0.542797	-2.939794	2.810117
C	0.658343	-3.312463	0.600382
C	-4.327190	2.320654	0.140387
O	0.221898	2.101468	-2.898428
H	2.272255	0.049047	-1.428923
H	-2.398553	1.682018	-2.712231
H	-3.513488	3.020713	-2.382891
H	-4.145296	1.354466	-2.509069
H	-5.236169	1.818932	-0.188491
H	-4.410112	3.399463	-0.023520
H	-4.193311	2.139988	1.214096
H	-0.022646	4.503572	0.808372

H	1.972900	5.007506	2.213748
H	-5.301940	-2.377975	-1.001172
H	0.826552	-2.913378	-0.404031
H	1.625361	-3.522116	1.068768
H	0.086176	-4.236692	0.512032
H	-1.200313	-3.787813	2.613609
H	0.345700	-3.275875	3.353318
H	-1.077136	-2.211357	3.431741
H	2.661390	0.791242	2.845985
H	3.300900	3.169959	3.222637
H	-4.716515	-3.534208	0.238170
H	-4.032892	-3.578835	-1.393832
H	3.014669	1.516039	-0.808205
H	3.054760	1.173966	-2.540335
H	5.315975	0.680471	-3.198211
H	7.473357	-0.489019	-2.867102
H	7.846757	-1.864277	-0.823628
H	6.030933	-2.054175	0.872647
H	3.883159	-0.887031	0.535161
H	0.091260	1.254955	-2.418570
H	0.025123	2.770400	-2.226684
H	-0.600786	-1.914956	-2.153171
O	-0.779780	-2.812169	-2.500442
H	-1.117351	-3.295981	-1.731785

Doublet TS1, 2 explicit H$_2$O, gas

C	-1.236271	2.634775	2.775031
C	-0.439488	2.020692	1.799939
C	-0.011648	2.755127	0.660105
C	-0.386664	4.096107	0.504647
C	-1.180834	4.695291	1.485646
C	-1.599723	3.973660	2.607462
N	0.031622	0.700450	1.783984
C	-0.058237	-0.221057	2.794038
O	-0.640421	-0.053586	3.865180
N	0.801668	1.986071	-0.177050
C	1.454108	2.387918	-1.304194
O	1.319623	3.479186	-1.865758
Fe	0.811848	0.142084	0.184151
N	2.243960	0.091740	-1.002959
C	3.031379	-0.993160	-1.276786
N	2.781561	-2.189139	-0.554417
C	3.469353	-3.391245	-1.041301
O	-0.543158	-0.432773	-0.711176
N	1.349085	-1.356307	1.156237
C	0.665614	-1.544153	2.458869
C	1.696907	-1.793476	3.580574
C	2.027806	-2.406359	0.617275
O	2.026568	-3.555422	1.090020

C	-0.405696	-2.660797	2.457441
C	2.428601	1.312985	-1.830661
C	2.095680	1.064245	-3.316879
C	3.846803	1.909259	-1.668711
O	3.920789	-0.996209	-2.135721
O	-1.408623	1.558694	-2.674169
O	-0.617162	-3.398969	-0.873721
C	-2.857856	0.088339	0.251222
C	-3.840739	-0.601031	-0.589263
C	-4.459765	-1.792402	-0.155491
C	-5.393806	-2.442020	-0.956118
C	-5.719304	-1.923724	-2.214070
C	-5.097070	-0.755138	-2.667877
C	-4.165081	-0.099124	-1.870030
H	-1.701122	-0.238102	-0.160193
H	-1.030195	-2.605130	1.560424
H	-1.035701	-2.542277	3.345139
H	0.071607	-3.641282	2.472630
H	2.196812	-2.749952	3.415298
H	1.184267	-1.802987	4.547223
H	2.447716	-0.994971	3.592726
H	-1.544885	2.063617	3.640281
H	-2.216898	4.454669	3.362790
H	2.736704	-4.179717	-1.230535
H	1.065406	0.709952	-3.425642
H	2.183224	2.010499	-3.860023
H	2.783165	0.329168	-3.737107
H	4.587305	1.239611	-2.106176
H	3.880180	2.884314	-2.164940
H	4.077959	2.050776	-0.606177
H	-0.048098	4.640630	-0.366974
H	-1.474012	5.736131	1.369409
H	4.178994	-3.759320	-0.294184
H	3.993876	-3.123152	-1.954159
H	-2.799656	1.169607	0.114388
H	-2.850118	-0.200635	1.303789
H	-4.199746	-2.198416	0.818803
H	-5.865583	-3.356059	-0.604490
H	-6.445689	-2.434258	-2.841777
H	-5.335624	-0.359563	-3.651950
H	-3.647946	0.785983	-2.232636
H	-1.055875	0.849906	-2.100085
H	-0.856922	2.328106	-2.461901
H	-0.570157	-2.424085	-0.879916
H	0.082353	-3.662590	-0.254970

Quartet Intermediate, 2 explicit H$_2$O, gas

C	-4.412759	-0.587499	-2.135634

C	-4.440628	-0.500120	-0.709598
C	-5.359925	-1.341457	-0.014457
C	-6.196280	-2.207815	-0.701886
C	-6.153258	-2.274839	-2.102614
C	-5.254962	-1.459540	-2.808329
C	-3.589081	0.392360	-0.028608
O	-0.339139	-0.568355	-0.816516
Fe	0.959996	0.163151	0.219015
N	1.837300	-1.310896	0.939318
C	2.690829	-2.103528	0.227293
O	2.944540	-3.284614	0.512035
N	0.099820	0.270360	1.872487
C	0.283314	-0.772231	2.748404
C	1.249427	-1.845202	2.193362
C	0.420454	-3.138208	1.996166
C	-0.655331	1.428526	2.082568
C	-1.554228	1.689940	3.126586
C	-2.222815	2.915083	3.151439
C	-2.007365	3.872144	2.152111
C	-1.113891	3.629559	1.108068
C	-0.427506	2.406940	1.072067
N	0.531754	1.986942	0.148966
C	1.000295	2.663798	-0.944027
C	2.184117	1.935744	-1.619246
C	3.434165	2.796857	-1.310666
O	-0.236996	-0.876475	3.856606
O	0.571466	3.741829	-1.361747
N	2.287838	0.583539	-1.011707
C	3.297925	-0.237335	-1.431273
O	4.153330	0.088796	-2.261491
N	3.330598	-1.556033	-0.903383
C	4.234468	-2.494934	-1.579342
C	2.346770	-2.065199	3.255953
C	1.916762	1.878375	-3.137127
O	-1.513644	1.314958	-2.630870
O	0.257677	-3.378323	-1.446677
H	-1.148315	-0.626913	-0.272911
H	-0.225826	-3.061920	1.115958
H	-0.198609	-3.299173	2.884804
H	1.083616	-3.991733	1.850580
H	3.016468	-2.865323	2.935170
H	1.877424	-2.329733	4.208094
H	2.928600	-1.147258	3.398783
H	-1.700852	0.942639	3.895209
H	-2.920010	3.124003	3.959373
H	3.682170	-3.396774	-1.852987
H	1.002398	1.314457	-3.346417
H	1.776561	2.897618	-3.510487
H	2.759725	1.409594	-3.645988
H	4.304164	2.384059	-1.821839

H	3.253740	3.823026	-1.646821
H	3.628386	2.811850	-0.231781
H	-0.933114	4.359569	0.330055
H	-2.540908	4.819008	2.185830
H	5.057033	-2.786129	-0.918578
H	4.627308	-1.997175	-2.461586
H	-2.925630	1.045613	-0.585472
H	-3.611210	0.482706	1.053191
H	-5.393712	-1.293768	1.071660
H	-6.887736	-2.841336	-0.150699
H	-6.807925	-2.958733	-2.636772
H	-5.213739	-1.514706	-3.893591
H	-3.707500	0.039870	-2.675057
H	-1.031797	0.646040	-2.099067
H	-1.145837	2.164173	-2.338125
H	0.095712	-2.425007	-1.307394
H	1.007472	-3.578938	-0.865268

Doublet Reactant, 3 explicit H$_2$O, gas

C	-4.650296	-0.126712	-1.938399
C	-4.589557	-1.347510	-1.251119
C	-5.783746	-2.055014	-1.041550
C	-7.004761	-1.561711	-1.501524
C	-7.054474	-0.343331	-2.184508
C	-5.873612	0.368598	-2.399841
C	-3.272570	-1.891391	-0.744048
O	0.062773	-0.275276	-1.034604
Fe	0.892344	0.236522	0.290060
N	2.173910	-1.069295	0.621257
C	3.385459	-1.136234	0.003283
O	4.138204	-2.123446	0.055745
N	-0.088651	-0.640721	1.665703
C	0.352591	-1.904478	2.024378
C	1.682914	-2.279316	1.336168
C	1.367878	-3.429589	0.351192
C	-1.132739	0.058022	2.184724
C	-2.077810	-0.383436	3.144706
C	-3.041475	0.499470	3.590541
C	-3.088648	1.837362	3.122416
C	-2.173591	2.309466	2.200998
C	-1.183308	1.428144	1.703609
N	-0.169355	1.715741	0.839915
C	0.178097	2.947658	0.314123
C	1.556939	2.927911	-0.376448
C	2.435768	3.938220	0.399222
O	-0.232170	-2.659263	2.792313
O	-0.516572	3.957206	0.378152
N	2.093109	1.541845	-0.285828
C	3.338995	1.309480	-0.795070

O	4.053904	2.179836	-1.306023
N	3.823564	-0.028128	-0.756757
C	5.098544	-0.266679	-1.454448
C	2.640158	-2.742650	2.455884
C	1.348832	3.382268	-1.838529
O	1.724551	-1.521371	-2.923354
O	-1.673153	1.583673	-2.217585
O	3.825220	-3.454930	-2.485760
H	0.637301	-3.098628	-0.393855
H	0.947779	-4.277622	0.902156
H	2.272287	-3.746069	-0.170696
H	3.553010	-3.151207	2.025700
H	2.134559	-3.499709	3.062480
H	2.903774	-1.897721	3.103811
H	-2.026050	-1.406285	3.492008
H	-3.784388	0.161647	4.308322
H	5.017075	-1.184491	-2.040102
H	0.643273	2.719381	-2.349044
H	0.928634	4.393344	-1.844055
H	2.306906	3.381149	-2.359912
H	3.399174	4.047369	-0.098086
H	1.922838	4.904036	0.440883
H	2.605203	3.587536	1.424565
H	-2.197898	3.326713	1.834274
H	-3.866468	2.501426	3.490251
H	5.919214	-0.382675	-0.738912
H	5.290530	0.592249	-2.091828
H	-3.276462	-1.988373	0.349663
H	-3.071667	-2.890760	-1.151530
H	-5.752932	-3.005468	-0.511008
H	-7.917427	-2.128311	-1.328280
H	-8.004598	0.044013	-2.545734
H	-5.898617	1.316467	-2.932865
H	-3.734217	0.435422	-2.115232
H	-1.068196	0.896333	-1.853757
H	-1.811767	2.183269	-1.469125
H	3.019015	-2.925429	-2.656203
H	4.076841	-3.174821	-1.587792
H	1.072359	-1.217107	-2.251537
H	2.344481	-0.777890	-2.967222
H	-2.432134	-1.246166	-1.014564

N	2.582108	-1.305711	-0.777619
C	1.941441	-0.089016	-0.806256
C	2.194613	0.691277	-2.103724
N	2.975869	-0.187409	-2.992395
C	3.258149	0.256134	-4.237926
O	2.937774	1.365723	-4.688402
N	3.789853	-3.376678	-1.327771
C	4.216687	-4.424874	-2.077875
C	4.501172	-4.002868	-3.532908
C	3.699824	-4.962334	-4.436401
Fe	3.808189	-1.652785	-2.120642
N	4.054824	-2.589546	-3.686170
C	4.240646	-2.000938	-4.918832
O	4.673734	-2.626598	-5.894748
O	5.199981	-1.065915	-1.651308
N	3.965966	-0.637439	-5.089494
C	4.297822	-0.130168	-6.424016
O	1.245994	0.359243	0.102356
O	4.354894	-5.589619	-1.699633
C	0.808744	1.041953	-2.688803
C	2.975843	1.970196	-1.723811
C	6.022246	-4.151062	-3.756597
H	3.957281	1.703053	-1.316413
H	2.419098	2.528345	-0.963713
H	3.117170	2.587678	-2.612640
H	0.920835	1.686328	-3.560711
H	0.214655	1.542980	-1.918535
H	0.285269	0.126622	-2.989698
H	1.318147	-1.220194	1.712416
H	1.385910	-3.111757	3.339270
H	4.158852	0.947623	-6.406701
H	6.565366	-3.435427	-3.128624
H	6.323327	-5.163962	-3.469506
H	6.272520	-3.969895	-4.802729
H	3.953927	-4.803235	-5.483933
H	3.927489	-5.990141	-4.138288
H	2.624624	-4.795382	-4.301418
H	3.782878	-5.410528	0.576020
H	2.610135	-5.199698	2.777327
H	3.648098	-0.574611	-7.186397
H	5.329337	-0.392198	-6.667993

Doublet catalyst

C	1.854237	-2.131254	1.486704
C	2.527085	-2.246150	0.262174
C	3.230664	-3.435851	-0.056055
C	3.255657	-4.505945	0.848643
C	2.588224	-4.375593	2.067538
C	1.897524	-3.200870	2.383564

Quartet catalyst

C	6.164681	12.289205	13.460940
C	4.905542	12.350671	14.064242
C	4.825648	12.414064	15.460559
C	6.007951	12.412356	16.244922
C	7.263219	12.347246	15.628350
C	7.329411	12.287512	14.233633

N	3.667507	12.464371	16.248224
C	2.380867	12.241491	15.843236
O	2.020509	12.026750	14.686345
N	5.732591	12.461490	17.618254
C	6.605427	12.234736	18.645825
O	7.810792	12.016817	18.527661
Fe	3.929227	12.834686	18.095777
N	2.132327	12.340882	18.276780
C	1.365109	12.269611	17.010983
C	0.480491	13.519470	16.801279
O	3.813179	14.454633	18.271404
N	4.460468	12.339149	19.821336
C	3.626588	12.493683	20.890061
N	2.244290	12.708495	20.635647
C	1.472318	12.495682	19.460845
O	0.242109	12.435372	19.575047
C	5.924708	12.262970	20.035763
C	6.312628	10.967323	20.773046
C	6.465665	13.510263	20.770857
O	3.999754	12.431445	22.067758
C	1.443228	12.939124	21.842628
C	0.531930	10.976091	16.937438
H	6.156318	14.419087	20.242931
H	7.559612	13.468742	20.788217
H	6.077876	13.542192	21.790184
H	5.932860	10.991740	21.795589
H	7.402747	10.873126	20.773582
H	5.889320	10.098012	20.256942
H	8.152657	12.332635	16.243829
H	8.302453	12.239172	13.749729
H	2.050659	13.490556	22.557834
H	1.089251	14.426685	16.883273
H	0.039205	13.481340	15.800001
H	-0.307915	13.551452	17.554822
H	-0.262329	11.000743	17.685073
H	0.107230	10.885140	15.933148
H	1.169971	10.104848	17.124757
H	3.992645	12.338722	13.484065
H	6.232122	12.242184	12.376251
H	1.130415	11.994857	22.305296
H	0.552658	13.498687	21.562486

Singlet Fe^{IV}(OH)

C	3.219779	1.445064	-2.988621
C	3.195680	0.066447	-3.333195
C	2.211869	-0.773741	-2.795128
C	1.253611	-0.237239	-1.932360
C	1.270634	1.121030	-1.602464
C	2.253373	1.969433	-2.119125

N	4.248131	-0.287707	-4.176396
C	4.860739	-1.495165	-4.190958
O	4.415492	-2.562661	-3.758621
N	4.294687	2.133171	-3.586461
C	4.531658	3.493964	-3.504176
O	3.825151	4.287469	-2.887685
Fe	5.251896	1.222688	-4.846336
N	6.351249	2.766057	-4.934132
C	7.553030	2.877594	-5.527777
N	8.160097	1.645492	-5.932181
C	9.433922	1.765170	-6.647279
O	4.324951	1.213641	-6.316081
N	6.609946	0.034604	-4.997204
C	6.278987	-1.412571	-4.808718
C	7.236890	-2.092230	-3.809866
C	7.834139	0.328975	-5.586272
O	8.648378	-0.558242	-5.870269
C	6.236434	-2.174867	-6.151748
C	5.766098	3.955941	-4.298081
C	5.288019	4.979530	-5.351860
C	6.717107	4.622478	-3.277473
O	8.172546	3.931619	-5.739237
H	3.729261	0.441056	-6.252981
H	5.600812	-1.642976	-6.870008
H	5.805214	-3.165910	-5.974832
H	7.236820	-2.273125	-6.574282
H	8.238710	-2.167421	-4.232309
H	6.845098	-3.085133	-3.571804
H	7.284060	-1.511711	-2.880868
H	2.230944	-1.826753	-3.045051
H	0.487496	-0.887788	-1.515561
H	9.436477	1.090805	-7.506502
H	4.617755	4.492488	-6.068978
H	4.746381	5.794901	-4.861147
H	6.154615	5.372262	-5.887860
H	7.577915	5.050096	-3.791886
H	6.173380	5.402448	-2.735547
H	7.072562	3.879886	-2.552721
H	2.282592	3.020546	-1.868804
H	0.514763	1.529200	-0.935286
H	10.276238	1.490700	-6.002220
H	9.534082	2.801854	-6.958130

Triplet Fe^{IV}(OH)

C	3.164092	1.495636	-2.987588
C	3.302821	0.086285	-3.149886
C	2.344419	-0.782195	-2.608513
C	1.259294	-0.245299	-1.912775
C	1.122345	1.138585	-1.754193

C	2.067288	2.017700	-2.287017	H	5.393080	-1.621151	-6.797746
N	4.457228	-0.248424	-3.863899	H	5.705611	-3.179584	-5.993967
C	4.978589	-1.496662	-4.071816	H	7.055275	-2.252337	-6.720261
O	4.478302	-2.559685	-3.703694	H	8.299870	-2.297844	-4.493104
N	4.216486	2.198268	-3.579906	H	6.953408	-3.187988	-3.709781
C	4.464940	3.541942	-3.515847	H	7.525061	-1.649411	-3.029015
O	3.769727	4.379488	-2.940289	H	2.474567	-1.849256	-2.732701
Fe	5.323946	1.185005	-4.702760	H	0.514565	-0.915718	-1.489342
N	6.410692	2.695053	-4.751088	H	9.435676	1.132281	-7.521513
C	7.604619	2.803309	-5.403804	H	4.759489	4.328023	-6.143674
N	8.197100	1.611007	-5.899214	H	4.776382	5.708056	-5.018078
C	9.443464	1.789703	-6.650871	H	6.261703	5.254282	-5.910436
O	4.405856	1.262782	-6.226327	H	7.538997	5.078142	-3.705541
N	6.693090	-0.029918	-5.034043	H	6.063610	5.478097	-2.766971
C	6.324369	-1.452652	-4.836333	H	6.959852	3.981196	-2.430623
C	7.353279	-2.200965	-3.961107	H	1.985283	3.089890	-2.166177
C	7.868211	0.251794	-5.668459	H	0.271286	1.539762	-1.208141
O	8.670943	-0.603254	-6.067105	H	10.314751	1.526779	-6.039331
C	6.108319	-2.178863	-6.182676	H	9.508509	2.834226	-6.943923
C	5.767825	3.937044	-4.253992				
C	5.366865	4.875093	-5.413942				
C	6.649551	4.673909	-3.222145				
O	8.195514	3.875307	-5.594178				
H	3.483517	1.053934	-5.992688				