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Hydrogen-atom Transfer Mechanism in the Oxidation of Alcohols by $[FeO4]^{2-}$ in Aqueous Solution

Jianhui Xie,[a,b] Po-Kam Lo,[b] Chow-Sing Lam, [b] Kai-Chung Lau,* [b] and Tai-Chu Lau* [b]

[a]Anhui Province Key Laboratory of Advanced Catalytic Materials and Reaction Engineering, School of Chemistry and Chemical Engineering, Hefei University of Technology, Hefei 230009, P. R. China.
[b]Department of Chemistry, City University of Hong Kong, Tat Chee Avenue, Kowloon Tong, Hong Kong, P.R. China.
E-mail: kaichung@cityu.edu.hk (K C Lau) bhtclau@cityu.edu.hk (T C Lau)

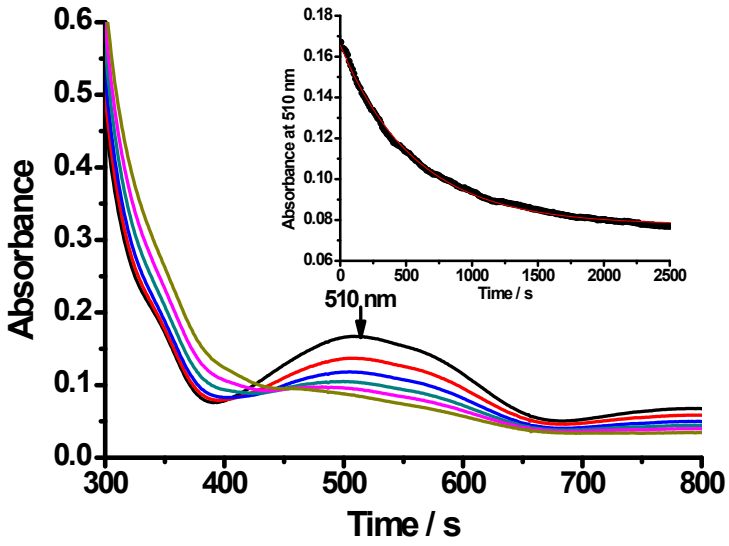


Fig. S1 Spectral changes at 200s intervals of the oxidation of benzyl alcohol (0.01 M) by ferrate (2.00×10^{-4} M) in the presence of 30% *tert*-butanol at pH 9.5, I = 0.1 M and 25 °C. Inset shows the absorbance-time trace and pseudo-first order fit at 510 nm, k_{obs} = $(1.77 \pm 0.02) \times 10^{-3}$ s^{-1}.

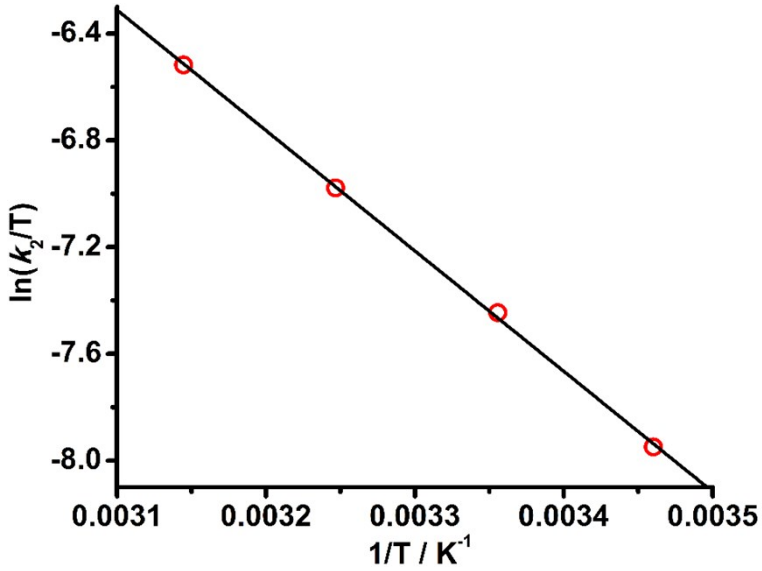


Fig. S2 Plot of ln(k_2/T) *vs*. 1/T for the oxidation of benzyl alcohol by ferrate at pH 9.5, I = 0.1 M.

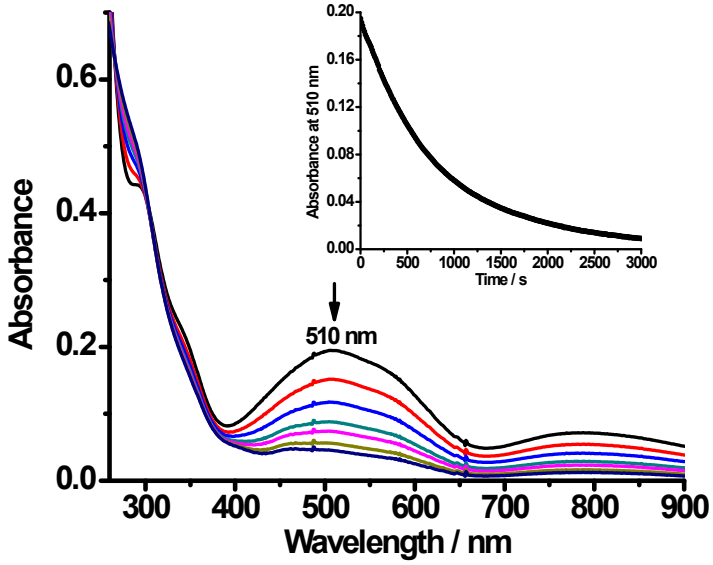


Fig. S3 Spectral changes at 200s intervals of the oxidation of methanol (0.136 M) by ferrate (2.00×10^{-4} M) at pH 9.5, I = 0.1 M and 25 °C. Inset shows the absorbance-time trace at 510 nm.

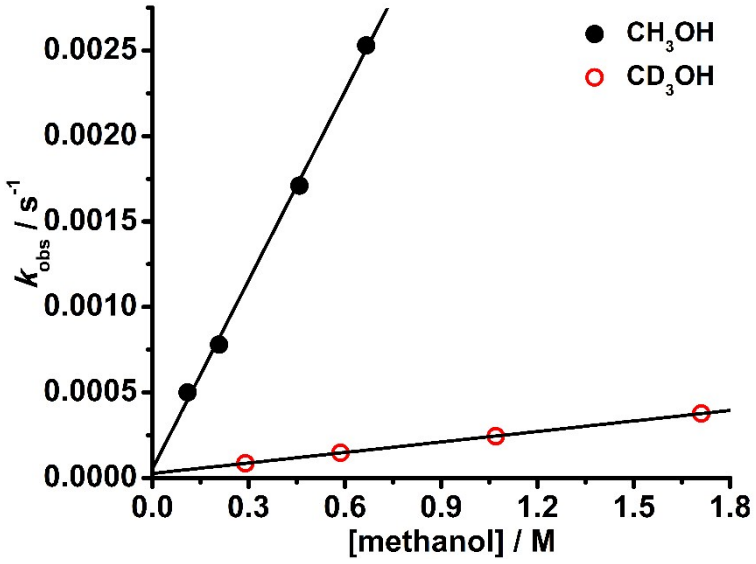


Fig. S4 Plot of k_{obs} *vs*. [methanol] for the oxidation of methanol by ferrate at pH = 9.5, I = 0.1 M and 25 °C. For methanol (solid cycle): slope = (3.68 ± 0.11) × 10^{-3}, y-intercept = – (5.24 ± 4.72) × 10^{-5}, r^2 = 0.997. For d_4-methanol (open cycle): slope = (2.05 ± 0.02) × 10^{-4}, y-intercept = – (2.62 ± 0.25) × 10^{-5}, r^2 = 0.999.

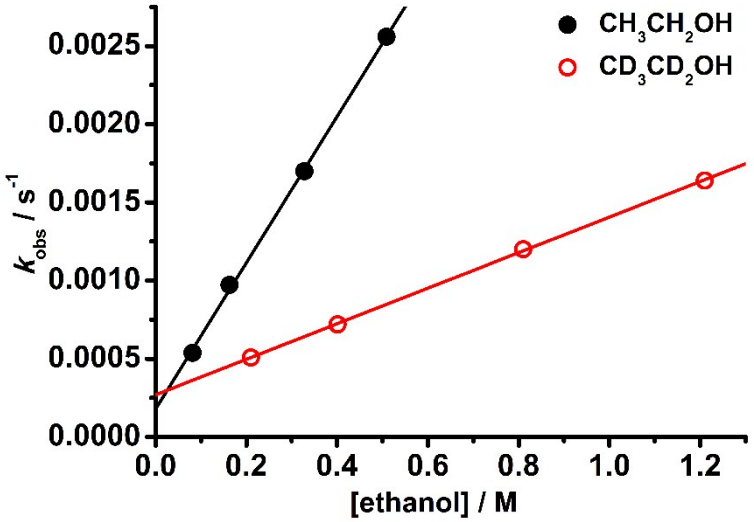


Fig. S5 Plot of k_{obs} *vs*. [ethanol] for the oxidation of ethanol by ferrate at pH = 9.5, *I* = 0.1 M and 25 °C. For ethanol (solid cycle): slope = (4.68 ± 0.09) × 10^{-3}, *y*-intercept = – (1.78 ± 0.28) × 10^{-4}, r^2 = 0.999. For d_6-ethanol (open cycle): slope = (1.14 ± 0.02) × 10^{-3}, *y*-intercept = – (2.69 ± 0.19) × 10^{-4}, r^2 = 0.999.

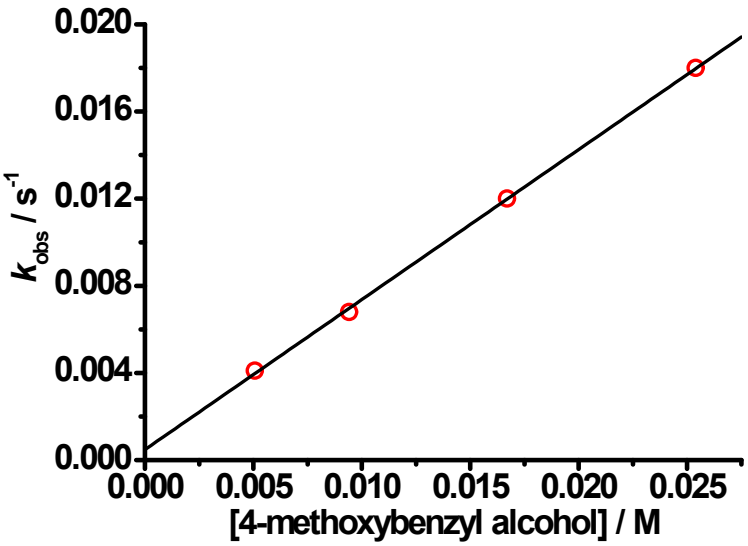


Fig. S6 Plot of k_{obs} *vs*. [4-methoxybenzyl alcohol] for the oxidation of 4-methoxybenzyl alcohol by ferrate (2.00 × 10^{-4} M) in the presence of 15% *tert*-butanol at pH 9.5, *I* = 0.1 M and 25 °C. [slope = (6.87 ± 0.10) × 10^{-1}, *y*-intercept = (6.74 ± 3.49) × 10^{-5}, r^2 = 0.999]

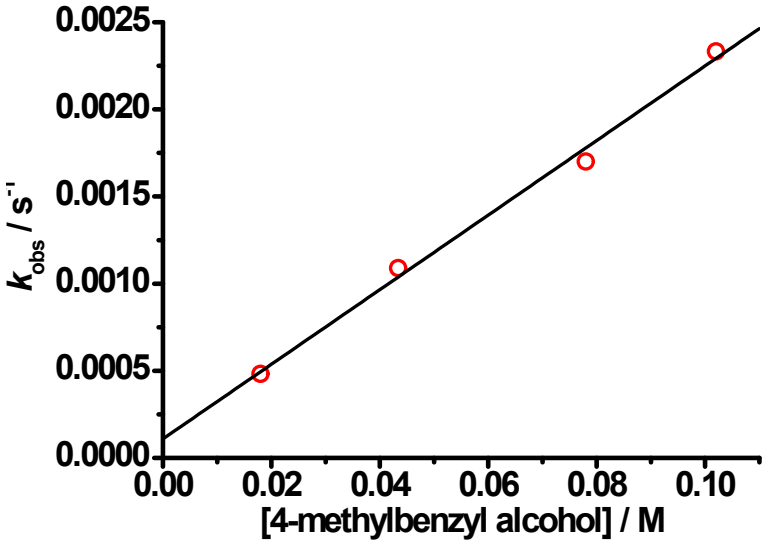


Fig. S7 Plot of k_{obs} *vs*. [4-methylbenzyl alcohol] for the oxidation of 4-methylbenzyl alcohol by ferrate (2.00×10^{-4} M) in the presence of 15% *tert*-butanol at pH 9.5, I = 0.1 M and 25 °C. [slope = $(2.14 \pm 0.11) \times 10^{-2}$, y-intercept = $(1.09 \pm 0.77) \times 10^{-4}$, $r^2 = 0.992$]

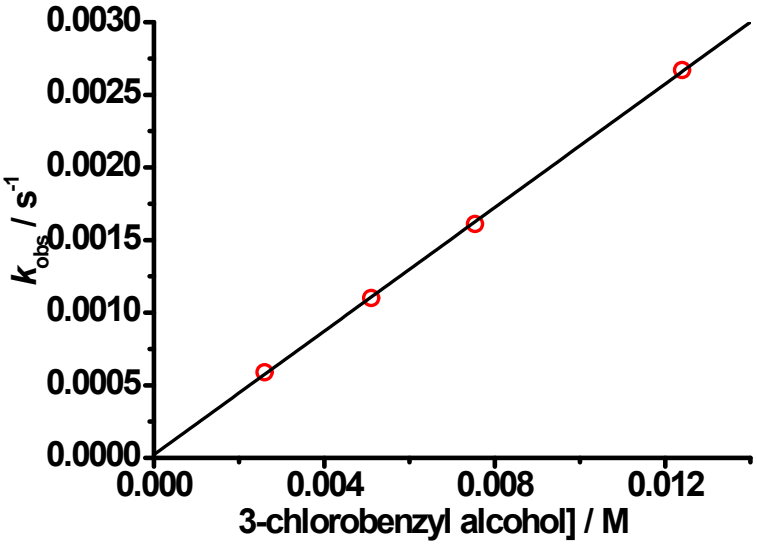


Fig. S8 Plot of k_{obs} *vs*. [3-chlorobenzyl alcohol] for the oxidation of 3-chlorobenzyl alcohol by ferrate (2.00×10^{-4} M) in the presence of 15% *tert*-butanol at pH 9.5, I = 0.1 M and 25 °C. [slope = $(2.13 \pm 0.02) \times 10^{-1}$, y-intercept = $(2.25 \pm 1.87) \times 10^{-5}$, $r^2 = 0.9996$]

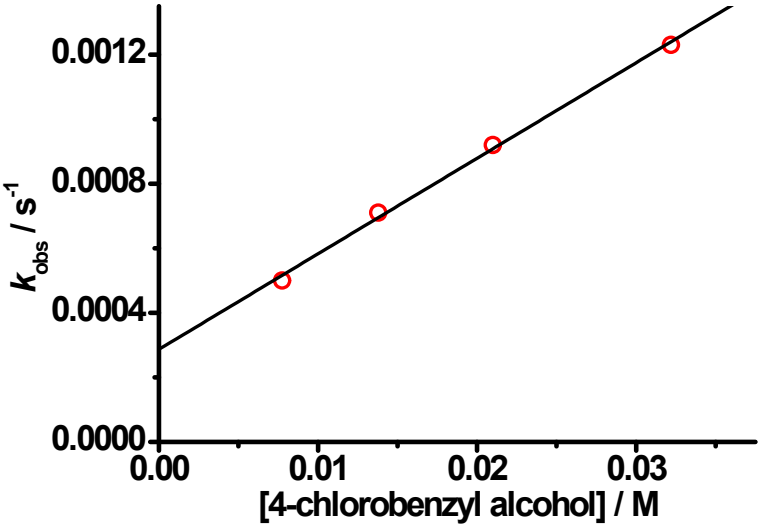


Fig. S9 Plot of k_{obs} *vs*. [4-chlorobenzyl alcohol] for the oxidation of 4-chlorobenzyl alcohol by ferrate (2.00×10^{-4} M) in the presence of 15% *tert*-butanol at pH 9.5, I = 0.1 M and 25 °C. [slope = $(2.96 \pm 0.01) \times 10^{-2}$, y-intercept = $(2.87 \pm 0.22) \times 10^{-4}$, $r^2 = 0.996$]

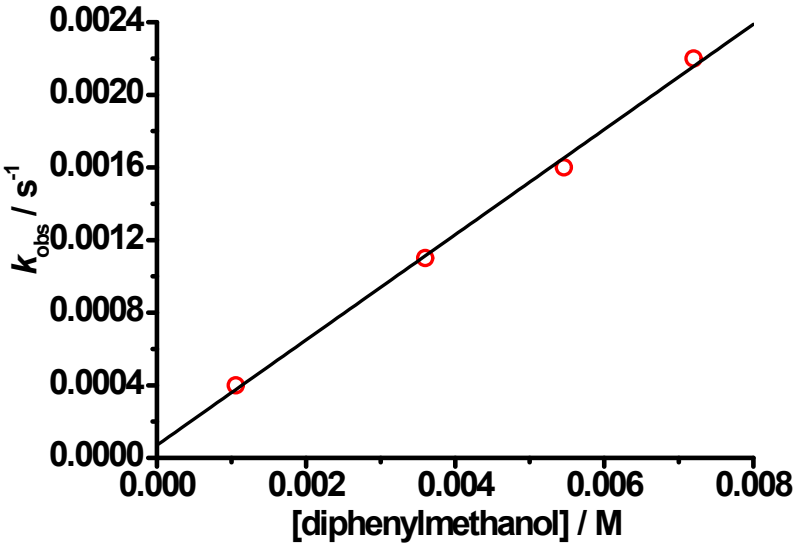


Fig. S10 Plot of k_{obs} *vs*. [diphenylmethanol] for the oxidation of diphenylmethanol by ferrate (2.00×10^{-4} M) in the presence of 15% *tert*-butanol at pH 9.5, I = 0.1 M and 25 °C. [slope = $(2.96 \pm 0.01) \times 10^{-1}$, y-intercept = $(2.87 \pm 0.22) \times 10^{-4}$, $r^2 = 0.996$]

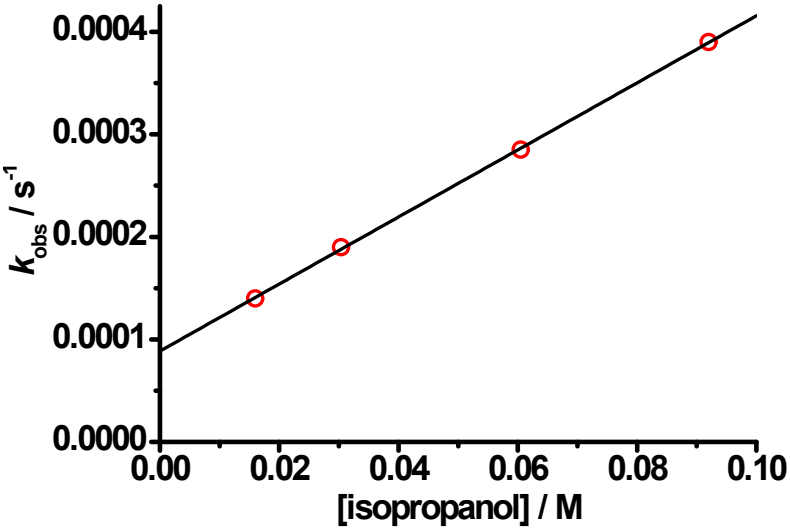


Fig. S11 Plot of k_{obs} *vs*. [isopropanol] for the oxidation of isopropanol by ferrate (2.00 × 10^{-4} M) at pH 9.5, *I* = 0.1 M and 25 °C. [slope = (3.27 ± 0.03) × 10^{-3}, *y*-intercept = (8.86 ± 0.19) × 10^{-5}, r^2 = 0.9997]

Table S1 Second-order rate constants for the oxidation of benzyl alcohols by ferrate(VI) at 25 °C, pH = 9.5 and *I* = 0.1 M

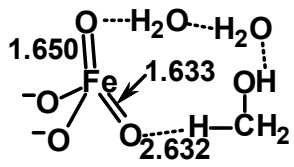
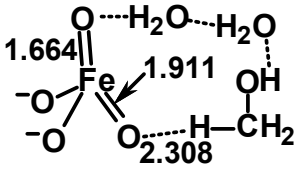
X- $C_6H_5CH_2OH$	k_2 / M^{-1} s^{-1}
4-MeO[a]	$(6.87 \pm 0.10) \times 10^{-1}$
4-Me[a]	$(2.14 \pm 0.11) \times 10^{-2}$
H	$(1.74 \pm 0.01) \times 10^{-1}$
4-Cl[a]	$(2.96 \pm 0.01) \times 10^{-2}$
3-Cl[a]	$(2.13 \pm 0.02) \times 10^{-1}$

[a] Experiments were carried out in the presence of 15% *tert*-butanol. The solutions were mixed and immediately sonicated to make them homogeneous.

Table S2 Second-order rate constants for the oxidation of benzyl alcohol by ferrate(VI) at 25 °C and *I* = 0.1 M

pH	k_2 / M^{-1} s^{-1}
6.67	1.77 ± 0.08
7.12	1.21 ± 0.03
7.40	(8.78± 0.13) × 10^{-1}
7.63	(6.61 ± 0.27) × 10^{-1}
7.95	(4.14 ± 0.21) × 10^{-1}
8.24	(3.57± 0.16) × 10^{-1}
8.54	(2.67 ± 0.17) × 10^{-1}
8.80	(2.62 ± 0.14) × 10^{-1}
9.27	(2.26± 0.14) × 10^{-1}
9.50	(1.74 ± 0.01) × 10^{-1}

Table S3 Cartesian coordinates of calculated intermediate and transition state structures in Schemes 3 and 4.

^{3}INT1				^{5}INT1			
							
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O	-0.59775796	-0.09177235	1.58862242	O	-0.61333000	-0.23327700	1.97300700
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H	3.28837297	0.86314265	-1.19950978	H	3.29018700	1.04848500	-1.30287700
O	1.80298760	0.88030123	-2.16510620	O	1.82038500	1.19762800	-2.27708300
H	1.75858052	1.54474854	-2.86155115	H	1.74858800	1.99367800	-2.81534400
H	0.99773182	1.01670877	-1.61669486	H	1.03496700	1.20743100	-1.67949700
O	4.11305694	0.83351319	-0.66464691	O	4.07570400	0.93989400	-0.71999100
H	3.87815293	-0.13574231	0.86916248	H	3.70439300	-0.15945300	0.68367300
H	4.68779945	0.19079617	-1.13020907	H	4.66833100	0.32260700	-1.19802800
O	5.40433585	-1.38984170	-1.77218155	O	5.44410200	-1.19435600	-1.89085700
H	4.74900275	-2.01176749	-1.37611721	H	4.77501600	-1.85861800	-1.59930900
H	5.38895038	-1.55244942	-2.72140054	H	5.52710900	-1.29770900	-2.84487800
O	3.57140527	-2.85749939	-0.33814085	O	3.51727600	-2.79307800	-0.75360100
H	2.65269440	-2.84154248	-0.67393980	H	2.64136000	-2.73463600	-1.18792900
H	3.57920855	-2.25257179	0.43330114	H	3.44389800	-2.25056100	0.05886200
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H	0.70243070	2.97782524	1.87277377	H	0.66112400	2.90812000	2.08366100
H	0.51428142	2.67511803	0.38147898	H	0.53204000	2.60168300	0.58259900
O	3.79044330	3.41285400	0.59731133	O	3.77656600	3.30908400	0.90867800
H	2.82445119	3.34707731	0.73384589	H	2.80542100	3.26045600	1.01665700
H	4.03977683	2.57411131	0.17487098	H	4.00629800	2.53406400	0.36956400
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H	0.40783371	1.75389822	4.02825299	H	0.36422200	1.77096600	4.28755200
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H	-3.86680227	-0.49754921	1.47333676	H	-3.68842400	-0.93344800	1.54983800
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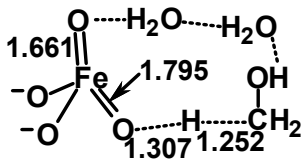
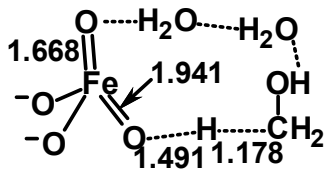
O	-4.67070360	-0.56125223	-1.72695723	O	-4.68475500	-0.44794800	-1.53985800
H	-3.99668379	-0.58417223	-2.43254202	H	-4.00467900	-0.37224500	-2.23916000
H	-4.16947530	-0.21525330	-0.97040611	H	-4.18390500	-0.26860400	-0.73080500
O	-2.33597701	-0.46599707	-3.36581016	O	-2.43711800	-0.16495600	-3.22956900
H	-2.19673957	0.50310686	-3.34130977	H	-2.28488500	0.79469900	-3.10956400
H	-1.84001292	-0.79116424	-2.59144379	H	-1.86683700	-0.58037900	-2.55056000
O	-1.86967391	2.29967890	-2.88444031	O	-1.90087900	2.52953000	-2.47312800
H	-2.63765823	2.65323350	-2.39619581	H	-2.61810400	2.80873600	-1.87343100
H	-1.25418280	2.07189404	-2.15993636	H	-1.22170500	2.20472400	-1.84647500
^{3}TS1				**^{5}TS1**			
							
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O	-1.08059688	-1.20679335	-0.93420958	O	-0.84805400	-1.23818700	-0.83639300
O	0.06717962	-0.37297862	1.51191228	O	-0.41274200	-0.12577900	1.99719900
C	2.49847385	-0.46241504	2.29811611	C	2.21302000	-0.30855200	2.33010400
H	2.68450288	0.55021847	2.66647398	H	2.49057300	0.71110200	2.61225000
H	2.46406298	-1.21044264	3.08952353	H	2.23710800	-0.98538100	3.18542200
H	-3.26060250	2.00946430	0.18102895	H	-3.25001100	2.01984900	-0.11497500
O	3.35472716	-0.85939642	1.29230972	O	2.99657500	-0.82175800	1.30300800
H	3.25702459	1.11283483	-1.17335054	H	3.24131600	0.96334400	-1.30264500
O	1.85868438	1.29145541	-2.20011976	O	1.88115100	1.09450800	-2.39243800
H	1.80363259	2.09890407	-2.72299545	H	1.83675500	1.88117000	-2.94698500
H	1.04751117	1.28002987	-1.63612115	H	1.09359200	1.13955300	-1.79585500
O	4.01683751	0.96837179	-0.56070621	O	3.92997600	0.84599100	-0.60692900
H	3.55582269	-0.10720344	0.67441207	H	3.25930200	-0.11772900	0.65821600
H	4.63936193	0.39537695	-1.05847920	H	4.57728400	0.20940600	-0.98009800

O	5.42913124	-1.07551480	-1.81029953	O	5.44582300	-1.31822100	-1.47856500
H	4.74942154	-1.75373822	-1.58668961	H	4.76192100	-1.98728300	-1.23858700
H	5.53565587	-1.10684666	-2.76711138	H	5.64123900	-1.45659800	-2.41158000
O	3.46995449	-2.75476719	-0.83668301	O	3.43657900	-2.93863300	-0.51666600
H	2.59981927	-2.70186015	-1.28702315	H	2.62673600	-2.92641900	-1.07031500
H	3.34053860	-2.29182687	0.00953402	H	3.20948500	-2.38306900	0.25061200
O	0.81918396	3.21702241	1.25924479	O	0.87308200	3.36562300	1.02302600
H	0.49905919	2.83549945	2.09883085	H	0.50747400	3.10908000	1.89263700
H	0.43489694	2.62339687	0.58196209	H	0.50295700	2.69473800	0.41275400
O	3.64056121	3.37724808	1.03848913	O	3.69740300	3.35373300	0.82163800
H	2.66816731	3.30597385	1.12009049	H	2.72288300	3.35603900	0.90997600
H	3.90442594	2.60251423	0.51627624	H	3.90084500	2.52832600	0.35077900
O	-2.24921891	-3.42812662	0.44749135	O	-2.11957500	-3.36138700	0.64614900
H	-1.57586650	-3.44872320	1.15650973	H	-1.57758300	-3.28952300	1.45772200
H	-1.91889280	-2.72357686	-0.14406070	H	-1.72137700	-2.70014900	0.04655800
O	-0.33383504	1.68901256	3.36131521	O	-0.39755700	2.26483300	3.29775100
H	-0.25030144	0.87635590	2.81407790	H	-0.42784000	1.35747700	2.90253300
H	0.06473582	1.47742380	4.21233704	H	0.02111300	2.16378600	4.15919700
O	0.99688664	-2.54673104	-2.10414348	O	1.10081100	-2.74064700	-2.02061200
H	0.57041726	-3.37370119	-2.35424261	H	0.62096500	-3.54923700	-2.23105800
H	0.29548859	-2.01614489	-1.65740529	H	0.44042700	-2.15117700	-1.58759900
O	-3.94378408	-1.65390353	1.95982241	O	-4.08136400	-1.58548400	1.77691800
H	-3.50201076	-2.38062277	1.48186377	H	-3.54975100	-2.31173300	1.39884200
H	-3.54402209	-0.86438606	1.55012131	H	-3.59631200	-0.79724000	1.47806200
O	-0.30135127	-2.96112464	2.42618544	O	-0.62736500	-2.68225700	2.93381800
H	-0.60761655	-2.94010030	3.33932801	H	-1.09495100	-2.69375600	3.77589200
H	-0.19347041	-2.01723486	2.15999274	H	-0.56552300	-1.72974100	2.67222300
O	-3.67766355	2.83836484	-0.15303042	O	-3.64751800	2.78452800	-0.58605100
H	-3.38295680	3.53436201	0.44427121	H	-3.48785100	3.54803300	-0.02052600
H	1.32564916	-0.40589671	1.86373066	H	1.07315100	-0.24598700	2.03918500
O	-4.62874921	-0.41516212	-1.39466536	O	-4.47064200	-0.64351300	-1.63506200
H	-4.03586942	-0.36811249	-2.16869602	H	-3.77811800	-0.62605900	-2.32489300
H	-4.03822308	-0.14980393	-0.66749156	H	-3.98745200	-0.36267200	-0.84294100
O	-2.46895403	-0.21366834	-3.22922464	O	-2.15820400	-0.45419600	-3.25636100
H	-2.30777192	0.74414514	-3.10763052	H	-2.05204200	0.51766800	-3.20265200
H	-1.92913223	-0.63190727	-2.52799658	H	-1.62287400	-0.79248400	-2.51004700
O	-2.02078852	2.49993114	-2.46486193	O	-1.78753000	2.31559900	-2.69848200
H	-2.73833010	2.76645996	-1.86043617	H	-2.54050900	2.61100300	-2.15281100
H	-1.33795255	2.17973812	-1.83642122	H	-1.12606600	2.06490400	-2.01942700
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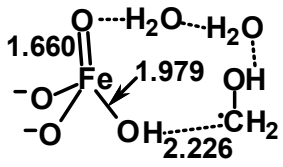

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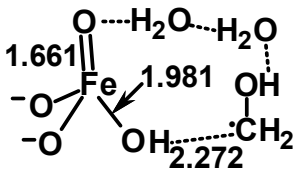
O	-1.05641804	-1.23270236	-0.90271999
O	-0.21136380	-0.40205899	1.89877411
C	2.93643661	-0.50642528	2.30352304
H	2.96245307	0.53877519	2.59376238
H	2.86061975	-1.28716607	3.04941848
H	-3.32908939	2.01031879	0.09521048
O	3.59672003	-0.86882022	1.17389218
H	3.27767438	1.14406917	-1.22635769
O	1.83964574	1.27147015	-2.20010356
H	1.74380096	2.07417612	-2.72449386
H	1.04631229	1.23684614	-1.61424573
O	4.07414026	1.01965287	-0.65711316
H	3.73583539	-0.09288773	0.56591267
H	4.68848991	0.48204745	-1.20235665
O	5.45239921	-0.95018548	-2.05360600
H	4.79651705	-1.64632625	-1.81609054
H	5.50222689	-0.94479786	-3.01555294
O	3.58508351	-2.70255051	-1.02065053
H	2.68351340	-2.67141503	-1.40545182
H	3.50070580	-2.27790911	-0.15001629
O	0.85827707	3.14557678	1.36551635
H	0.50714310	2.79051320	2.20626678
H	0.46735561	2.55622682	0.68975613
O	3.66860400	3.34734983	1.07344897
H	2.70079219	3.25428151	1.18304662
H	3.93027467	2.61070722	0.49842697
O	-2.32088458	-3.42023394	0.52588887
H	-1.72442779	-3.40376891	1.30276480
H	-1.94067988	-2.74414968	-0.06652979
O	-0.39533645	1.77621261	3.50083337
H	-0.37806992	0.92275239	2.99486482
H	0.02193376	1.58899663	4.34838784
O	1.01966183	-2.57412359	-2.10994034
H	0.60195619	-3.41598275	-2.32246325
H	0.32629409	-2.04874085	-1.64988747
O	-4.15215714	-1.64029418	1.85742481



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O	-1.04596500	-1.23603500	-0.87049700
O	-0.31139100	-0.30416300	1.92742300
C	2.86942400	-0.51411500	2.40471200
H	2.89051500	0.54140800	2.65526200
H	2.74660500	-1.26543500	3.17418800
H	-3.27207200	2.10312000	-0.12898100
O	3.58041700	-0.92546900	1.32301500
H	3.36101700	1.00173800	-1.15713300
O	1.95427100	1.12078800	-2.17609900
H	1.90084800	1.89625900	-2.74555300
H	1.13840400	1.13838300	-1.62081600
O	4.14070600	0.88530200	-0.56344300
H	3.75121200	-0.17511400	0.69186700
H	4.75734900	0.31494800	-1.07137800
O	5.51013000	-1.16796900	-1.84500800
H	4.83004800	-1.83855500	-1.60226200
H	5.59083100	-1.20190500	-2.80425800
O	3.57033200	-2.83397700	-0.80193500
H	2.67884100	-2.79339700	-1.20840000
H	3.47834200	-2.37361700	0.04978700
O	0.91013800	3.18055700	1.25213100
H	0.51858000	2.87644600	2.09508700
H	0.52068200	2.57589000	0.58919000
O	3.73350100	3.29067000	1.05728800
H	2.75998800	3.22831700	1.13301200
H	3.99574400	2.52458600	0.52240600
O	-2.44114100	-3.32074800	0.58875100
H	-1.88668100	-3.28371100	1.39538300
H	-2.01191700	-2.68199300	-0.01163100
O	-0.45857900	1.95974900	3.40544200
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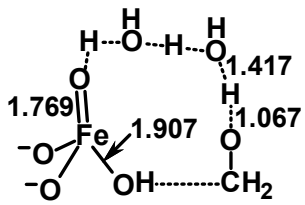
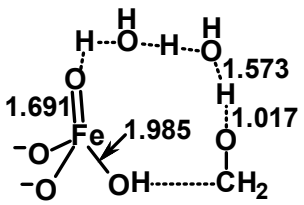
H	-0.07663400	1.80224100	4.27538300
O	1.03164000	-2.68155100	-1.95318300
H	0.59694000	-3.52069800	-2.14089100
H	0.34010900	-2.11789800	-1.53831200
O	-4.28090500	-1.43606300	1.75681900

H	-3.67031237	-2.36504832	1.41571077	H	-3.80200800	-2.19190400	1.36717700
H	-3.67110774	-0.85327321	1.54718111	H	-3.75862800	-0.67712200	1.44345700
O	-0.65284395	-2.93383564	2.72600611	O	-0.88631000	-2.77176200	2.85695700
H	-1.07517051	-2.93805344	3.59159866	H	-1.36138300	-2.71818600	3.69305700
H	-0.51638125	-1.97697914	2.49399116	H	-0.70683200	-1.83281100	2.58481900
O	-3.71537164	2.82898322	-0.29051412	O	-3.62256800	2.90605600	-0.57627100
H	-3.51325829	3.53157671	0.33687961	H	-3.42870500	3.63911900	0.01800400
H	0.76211654	-0.42656295	1.83401082	H	0.65987000	-0.38128100	1.89439400
O	-4.60608593	-0.49727959	-1.52791248	O	-4.55159400	-0.44846000	-1.68266600
H	-3.96774213	-0.44152335	-2.26462983	H	-3.87733300	-0.44821700	-2.38913800
H	-4.06189797	-0.25335085	-0.76084621	H	-4.03831400	-0.18417600	-0.90177400
O	-2.36108702	-0.21599449	-3.25100722	O	-2.23238100	-0.32053900	-3.32083800
H	-2.22936120	0.74432180	-3.11278668	H	-2.08079800	0.64245200	-3.22827000
H	-1.83162410	-0.63129243	-2.54161285	H	-1.73934800	-0.70999600	-2.57171200
O	-1.90226389	2.48367407	-2.46026293	O	-1.73890000	2.40443000	-2.65482200
H	-2.63915928	2.75564653	-1.88095854	H	-2.49124800	2.72303900	-2.12107700
H	-1.23659276	2.17021344	-1.81325153	H	-1.10759700	2.11056100	-1.96515000
^{3}TS2				**^{5}TS2**			
							
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O	-2.48801000	0.43961100	0.46650600	O	-2.66004100	0.51597700	0.46892700
O	-0.76132400	-1.18977500	-0.87787400	O	-1.02988300	-1.27272800	-0.86624900
O	-0.27890700	-0.37908800	1.89338200	O	-0.30760200	-0.23658700	1.91026900
C	2.71490900	-0.48375000	2.38388100	C	2.87589700	-0.25999000	2.43343200
H	2.73793500	0.56427100	2.67461600	H	2.82705200	0.81819800	2.53037300
H	2.65915400	-1.25272800	3.14751700	H	2.65786500	-0.93120400	3.25252600
H	-3.34159900	1.99313100	-0.09312700	H	-3.27972600	2.04168800	-0.15429600
O	3.32578500	-0.83548200	1.24227800	O	3.43567000	-0.79763300	1.36345700
H	2.78390000	1.07601800	-1.20455200	H	3.31674000	0.93553600	-1.17873300
O	1.86565400	1.12971800	-1.93583300	O	1.97503000	1.06544900	-2.21504500
H	1.98822500	1.87863200	-2.52899700	H	1.95328700	1.84220300	-2.78462100
H	0.67510300	1.26374300	-1.23469400	H	1.14265000	1.10312700	-1.66927200
O	3.72349600	0.99162700	-0.38924900	O	4.07740800	0.81333100	-0.55347700
H	3.47551900	-0.01440700	0.57773500	H	3.65822700	-0.10866800	0.64948900
H	4.47950300	0.62820400	-0.87934900	H	4.71310100	0.23766200	-1.03544600
O	5.59951900	-0.85569600	-1.73382900	O	5.50034100	-1.23976000	-1.72223500
H	4.97555800	-1.57891100	-1.50071700	H	4.81632900	-1.90755500	-1.48384300

H	5.70125800	-0.89759900	-2.69062100	H	5.61980100	-1.30429300	-2.67592500
O	3.77946400	-2.73695900	-0.76692500	O	3.52529200	-2.88297600	-0.70831100
H	2.92895900	-2.76948600	-1.24949700	H	2.64169100	-2.81918800	-1.13421900
H	3.57236500	-2.25772100	0.05664800	H	3.41378100	-2.46211900	0.15688000
O	0.57966100	3.37160000	1.28852200	O	0.86973000	3.21317100	1.06875600
H	0.22371800	2.96997500	2.10521500	H	0.47317700	2.95035900	1.92238600
H	0.27175900	2.77208400	0.58098400	H	0.50002400	2.56291900	0.43220200
O	3.43479000	3.40640800	0.99179100	O	3.68346100	3.32350900	0.94204800
H	2.46839800	3.40420800	1.12749500	H	2.70648400	3.26987300	0.98907300
H	3.62045500	2.58009000	0.49710200	H	3.95505200	2.54564000	0.43077800
O	-2.24016900	-3.44266000	0.45895500	O	-2.32159100	-3.31457900	0.67352400
H	-1.69630500	-3.41735400	1.27381900	H	-1.75686700	-3.26314300	1.47089000
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O	-0.61302400	1.89736300	3.41080900	O	-0.49689200	2.08684500	3.29171200
H	-0.53805700	1.02383100	2.95993500	H	-0.48239900	1.18770300	2.87184900
H	-0.20058800	1.78341900	4.27387300	H	-0.10995600	1.97607700	4.16660900
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H	0.83942000	-3.55074500	-2.21404500	H	0.61309100	-3.50263600	-2.14752700
H	0.63606700	-2.13098300	-1.64869700	H	0.33168400	-2.11394700	-1.51142800
O	-4.13261300	-1.66204000	1.70461600	O	-4.16654300	-1.43737100	1.87819700
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H	-3.62816300	-0.86371600	1.48042500	H	-3.68552600	-0.67577900	1.50037600
O	-0.76364300	-2.92244100	2.77314700	O	-0.74255800	-2.69949800	2.92188800
H	-1.26105100	-2.93217800	3.59809500	H	-1.20865100	-2.64612800	3.76300300
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H	0.70574200	-0.44041200	1.91399900	H	0.66313500	-0.27003800	1.85170200
O	-4.39341600	-0.69196300	-1.70519500	O	-4.54256500	-0.51218100	-1.58397500
H	-3.70294800	-0.58399500	-2.38882800	H	-3.88675000	-0.54761800	-2.30636500
H	-3.94030200	-0.42454400	-0.89286000	H	-4.00729000	-0.21202200	-0.82808000
O	-2.13281400	-0.26790200	-3.36068700	O	-2.25775600	-0.46063300	-3.28474100
H	-2.06692400	0.70327400	-3.23733600	H	-2.10818100	0.50528400	-3.23179300
H	-1.53984400	-0.63609600	-2.68399300	H	-1.75673400	-0.81692400	-2.52052900
O	-1.90081300	2.45339300	-2.65248100	O	-1.75265700	2.29255100	-2.71628200
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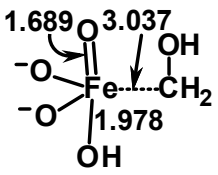
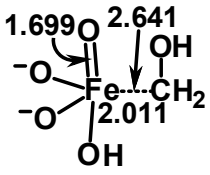
^{3}TS1front



^{3}INT1front



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O	2.18244696	0.55044113	0.42860481	O	2.13634118	0.67676990	0.35993944
O	0.69590370	-1.75856815	0.12028285	O	0.66871964	-1.70613567	0.02959518
O	1.57925240	-0.06323068	-2.03600252	O	1.65765176	0.01943801	-2.07302690
C	-1.43227143	0.09923358	-2.26026039	C	-1.23308174	-0.00024979	-2.01655249
H	-1.18607347	1.13907759	-2.09855174	H	-1.06848954	1.07031811	-2.04279811
H	-0.96332625	-0.47266384	-3.04894168	H	-0.71609176	-0.65831106	-2.70023543
H	1.97204580	2.05654818	1.38080227	H	1.93751882	2.09644611	1.34184242
O	-2.63420175	-0.35033196	-1.90308505	O	-2.36757068	-0.47435030	-1.58129217
H	-3.72806208	0.73669655	0.68063497	H	-3.66874367	0.73144007	0.75692137
O	-2.73737025	0.09953525	1.93888907	O	-2.70033192	0.13822490	2.04433551
H	-2.61652997	0.57559710	2.76831242	H	-2.55787369	0.62974018	2.86105277
H	-1.86575316	0.16733377	1.46882511	H	-1.84211610	0.20595074	1.54489164
O	-4.14754551	0.95537634	-0.18735089	O	-4.02316622	0.89335892	-0.15301989
H	-3.12209169	0.25309155	-1.26621836	H	-2.93941248	0.17268007	-1.03936223
H	-4.91670192	0.34721032	-0.24222285	H	-4.79866732	0.29162083	-0.22604989
O	-5.90300844	-1.20250321	-0.34291040	O	-5.83339586	-1.19272742	-0.33890855
H	-5.20798467	-1.88793908	-0.46601688	H	-5.17492489	-1.91740657	-0.43332262
H	-6.41041011	-1.47063243	0.43050529	H	-6.38041543	-1.42253136	0.42004424
O	-3.75091773	-2.82435356	-1.01098243	O	-3.76578156	-2.94929878	-0.93071412
H	-3.04217284	-3.07245036	-0.38100092	H	-3.04240831	-3.13225221	-0.29296650
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O	-0.44273993	3.21562120	-0.13580575	O	-0.47324562	3.25137825	-0.10513734
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O	1.21762454	2.63487768	-2.39280270	O	1.25510150	2.71404656	-2.33296682
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O	-1.52691085	-3.32089120	0.62021063	O	-1.50307693	-3.26287719	0.67153759
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O	4.63990375	1.13935603	-0.64443639	O	4.76511800	0.88058104	-0.28673083
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H	4.58827448	-0.47885904	-1.75881781	H	4.63172826	-0.51265465	-1.63281192
H	3.16637766	-0.72272917	-2.25229234	H	3.23240670	-0.64227423	-2.23066420

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H	1.05824867	-0.59095345	-2.65095505	H	1.21168185	-0.47586384	-2.76815346
O	3.68837005	-0.87406303	2.36995549	O	3.66982312	-0.63347170	2.27389171
H	2.94469093	-1.34503858	2.78678402	H	3.03190304	-1.22349425	2.70978027
H	3.23539492	-0.38008990	1.65796607	H	3.10088091	-0.18422711	1.60980725
O	1.07836001	-1.83972148	3.05879844	O	1.14610059	-1.84558385	2.95750254
H	0.77565712	-0.94044897	3.29513423	H	0.83879673	-0.95611792	3.22231786
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O	0.17424936	0.86340092	3.30591914	O	0.22513403	0.84920670	3.28150769
H	0.81005658	1.59666784	3.28177983	H	0.85624849	1.58681113	3.25212190
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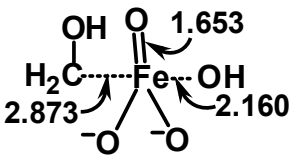

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O	0.65749697	1.29537464	-0.44068631	O	0.31743151	1.33920689	-0.49588965
O	1.21919410	-0.25762417	1.94863672	O	1.19758298	-0.36979283	1.53315248
C	-1.56258980	0.35689359	1.74002389	C	-1.49607456	0.39685133	1.58297512
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H	-0.94870921	1.02817461	2.31919532	H	-0.96395770	1.12588818	2.18462107
H	3.39329429	-1.78905864	-1.02639548	H	4.07752605	-1.58712061	-0.82814076
O	-2.68559547	0.88437811	1.25796696	O	-2.50794587	0.89359244	0.90970062
H	-3.50515757	-1.03798966	-0.85844360	H	-3.72661121	-1.12833584	-0.99297020
O	-2.18030854	-1.38736890	-1.90448722	O	-2.58616227	-1.66723453	-2.21091699
H	-2.17848829	-2.24936222	-2.33516793	H	-2.61501021	-2.58775801	-2.49550478
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O	-4.14066897	-0.76650468	-0.15221215	O	-4.16848922	-0.74296045	-0.19942834
H	-3.26118289	0.20283632	0.79331668	H	-3.12028929	0.18758757	0.50407432
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H	-4.96710248	2.05397928	-0.95843662	H	-5.20860158	2.03236143	-0.90838241
H	-5.93485777	1.43209408	-2.01045156	H	-6.16482881	1.31797668	-1.91190208
O	-3.61774805	3.08299652	-0.36050341	O	-3.94372052	3.19630802	-0.39902799
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H	-3.33388584	2.55583828	0.40297132	H	-3.64708612	2.82574376	0.44232555
O	-1.05277740	-3.37469649	1.26390038	O	-1.32853056	-3.45759873	1.27425901
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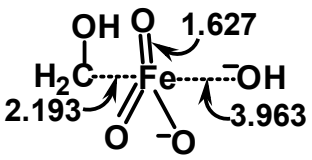

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H	-4.10507974	-2.37234461	0.99474803	H	-4.24786150	-2.21726941	1.10351164
O	1.73684448	3.42774598	1.10951983	O	2.16694331	3.16603187	0.92571705
H	1.54019271	3.09342734	2.00629496	H	1.94256724	2.83441220	1.81618399
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O	0.76299823	-2.60228865	3.29454818	O	0.82843509	-2.74869760	2.97319497
H	0.95337809	-1.73452281	2.86839517	H	1.02985201	-1.89715664	2.53284193
H	0.49628062	-2.39526643	4.19679460	H	0.71328256	-2.53671528	3.90599184
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H	3.46560844	2.63385351	0.94398031	H	4.05453404	2.53973484	0.91372556
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