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Analysis of an alternative to the H-atom abstraction mechanism in methane C−H bond activation by nonheme iron(IV)–oxo oxidants

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Part 3

All xyz coordinates.

Table S1. Energy data in solution for $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^-, OH^-, F^-, and $CF_3CO_2^-$.

solution	Point	ΔG (au) (B3LYP/B1)	ΔG (au) (B3LYP/B2// B3LYP/B1)	ΔG (au) (B3LYP/G/B2// B3LYP/B1)	ΔG (au) (PBE0/B2//B3LYP/B1)	ΔG (au) (B3LYP+VDW/B2// B3LYP/B1)
L = SR^-	S = 1	-2546.64479	-2547.07086	-2547.81611	-2546.34823	-2547.16924
	S = 2	-2546.65076	-2547.07423	-2547.81884	-2546.35563	-2547.17583
L = OH^-	S = 1	-2185.63216	-2186.04722	-2186.73876	-2185.38123	-2186.14063
	S = 2	-2185.63686	-2186.04896	-2186.73987	-2185.38737	-2186.14506
L = F^-	S = 1	-2209.70416	-2210.10738	-2210.79951	-2209.42714	-2210.19825
	S = 2	-2209.70348	-2210.10338	-2210.79488	-2209.42752	-2210.19661
L = $CF_3CO_2^-$	S = 1	-2636.01778	-2636.45163	-2637.31753	-2635.52283	-2636.55664
	S = 2	-2636.01807	-2636.45035	-2637.31563	-2635.52610	-2636.55770

solution	Point	ΔG (kcal/mol) (B3LYP/B1)	ΔG (kcal/mol) (B3LYP/B2// B3LYP/B1)	ΔG (kcal/mol) (B3LYP/G/B2// B3LYP/B1)	ΔG (kcal/mol) (PBE0/B2//B3LYP/B1)	ΔG (kcal/mol) (B3LYP+ VDW/B2// B3LYP/B1)
L = SR^-	S = 1	3.7	2.1	1.7	4.6	4.1
	S = 2	0.0	0.0	0.0	0.0	0.0
L = OH^-	S = 1	3.0	1.1	0.7	3.9	2.8
	S = 2	0.0	0.0	0.0	0.0	0.0
L = F^-	S = 1	0.0	0.0	0.0	0.2	0.0
	S = 2	0.4	2.5	2.9	0.0	1.0
L = $CF_3CO_2^-$	S = 1	0.2	0.0	0.0	2.0	0.7
	S = 2	0.0	0.8	1.2	0.0	0.0

Table S2. Energy data in gas for $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^{-}, and OH^{-}.

gas	Point	ΔG (au) (B3LYP/B1)	ΔG (au) (B3LYP/B2// B3LYP/B1)	ΔG (au) (B3LYP/G/B2// B3LYP/B1)	ΔG (au) (PBE0/B2//B3LYP/B1)	ΔG (au) (B3LYP+VDW/B2// B3LYP/B1)
L = SR^{-}	S = 1	-2546.57403	-2547.07117	-2547.81642	-2546.34856	-2547.16963
	S = 2	-2546.57914	-2547.07441	-2547.81901	-2546.35568	-2547.17609
L = OH^{-}	S = 1	-2185.56137	-2186.04763	-2186.73916	-2185.38143	-2186.14108
	S = 2	-2185.56804	-2186.04938	-2186.74028	-2185.38749	-2186.14542

gas	Point	ΔG (kcal/mol) (B3LYP/B1)	ΔG (kcal/mol) (B3LYP/B2// B3LYP/B1)	ΔG (kcal/mol) (B3LYP/G/B2// B3LYP/B1)	ΔG (kcal/mol) (PBE0/B2//B3LYP/B1)	ΔG (kcal/mol) (B3LYP+VDW/B2// B3LYP/B1)
L = SR^{-}	S = 1	3.2	2.0	1.6	4.5	4.1
	S = 2	0.0	0.0	0.0	0.0	0.0
L = OH^{-}	S = 1	4.2	1.1	0.7	3.8	2.7
	S = 2	0.0	0.0	0.0	0.0	0.0

Table S3. Energies data in solution for $[Fe^{IV}=O(TMC)(SR)]^{+}$. (a) B3LYP/B1, B3LYP-G/B1, B3LYP+VDW/B1 and PBE0/B1; (b) B3LYP/B2//B1, B3LYP-G/B2//B1, B3LYP+VDW/B2//B1 and PBE0/B2//B1.

(a)

B1	Point	ΔG (au) (B3LYP)	ΔG (au) (B3LYP-G)	ΔG (au) (B3LYP+VDW)	ΔG (au) (PBE0)
ΔG (au)	S = 1	-2546.644791	-2547.389721	-2546.741274	-2545.925074
	S = 2	-2546.650761	-2547.394991	-2546.750265	-2545.934548
ΔG (kcal/mol)	S = 1	3.7	3.3	5.6	5.9
	S = 2	0.0	0.0	0.0	0.0

(b)

B2	Point	ΔG (kcal/mol) (B3LYP)	ΔG (kcal/mol) (B3LYP-G)	ΔG (kcal/mol) (B3LYP+VDW)	ΔG (kcal/mol) (PBE0)
ΔG (au)	S = 1	-2547.070864	-2547.816144	-2547.169728	-2546.352464
	S = 2	-2547.074229	-2547.818868	-2547.176494	-2546.359232
ΔG (kcal/mol)	S = 1	2.1	1.7	4.2	4.2
	S = 2	0.0	0.0	0.0	0.0

Table S4. Relative energies data in solution of B3LYP, B3LYP-G, PBE0 and B3LYP+VDW for methane C−H bond hydroxylation by $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^{-}, OH^{-}, F^{-}, and $CF_3CO_2^{-}$. The energy values in solution are relative to ^{3,5}**R** + **CH$_4$**.

solution	Point	ΔG (kcal/mol) (B3LYP/B1)	ΔG (kcal/mol) (B3LYP/B2// B3LYP/B1)	ΔG (kcal/mol) (B3LYP/G/B2// B3LYP/B1)	ΔG (kcal/mol) (PBE0/B2//B3LYP/B1)	ΔG (kcal/mol) (B3LYP+VDW/B2// B3LYP/B1)
L = SR^{-}	$^{3\delta}$**R+CH$_4$**	3.7	2.1	1.7	4.6	4.1
	$^{3\delta}$**TS**	45.2	35.7	35.6	32.9	30.5
	$^{3\delta}$**I**	33.4	22.4	22.4	19.2	19.0
	$^{3\pi}$**R+CH$_4$**	3.7	2.1	1.7	4.6	4.1
	$^{3\pi}$**TS**	46.2	35.4	34.9	34.6	32.2
	$^{3\pi}$**I**	35.2	22.9	22.5	22.1	21.6
	$^{5\sigma}$**R+CH$_4$**	0.0	0.0	0.0	0.0	0.0
	$^{5\sigma}$**TS**	34.3	28.6	28.8	23.4	24.4
	$^{5\sigma}$**I**	28.1	20.9	21.3	15.1	17.9
	$^{5\pi}$**R+CH$_4$**	0.0	0.0	0.0	0.0	0.0
	$^{5\pi}$**TS**	42.2	33.2	33.1	30.2	27.8
	$^{5\pi}$**I**	30.3	20.8	20.8	17.7	17.3
L = OH^{-}	$^{3\delta}$**R+CH$_4$**	3.0	1.1	0.7	3.9	2.8
	$^{3\delta}$**TS**	45.1	35.1	34.9	32.1	29.9
	$^{3\delta}$**I**	31.8	20.5	20.5	17.1	17.0
	$^{3\pi}$**R+CH$_4$**	3.0	1.1	0.7	3.9	2.8
	$^{3\pi}$**TS**	46.3	34.8	34.4	34.5	31.4
	$^{3\pi}$**I**	34.4	22.6	22.2	22.4	21.1
	$^{5\sigma}$**R+CH$_4$**	0.0	0.0	0.0	0.0	0.0
	$^{5\sigma}$**TS**	33.4	27.2	27.4	21.7	23.1
	$^{5\sigma}$**I**	27.3	19.3	19.7	13.2	16.4
	$^{5\pi}$**R+CH$_4$**	0.0	0.0	0.0	0.0	0.0
	$^{5\pi}$**TS**	44.9	35.6	35.5	32.9	30.3
	$^{5\pi}$**I**	30.4	20.5	20.5	17.3	17.1
L = F^{-}	$^{3\sigma}$**R+CH$_4$**	0.0	0.0	0.0	0.2	0.0
	$^{3\sigma}$**TS**	44.3	39.2	39.4	34.8	35.4

	$^{3\sigma}$**I**	34.2	24.5	24.9	18.4	19.3
	$^{3\pi}$**R+CH$_4$**	0.0	0.0	0.0	0.2	0.0
	$^{3\pi}$**TS**	44.4	35.8	35.8	32.8	30.6
	$^{3\pi}$**I**	34.0	24.7	24.7	21.8	21.3
	$^{5\sigma}$**R+CH$_4$**	0.4	2.5	2.9	0.0	1.0
	$^{5\sigma}$**TS**	32.3	28.7	29.3	20.6	23.3
	$^{5\sigma}$**I**	26.6	21.4	22.2	12.5	17.1
	$^{5\pi}$**R+CH$_4$**	0.4	2.5	2.9	0.0	1.0
	$^{5\pi}$**TS**	46.3	40.0	40.3	34.5	33.0
	$^{5\pi}$**I**	32.7	24.3	24.6	18.2	19.1
L = $CF_3CO_2^-$	$^{3\sigma}$**R+CH$_4$**	0.2	0.0	0.0	2.0	0.7
	$^{3\sigma}$**TS**	40.0	36.9	37.1	34.2	29.9
	$^{3\sigma}$**I**	36.6	31.4	31.8	28.1	25.5
	$^{3\pi}$**R+CH$_4$**	0.2	0.0	0.0	2.0	0.7
	$^{3\pi}$**TS**	45.3	36.5	36.5	35.1	31.6
	$^{3\pi}$**I**	35.4	24.5	24.5	23.1	21.3
	$^{5\sigma}$**R+CH$_4$**	0.0	0.8	1.2	0.0	0.0
	$^{5\sigma}$**TS**	29.6	25.9	26.5	19.6	20.8
	$^{5\sigma}$**I**	25.5	18.6	19.4	11.4	14.3
	$^{5\pi}$**R+CH$_4$**	0.0	0.8	1.2	0.0	0.0
	$^{5\pi}$**TS**	45.5	38.8	39.1	35.3	32.2
	$^{5\pi}$**I**	35.7	26.8	27.2	22.7	21.9

Table S5. Relative energies data in the gas phase of B3LYP, B3LYP-G, PBE0 and B3LYP+VDW for methane C-H bond hydroxylation by $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^{-}, and OH^{-}. The gas-phase energies are relative to ^{3,5}**RC**.

gas	Point	ΔG (kcal/mol) (B3LYP/B1)	ΔG (kcal/mol) (B3LYP/B2// B3LYP/B1)	ΔG (kcal/mol) (PBE0/B2//B3LYP/B1)	ΔG (kcal/mol) (B3LYP+VDW/B2// B3LYP/B1)
L = SR^{-}	$^{3\delta}$**R+CH$_4$**	-4.8	2.2	5.1	5.8
	$^{3\delta}$**RC**	5.1	2.4	5.1	5.2
	$^{3\delta}$**TS**	32.1	35.8	33.6	32.3
	$^{3\delta}$**I**	19.3	21.0	18.4	19.1
	$^{3\pi}$**R+CH$_4$**	-4.8	2.2	5.1	5.8
	$^{3\pi}$**RC**	4.8	2.1	4.5	4.3
	$^{3\pi}$**TS**	34.6	35.4	35.1	33.8
	$^{3\pi}$**I**	23.7	22.9	22.4	23.0
	$^{5\sigma}$**R+CH$_4$**	-8.0	0.2	0.7	1.7
	$^{5\sigma}$**RC**	0.2	0.2	0.4	0.9
	$^{5\sigma}$**TS**	22.8	28.6	23.9	26.0
	$^{5\sigma}$**I**	16.7	21.0	15.8	19.7
	$^{5\pi}$**R+CH$_4$**	-8.0	0.2	0.7	1.7
	$^{5\pi}$**RC**	0.0	0.0	0.0	0.0
	$^{5\pi}$**TS**	29.7	33.3	30.9	29.5
	$^{5\pi}$**I**	18.7	20.8	18.2	18.9
L = OH^{-}	$^{3\delta}$**R+CH$_4$**	-5.5	1.4	4.6	4.8
	$^{3\delta}$**RC**	3.7	0.3	2.9	2.0
	$^{3\delta}$**TS**	33.3	35.4	32.9	32.0
	$^{3\delta}$**I**	19.1	20.7	17.8	19.0
	$^{3\pi}$**R+CH$_4$**	-5.5	1.4	4.6	4.8
	$^{3\pi}$**RC**	5.1	0.3	2.8	2.0
	$^{3\pi}$**TS**	34.9	35.2	35.4	33.6
	$^{3\pi}$**I**	23.9	22.8	22.9	23.0
	$^{5\sigma}$**R+CH$_4$**	-9.7	0.3	0.8	2.1
	$^{5\sigma}$**RC**	1.1	0.3	0.3	0.7
	$^{5\sigma}$**TS**	20.8	27.2	22.4	24.9
	$^{5\sigma}$**I**	14.9	19.3	13.7	18.2

$^{5\pi}$**R+CH$_4$**	-9.7	0.3	0.8	2.1
$^{5\pi}$**RC**	0.0	0.0	0.0	0.0
$^{5\pi}$**TS**	32.9	36.0	33.8	32.5
$^{5\pi}$**I**	19.3	20.8	18.0	19.0

Table S6. Spin populations in solution of the reactants, transition states, and intermediates for (a) $^{3}\delta$ and $^{3}\pi$-pathways; (b) $^{5}\sigma$ and $^{5}\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^{-}, and OH^{-}.[a]

(a)

solution		Fe		O		CH_3		H[b]	
		3δ	3π	3δ	3π	3δ	3π	3δ	3π
L = SR^{-}	**R**	2.25	2.25	0.45	0.45	0.00	0.00	0.00	0.00
	TS_H	2.28	1.18	0.15	0.57	-0.35	0.42	0.03	-0.05
	I	2.89	0.96	0.06	0.07	-0.98	0.98	0.00	0.00
L = OH^{-}	**R**	1.49	1.49	0.66	0.66	0.00	0.00	0.00	0.00
	TS_H	2.20	1.08	0.18	0.46	-0.30	0.57	0.03	-0.05
	I	2.81	0.97	0.03	0.06	-0.98	0.98	0.00	0.00

(b)

solution		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = SR^{-}	**R**	2.97	2.97	0.56	0.56	0.00	0.00	0.00	0.00
	TS_H	3.91	2.97	0.08	0.40	-0.56	0.53	0.03	-0.04
	I	4.08	2.90	0.23	0.03	-0.97	0.98	0.00	0.00
L = OH^{-}	**R**	3.19	3.19	0.56	0.56	0.00	0.00	0.00	0.00
	TS_H	3.97	2.91	0.02	0.38	-0.53	0.53	0.04	-0.05
	I	4.17	2.82	0.20	0.04	-0.98	0.99	0.01	0.01

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

Table S7. Spin populations in the gas phase of the reactants, transition states, and intermediates for (a) $^3\delta$ and $^3\pi$-pathways; (b) $^5\sigma$ and $^5\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^+$ with L = SR^-, and OH^-.[a]

(a)

gas		Fe		O		CH_3		H[b]	
		3δ	3π	3δ	3π	3δ	3π	3δ	3π
L = SR^-	**R**	1.35	1.35	0.73	0.73	0.00	0.00	0.00	0.00
	RC	1.35	1.35	0.73	0.73	0.00	0.00	0.00	0.00
	TS_H	2.82	1.03	-0.31	0.46	-0.50	0.57	0.03	-0.04
	I	2.90	0.93	0.02	0.07	-0.98	0.98	-0.01	0.00
L = OH^-	**R**	1.37	1.37	0.69	0.69	0.00	0.00	0.00	0.00
	RC	1.37	1.37	0.69	0.69	0.00	0.00	0.00	0.00
	TS_H	2.74	1.02	-0.39	0.45	-0.51	0.58	0.03	-0.04
	I	2.80	0.95	0.04	0.06	-0.97	0.98	0.00	0.00

(b)

gas		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = SR^-	**R**	3.15	3.15	0.67	0.67	0.00	0.00	0.00	0.00
	RC	3.19	3.19	0.64	0.64	0.00	0.00	0.00	0.00
	TS_H	3.91	2.98	0.06	0.40	-0.56	0.56	0.02	-0.03
	I	4.06	2.90	0.21	0.03	-0.97	0.97	0.00	0.01
L = OH^-	**R**	3.17	3.17	0.56	0.56	0.00	0.00	0.00	0.00
	RC	3.18	3.18	0.55	0.55	0.00	0.00	0.00	0.00
	TS_H	3.99	2.91	0.02	0.36	-0.57	0.58	0.03	-0.03
	I	4.16	2.81	0.19	0.04	-0.97	0.97	0.00	0.02

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

Table S8. Spin populations in solution of the reactants, transition states, and intermediates for (a) $^3\delta$ and $^3\pi$-pathways; (b) $^5\sigma$ and $^5\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^+$ with L = F^-, and $CF_3CO_2^-$.[a]

(a)

solution		Fe		O		CH_3		H[b]	
		3σ	3π	3σ	3π	3σ	3π	3σ	3π
L = F^-	**R**	1.52	1.52	0.66	0.66	0.00	0.00	0.00	0.00
	TS_H	2.69	1.11	0.07	0.46	-0.70	0.58	0.05	-0.05
	I	2.82	1.01	0.05	0.07	-0.98	0.98	0.00	0.00
L = $CF_3CO_2^-$	**R**	1.51	1.51	0.70	0.70	0.00	0.00	0.00	0.00
	TS_H	2.71	1.09	0.08	0.45	-0.63	0.59	0.04	-0.04
	I	2.95	1.03	0.23	0.08	-0.97	0.98	0.01	0.00

(b)

solution		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = F^-	**R**	3.19	3.19	0.53	0.53	0.00	0.00	0.00	0.00
	TS_H	3.99	2.91	0.05	0.36	-0.53	0.55	0.03	-0.04
	I	4.20	2.82	0.23	0.05	-0.97	0.98	0.00	0.01
L = $CF_3CO_2^-$	**R**	3.16	3.16	0.57	0.57	0.00	0.00	0.00	0.00
	TS_H	4.02	2.96	0.11	0.34	-0.57	0.51	0.02	-0.02
	I	4.17	2.87	0.29	0.02	-0.96	0.97	0.00	0.01

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

Table S9. Mulliken charge analysis of the reactants, transition states, and intermediates in solution for (a) $^3\delta$ and $^3\pi$-pathways; (b) $^5\sigma$ and $^5\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^+$ with L = SR^-, and OH^-.[a]

(a)

solution		Fe		O		CH_3		H[b]	
		3δ	3π	3δ	3π	3δ	3π	3δ	3π
L = SR^-	**R**	0.51	0.51	-0.66	-0.66	-0.13	-0.13	0.13	0.13
	TS_H	0.51	0.58	-0.67	-0.63	-0.26	-0.08	0.31	0.24
	I	0.65	0.45	-0.71	-0.71	0.02	0.01	0.28	0.27
L = OH^-	**R**	0.80	0.80	-0.60	-0.60	-0.13	-0.13	0.13	0.13
	TS_H	0.63	0.78	-0.67	-0.68	-0.36	-0.12	0.34	0.30
	I	0.85	0.59	-0.70	-0.71	0.02	0.01	0.28	0.27

(b)

solution		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = SR^-	**R**	0.56	0.56	-0.58	-0.58	-0.13	-0.13	0.13	0.13
	TS_H	0.84	0.56	-0.68	-0.67	-0.06	-0.10	0.27	0.27
	I	0.89	0.69	-0.76	-0.71	0.01	0.01	0.28	0.27
L = OH^-	**R**	0.90	0.90	-0.57	-0.57	-0.13	-0.13	0.13	0.13
	TS_H	0.98	0.69	-0.66	-0.66	-0.08	-0.11	0.27	0.28
	I	1.03	0.84	-0.74	-0.68	0.01	0.01	0.28	0.29

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

Table S10. Mulliken charge analysis of the reactants, transition states, and intermediates in the gas phase for (a) $^{3}\delta$ and $^{3}\pi$-pathways; (b) $^{5}\sigma$ and $^{5}\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^{+}$ with L = SR^{-}, and OH^{-}.[a]

(a)

gas		Fe		O		CH_3		H[b]	
		3δ	3π	3δ	3π	3δ	3π	3δ	3π
L = SR^{-}	**R**	0.38	0.38	-0.55	-0.55	-0.12	-0.12	0.12	0.12
	RC	0.41	0.40	-0.56	-0.56	-0.13	-0.12	0.12	0.11
	TS_H	0.66	0.44	-0.70	-0.69	0.00	-0.05	0.23	0.25
	I	0.66	0.41	-0.71	-0.71	0.02	0.02	0.27	0.26
L = OH^{-}	**R**	0.59	0.59	-0.56	-0.56	-0.12	-0.12	0.12	0.12
	RC	0.60	0.60	-0.58	-0.58	-0.13	-0.12	0.12	0.11
	TS_H	0.84	0.57	-0.67	-0.69	-0.01	-0.07	0.25	0.27
	I	0.85	0.57	-0.69	-0.70	0.03	0.02	0.28	0.26

(b)

gas		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = SR^{-}	**R**	0.46	0.46	-0.40	-0.40	-0.12	-0.12	0.12	0.12
	RC	0.67	0.66	-0.55	-0.55	-0.12	-0.12	0.12	0.12
	TS_H	0.80	0.68	-0.69	-0.68	-0.03	-0.04	0.25	0.25
	I	0.84	0.66	-0.78	-0.71	0.02	0.02	0.28	0.27
L = OH^{-}	**R**	0.85	0.85	-0.54	-0.54	-0.12	-0.12	0.12	0.12
	RC	0.88	0.88	-0.55	-0.56	-0.12	-0.12	0.11	0.11
	TS_H	0.96	0.84	-0.68	-0.67	-0.03	-0.05	0.25	0.26
	I	1.00	0.86	-0.74	-0.69	0.02	0.02	0.28	0.28

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

Table S11. Mulliken charge analysis of the reactants, transition states, and intermediates in solution for (a) $^3\delta$ and $^3\pi$-pathways; (b) $^5\sigma$ and $^5\pi$-pathways; for methane hydroxylation by $[Fe^{IV}=O(TMC)(L)]^+$ with L = F^-, and $CF_3CO_2^-$.[a]

(a)

solution		Fe		O		CH_3		H[b]	
		3σ	3π	3σ	3π	3σ	3π	3σ	3π
L = F^-	**R**	0.85	0.85	-0.60	-0.60	-0.13	-0.13	0.13	0.13
	TS_H	0.73	0.70	-0.74	-0.66	-0.09	-0.07	0.31	0.28
	I	0.86	0.63	-0.68	-0.69	0.02	0.01	0.28	0.27
L = $CF_3CO_2^-$	**R**	0.87	0.87	-0.53	-0.53	-0.13	-0.13	0.13	0.13
	TS_H	0.85	0.79	-0.69	-0.59	-0.04	0.03	0.29	0.27
	I	0.91	0.69	-0.74	-0.62	0.02	0.02	0.28	0.28

(b)

solution		Fe		O		CH_3		H[b]	
		5σ	5π	5σ	5π	5σ	5π	5σ	5π
L = F^-	**R**	0.96	-0.56	-0.56	-0.56	-0.13	-0.13	0.13	0.13
	TS_H	0.97	-0.65	-0.65	-0.64	-0.06	-0.09	0.27	0.28
	I	1.03	-0.75	-0.75	-0.68	0.02	0.02	0.29	0.29
L = $CF_3CO_2^-$	**R**	0.98	0.98	-0.49	-0.49	-0.13	-0.13	0.13	0.13
	TS_H	1.14	0.83	-0.62	-0.58	0.01	-0.01	0.26	0.25
	I	1.20	0.96	-0.70	-0.61	0.03	0.02	0.29	0.28

[a] Values from Mulliken population analysis. [b] The transferred hydrogen.

1. Schematic MO diagrams of $^{5}\boldsymbol{\sigma}$, and $^{3,5}\boldsymbol{\pi}$**-pathways** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^{+}$ in solution.

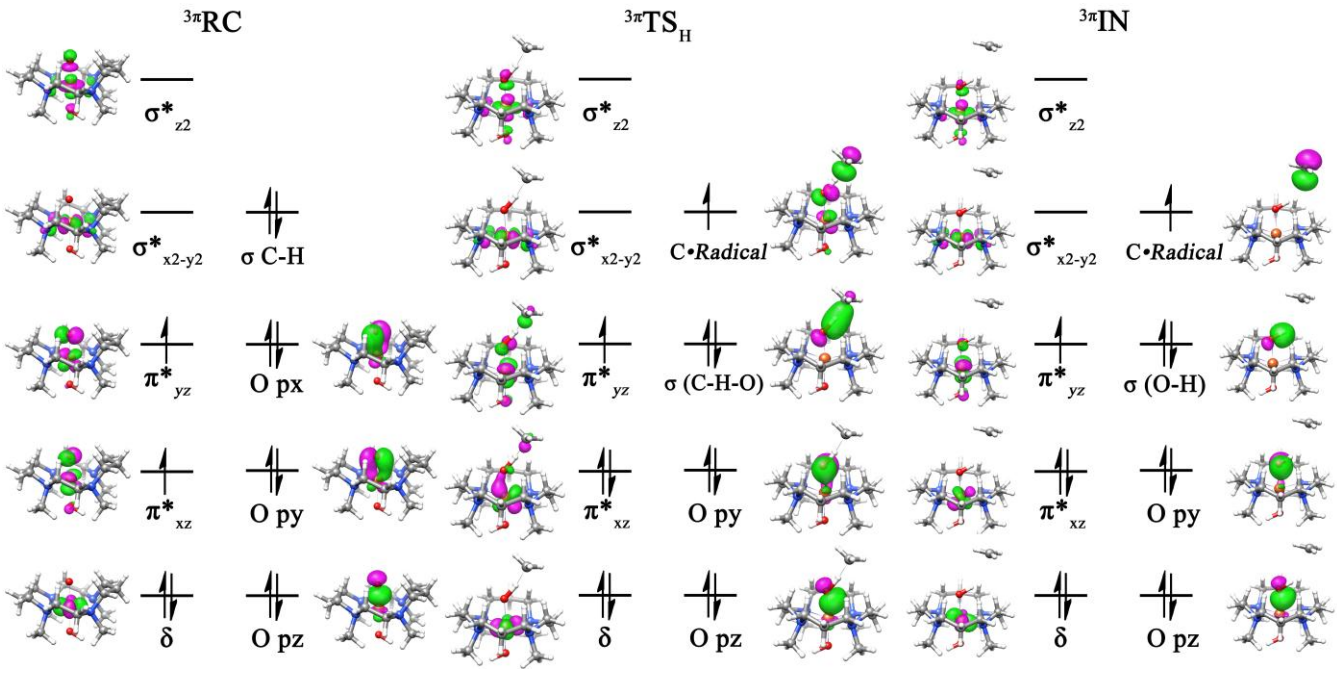

Figure S1. Schematic MO diagram of $^{3}\boldsymbol{\pi}$**-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^{+}$ in solution.

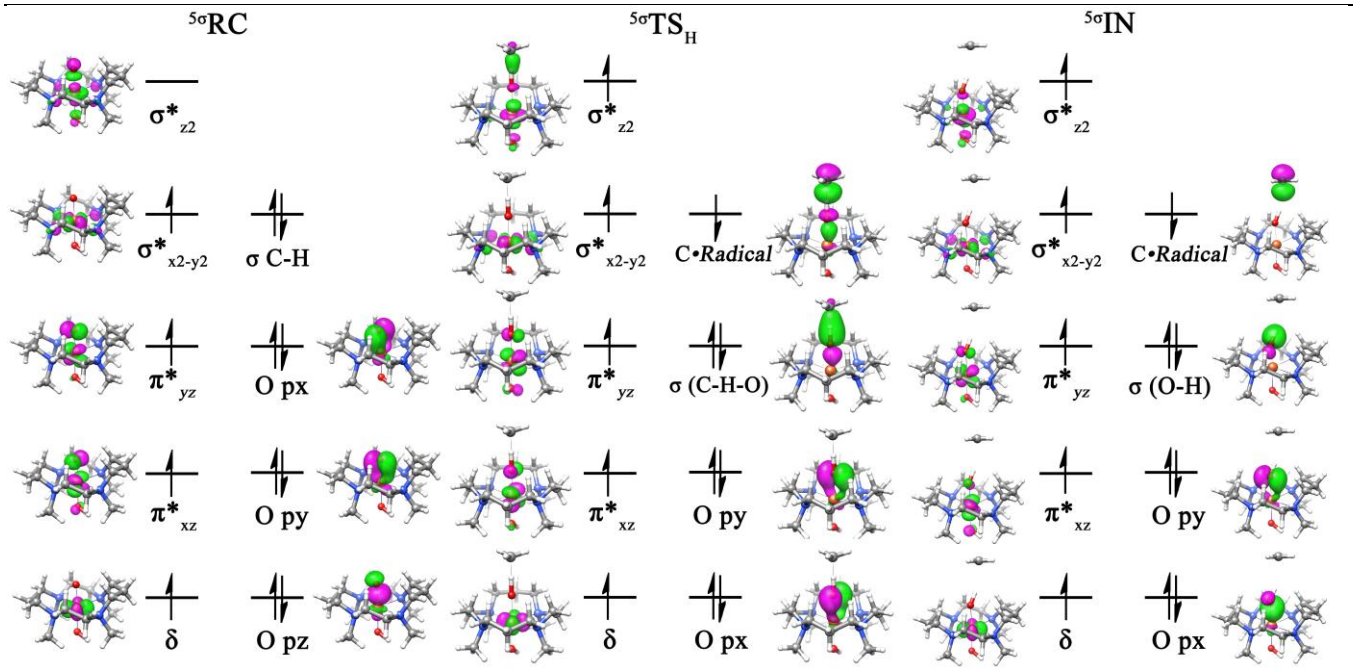

Figure S2. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^{+}$ in solution.

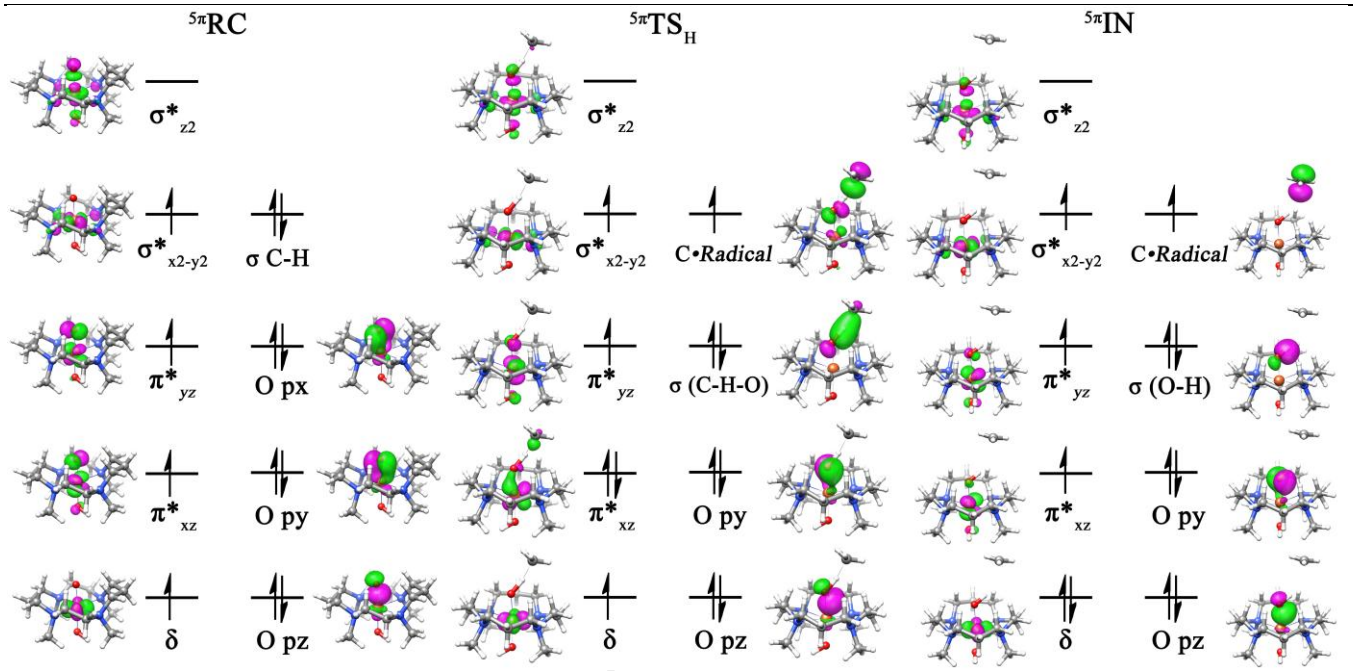

Figure S3. Schematic MO diagram of **^{5}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^{+}$ in solution.

2. Schematic MO diagrams of **$^{5}\sigma$**, and **$^{3,5}\pi$-pathways** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^{+}$ in solution.

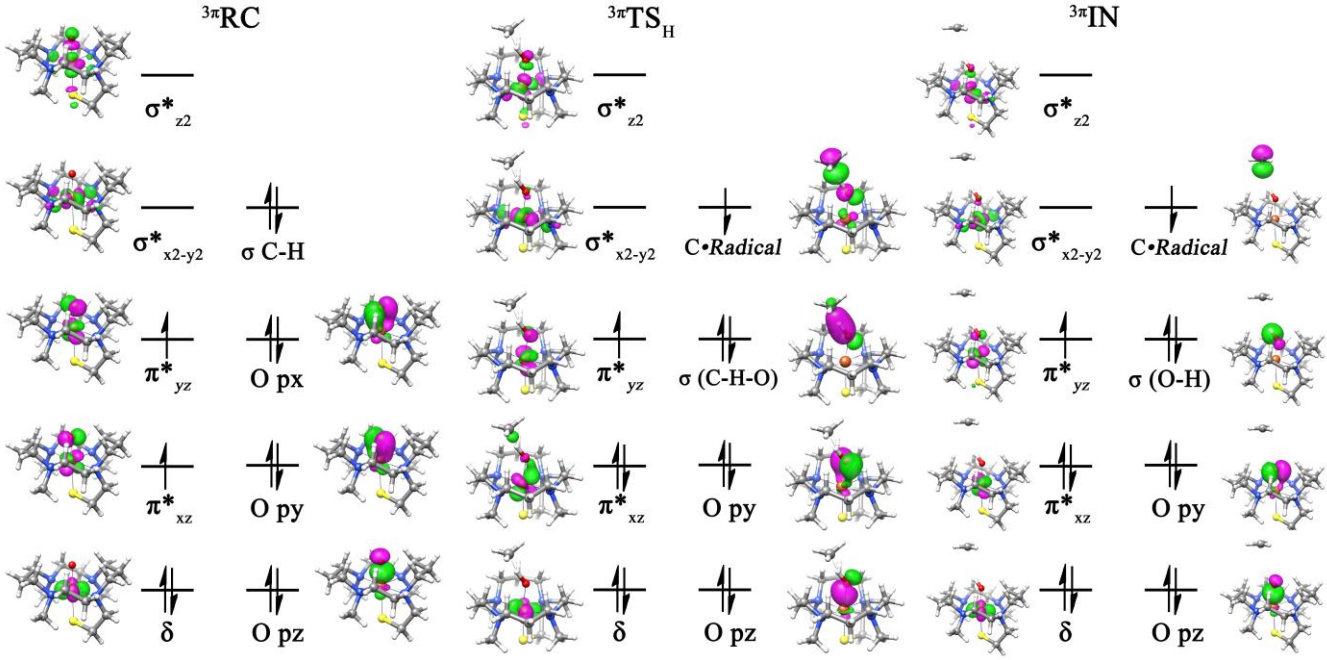

Figure S4. Schematic MO diagram of **$^{3}\pi$-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^{+}$ in solution.

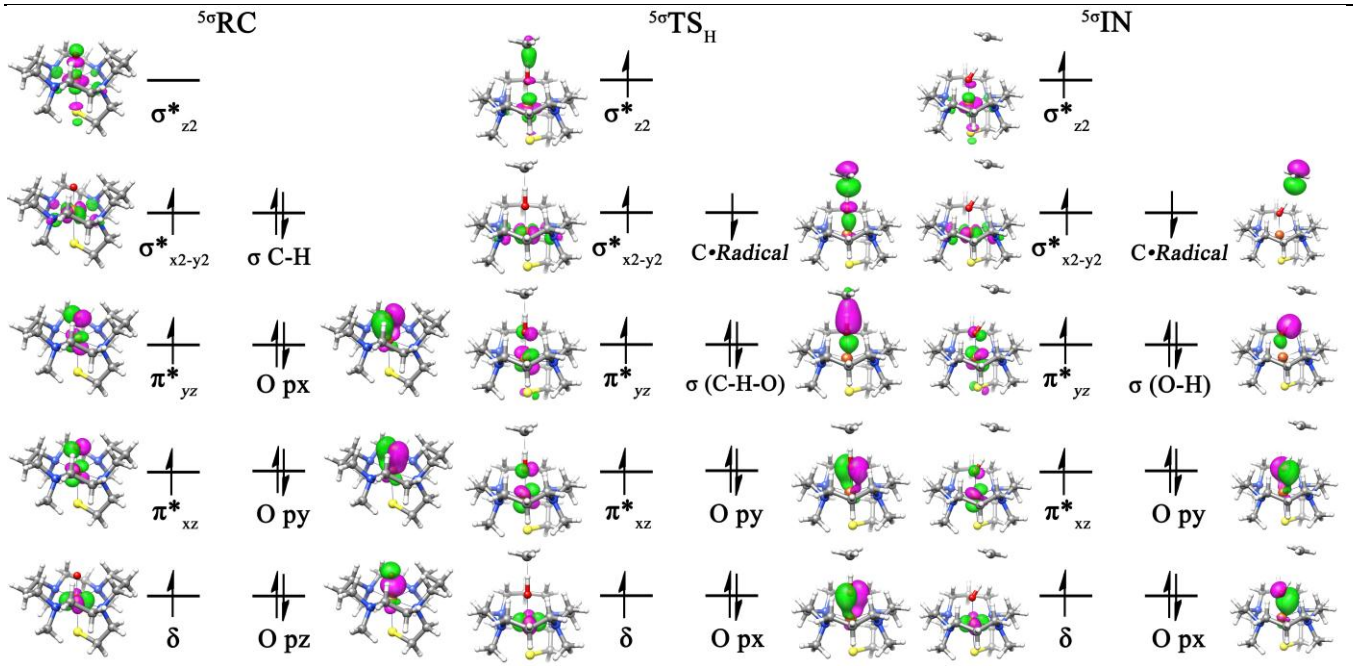

Figure S5. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^+$ in solution.

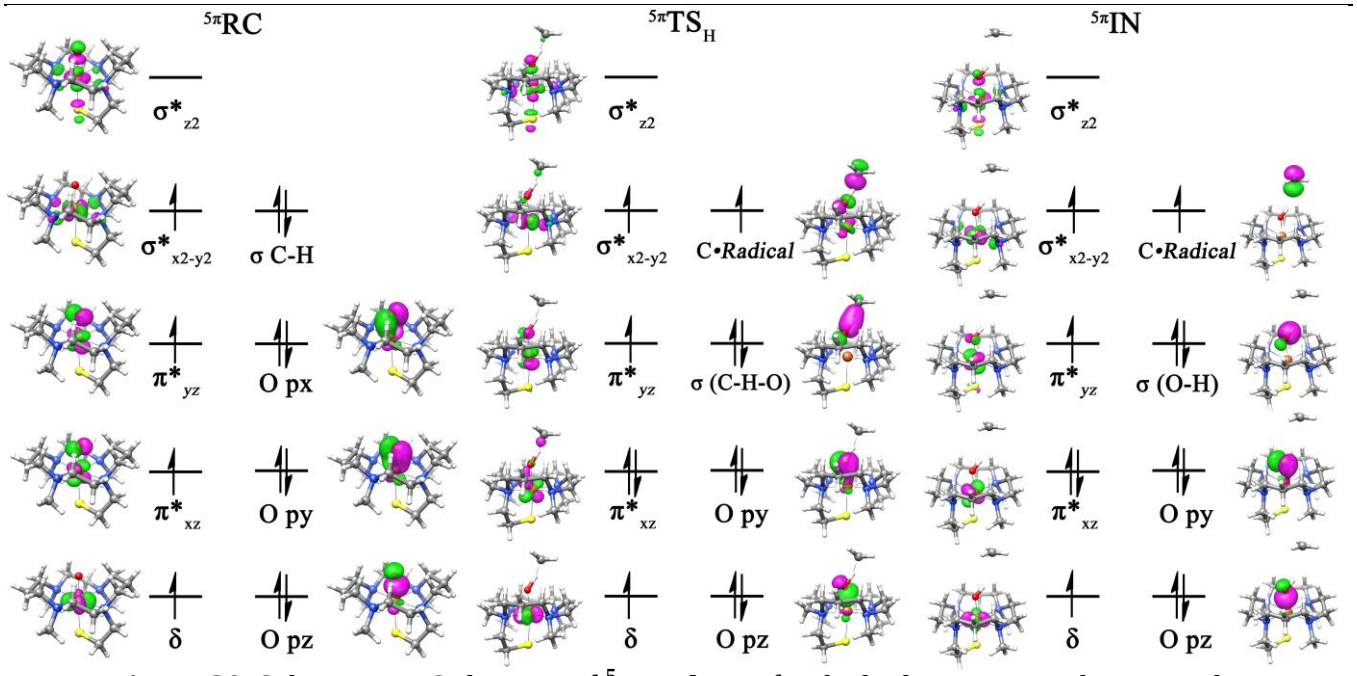

Figure S6. Schematic MO diagram of **^{5}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^+$ in solution.

3. Schematic MO diagrams of $^{3,5}\sigma$ and $^{3,5}\pi$**-pathways** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(F)]^{+}$ in solution.

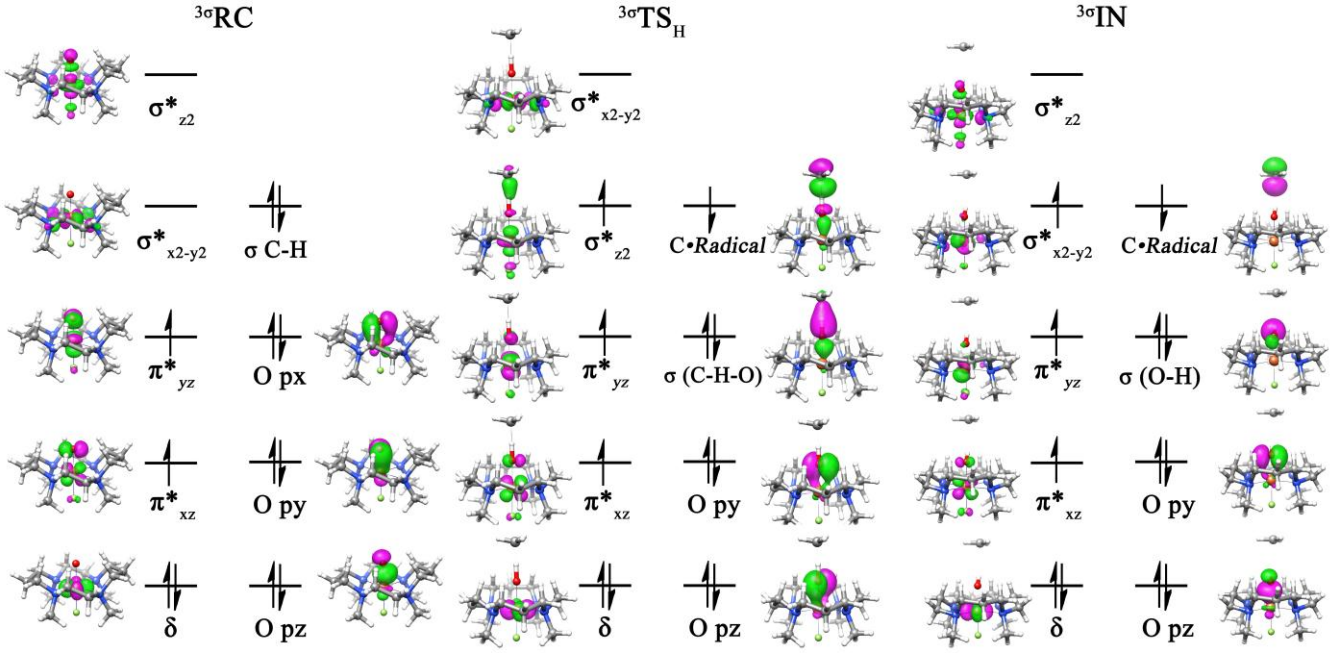

Figure S7. Schematic MO diagram of $^{3}\sigma$**-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(F)]^{+}$ in solution.

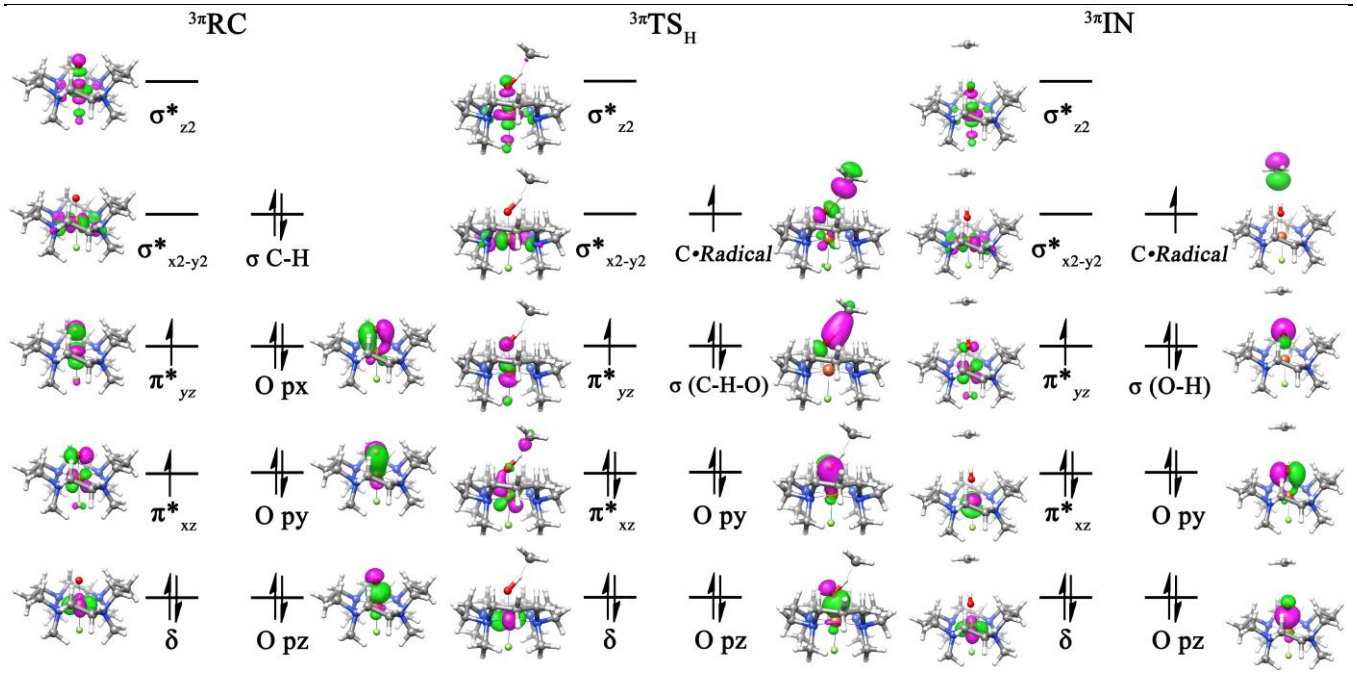

Figure S8. Schematic MO diagram of **^{3}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(F)]^+$ in solution.

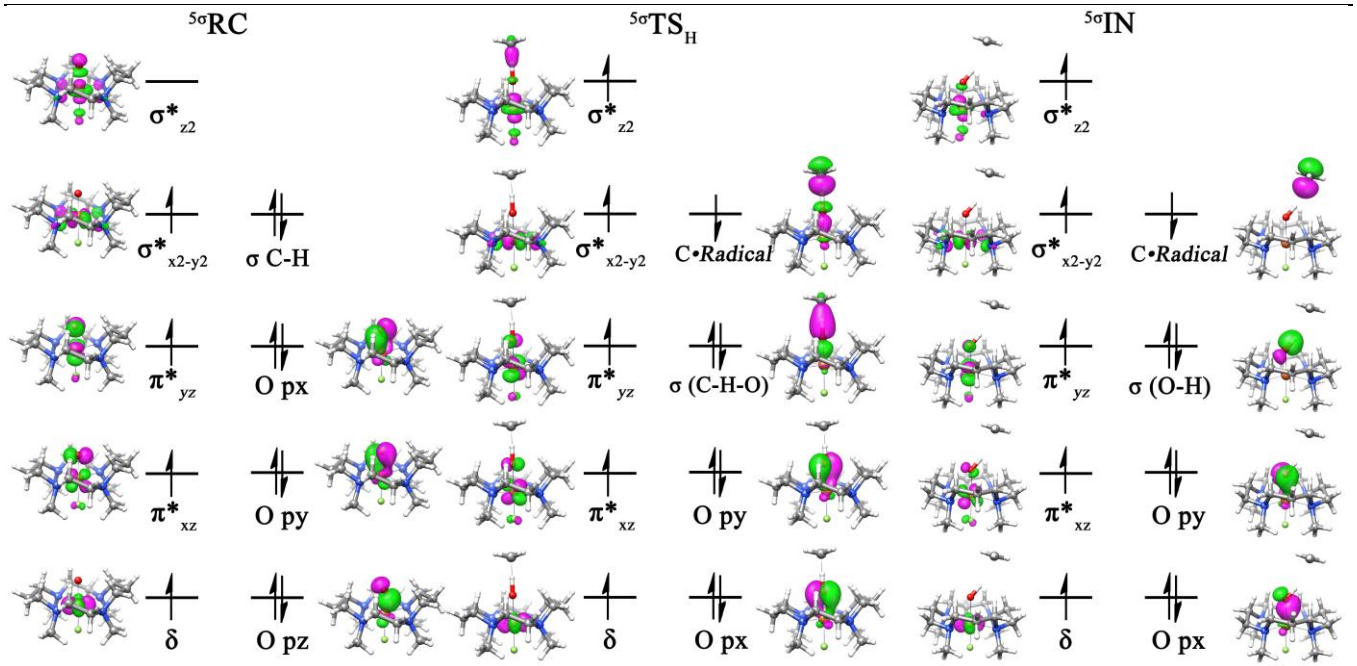

Figure S9. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(F)]^+$ in solution.

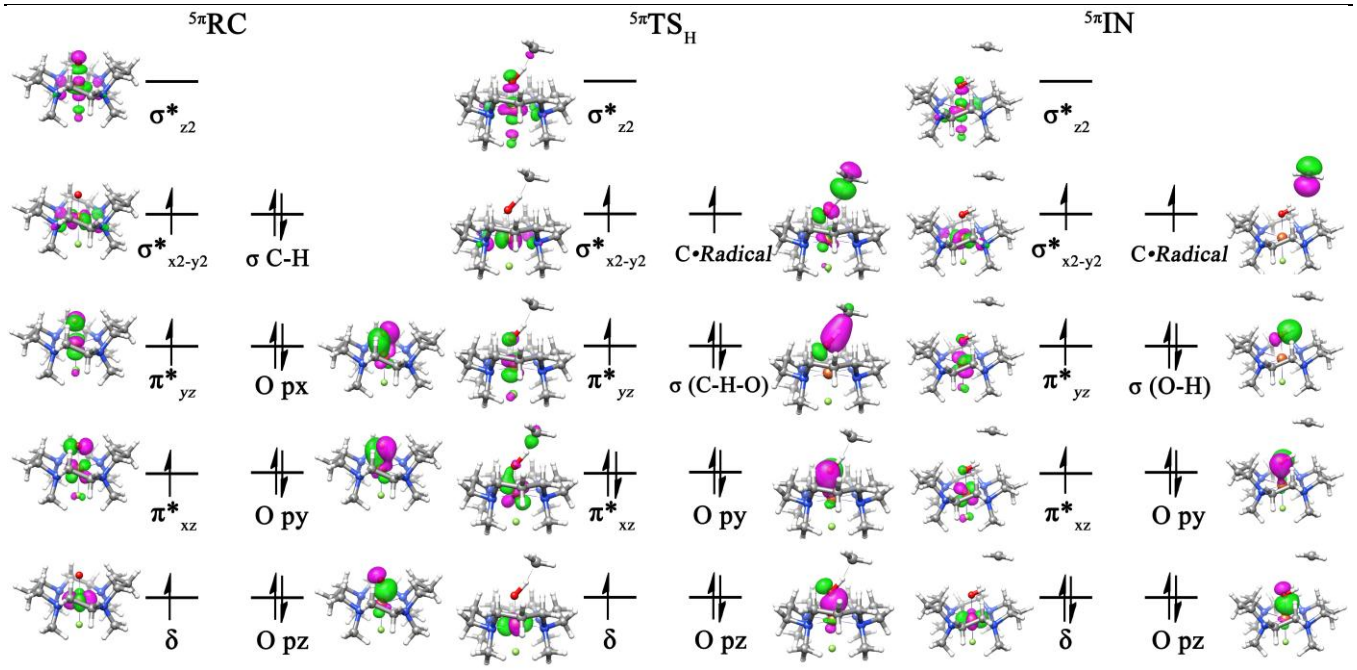

Figure S10. Schematic MO diagram of **$^5\pi$-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(F)]^+$ in solution.

4. Schematic MO diagrams of ^{3,5}**σ** and ^{3,5}**π-pathways** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$ in solution.

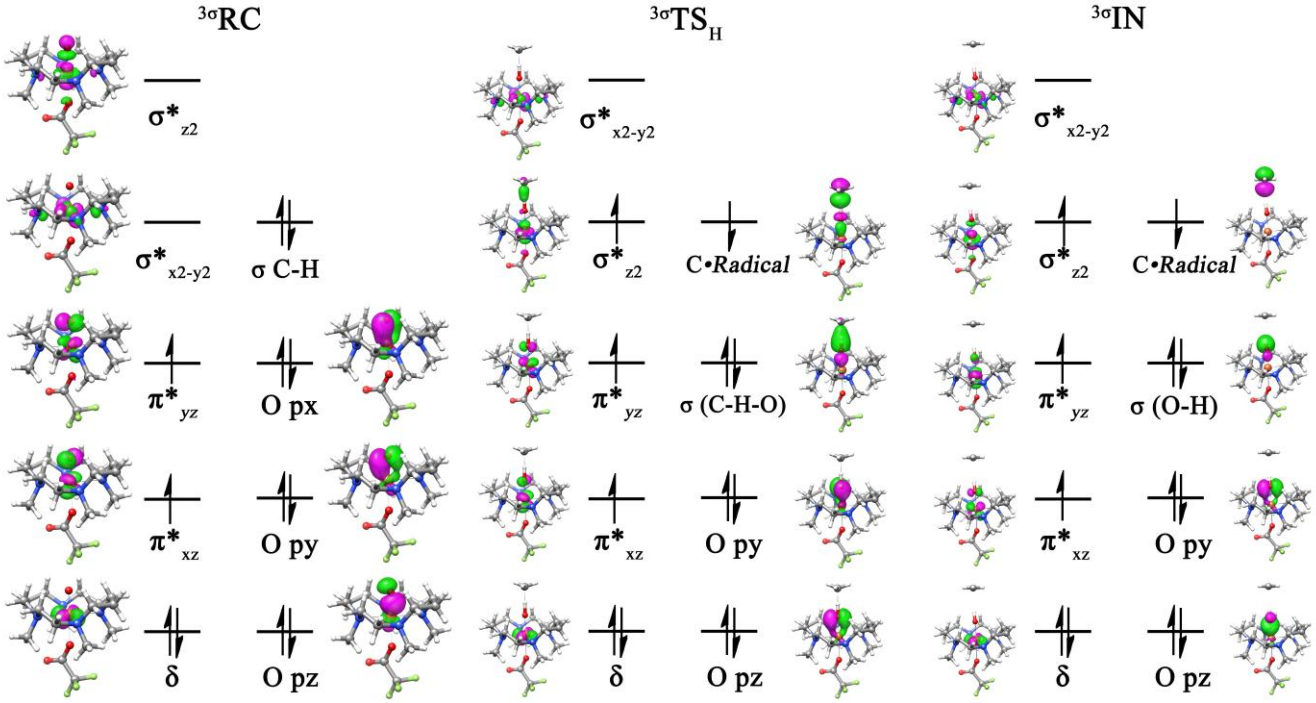

Figure S11. Schematic MO diagram of ^{3}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$ in solution.

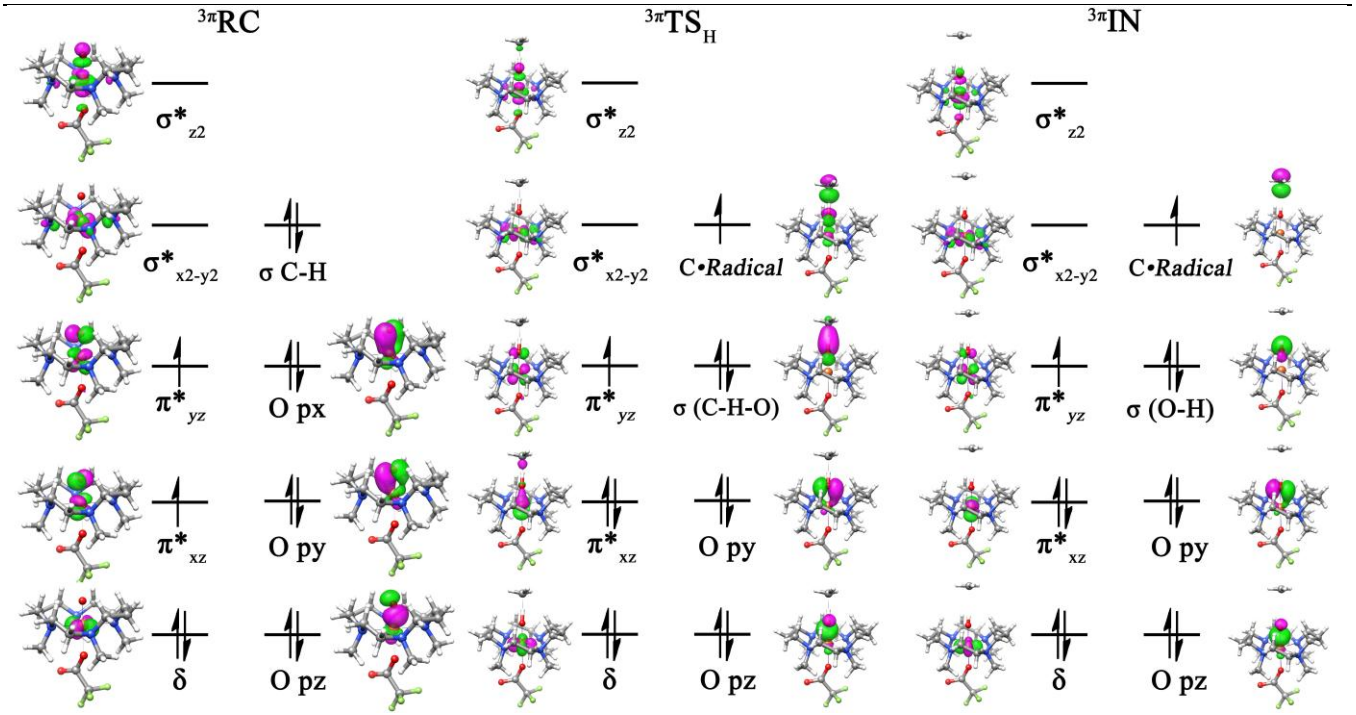

Figure S12. Schematic MO diagram of ^{3}**π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$ in solution.

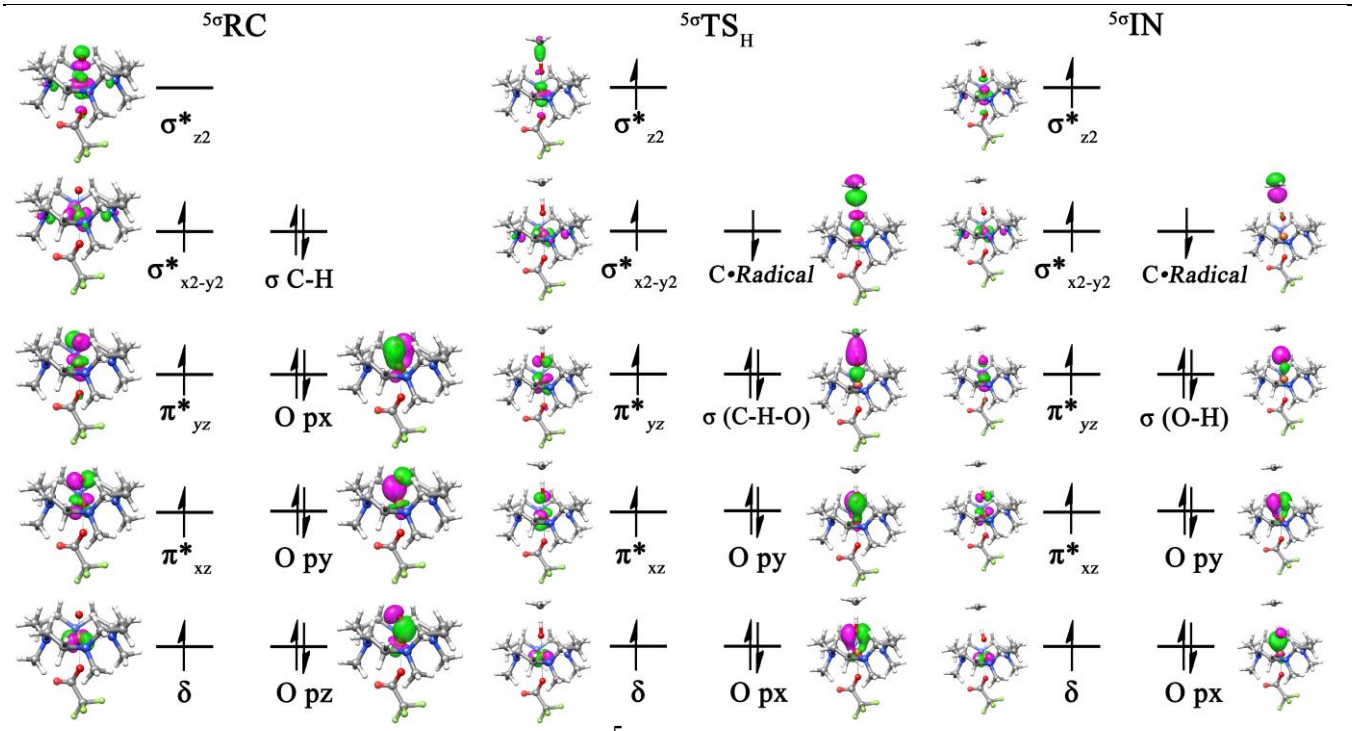

Figure S13. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$ in solution.

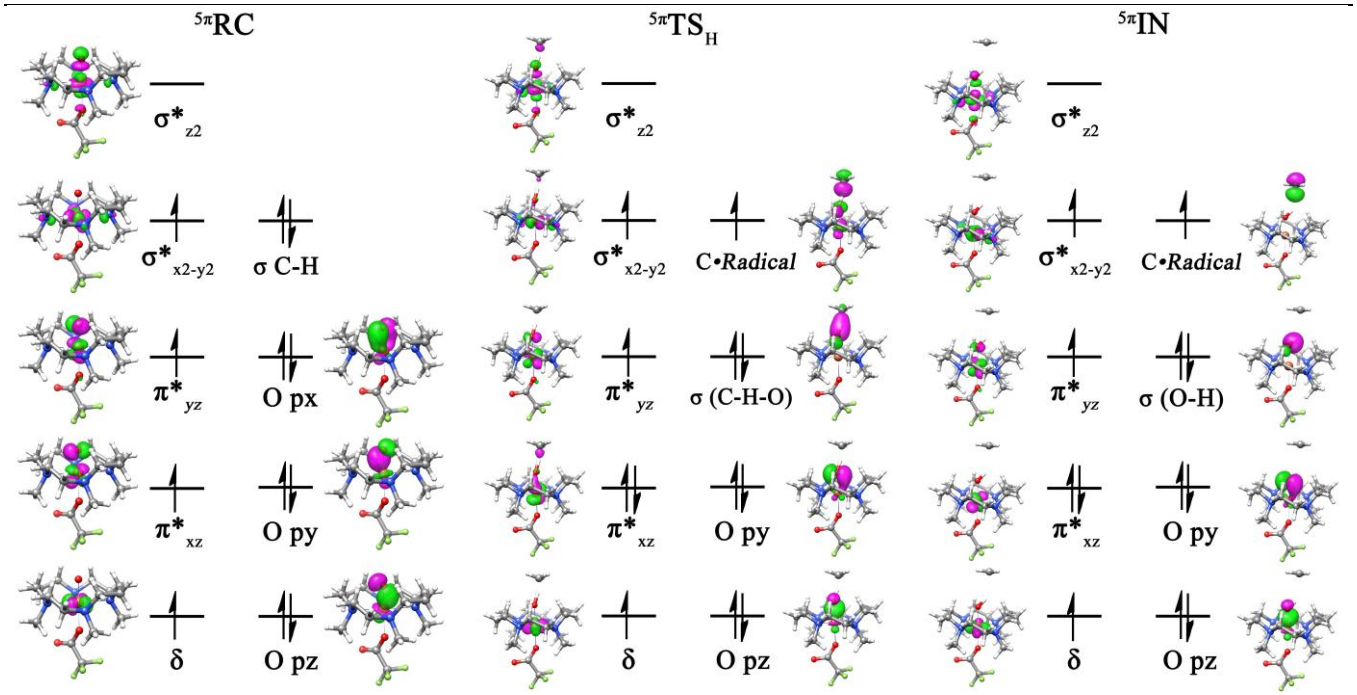

Figure S14. Schematic MO diagram of $^{5}\pi$**-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$ in solution.

5. The gas-phase schematic MO diagrams of $^{3}\delta$, $^{5}\sigma$ and $^{3,5}\pi$**-pathways** for the hydrogen-atom abstraction by **1**.

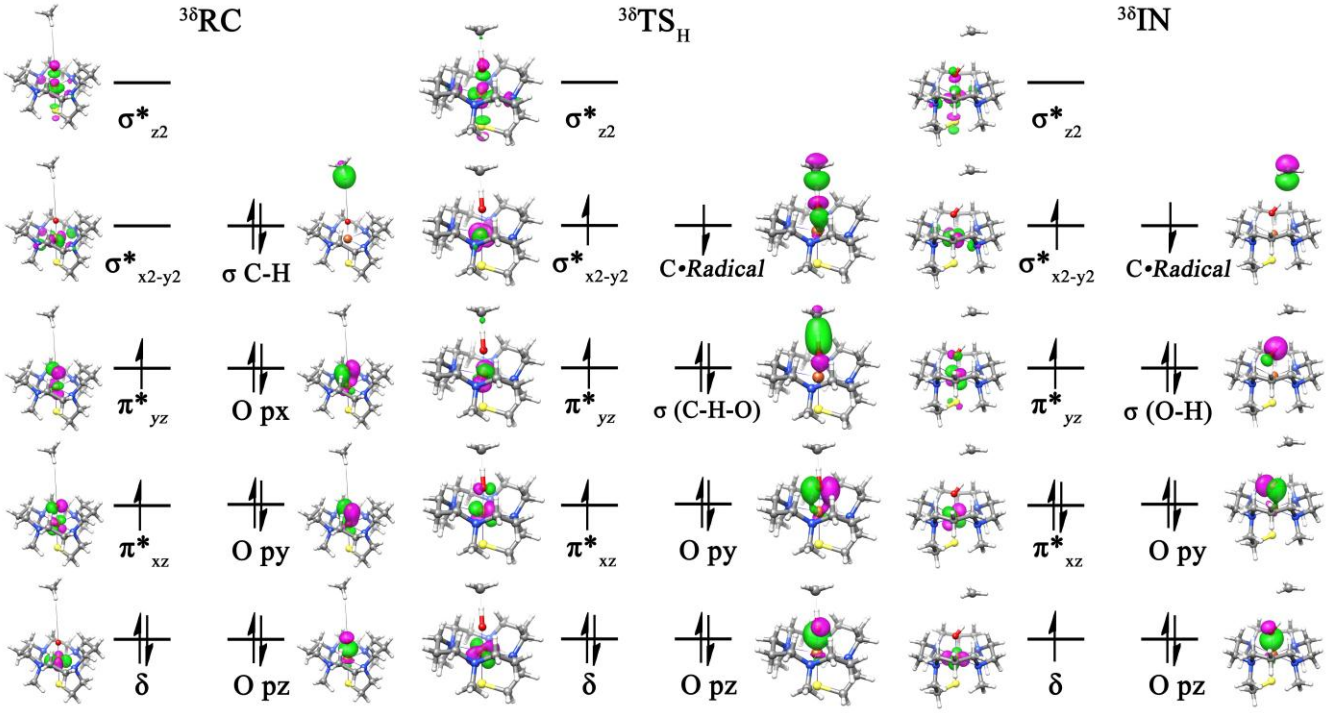

Figure S15. Schematic MO diagram of $^{3}\delta$**-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^{+}$ in the gas phase.

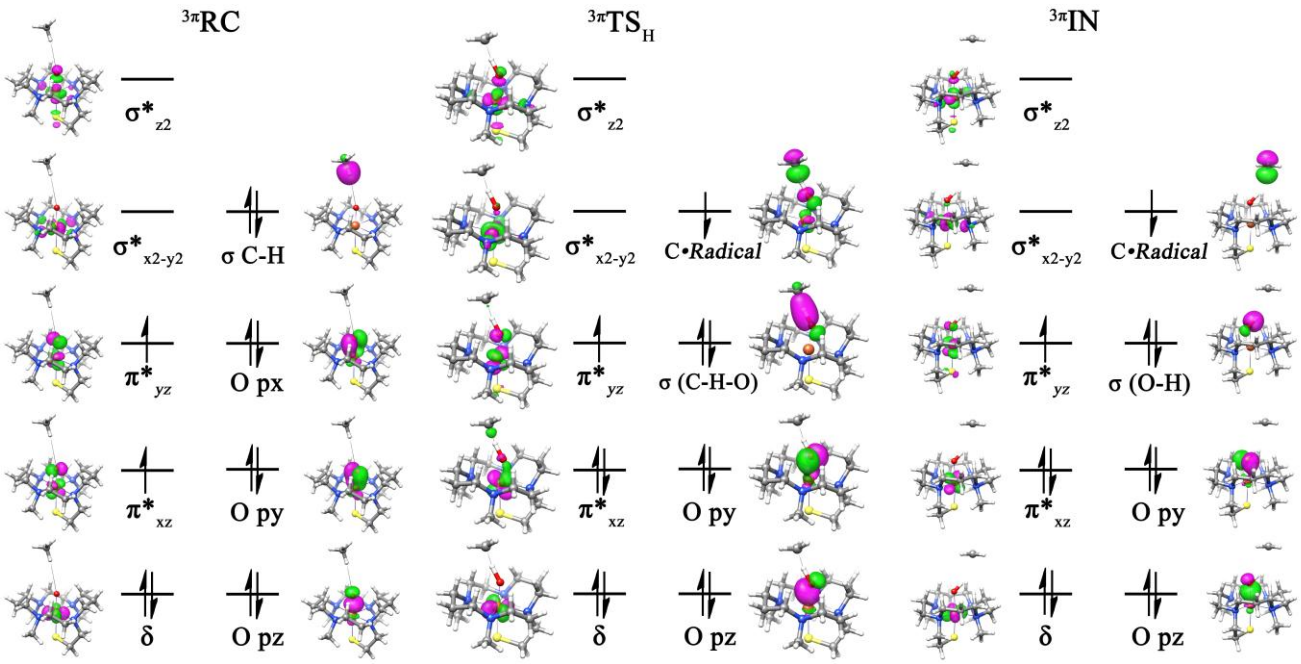

Figure S16. Schematic MO diagram of ^{3}**π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^{+}$ in the gas phase.

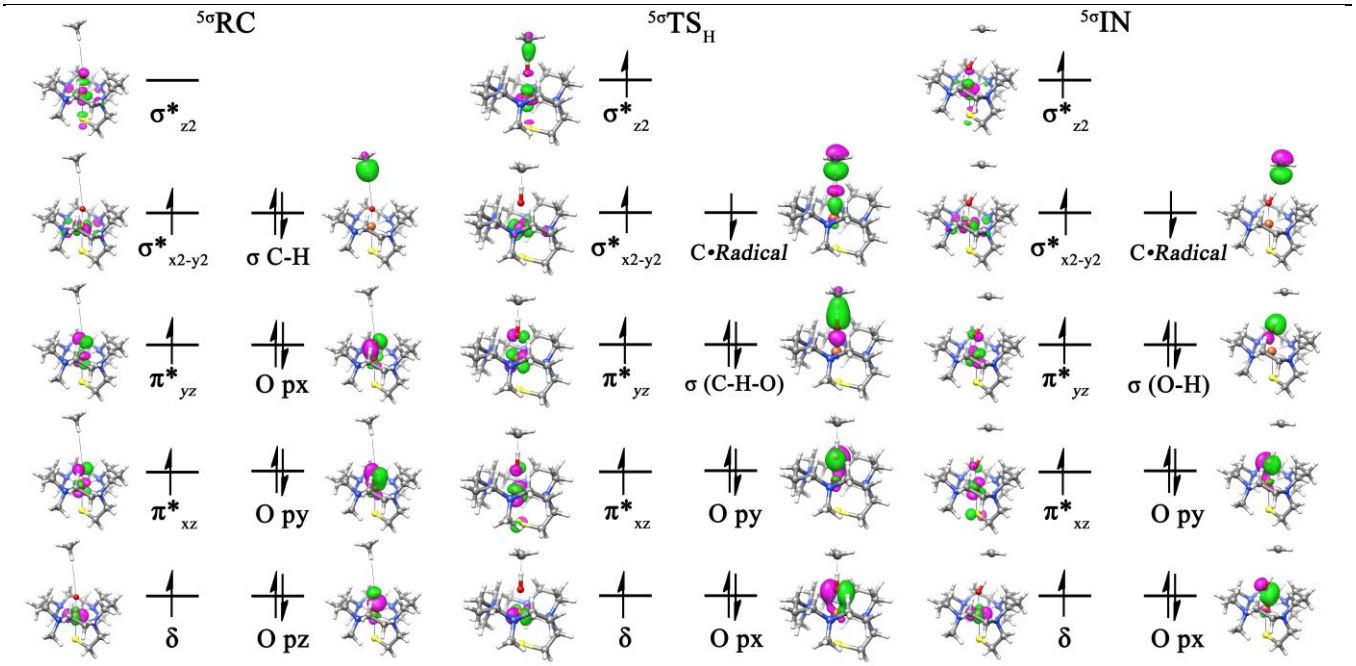

Figure S17. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^{+}$ in the gas phase.

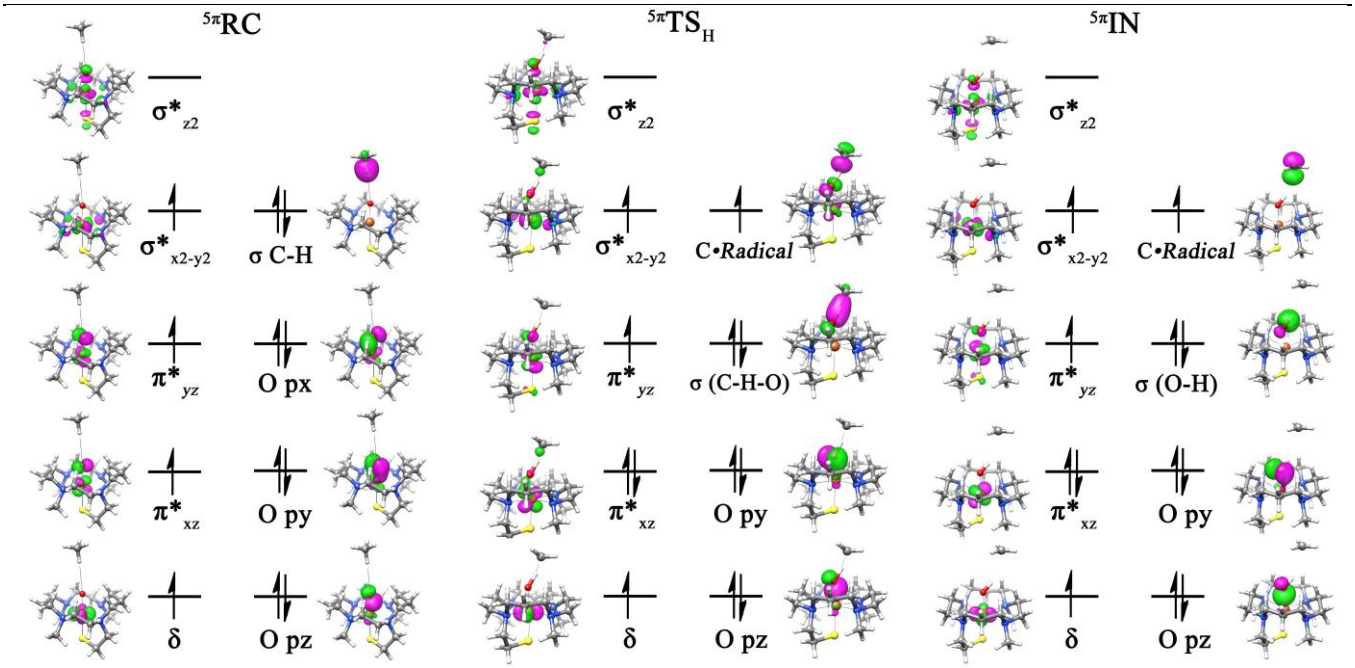

Figure S18. Schematic MO diagram of **^{5}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(SR)]^+$ in the gas phase.

6. The gas-phase schematic MO diagrams of $^{3}\delta$, $^{5}\sigma$ and $^{3,5}\pi$**-pathways** for the hydrogen-atom abstraction by **2**.

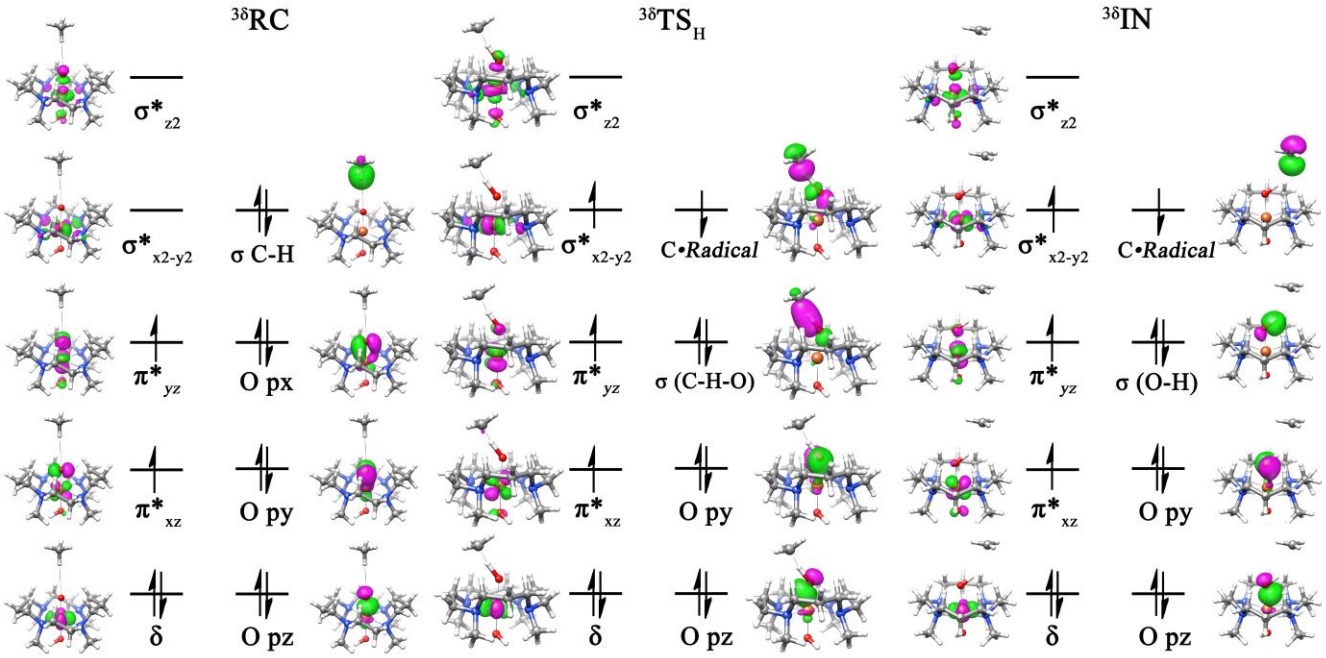

Figure S19. Schematic MO diagram of $^{3}\delta$**-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^{+}$ in the gas phase.

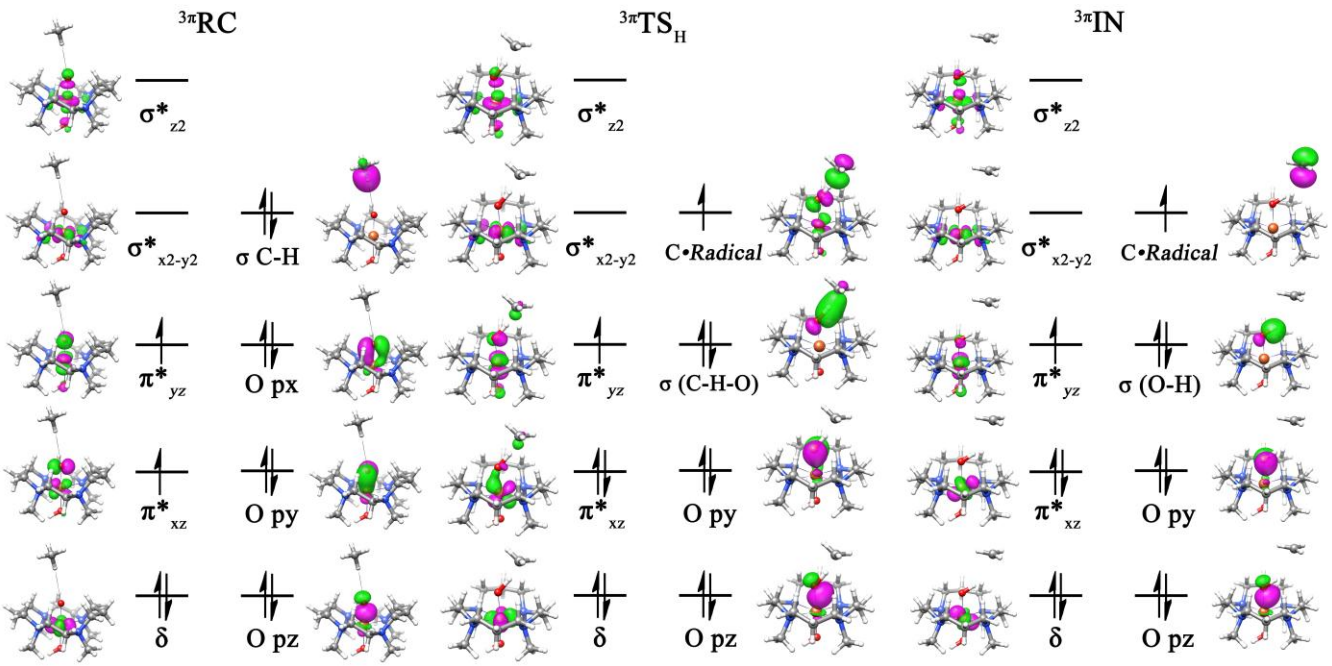

Figure S20. Schematic MO diagram of **^{3}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^+$ in the gas phase.

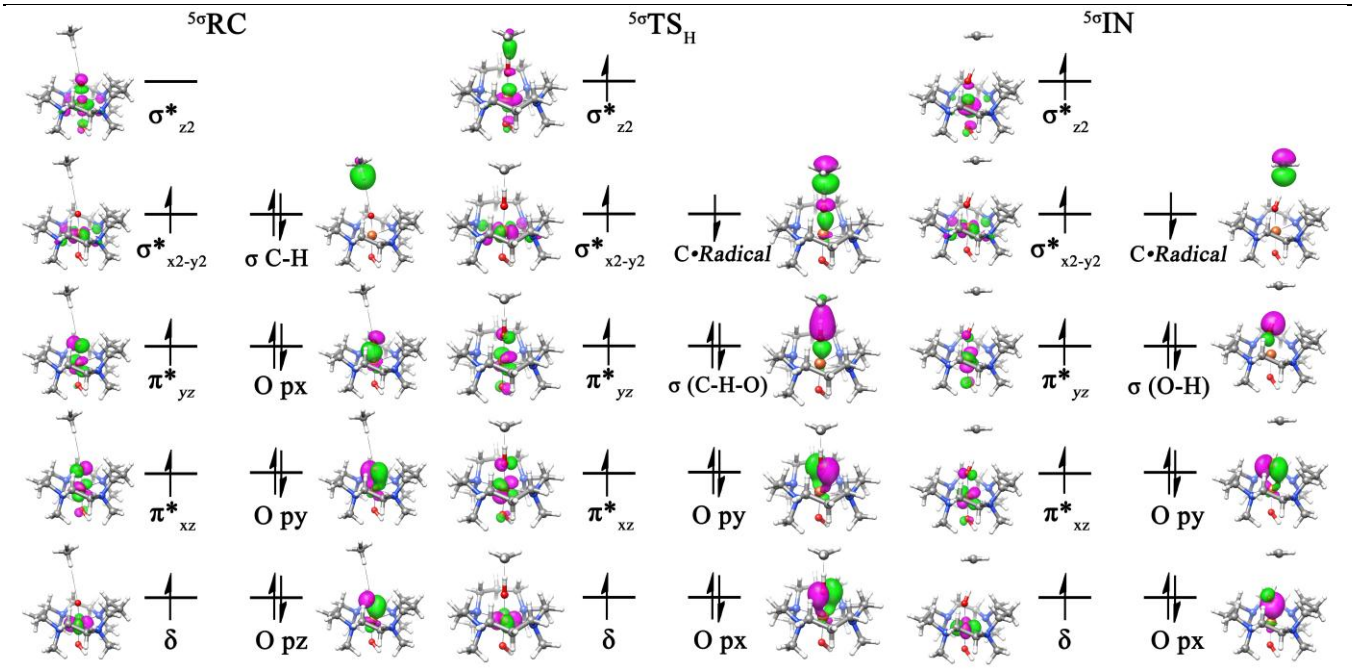

Figure S21. Schematic MO diagram of ^{5}**σ-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^+$ in the gas phase.

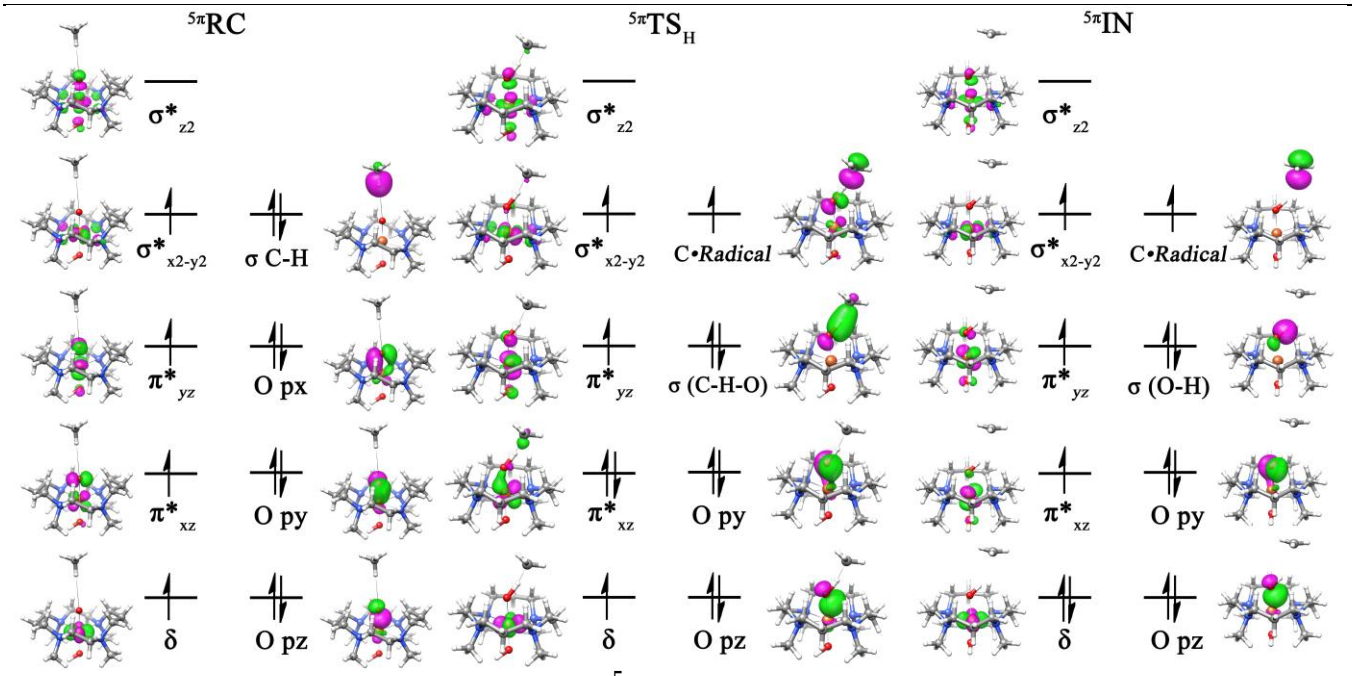

Figure S22. Schematic MO diagram of **^{5}π-pathway** for the hydrogen-atom abstraction by $[Fe^{IV}=O(TMC)(OH)]^+$ in the gas phase.

Part 3 All xyz coordinates

The gas-phase optimized geometries

Cat

^{3}[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.136058	0.651908	0.206703
O	-0.181340	0.630394	1.865474
N	-2.286341	0.610485	0.305146
C	-2.819622	1.680109	1.202806
C	-2.503745	-0.705493	0.975897
C	-3.052791	0.654912	-0.969606
N	0.084682	2.757949	0.347352
C	1.365066	2.881039	1.112401
C	-0.970344	3.418168	1.182179
C	0.185276	3.477686	-0.950693
C	-2.409798	3.094168	0.811425
N	2.071200	0.616099	0.286857
C	2.461416	2.048666	0.495798
C	2.415293	-0.213939	1.485204
C	2.902676	0.158055	-0.864602
N	-0.263638	-1.434802	0.128938
C	-1.718023	-1.790954	0.274797
C	0.494881	-2.011157	1.291808
C	0.224723	-2.021386	-1.162230
C	1.989163	-1.681494	1.379292
H	1.677950	3.930977	1.143582
H	1.161686	2.551579	2.127018
H	3.359025	2.100477	1.120021
H	2.733315	2.454259	-0.477075
H	2.337578	-2.163903	2.297262
H	2.538493	-2.181514	0.580575
H	-0.004584	-1.658544	2.190828
H	0.391863	-3.101658	1.244722
H	-0.802998	3.106597	2.211331
H	-0.804131	4.499384	1.127460
H	-2.621612	3.307165	-0.237895
H	-3.042006	3.781222	1.380381
H	-2.456399	1.470717	2.206671
H	-3.911773	1.595800	1.210936
H	-2.757913	-0.150726	-1.630047
H	-4.121827	0.572035	-0.748613
H	-2.860038	1.583129	-1.495886
H	-2.176041	-0.601588	2.006571
H	-3.569549	-0.959412	0.972771
H	-2.122980	-1.964869	-0.719172
H	-1.810941	-2.732908	0.821639
H	2.809996	-0.908446	-1.023344
H	2.581132	0.662077	-1.770012
H	3.954481	0.378629	-0.655374
H	0.945883	3.029690	-1.582249
H	-0.759892	3.414881	-1.482739
H	0.430263	4.529559	-0.774778
H	3.503600	-0.182026	1.617602
H	1.946838	0.243835	2.351599

S	-0.082874	0.571014	-2.148538
C	-0.267052	-1.250260	-2.375819
H	0.317374	-1.551650	-3.245916
H	-1.306999	-1.487087	-2.609140
H	1.307495	-2.016641	-1.143897
H	-0.090637	-3.071448	-1.208303

^{5}[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.159156	0.669259	0.189742
O	-0.202628	0.646483	1.857545
N	-2.420155	0.575757	0.297874
C	-2.883159	1.693333	1.171173
C	-2.549660	-0.728057	1.001181
C	-3.216117	0.574687	-0.949990
N	0.131926	2.822300	0.338839
C	1.392576	2.895462	1.142329
C	-0.972030	3.434964	1.150687
C	0.275925	3.559836	-0.940183
C	-2.400770	3.080542	0.732026
N	2.186020	0.636119	0.293045
C	2.526139	2.065891	0.555623
C	2.468388	-0.231755	1.474505
C	3.014641	0.207424	-0.859819
N	-0.281386	-1.489324	0.129208
C	-1.735133	-1.823553	0.315302
C	0.517632	-2.032726	1.279288
C	0.189688	-2.046625	-1.176506
C	2.016845	-1.693426	1.325373
H	1.723419	3.938604	1.209465
H	1.150796	2.548348	2.142654
H	3.387296	2.130998	1.230194
H	2.843199	2.500741	-0.391123
H	2.389392	-2.208440	2.216105
H	2.541614	-2.170398	0.496653
H	0.040585	-1.665595	2.185480
H	0.423771	-3.125663	1.262639
H	-0.824437	3.117136	2.181038
H	-0.841417	4.522338	1.115021
H	-2.556392	3.238605	-0.337520
H	-3.049385	3.809386	1.225300
H	-2.522472	1.494548	2.178541
H	-3.979284	1.680076	1.197640
H	-2.910510	-0.233942	-1.604940
H	-4.280227	0.462188	-0.713489
H	-3.064978	1.500752	-1.496691
H	-2.203818	-0.585808	2.021496
H	-3.598812	-1.045892	1.034162
H	-2.155568	-2.033188	-0.665719
H	-1.821895	-2.746111	0.895972
H	2.881067	-0.848030	-1.068753
H	2.718983	0.757741	-1.748711
H	4.076013	0.381082	-0.647166
H	1.048675	3.110178	-1.557210
H	-0.655883	3.518454	-1.499151
H	0.530638	4.606638	-0.745275
H	3.551514	-0.231263	1.656339
H	1.977848	0.211808	2.337404

S	-0.105659	0.564832	-2.138560
C	-0.332982	-1.256568	-2.364500
H	0.216525	-1.552041	-3.259055
H	-1.384463	-1.468478	-2.562705
H	1.273928	-2.017730	-1.178059
H	-0.107268	-3.101137	-1.247592

$^{3}[Fe^{IV}=O(TMC)(OH)]^{+}$

Fe	-0.113166	0.648090	0.217556
O	-0.164745	0.606816	1.871753
N	-2.232008	0.583084	0.260753
C	-2.845557	1.662502	1.092099
C	-2.486400	-0.709690	0.962106
C	-2.867833	0.583845	-1.081791
N	0.086375	2.747303	0.372220
C	1.359253	2.874692	1.142982
C	-0.989329	3.390673	1.185526
C	0.196185	3.455490	-0.931215
C	-2.410919	3.077927	0.739901
N	2.042911	0.624385	0.270860
C	2.455171	2.049232	0.511912
C	2.452451	-0.233752	1.428629
C	2.767232	0.197067	-0.955775
N	-0.245357	-1.511563	0.161373
C	-1.704740	-1.835921	0.326960
C	0.528021	-2.023143	1.341663
C	0.192745	-2.230255	-1.063977
C	2.025143	-1.701376	1.338303
H	1.668740	3.925391	1.181448
H	1.156584	2.534231	2.154241
H	3.349585	2.073261	1.140933
H	2.734648	2.476576	-0.449017
H	2.434113	-2.185328	2.230063
H	2.522827	-2.196059	0.502534
H	0.066863	-1.602068	2.230931
H	0.411476	-3.113346	1.369503
H	-0.861316	3.050642	2.211933
H	-0.820496	4.472770	1.163917
H	-2.568046	3.303357	-0.316263
H	-3.071862	3.757882	1.284043
H	-2.573803	1.461263	2.126749
H	-3.934054	1.572777	1.004267
H	-2.450694	-0.197897	-1.704969
H	-3.948004	0.440814	-0.974215
H	-2.668622	1.522754	-1.586652
H	-2.187954	-0.574816	1.997680
H	-3.555922	-0.947446	0.933221
H	-2.106765	-2.056862	-0.660029
H	-1.815435	-2.746826	0.922195
H	1.252887	-2.103035	-1.242904
H	-0.007934	-3.301257	-0.957899
H	-0.356156	-1.859709	-1.926116
H	2.628836	-0.859176	-1.149464
H	2.395348	0.760582	-1.806494
H	3.839746	0.378581	-0.833171
H	0.948027	2.991552	-1.556637
H	-0.741270	3.384110	-1.472413

H	0.439585	4.507244	-0.751691
H	3.546291	-0.198671	1.503039
H	2.029626	0.214134	2.324086
O	-0.103104	0.812039	-1.660146
H	0.232069	0.097880	-2.206103

^{5}[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.126136	0.683291	0.184678
O	-0.185399	0.642649	1.834884
N	-2.323537	0.535398	0.245402
C	-2.870572	1.660016	1.065580
C	-2.515005	-0.747374	0.975031
C	-2.986924	0.507435	-1.076346
N	0.139900	2.859475	0.374593
C	1.395267	2.911327	1.174320
C	-0.987412	3.437081	1.165723
C	0.290585	3.593643	-0.903251
C	-2.389674	3.061532	0.674980
N	2.124357	0.638215	0.283356
C	2.503645	2.062167	0.560387
C	2.485874	-0.248918	1.429623
C	2.837794	0.227846	-0.950331
N	-0.262135	-1.592918	0.150048
C	-1.717026	-1.890641	0.355803
C	0.540770	-2.050382	1.330674
C	0.172176	-2.311548	-1.070550
C	2.039076	-1.713195	1.303947
H	1.753277	3.945474	1.247971
H	1.157027	2.559499	2.174237
H	3.375242	2.089180	1.221914
H	2.815689	2.502856	-0.384715
H	2.462833	-2.220704	2.175759
H	2.522051	-2.188591	0.448886
H	0.087605	-1.610778	2.215868
H	0.442514	-3.141548	1.400476
H	-0.871197	3.096222	2.193431
H	-0.882033	4.528268	1.161846
H	-2.497202	3.236860	-0.397576
H	-3.079993	3.764025	1.149495
H	-2.590581	1.468464	2.099782
H	-3.964576	1.621748	1.001994
H	-2.614108	-0.318181	-1.675610
H	-4.070087	0.397056	-0.953886
H	-2.771447	1.421830	-1.620979
H	-2.201389	-0.582037	2.002057
H	-3.575366	-1.027381	0.979312
H	-2.138854	-2.147028	-0.614871
H	-1.829299	-2.778879	0.985615
H	1.216791	-2.119657	-1.287679
H	0.035280	-3.392528	-0.952476
H	-0.418419	-1.985450	-1.925208
H	2.691324	-0.827819	-1.150474
H	2.444649	0.789597	-1.793528
H	3.913619	0.407093	-0.846238
H	1.042257	3.123926	-1.527716
H	-0.640212	3.562036	-1.461694
H	0.561350	4.635946	-0.703074

H	3.577962	-0.237198	1.541980
H	2.047788	0.186166	2.325148
O	-0.065386	0.893463	-1.670605
H	-0.171478	0.133722	-2.249553

RC

$^{3\delta}$RC−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.236921	0.549801	0.132982
O	-0.410935	0.393913	1.775807
C	0.483047	2.020353	6.262615
H	0.191048	1.369935	5.437943
N	-2.388670	0.483743	0.055929
C	-3.006879	1.476047	0.987574
C	-2.640441	-0.882487	0.603630
C	-3.052965	0.622238	-1.268656
N	-0.055700	2.638449	0.459268
C	1.158165	2.709565	1.332541
C	-1.183495	3.220729	1.256080
C	0.138840	3.462401	-0.764864
C	-2.583751	2.918580	0.743667
N	1.957051	0.524059	0.384261
C	2.311346	1.936837	0.741678
C	2.219049	-0.399327	1.534881
C	2.881181	0.168506	-0.732398
N	-0.330190	-1.524758	-0.118281
C	-1.785924	-1.905514	-0.111172
C	0.347273	-2.188672	1.048216
C	0.262810	-1.999690	-1.411609
C	1.825579	-1.856728	1.276704
H	1.453544	3.755948	1.470807
H	0.879243	2.300585	2.299041
H	3.153791	1.941051	1.440162
H	2.657037	2.423105	-0.168660
H	2.109249	-2.410700	2.176661
H	2.442266	-2.284989	0.485288
H	-0.223049	-1.914535	1.932318
H	0.262489	-3.272089	0.904433
H	-1.095852	2.827529	2.267298
H	-1.028202	4.303814	1.303079
H	-2.711974	3.212139	-0.299591
H	-3.268766	3.554659	1.310800
H	-2.724588	1.190958	1.998575
H	-4.094857	1.384529	0.898197
H	-2.696623	-0.126990	-1.964218
H	-4.134852	0.513630	-1.140307
H	-2.832613	1.590232	-1.703852
H	-2.397571	-0.856431	1.662342
H	-3.698766	-1.143730	0.494416
H	-2.111319	-2.012062	-1.142961
H	-1.905341	-2.885377	0.358596
H	2.815866	-0.882049	-0.983261
H	2.622968	0.742748	-1.616076
H	3.910584	0.379297	-0.425150
H	0.952978	3.071522	-1.366649
H	-0.760010	3.437191	-1.374544
H	0.356090	4.497988	-0.485632

H	3.292605	-0.368171	1.755723
H	1.676557	-0.017184	2.394777
S	-0.000928	0.661260	-2.209974
C	-0.149388	-1.136898	-2.592257
H	0.498203	-1.365390	-3.439595
H	-1.167706	-1.360153	-2.916630
H	1.340906	-1.984312	-1.310734
H	-0.030242	-3.045598	-1.566033
H	1.374640	2.585018	5.991269
H	-0.328975	2.710593	6.487768
H	0.693853	1.415231	7.143096

$^{3\pi}$RC−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.087990	0.614119	0.119832
O	-0.058602	0.577368	1.779198
C	-0.246929	1.595528	5.727989
H	-0.171441	1.233290	4.702510
N	-2.232666	0.586645	0.314311
C	-2.716948	1.653841	1.242298
C	-2.428334	-0.732561	0.984910
C	-3.056503	0.645190	-0.923867
N	0.154014	2.718560	0.268325
C	1.466198	2.825782	0.979355
C	-0.859888	3.382075	1.149977
C	0.205991	3.446257	-1.028080
C	-2.315848	3.067682	0.840851
N	2.119046	0.563671	0.102286
C	2.529033	1.991137	0.309521
C	2.510833	-0.281396	1.275323
C	2.893152	0.112350	-1.090690
N	-0.235689	-1.470525	0.029895
C	-1.684520	-1.817853	0.239364
C	0.570298	-2.063386	1.151984
C	0.189394	-2.048697	-1.287298
C	2.069063	-1.744559	1.175232
H	1.788636	3.873001	1.005354
H	1.303139	2.490972	1.999461
H	3.452262	2.029655	0.896210
H	2.763529	2.405085	-0.669660
H	2.454963	-2.238138	2.072085
H	2.578101	-2.240340	0.347826
H	0.114076	-1.716434	2.075754
H	0.457544	-3.152615	1.098802
H	-0.650802	3.069842	2.171125
H	-0.690198	4.462536	1.090025
H	-2.571502	3.287407	-0.197148
H	-2.918776	3.755132	1.440393
H	-2.310297	1.435382	2.227288
H	-3.808124	1.576843	1.299502
H	-2.797104	-0.156931	-1.603137
H	-4.114723	0.566561	-0.654701
H	-2.882606	1.576292	-1.451467
H	-2.050792	-0.639006	1.999375
H	-3.494904	-0.979099	1.031055
H	-2.136007	-1.980721	-0.736352
H	-1.759080	-2.763553	0.782404
H	2.784073	-0.951563	-1.256693

H	2.534985	0.628889	-1.975111
H	3.955282	0.322332	-0.927646
H	0.934538	2.995684	-1.694720
H	-0.761682	3.395933	-1.519292
H	0.468194	4.494580	-0.855917
H	3.604404	-0.259230	1.357697
H	2.086145	0.173576	2.165205
S	-0.144385	0.554966	-2.236072
C	-0.350657	-1.263224	-2.470774
H	0.192396	-1.559957	-3.368754
H	-1.401565	-1.491181	-2.659670
H	1.271939	-2.051852	-1.317879
H	-0.135548	-3.096033	-1.328596
H	0.749317	1.682872	6.160122
H	-0.731325	2.571724	5.741998
H	-0.834746	0.895286	6.320248

$^{5\sigma}$RC−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.167067	0.602017	0.129990
O	-0.226555	0.494022	1.789022
C	-0.231412	1.354325	6.147544
H	-0.246683	1.029542	5.106862
N	-2.429565	0.498125	0.210909
C	-2.900405	1.569623	1.136827
C	-2.563381	-0.840125	0.845030
C	-3.214476	0.560189	-1.042446
N	0.123050	2.744423	0.390345
C	1.378969	2.778658	1.204035
C	-0.988479	3.310768	1.225188
C	0.274480	3.547525	-0.848237
C	-2.413404	2.977863	0.775674
N	2.179759	0.560994	0.250990
C	2.515956	1.976262	0.586168
C	2.448986	-0.362621	1.392892
C	3.020968	0.189244	-0.912432
N	-0.284529	-1.551515	-0.041764
C	-1.739156	-1.897799	0.112966
C	0.504424	-2.154479	1.085483
C	0.200230	-2.038471	-1.370492
C	2.002142	-1.815901	1.167055
H	1.710996	3.817378	1.318718
H	1.130502	2.391882	2.188096
H	3.372836	2.008777	1.268566
H	2.838891	2.456691	-0.336366
H	2.364232	-2.373274	2.036457
H	2.538264	-2.251256	0.322834
H	0.016408	-1.838797	2.005055
H	0.413256	-3.245038	1.007973
H	-0.848180	2.937388	2.237834
H	-0.859863	4.398648	1.250201
H	-2.560092	3.191800	-0.285238
H	-3.066672	3.679386	1.301449
H	-2.548819	1.317251	2.135171
H	-3.996757	1.556446	1.152262
H	-2.901933	-0.213506	-1.735383
H	-4.280382	0.434023	-0.821351
H	-3.060262	1.513367	-1.539028

H	-2.229411	-0.750369	1.875222
H	-3.612064	-1.161103	0.850072
H	-2.149731	-2.058792	-0.881473
H	-1.829240	-2.848799	0.645413
H	2.893052	-0.855553	-1.171448
H	2.732587	0.780281	-1.777393
H	4.079718	0.355617	-0.681781
H	1.053427	3.131981	-1.481166
H	-0.652946	3.533101	-1.415432
H	0.525203	4.583367	-0.597253
H	3.529454	-0.369539	1.589624
H	1.945235	0.041060	2.267626
S	-0.091614	0.619243	-2.202611
C	-0.313252	-1.189080	-2.521195
H	0.244397	-1.438312	-3.424738
H	-1.362705	-1.391924	-2.738638
H	1.284338	-2.006556	-1.359782
H	-0.092473	-3.088600	-1.499698
H	0.644567	1.977420	6.325590
H	-1.132081	1.926746	6.366908
H	-0.191682	0.483305	6.800055

$^{5\pi}$RC−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.111768	0.667323	0.112303
O	-0.094358	0.681047	1.775865
C	-0.226556	1.219985	5.627148
H	-0.168864	1.039888	4.553232
N	-2.368884	0.606356	0.301306
C	-2.786941	1.750258	1.163561
C	-2.490545	-0.679229	1.038988
C	-3.209910	0.587356	-0.917078
N	0.209696	2.820210	0.200603
C	1.497396	2.895210	0.959505
C	-0.858525	3.467467	1.033328
C	0.319583	3.524084	-1.100504
C	-2.305099	3.120581	0.673437
N	2.231455	0.605576	0.133130
C	2.599964	2.035400	0.357034
C	2.550887	-0.246685	1.316530
C	3.009554	0.145721	-1.043127
N	-0.265573	-1.491804	0.100907
C	-1.715193	-1.801514	0.350591
C	0.570328	-2.023315	1.230462
C	0.147033	-2.083622	-1.209546
C	2.074452	-1.704109	1.211313
H	1.845041	3.934749	0.987983
H	1.283538	2.579321	1.976271
H	3.481965	2.100632	1.004028
H	2.894746	2.446689	-0.607331
H	2.475676	-2.208628	2.095561
H	2.559155	-2.202327	0.370846
H	0.133023	-1.632612	2.146770
H	0.461488	-3.114948	1.239559
H	-0.679904	3.174767	2.066034
H	-0.716168	4.551818	0.964902
H	-2.496482	3.254699	-0.393501
H	-2.927642	3.868892	1.171226

H	-2.392860	1.572404	2.162330
H	-3.881435	1.750957	1.229779
H	-2.938365	-0.240111	-1.563286
H	-4.265969	0.494005	-0.639574
H	-3.068039	1.498862	-1.489971
H	-2.110045	-0.517794	2.043921
H	-3.542027	-0.982124	1.114662
H	-2.175459	-2.029903	-0.608201
H	-1.790939	-2.708146	0.957219
H	2.850157	-0.910204	-1.230836
H	2.690586	0.687569	-1.929012
H	4.080837	0.304267	-0.872138
H	1.066533	3.050040	-1.730990
H	-0.630669	3.480076	-1.627197
H	0.592337	4.572276	-0.940510
H	3.640920	-0.258420	1.451500
H	2.105965	0.215955	2.193853
S	-0.145413	0.511497	-2.216832
C	-0.407944	-1.311028	-2.394471
H	0.103523	-1.633584	-3.301959
H	-1.469222	-1.510375	-2.548763
H	1.230761	-2.071585	-1.252494
H	-0.167784	-3.134794	-1.246583
H	0.619239	1.829182	5.944852
H	-1.153508	1.741059	5.865388
H	-0.203381	0.269875	6.159555

$^{3\delta}$RC−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.201082	0.725841	0.044501
O	-0.468346	0.911753	1.666773
C	-1.211772	1.549590	5.432099
H	-1.018738	1.382288	4.371913
N	-2.315216	0.649623	-0.176756
C	-3.022872	1.807051	0.450466
C	-2.646598	-0.567471	0.625091
C	-2.795996	0.486881	-1.572791
N	-0.021807	2.843890	-0.045953
C	1.159949	3.071386	0.840897
C	-1.183472	3.563173	0.560055
C	0.242797	3.401077	-1.397698
C	-2.546382	3.181066	-0.001323
N	1.913647	0.724282	0.370642
C	2.305925	2.171619	0.443837
C	2.173127	0.051670	1.684421
C	2.771308	0.125333	-0.691556
N	-0.310796	-1.405506	0.246230
C	-1.776355	-1.731633	0.214982
C	0.271307	-1.766951	1.579181
C	0.311044	-2.234520	-0.825916
C	1.752158	-1.418953	1.764284
H	1.476804	4.118713	0.779860
H	0.840083	2.864379	1.857828
H	3.136103	2.293258	1.145838
H	2.679251	2.456916	-0.537465
H	2.012373	-1.748685	2.774022
H	2.372990	-2.029326	1.106602
H	-0.319030	-1.260314	2.338360

H	0.156356	-2.849231	1.713285
H	-1.173777	3.344320	1.626419
H	-1.015248	4.638294	0.432686
H	-2.588113	3.292648	-1.087212
H	-3.264453	3.908121	0.387497
H	-2.877158	1.725208	1.526089
H	-4.093376	1.696841	0.244136
H	-2.257766	-0.310047	-2.073392
H	-3.869053	0.270108	-1.573940
H	-2.630732	1.404571	-2.132211
H	-2.486188	-0.314420	1.668985
H	-3.701214	-0.830773	0.486268
H	-2.019273	-2.037848	-0.800330
H	-1.976490	-2.592258	0.860534
H	1.387825	-2.260723	-0.723576
H	-0.057272	-3.261807	-0.751103
H	0.068288	-1.801553	-1.791487
H	2.725334	-0.955264	-0.667247
H	2.414953	0.459310	-1.660922
H	3.811540	0.422722	-0.529514
H	1.042338	2.856727	-1.887235
H	-0.646794	3.315814	-2.017051
H	0.507323	4.460067	-1.317119
H	3.250193	0.108830	1.882698
H	1.650625	0.621007	2.448899
O	0.127176	0.491415	-1.803492
H	-0.349144	1.017447	-2.449755
H	-0.440719	2.196850	5.849157
H	-2.184837	2.022929	5.560955
H	-1.204533	0.597200	5.961226

$^{3\pi}$RC−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.143005	0.737533	0.042233
O	-0.358076	0.919697	1.672423
C	-1.990610	1.195629	5.293341
H	-1.461094	1.157563	4.341079
N	-2.263368	0.689839	-0.113156
C	-2.936169	1.851813	0.543223
C	-2.586766	-0.528490	0.690034
C	-2.788455	0.542876	-1.494884
N	0.061051	2.853103	-0.043125
C	1.275116	3.060622	0.803702
C	-1.069932	3.583388	0.605803
C	0.286808	3.414236	-1.400218
C	-2.455816	3.223187	0.087583
N	1.981567	0.706807	0.301696
C	2.394940	2.148544	0.362487
C	2.270356	0.030520	1.607298
C	2.798685	0.096864	-0.785718
N	-0.272453	-1.392646	0.240670
C	-1.742065	-1.700220	0.248981
C	0.342551	-1.764180	1.555710
C	0.308206	-2.226645	-0.850848
C	1.832322	-1.434578	1.699124
H	1.602116	4.104546	0.738821
H	0.989219	2.848816	1.829617
H	3.252171	2.258339	1.033399

H	2.735289	2.431031	-0.631532
H	2.116698	-1.768106	2.701072
H	2.426696	-2.052513	1.024270
H	-0.219565	-1.251190	2.331596
H	0.217972	-2.845177	1.691351
H	-1.026200	3.357126	1.669566
H	-0.891682	4.656993	0.479360
H	-2.532379	3.344998	-0.995306
H	-3.150797	3.956061	0.506216
H	-2.760841	1.758556	1.613297
H	-4.013740	1.757640	0.367578
H	-2.276070	-0.257603	-2.016430
H	-3.863818	0.340161	-1.464958
H	-2.628138	1.462032	-2.053414
H	-2.397451	-0.284215	1.730929
H	-3.647716	-0.778754	0.577421
H	-2.016820	-1.996442	-0.761185
H	-1.934606	-2.562809	0.894177
H	1.386585	-2.271544	-0.776167
H	-0.074789	-3.248181	-0.771374
H	0.047601	-1.785093	-1.807893
H	2.741635	-0.983110	-0.757947
H	2.416437	0.433898	-1.744159
H	3.846795	0.382760	-0.656951
H	1.062136	2.862225	-1.919207
H	-0.624248	3.343436	-1.989440
H	0.567671	4.469342	-1.323904
H	3.353320	0.073460	1.774961
H	1.776483	0.608082	2.384294
O	0.125031	0.506445	-1.815915
H	-0.359930	1.044290	-2.445831
H	-1.706415	2.097613	5.834117
H	-3.066579	1.205028	5.120253
H	-1.731426	0.322570	5.891391

$^{5\sigma}$RC−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.143354	0.608412	0.157946
O	-0.228879	0.465817	1.801196
C	-0.132024	1.426804	5.762192
H	-0.204106	1.048940	4.742114
N	-2.338916	0.447860	0.174260
C	-2.907000	1.515338	1.053999
C	-2.534674	-0.879643	0.817639
C	-2.978627	0.499565	-1.158723
N	0.105797	2.769631	0.484610
C	1.348827	2.781227	1.305519
C	-1.036494	3.294605	1.291415
C	0.271763	3.579412	-0.745162
C	-2.429379	2.941120	0.759744
N	2.104803	0.568518	0.289522
C	2.471745	1.974160	0.661920
C	2.453397	-0.387439	1.383875
C	2.842528	0.239932	-0.954037
N	-0.263555	-1.663405	-0.020909
C	-1.720792	-1.977942	0.140897
C	0.522663	-2.189649	1.141493
C	0.193466	-2.305757	-1.275469

C	2.019107	-1.843796	1.158891
H	1.700245	3.811331	1.441524
H	1.097721	2.375728	2.281597
H	3.330568	1.962977	1.340297
H	2.799831	2.473708	-0.247842
H	2.433297	-2.402600	2.003568
H	2.518165	-2.261809	0.283282
H	0.053592	-1.808044	2.044991
H	0.429693	-3.283609	1.142068
H	-0.930262	2.899463	2.300568
H	-0.938223	4.384876	1.349996
H	-2.523480	3.182600	-0.300977
H	-3.130402	3.608544	1.268114
H	-2.643900	1.262124	2.079183
H	-3.999547	1.475362	0.969348
H	-2.579567	-0.275570	-1.806091
H	-4.061778	0.364824	-1.062736
H	-2.768549	1.451731	-1.635848
H	-2.240138	-0.778837	1.858593
H	-3.593281	-1.164196	0.785215
H	-2.125117	-2.172360	-0.851435
H	-1.839716	-2.905356	0.710301
H	1.242714	-2.103383	-1.460127
H	0.055174	-3.391996	-1.226916
H	-0.381635	-1.927715	-2.119027
H	2.698327	-0.799138	-1.227899
H	2.469861	0.860099	-1.765228
H	3.916263	0.408598	-0.816866
H	1.035975	3.151113	-1.383964
H	-0.650277	3.576631	-1.318818
H	0.533475	4.609327	-0.479275
H	3.543268	-0.376207	1.515284
H	1.997746	-0.012938	2.297787
O	-0.067012	0.925854	-1.681663
H	-0.032501	0.187934	-2.296554
H	-0.537260	2.437230	5.812081
H	-0.699286	0.780366	6.430533
H	0.910871	1.441687	6.077291

$^{5\pi}$RC−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.216165	0.727766	0.000481
O	-0.499529	0.870657	1.620905
C	-1.296363	1.497724	5.383778
H	-1.084952	1.326136	4.327748
N	-2.414621	0.604453	-0.232570
C	-3.067809	1.789249	0.402096
C	-2.692648	-0.614841	0.580922
C	-2.909914	0.434354	-1.617038
N	0.015046	2.930926	-0.009402
C	1.162115	3.072945	0.934108
C	-1.198168	3.576839	0.576820
C	0.334875	3.542775	-1.319157
C	-2.533815	3.154447	-0.043353
N	1.990082	0.723388	0.402754
C	2.334850	2.172244	0.561451
C	2.188423	-0.024675	1.682235
C	2.858982	0.180111	-0.671249

N	-0.340377	-1.509520	0.188432
C	-1.810982	-1.793242	0.181074
C	0.273351	-1.859105	1.506291
C	0.265525	-2.305556	-0.908040
C	1.759450	-1.500193	1.670177
H	1.513234	4.111930	0.942606
H	0.794427	2.829140	1.926602
H	3.117563	2.284870	1.318497
H	2.763465	2.506534	-0.381559
H	2.044766	-1.891538	2.650979
H	2.367585	-2.066237	0.962888
H	-0.305357	-1.356451	2.278244
H	0.171449	-2.942006	1.654785
H	-1.213726	3.332595	1.637842
H	-1.083620	4.663601	0.486357
H	-2.514707	3.241505	-1.132684
H	-3.271265	3.892750	0.283340
H	-2.930942	1.696249	1.478167
H	-4.143653	1.735734	0.196632
H	-2.368999	-0.359921	-2.122490
H	-3.980986	0.203602	-1.613059
H	-2.760092	1.351856	-2.182781
H	-2.526113	-0.351618	1.621450
H	-3.741577	-0.911708	0.463209
H	-2.071503	-2.117371	-0.824834
H	-2.029138	-2.635501	0.846275
H	1.347475	-2.259521	-0.866550
H	-0.034517	-3.355629	-0.823856
H	-0.046785	-1.894186	-1.863739
H	2.744393	-0.894007	-0.754917
H	2.566717	0.616666	-1.621922
H	3.910100	0.398030	-0.453378
H	1.146494	3.008157	-1.802789
H	-0.531295	3.494007	-1.975939
H	0.611240	4.594872	-1.189824
H	3.255632	0.012050	1.936789
H	1.637691	0.503624	2.457595
O	0.134233	0.543606	-1.830076
H	-0.362934	1.058544	-2.471520
H	-0.368457	1.464648	5.953708
H	-1.762250	2.474146	5.514020
H	-1.971470	0.726265	5.752976

TS_H

$^{3\delta}TS_H$–[Fe^{IV}=O(TMC)(SR)]$^+$

Fe	-0.207345	0.662563	0.326034
O	-0.571993	0.584820	2.086177
C	0.290382	0.985385	4.413419
H	-0.066856	0.800727	3.164558
N	-2.581734	0.573570	0.290818
C	-3.077057	1.703714	1.115977
C	-2.729838	-0.735790	0.964500
C	-3.294148	0.572430	-1.000307
N	0.070503	2.763441	0.475337
C	1.295422	2.868663	1.329188
C	-1.082715	3.380455	1.221711

C	0.272058	3.504335	-0.796057
C	-2.493337	3.065314	0.710717
N	2.175110	0.630533	0.503623
C	2.479256	2.054474	0.811605
C	2.393475	-0.270630	1.666197
C	3.050472	0.226685	-0.619270
N	-0.362236	-1.447840	0.224683
C	-1.826329	-1.803916	0.338484
C	0.399852	-2.032296	1.379930
C	0.164110	-1.993084	-1.068328
C	1.904652	-1.717369	1.475009
H	1.604139	3.918921	1.399173
H	1.016555	2.542606	2.324956
H	3.293107	2.130328	1.543567
H	2.853038	2.510087	-0.104229
H	2.243668	-2.262525	2.361690
H	2.442969	-2.185454	0.650073
H	-0.103991	-1.692123	2.280427
H	0.297855	-3.123409	1.326029
H	-1.005568	3.052291	2.255119
H	-0.931193	4.465781	1.203393
H	-2.565608	3.216990	-0.368577
H	-3.142638	3.829087	1.148292
H	-2.820717	1.500636	2.153066
H	-4.171894	1.751996	1.045127
H	-2.947697	-0.234949	-1.637463
H	-4.373637	0.454948	-0.839463
H	-3.114243	1.499785	-1.537145
H	-2.482155	-0.602357	2.012701
H	-3.763674	-1.102667	0.900116
H	-2.182789	-2.029928	-0.663886
H	-1.921760	-2.727566	0.916066
H	2.915476	-0.822267	-0.861838
H	2.798844	0.801667	-1.506835
H	4.106245	0.382866	-0.364007
H	1.085441	3.068529	-1.368691
H	-0.627011	3.451580	-1.404238
H	0.501198	4.553449	-0.582909
H	3.468939	-0.312347	1.892735
H	1.900790	0.167057	2.528493
S	-0.112739	0.611721	-1.977710
C	-0.319515	-1.198291	-2.265219
H	0.269999	-1.467677	-3.142758
H	-1.360629	-1.410607	-2.508750
H	1.246894	-1.947308	-1.030651
H	-0.116892	-3.050805	-1.154003
H	1.266636	1.461182	4.432728
H	-0.506898	1.612729	4.801521
H	0.288512	-0.019793	4.824407

$^{3\pi}TS_H$–[Fe^{IV}=O(TMC)(SR)]$^+$

Fe	-0.120773	0.635853	0.267821
O	-0.223724	0.431006	2.074315
C	0.222647	1.529442	4.319129
H	0.004857	1.038694	3.021855
N	-2.283544	0.587738	0.382456
C	-2.803234	1.662368	1.280538

C	-2.513035	-0.731760	1.043097
C	-3.060848	0.642457	-0.885310
N	0.112925	2.732866	0.432914
C	1.396276	2.860444	1.187913
C	-0.947143	3.410962	1.247668
C	0.222545	3.451594	-0.865840
C	-2.385818	3.073625	0.879906
N	2.081783	0.596481	0.324579
C	2.493226	2.016125	0.581077
C	2.454042	-0.290854	1.475759
C	2.884782	0.172290	-0.860535
N	-0.272885	-1.468309	0.167010
C	-1.725430	-1.821171	0.345115
C	0.524004	-2.090216	1.277634
C	0.167883	-2.029799	-1.151523
C	2.019923	-1.753532	1.324576
H	1.717424	3.908950	1.204424
H	1.205786	2.557035	2.210410
H	3.374828	2.039198	1.229311
H	2.798326	2.441807	-0.373003
H	2.404724	-2.271409	2.208436
H	2.543287	-2.216540	0.487205
H	0.056048	-1.776862	2.205974
H	0.427334	-3.179033	1.188014
H	-0.785882	3.135535	2.286129
H	-0.788062	4.491947	1.167131
H	-2.594270	3.275916	-0.172123
H	-3.020013	3.767553	1.438559
H	-2.439062	1.450076	2.282587
H	-3.896526	1.590926	1.295515
H	-2.790383	-0.174780	-1.542131
H	-4.129633	0.578979	-0.656182
H	-2.857031	1.563706	-1.419504
H	-2.192364	-0.636148	2.075006
H	-3.579780	-0.982606	1.024048
H	-2.146898	-2.012277	-0.639303
H	-1.810551	-2.755532	0.906287
H	2.734327	-0.875005	-1.086991
H	2.587464	0.745859	-1.731518
H	3.947521	0.327988	-0.647120
H	0.985149	3.001830	-1.493603
H	-0.719630	3.393122	-1.403445
H	0.471598	4.502607	-0.688840
H	3.546550	-0.270880	1.574602
H	2.020392	0.129597	2.375678
S	-0.096382	0.586189	-2.029010
C	-0.342362	-1.215220	-2.326937
H	0.211087	-1.492743	-3.224728
H	-1.393641	-1.419784	-2.537723
H	1.251389	-2.043868	-1.166635
H	-0.165472	-3.073010	-1.220291
H	1.299673	1.537316	4.461970
H	-0.236296	2.510501	4.395647
H	-0.286765	0.761953	4.893570

$^{5\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.147923	0.675182	0.264216

O	-0.220447	0.639507	2.069265
C	-0.273537	0.593085	4.601409
H	-0.246807	0.606795	3.215041
N	-2.423213	0.572684	0.388656
C	-2.889422	1.698753	1.248727
C	-2.559450	-0.734790	1.087876
C	-3.212827	0.568489	-0.863442
N	0.143168	2.865510	0.453962
C	1.394056	2.924265	1.270216
C	-0.979270	3.468890	1.241551
C	0.308147	3.597641	-0.824403
C	-2.398398	3.085217	0.805160
N	2.179727	0.654839	0.397158
C	2.529435	2.078755	0.700952
C	2.480206	-0.256027	1.542817
C	2.992398	0.256081	-0.779379
N	-0.291284	-1.531366	0.205791
C	-1.746780	-1.843370	0.411598
C	0.531675	-2.082402	1.330169
C	0.154723	-2.077938	-1.108361
C	2.028016	-1.716584	1.359782
H	1.742997	3.962154	1.341520
H	1.136664	2.581895	2.266961
H	3.372680	2.118379	1.399324
H	2.879954	2.526404	-0.227716
H	2.426519	-2.253290	2.226426
H	2.541811	-2.162156	0.507340
H	0.061162	-1.746850	2.250205
H	0.464020	-3.177611	1.295893
H	-0.841786	3.168628	2.278207
H	-0.873640	4.559183	1.195368
H	-2.533488	3.227155	-0.269547
H	-3.064020	3.815435	1.273261
H	-2.544313	1.505477	2.261558
H	-3.986160	1.695441	1.261401
H	-2.904553	-0.243373	-1.512851
H	-4.278892	0.458325	-0.633321
H	-3.057193	1.491896	-1.413413
H	-2.222920	-0.595053	2.110110
H	-3.610334	-1.049817	1.111489
H	-2.176403	-2.063627	-0.563596
H	-1.843624	-2.757729	1.004861
H	2.823923	-0.783846	-1.035308
H	2.708700	0.852184	-1.641876
H	4.059101	0.390965	-0.565057
H	1.083799	3.138572	-1.431478
H	-0.616991	3.560592	-1.395180
H	0.569237	4.644419	-0.634554
H	3.567155	-0.265738	1.700919
H	2.013714	0.164371	2.428376
S	-0.111504	0.545353	-2.100428
C	-0.360522	-1.276357	-2.296882
H	0.174114	-1.594782	-3.192178
H	-1.417563	-1.470102	-2.486086
H	1.240206	-2.066652	-1.121064
H	-0.156991	-3.127696	-1.192240
H	0.625766	1.129315	4.888354

H	-1.197478	1.104553	4.852549
H	-0.264283	-0.461907	4.856658

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.125032	0.648296	0.260943
O	-0.158218	0.419604	2.065625
C	-0.092982	1.587202	4.316768
H	-0.118037	1.068801	3.009151
N	-2.415591	0.570900	0.412908
C	-2.835113	1.691651	1.298523
C	-2.539939	-0.741650	1.098100
C	-3.242570	0.590954	-0.813163
N	0.198377	2.771590	0.425473
C	1.480336	2.836659	1.194914
C	-0.887425	3.417327	1.237656
C	0.334214	3.506087	-0.857717
C	-2.329343	3.070680	0.850775
N	2.245903	0.581582	0.292820
C	2.602484	1.999204	0.588449
C	2.561596	-0.334278	1.427974
C	3.026334	0.182908	-0.902766
N	-0.273703	-1.501218	0.168162
C	-1.726191	-1.830794	0.394929
C	0.569572	-2.106485	1.254512
C	0.139153	-2.034032	-1.169071
C	2.074943	-1.782698	1.247526
H	1.821408	3.877799	1.250504
H	1.268379	2.502754	2.203467
H	3.465189	2.044210	1.263360
H	2.923659	2.453467	-0.347741
H	2.479022	-2.335609	2.101398
H	2.557772	-2.234805	0.380335
H	0.137424	-1.780331	2.196042
H	0.466044	-3.196729	1.184676
H	-0.727524	3.140545	2.276036
H	-0.750403	4.502437	1.167368
H	-2.499998	3.225031	-0.216782
H	-2.957775	3.813835	1.349332
H	-2.465663	1.477977	2.298921
H	-3.930959	1.711889	1.348335
H	-2.973179	-0.225324	-1.475114
H	-4.303659	0.500367	-0.552689
H	-3.085884	1.513676	-1.364227
H	-2.188605	-0.617004	2.116900
H	-3.587832	-1.066374	1.126510
H	-2.169404	-2.044302	-0.575608
H	-1.797727	-2.752962	0.978085
H	2.858086	-0.859383	-1.150046
H	2.717046	0.775757	-1.759239
H	4.099169	0.321754	-0.722023
H	1.089822	3.044624	-1.486497
H	-0.606593	3.481026	-1.401893
H	0.609511	4.548297	-0.665238
H	3.652106	-0.363199	1.561797
H	2.120013	0.083913	2.327464
S	-0.150314	0.596283	-2.020270
C	-0.410408	-1.207894	-2.316790

H	0.110492	-1.475138	-3.236997
H	-1.469962	-1.399537	-2.490188
H	1.222957	-2.020605	-1.210764
H	-0.175692	-3.082388	-1.252820
H	0.802801	2.192938	4.414734
H	-1.018361	2.141487	4.441081
H	-0.059364	0.658423	4.877663

$^{3\delta}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.257478	0.807548	0.184613
O	-0.308877	1.227061	1.920124
C	-1.457392	0.638216	4.080957
H	-0.916145	0.861492	2.908844
N	-2.508324	0.721367	0.043015
C	-3.096727	1.981725	0.572831
C	-2.781585	-0.418166	0.947686
C	-3.030595	0.450879	-1.312804
N	0.047145	2.967409	-0.013776
C	1.236780	3.211838	0.850186
C	-1.133533	3.696131	0.542157
C	0.306886	3.427221	-1.396777
C	-2.501403	3.271044	-0.006424
N	2.099367	0.843465	0.419624
C	2.422338	2.298308	0.525690
C	2.337716	0.121803	1.702194
C	2.946697	0.267933	-0.645132
N	-0.420777	-1.341022	0.515280
C	-1.888336	-1.633604	0.672063
C	0.351456	-1.668475	1.757772
C	0.075011	-2.179088	-0.606597
C	1.855831	-1.339508	1.744420
H	1.570538	4.251532	0.744200
H	0.920619	3.062281	1.878056
H	3.195598	2.462563	1.284922
H	2.860220	2.604972	-0.423138
H	2.237690	-1.742993	2.687224
H	2.360694	-1.927607	0.976221
H	-0.124808	-1.154458	2.585621
H	0.253683	-2.746838	1.938933
H	-1.122743	3.547553	1.620176
H	-0.990829	4.767025	0.352305
H	-2.499697	3.245332	-1.097990
H	-3.196190	4.073983	0.256674
H	-2.952938	1.986834	1.652662
H	-4.179346	1.973901	0.388851
H	-2.564259	-0.435361	-1.731789
H	-4.118790	0.314689	-1.282682
H	-2.790604	1.275157	-1.978549
H	-2.638973	-0.072135	1.965290
H	-3.825306	-0.749487	0.860666
H	-2.219816	-2.113637	-0.246558
H	-2.036107	-2.363616	1.473660
H	1.137220	-2.025587	-0.761312
H	-0.093240	-3.239274	-0.388032
H	-0.440973	-1.903765	-1.521131
H	2.743817	-0.790672	-0.780189
H	2.757467	0.774761	-1.591424

H	4.012776	0.379687	-0.410294
H	1.180279	2.930309	-1.807291
H	-0.532574	3.181592	-2.039527
H	0.474304	4.510322	-1.406777
H	3.417502	0.120049	1.909523
H	1.846401	0.686914	2.489336
O	-0.154214	0.580888	-1.612208
H	0.704671	0.352771	-1.981557
H	-0.643485	0.908068	4.748173
H	-2.299594	1.322088	4.130059
H	-1.740837	-0.408479	4.143621

$^{3\pi}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.223119	0.780947	0.185225
O	-0.330163	1.193670	1.949430
C	-1.535545	0.604213	4.106772
H	-0.932379	0.840533	2.861747
N	-2.332140	0.713875	0.028899
C	-3.013885	1.923191	0.583341
C	-2.685322	-0.449708	0.890797
C	-2.834589	0.482828	-1.353555
N	0.010189	2.900020	-0.007134
C	1.206347	3.179302	0.843540
C	-1.142055	3.658241	0.571007
C	0.247846	3.385553	-1.389585
C	-2.512457	3.255923	0.041197
N	1.926601	0.802125	0.428677
C	2.348229	2.244265	0.505651
C	2.238949	0.110385	1.723520
C	2.742205	0.188513	-0.653963
N	-0.374019	-1.338902	0.458173
C	-1.841242	-1.654944	0.542318
C	0.313811	-1.693939	1.741253
C	0.156468	-2.201187	-0.637787
C	1.807826	-1.356999	1.807134
H	1.531988	4.217131	0.707371
H	0.898666	3.039036	1.874070
H	3.146115	2.359966	1.244420
H	2.779257	2.513379	-0.457100
H	2.147886	-1.709911	2.785088
H	2.365381	-1.960026	1.088657
H	-0.210463	-1.189242	2.545540
H	0.204998	-2.774764	1.893692
H	-1.119233	3.495399	1.645886
H	-0.970845	4.724163	0.383495
H	-2.553880	3.289819	-1.049440
H	-3.218943	4.019089	0.379369
H	-2.873942	1.911812	1.662141
H	-4.086894	1.824004	0.383787
H	-2.331425	-0.359754	-1.810759
H	-3.915525	0.311093	-1.320991
H	-2.623503	1.346229	-1.975472
H	-2.529107	-0.155000	1.921946
H	-3.745283	-0.702229	0.769422
H	-2.145677	-2.045706	-0.425935
H	-2.010244	-2.453159	1.271192
H	1.238850	-2.195834	-0.650959

H	-0.171006	-3.233269	-0.479005
H	-0.195617	-1.823454	-1.591704
H	2.507751	-0.859315	-0.780107
H	2.546964	0.685330	-1.599337
H	3.806525	0.286318	-0.415901
H	1.152911	2.948384	-1.802906
H	-0.583303	3.115761	-2.034171
H	0.366688	4.473793	-1.389882
H	3.324942	0.152889	1.871553
H	1.756709	0.681181	2.510785
O	-0.092620	0.467961	-1.640491
H	0.506827	1.008035	-2.161180
H	-0.747895	0.946281	4.771244
H	-2.417246	1.238186	4.117598
H	-1.756927	-0.455305	4.200938

$^{5\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.120948	0.672062	0.258874
O	-0.208150	0.633617	2.062063
C	-0.291880	0.586323	4.587288
H	-0.248728	0.605803	3.211997
N	-2.357113	0.518432	0.340890
C	-2.892392	1.660523	1.140893
C	-2.536456	-0.761411	1.078817
C	-3.028629	0.471452	-0.974600
N	0.157648	2.874437	0.478145
C	1.403513	2.920013	1.293140
C	-0.988445	3.444077	1.245729
C	0.330487	3.614642	-0.793060
C	-2.383020	3.051830	0.735264
N	2.148490	0.648320	0.382007
C	2.523097	2.067583	0.696298
C	2.516237	-0.273301	1.497941
C	2.856070	0.267535	-0.864819
N	-0.269903	-1.614120	0.246770
C	-1.723642	-1.909619	0.477054
C	0.565048	-2.089158	1.394778
C	0.142043	-2.304778	-0.997551
C	2.061287	-1.734937	1.342088
H	1.767033	3.952463	1.374384
H	1.151143	2.567446	2.287998
H	3.376955	2.082861	1.381341
H	2.864214	2.522363	-0.232053
H	2.509665	-2.266144	2.187363
H	2.524439	-2.183104	0.462092
H	0.126228	-1.679459	2.299645
H	0.485634	-3.183577	1.441129
H	-0.885232	3.114630	2.277855
H	-0.900332	4.537201	1.234675
H	-2.462828	3.201910	-0.343775
H	-3.081249	3.769730	1.173958
H	-2.628709	1.478346	2.180446
H	-3.986843	1.647590	1.066803
H	-2.650630	-0.356989	-1.567880
H	-4.110789	0.349749	-0.849022
H	-2.829558	1.385002	-1.528024
H	-2.230905	-0.584635	2.104739

H	-3.593264	-1.057850	1.079653
H	-2.152699	-2.190628	-0.483680
H	-1.827680	-2.785138	1.126106
H	1.179627	-2.095630	-1.233249
H	0.017192	-3.389554	-0.899833
H	-0.465252	-1.959685	-1.831321
H	2.687506	-0.777828	-1.100231
H	2.470098	0.859055	-1.690556
H	3.935401	0.424498	-0.757116
H	1.095378	3.148851	-1.404977
H	-0.589656	3.582545	-1.369113
H	0.596553	4.657813	-0.587488
H	3.610128	-0.275485	1.597094
H	2.095701	0.142269	2.409544
O	-0.062152	0.866401	-1.611986
H	-0.346143	0.277439	-2.313829
H	-0.839142	1.487542	4.845999
H	-0.813918	-0.334890	4.827213
H	0.750627	0.597626	4.889376

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.252801	0.791490	0.163194
O	-0.443432	1.256418	1.890874
C	-1.326811	0.470957	4.140234
H	-0.873783	0.779348	2.832843
N	-2.464384	0.697399	-0.015479
C	-3.082840	1.947161	0.514719
C	-2.749596	-0.448349	0.886381
C	-2.971237	0.423600	-1.379711
N	0.037992	2.985827	-0.044884
C	1.204887	3.214077	0.856799
C	-1.160992	3.701117	0.496716
C	0.332274	3.485694	-1.405404
C	-2.515547	3.249860	-0.061773
N	2.007612	0.820967	0.473202
C	2.371658	2.270526	0.566240
C	2.240280	0.114426	1.769225
C	2.839402	0.217819	-0.594881
N	-0.404816	-1.396229	0.479250
C	-1.878079	-1.668017	0.582993
C	0.305895	-1.720529	1.754902
C	0.116812	-2.248447	-0.621505
C	1.799839	-1.358440	1.814444
H	1.563137	4.245792	0.755008
H	0.852259	3.068231	1.871988
H	3.132924	2.417037	1.339424
H	2.839252	2.548828	-0.377241
H	2.146122	-1.734421	2.781752
H	2.357751	-1.942126	1.080788
H	-0.221111	-1.220948	2.561124
H	0.221145	-2.801491	1.927873
H	-1.159239	3.553793	1.573812
H	-1.031566	4.772404	0.301335
H	-2.510779	3.229012	-1.154130
H	-3.228802	4.036234	0.201089
H	-2.940573	1.951688	1.593804
H	-4.161939	1.908677	0.320464

H	-2.448572	-0.418480	-1.820511
H	-4.048465	0.222941	-1.347006
H	-2.789255	1.279025	-2.024219
H	-2.590851	-0.110707	1.904684
H	-3.799773	-0.753824	0.796455
H	-2.190971	-2.100670	-0.365008
H	-2.062280	-2.428832	1.348261
H	1.196903	-2.181229	-0.681836
H	-0.153586	-3.295181	-0.444765
H	-0.285833	-1.903437	-1.568484
H	2.619986	-0.836667	-0.711639
H	2.625272	0.698017	-1.545580
H	3.904806	0.330594	-0.362256
H	1.220168	3.004452	-1.811163
H	-0.503961	3.285998	-2.072552
H	0.511266	4.566459	-1.387594
H	3.315676	0.145267	1.990230
H	1.719360	0.678248	2.538521
O	-0.062626	0.443826	-1.638842
H	0.267115	1.158867	-2.190796
H	-0.398919	0.455987	4.704041
H	-1.959580	1.325282	4.358766
H	-1.852359	-0.479150	4.125333

IN

$^{3\delta}$I−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.180030	0.578801	0.228349
O	-0.278023	0.340279	2.092612
C	-0.356762	2.030754	5.283423
H	-0.307478	1.106628	2.672540
N	-2.484771	0.559642	0.337314
C	-2.912466	1.648490	1.257043
C	-2.644355	-0.777931	0.963767
C	-3.275135	0.644108	-0.909379
N	0.179067	2.687212	0.537922
C	1.440955	2.704495	1.344247
C	-0.918274	3.324749	1.342935
C	0.366174	3.475150	-0.708400
C	-2.354797	3.032719	0.896082
N	2.195233	0.475305	0.371263
C	2.565081	1.871953	0.734897
C	2.440788	-0.483423	1.488181
C	3.020268	0.103133	-0.802144
N	-0.365431	-1.535394	0.072635
C	-1.831554	-1.846456	0.230753
C	0.415636	-2.187789	1.178794
C	0.092578	-2.033774	-1.263957
C	1.928440	-1.911741	1.238712
H	1.795106	3.737671	1.445760
H	1.206831	2.345959	2.342237
H	3.410126	1.875724	1.433611
H	2.918288	2.359672	-0.172547
H	2.281860	-2.502723	2.089604
H	2.433399	-2.349869	0.376767
H	-0.042476	-1.865459	2.109454
H	0.279903	-3.272019	1.081617

H	-0.800658	3.016477	2.382105
H	-0.752787	4.407857	1.324100
H	-2.483434	3.241004	-0.168094
H	-2.980636	3.768826	1.408300
H	-2.595629	1.379523	2.262636
H	-4.008624	1.697962	1.263293
H	-2.986263	-0.137034	-1.604993
H	-4.344156	0.544135	-0.686911
H	-3.100335	1.593687	-1.407074
H	-2.310021	-0.701956	1.993398
H	-3.697088	-1.087776	0.957489
H	-2.244090	-1.998782	-0.764436
H	-1.939870	-2.796607	0.761121
H	2.849402	-0.929062	-1.087330
H	2.754230	0.726603	-1.651803
H	4.086737	0.220836	-0.574715
H	1.133234	3.026681	-1.332307
H	-0.557512	3.487874	-1.281197
H	0.651810	4.503573	-0.463800
H	3.523128	-0.541491	1.670054
H	1.963726	-0.085990	2.379272
S	-0.129832	0.631488	-2.035571
C	-0.396955	-1.160018	-2.404255
H	0.157998	-1.403643	-3.311004
H	-1.451075	-1.329275	-2.627175
H	1.177248	-2.037415	-1.261453
H	-0.235412	-3.073043	-1.394313
H	-1.273113	2.586005	5.419734
H	-0.388870	0.953028	5.220924
H	0.591423	2.531011	5.415223

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.127664	0.572851	0.192208
O	-0.208929	0.383771	2.062591
C	0.298332	2.209209	5.182019
H	-0.047990	1.144305	2.628073
N	-2.282074	0.538126	0.332427
C	-2.797410	1.592531	1.258656
C	-2.508730	-0.792616	0.971749
C	-3.068795	0.621240	-0.927975
N	0.115954	2.682482	0.444135
C	1.407908	2.791543	1.185670
C	-0.937876	3.344180	1.279077
C	0.218091	3.434198	-0.836864
C	-2.376607	3.014804	0.903133
N	2.073685	0.535903	0.269720
C	2.491318	1.948483	0.551576
C	2.441050	-0.369049	1.409838
C	2.882208	0.129457	-0.918024
N	-0.283529	-1.513775	0.071148
C	-1.735472	-1.868652	0.240668
C	0.504565	-2.149411	1.180580
C	0.160733	-2.051664	-1.255341
C	2.002715	-1.826891	1.234257
H	1.738706	3.836992	1.211727
H	1.239968	2.489251	2.215832
H	3.381015	1.954743	1.189105

H	2.786629	2.393117	-0.396984
H	2.381432	-2.359779	2.111803
H	2.525050	-2.281077	0.391302
H	0.038733	-1.834920	2.109684
H	0.397306	-3.236650	1.085230
H	-0.776146	3.057350	2.317768
H	-0.779486	4.427078	1.224217
H	-2.582066	3.248104	-0.143013
H	-3.012671	3.691699	1.480349
H	-2.440177	1.348766	2.256004
H	-3.891019	1.525487	1.268505
H	-2.795332	-0.174345	-1.609781
H	-4.135683	0.542975	-0.694828
H	-2.875242	1.559464	-1.436285
H	-2.167597	-0.716696	1.999041
H	-3.576901	-1.037301	0.966710
H	-2.160779	-2.030199	-0.747530
H	-1.823349	-2.817655	0.776467
H	2.733653	-0.914800	-1.159017
H	2.587492	0.715570	-1.781735
H	3.944123	0.282596	-0.699088
H	0.977302	2.999525	-1.479168
H	-0.726565	3.386482	-1.370946
H	0.466961	4.481631	-0.638047
H	3.533010	-0.350972	1.513528
H	1.999068	0.035133	2.313913
S	-0.098915	0.588601	-2.081473
C	-0.340972	-1.209467	-2.416180
H	0.217163	-1.467641	-3.316807
H	-1.391330	-1.407713	-2.637249
H	1.244206	-2.071097	-1.265997
H	-0.177258	-3.091362	-1.348482
H	1.374847	2.262556	5.252620
H	-0.283797	3.114374	5.273667
H	-0.192495	1.248355	5.227386

$^{5\sigma}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.214688	0.683721	0.209219
O	-0.469966	0.662810	2.094272
C	0.600056	0.525101	5.323682
H	0.009012	0.551295	2.921210
N	-2.496348	0.601546	0.231151
C	-2.994462	1.739120	1.059621
C	-2.683033	-0.701564	0.929774
C	-3.218667	0.598798	-1.060129
N	0.094842	2.882116	0.422530
C	1.296786	2.920072	1.309029
C	-1.066347	3.490743	1.149265
C	0.341038	3.617765	-0.839925
C	-2.461938	3.116813	0.633104
N	2.109713	0.640743	0.478371
C	2.455503	2.061564	0.807107
C	2.354224	-0.283157	1.625082
C	2.972720	0.238263	-0.661275
N	-0.383980	-1.537102	0.161673
C	-1.853526	-1.825263	0.298587
C	0.375108	-2.079829	1.331574

C	0.119479	-2.097901	-1.122190
C	1.875073	-1.734536	1.427838
H	1.656744	3.952380	1.406856
H	0.975465	2.584252	2.289672
H	3.257032	2.092023	1.553510
H	2.864793	2.507113	-0.097999
H	2.227683	-2.276370	2.311073
H	2.418879	-2.189737	0.599388
H	-0.138218	-1.726962	2.222591
H	0.297628	-3.174925	1.313141
H	-0.990798	3.181471	2.189500
H	-0.951612	4.580557	1.113300
H	-2.532499	3.252104	-0.448934
H	-3.145756	3.857866	1.055808
H	-2.702315	1.547350	2.088892
H	-4.090166	1.749917	1.011105
H	-2.884990	-0.219060	-1.689554
H	-4.296605	0.499061	-0.887323
H	-3.027186	1.519070	-1.604453
H	-2.390399	-0.556692	1.964603
H	-3.737910	-1.002865	0.902871
H	-2.236636	-2.045799	-0.695900
H	-1.993653	-2.735283	0.890507
H	2.797194	-0.796338	-0.934586
H	2.742418	0.846827	-1.530617
H	4.030067	0.352391	-0.394750
H	1.142645	3.150279	-1.405992
H	-0.551919	3.596932	-1.460899
H	0.606198	4.660456	-0.632739
H	3.435981	-0.322381	1.813018
H	1.897085	0.146590	2.512077
S	-0.042119	0.528068	-2.140464
C	-0.313248	-1.290161	-2.340680
H	0.261592	-1.623143	-3.205133
H	-1.362885	-1.459675	-2.585079
H	1.204442	-2.109796	-1.078471
H	-0.208672	-3.140940	-1.224573
H	1.202387	1.420270	5.378649
H	-0.474090	0.601861	5.406361
H	1.073902	-0.440502	5.422421

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.118290	0.585676	0.178757
O	-0.139173	0.385976	2.050139
C	-0.170779	2.229711	5.161874
H	-0.156618	1.163440	2.615933
N	-2.416659	0.527452	0.376431
C	-2.831522	1.625742	1.290433
C	-2.526435	-0.799283	1.035800
C	-3.254585	0.571160	-0.841125
N	0.206469	2.707733	0.428712
C	1.498164	2.767378	1.183895
C	-0.870671	3.341961	1.263019
C	0.328276	3.471474	-0.840187
C	-2.317872	3.013293	0.880701
N	2.259940	0.531070	0.232531
C	2.614331	1.942924	0.549458

C	2.567510	-0.397521	1.359218
C	3.046666	0.148206	-0.963488
N	-0.269683	-1.534488	0.074284
C	-1.722581	-1.868217	0.293992
C	0.564970	-2.147017	1.164123
C	0.147330	-2.054285	-1.267579
C	2.073293	-1.840259	1.160561
H	1.835431	3.809118	1.248447
H	1.310162	2.427330	2.197896
H	3.486143	1.980326	1.213459
H	2.920963	2.416117	-0.382413
H	2.470302	-2.405361	2.009731
H	2.553523	-2.287603	0.289370
H	0.135419	-1.813004	2.104187
H	0.447884	-3.235668	1.095606
H	-0.705889	3.058503	2.302628
H	-0.727522	4.427441	1.214284
H	-2.493911	3.198357	-0.180969
H	-2.937264	3.746928	1.404182
H	-2.469866	1.383831	2.287871
H	-3.927410	1.652649	1.339165
H	-2.976046	-0.218240	-1.531504
H	-4.312434	0.455441	-0.576822
H	-3.117380	1.513498	-1.363933
H	-2.153769	-0.694845	2.049652
H	-3.572707	-1.128045	1.077464
H	-2.169328	-2.048118	-0.681674
H	-1.793433	-2.808945	0.846936
H	2.883077	-0.892376	-1.221426
H	2.738154	0.749033	-1.815051
H	4.118711	0.288426	-0.778705
H	1.080825	3.026166	-1.483902
H	-0.616622	3.451739	-1.377088
H	0.599960	4.510957	-0.628857
H	3.657165	-0.431832	1.498909
H	2.118538	0.010472	2.259907
S	-0.154083	0.589372	-2.086124
C	-0.399678	-1.214482	-2.407395
H	0.126902	-1.467243	-3.328397
H	-1.457663	-1.407969	-2.588585
H	1.231246	-2.039609	-1.305718
H	-0.166900	-3.101619	-1.363197
H	0.744519	2.795927	5.253542
H	-1.120047	2.739387	5.238263
H	-0.138686	1.151011	5.204349

$^{3\delta}$I−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.215654	0.851023	0.088907
O	-0.351434	1.265466	1.861274
C	-1.824004	0.224510	4.896326
H	-0.851510	0.722413	2.477561
N	-2.483839	0.767408	0.012245
C	-3.056733	2.039440	0.532373
C	-2.755700	-0.355612	0.937806
C	-3.030032	0.479199	-1.330962
N	0.088164	2.995070	-0.101195
C	1.282142	3.235964	0.758910

C	-1.084437	3.735714	0.458855
C	0.344326	3.447346	-1.487990
C	-2.459029	3.314295	-0.074060
N	2.119364	0.860984	0.356652
C	2.456983	2.314141	0.427314
C	2.336061	0.180687	1.666176
C	2.974181	0.247764	-0.680963
N	-0.406688	-1.302144	0.504226
C	-1.875946	-1.580220	0.664810
C	0.354835	-1.613309	1.756071
C	0.085292	-2.173583	-0.594223
C	1.857499	-1.279436	1.749520
H	1.620749	4.273152	0.647043
H	0.968229	3.089013	1.787268
H	3.247056	2.486097	1.167539
H	2.876533	2.598544	-0.536624
H	2.232484	-1.653848	2.706799
H	2.369176	-1.889438	1.003074
H	-0.130554	-1.103809	2.585383
H	0.258806	-2.689837	1.949080
H	-1.065428	3.594156	1.537339
H	-0.934629	4.803388	0.257533
H	-2.466325	3.270584	-1.165169
H	-3.145557	4.126744	0.181278
H	-2.895922	2.060157	1.609808
H	-4.141727	2.035665	0.362961
H	-2.572795	-0.413679	-1.745946
H	-4.118047	0.347581	-1.282614
H	-2.798245	1.294168	-2.011085
H	-2.613613	-0.000084	1.956358
H	-3.802643	-0.680183	0.866166
H	-2.214884	-2.056445	-0.252917
H	-2.029801	-2.308149	1.467291
H	1.149602	-2.033406	-0.748848
H	-0.092325	-3.226915	-0.351261
H	-0.426602	-1.917242	-1.516712
H	2.765415	-0.813215	-0.785942
H	2.796125	0.726993	-1.643555
H	4.038411	0.359628	-0.438241
H	1.202279	2.930812	-1.906820
H	-0.507145	3.218046	-2.121236
H	0.532720	4.526777	-1.501924
H	3.412332	0.188448	1.890208
H	1.830140	0.771313	2.424915
O	-0.144081	0.578271	-1.694440
H	0.696723	0.283102	-2.059007
H	-0.940829	0.824153	5.061072
H	-2.777556	0.711115	4.752557
H	-1.795705	-0.835832	5.100706

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.174935	0.811734	0.112102
O	-0.309138	1.232969	1.936767
C	-2.074819	0.268160	4.915544
H	-0.913536	0.752350	2.509172
N	-2.300127	0.749695	0.013636
C	-2.966751	1.969935	0.563175

C	-2.651010	-0.403038	0.890046
C	-2.827838	0.504731	-1.357484
N	0.059543	2.916310	-0.083884
C	1.262140	3.193637	0.757982
C	-1.081476	3.686990	0.502233
C	0.286577	3.392727	-1.471097
C	-2.462170	3.290493	-0.004510
N	1.965034	0.821136	0.347940
C	2.397697	2.259905	0.402374
C	2.276899	0.153314	1.656479
C	2.771825	0.183186	-0.726797
N	-0.345575	-1.308584	0.443822
C	-1.812682	-1.614987	0.548584
C	0.351532	-1.649896	1.724955
C	0.168430	-2.194937	-0.641198
C	1.845708	-1.311761	1.772366
H	1.584655	4.232844	0.625901
H	0.962758	3.045186	1.790044
H	3.211817	2.378440	1.122947
H	2.808099	2.519518	-0.571972
H	2.195368	-1.646196	2.753397
H	2.394965	-1.929360	1.059850
H	-0.164276	-1.142384	2.535648
H	0.243448	-2.728727	1.891615
H	-1.045323	3.532069	1.577775
H	-0.904959	4.749799	0.302416
H	-2.518332	3.309139	-1.094891
H	-3.157145	4.064745	0.332394
H	-2.810320	1.974635	1.640454
H	-4.043605	1.876006	0.381976
H	-2.336784	-0.346197	-1.812427
H	-3.909436	0.341420	-1.306874
H	-2.620299	1.359117	-1.992886
H	-2.507270	-0.103502	1.925279
H	-3.711946	-0.655648	0.777209
H	-2.131021	-2.012795	-0.412209
H	-1.978848	-2.405219	1.286895
H	1.250769	-2.196580	-0.664539
H	-0.163803	-3.222264	-0.462196
H	-0.189843	-1.830272	-1.597921
H	2.527800	-0.864642	-0.835251
H	2.576449	0.666550	-1.679418
H	3.838028	0.275735	-0.494953
H	1.176324	2.936330	-1.896799
H	-0.559153	3.135229	-2.101879
H	0.425013	4.478686	-1.478573
H	3.363224	0.197243	1.801509
H	1.794264	0.739553	2.432100
O	-0.089528	0.455238	-1.701202
H	0.511537	0.985278	-2.231300
H	-1.201335	0.888745	5.050940
H	-3.038274	0.730000	4.757040
H	-2.023909	-0.785612	5.147210

$^{5\sigma}$IN–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.203227	0.651643	0.202622
O	-0.480674	0.562536	2.085676

C	0.712651	0.847901	5.296746
H	0.051175	0.640455	2.882946
N	-2.440701	0.528199	0.172876
C	-3.017030	1.660540	0.958061
C	-2.673909	-0.763101	0.879332
C	-3.030011	0.506013	-1.183355
N	0.078221	2.858173	0.485628
C	1.273362	2.879385	1.374013
C	-1.107200	3.423518	1.198348
C	0.333020	3.621561	-0.757860
C	-2.473681	3.053159	0.602917
N	2.067813	0.607589	0.484327
C	2.426883	2.019058	0.852407
C	2.369946	-0.351610	1.587753
C	2.847321	0.248923	-0.725446
N	-0.375633	-1.640205	0.156345
C	-1.847122	-1.912555	0.299464
C	0.385537	-2.131985	1.346467
C	0.092946	-2.328830	-1.067738
C	1.889251	-1.800053	1.378937
H	1.645217	3.906452	1.485686
H	0.955465	2.539267	2.354816
H	3.225629	2.017800	1.601300
H	2.842559	2.486427	-0.038306
H	2.285856	-2.356858	2.233589
H	2.391033	-2.237181	0.514506
H	-0.100907	-1.719572	2.226143
H	0.291195	-3.225656	1.383467
H	-1.068276	3.069527	2.226767
H	-1.009503	4.515770	1.214778
H	-2.491255	3.221598	-0.476316
H	-3.188706	3.771249	1.013609
H	-2.813283	1.460507	2.007542
H	-4.104876	1.657594	0.816631
H	-2.588348	-0.287035	-1.779314
H	-4.114403	0.354356	-1.125921
H	-2.822785	1.441309	-1.695425
H	-2.415485	-0.605556	1.921287
H	-3.733118	-1.043874	0.817322
H	-2.223829	-2.166274	-0.690283
H	-2.001627	-2.799298	0.923256
H	1.151143	-2.151784	-1.233587
H	-0.067575	-3.410984	-0.994423
H	-0.452330	-1.954921	-1.931710
H	2.651728	-0.777250	-1.018928
H	2.553179	0.895468	-1.547756
H	3.922112	0.353469	-0.538132
H	1.138911	3.166814	-1.324148
H	-0.547560	3.599344	-1.393502
H	0.583824	4.661856	-0.519780
H	3.458991	-0.384810	1.728538
H	1.944438	0.047827	2.504986
O	-0.043889	0.853099	-1.650864
H	0.164358	0.244285	-2.362363
H	-0.360375	0.922624	5.393623
H	1.192873	-0.110689	5.427339
H	1.311833	1.746843	5.298394

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.196417	0.825924	0.069488
O	-0.435958	1.256046	1.825707
C	-1.605943	0.149525	4.958257
H	-0.752929	0.614689	2.467627
N	-2.388013	0.721352	-0.073598
C	-3.008256	1.979481	0.447943
C	-2.708133	-0.412854	0.837879
C	-2.908129	0.436857	-1.430801
N	0.076591	3.074843	-0.114021
C	1.235552	3.263904	0.797230
C	-1.124694	3.777366	0.417829
C	0.392474	3.571473	-1.468171
C	-2.466146	3.287250	-0.141411
N	1.994938	0.849399	0.426452
C	2.381660	2.295954	0.500307
C	2.230541	0.157546	1.731082
C	2.814867	0.224931	-0.640384
N	-0.394082	-1.426767	0.473842
C	-1.865749	-1.662387	0.567659
C	0.309555	-1.712592	1.755997
C	0.132469	-2.306285	-0.598193
C	1.797071	-1.318144	1.811926
H	1.627080	4.286374	0.715501
H	0.876165	3.116558	1.810480
H	3.157499	2.434762	1.260256
H	2.836222	2.556652	-0.454148
H	2.151244	-1.667061	2.786608
H	2.360818	-1.912355	1.091446
H	-0.233693	-1.224447	2.565156
H	0.248278	-2.791297	1.958250
H	-1.127772	3.642249	1.497594
H	-1.023314	4.851921	0.217507
H	-2.453540	3.255731	-1.233895
H	-3.202823	4.057207	0.105714
H	-2.850625	1.994619	1.524392
H	-4.089461	1.924914	0.269101
H	-2.406593	-0.425053	-1.860368
H	-3.987694	0.251770	-1.394445
H	-2.730790	1.287067	-2.086135
H	-2.568730	-0.065703	1.858278
H	-3.765034	-0.689949	0.738206
H	-2.184063	-2.105513	-0.374358
H	-2.087665	-2.402667	1.344822
H	1.213283	-2.240674	-0.655782
H	-0.137459	-3.351431	-0.405956
H	-0.263659	-1.985637	-1.557313
H	2.605368	-0.835495	-0.719788
H	2.567383	0.674395	-1.596937
H	3.881619	0.355522	-0.425804
H	1.209382	3.003974	-1.906577
H	-0.473950	3.466599	-2.119969
H	0.668749	4.632492	-1.440138
H	3.307533	0.190171	1.943863
H	1.721156	0.736534	2.496772
O	0.081153	0.487218	-1.683418

H	-0.351390	1.070278	-2.315341
H	-0.567291	0.229848	5.243133
H	-2.182204	1.049338	4.800280
H	-2.112015	-0.800258	5.049877

The optimized geometries in acetonitrile.

Cat

^{3}[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.133914	0.654682	0.213278
O	-0.180311	0.630706	1.868574
N	-2.279916	0.612160	0.306411
C	-2.820188	1.683067	1.198534
C	-2.504151	-0.705004	0.975023
C	-3.044233	0.655421	-0.969573
N	0.084869	2.755703	0.353456
C	1.365609	2.886638	1.117926
C	-0.972104	3.421023	1.181723
C	0.187145	3.471638	-0.946065
C	-2.409179	3.095705	0.807175
N	2.065673	0.622426	0.289151
C	2.461598	2.054104	0.504713
C	2.417157	-0.214603	1.481155
C	2.896920	0.166030	-0.862651
N	-0.263330	-1.431238	0.128798
C	-1.718350	-1.789946	0.277098
C	0.498765	-2.013684	1.286312
C	0.222984	-2.023917	-1.159365
C	1.991548	-1.680914	1.369659
H	1.674631	3.936824	1.139472
H	1.164422	2.566057	2.135386
H	3.354624	2.098268	1.134161
H	2.739212	2.462538	-0.464877
H	2.344499	-2.167678	2.283386
H	2.536401	-2.172915	0.563390
H	-0.002866	-1.674029	2.188597
H	0.397481	-3.102806	1.228093
H	-0.807360	3.117577	2.213468
H	-0.803476	4.500692	1.118847
H	-2.616740	3.306640	-0.243430
H	-3.042419	3.782315	1.374946
H	-2.467092	1.475811	2.206140
H	-3.911417	1.595718	1.196475
H	-2.749194	-0.152437	-1.627160
H	-4.111820	0.568080	-0.745899
H	-2.856955	1.588408	-1.489838
H	-2.186171	-0.604150	2.008579
H	-3.569736	-0.954910	0.961782
H	-2.124967	-1.968238	-0.714870
H	-1.806632	-2.729047	0.827415
H	2.779439	-0.893900	-1.045375
H	2.601904	0.700507	-1.758796
H	3.949727	0.359564	-0.634397
H	0.957476	3.027916	-1.568797
H	-0.757792	3.405706	-1.478489
H	0.427508	4.523756	-0.768519

H	3.505941	-0.181780	1.602498
H	1.960680	0.242681	2.353610
S	-0.077229	0.558757	-2.172176
C	-0.277008	-1.267034	-2.376997
H	0.298634	-1.587607	-3.245961
H	-1.322000	-1.497220	-2.590329
H	1.305708	-2.020804	-1.147345
H	-0.094606	-3.072497	-1.197200

$^{5}[Fe^{IV}=O(TMC)(SR)]^{+}$

Fe	-0.157119	0.669649	0.196936
O	-0.202392	0.645405	1.857635
N	-2.416873	0.577917	0.297292
C	-2.886344	1.696920	1.165013
C	-2.551720	-0.726841	0.999508
C	-3.210211	0.574459	-0.952085
N	0.132070	2.818399	0.344198
C	1.393383	2.898641	1.146584
C	-0.973337	3.434947	1.151161
C	0.277245	3.554284	-0.935535
C	-2.399925	3.082179	0.727542
N	2.183152	0.640502	0.294441
C	2.526342	2.069724	0.561147
C	2.472426	-0.232419	1.470695
C	3.010435	0.212507	-0.858930
N	-0.279949	-1.484440	0.131274
C	-1.734523	-1.821596	0.319178
C	0.522540	-2.035052	1.275452
C	0.188116	-2.047482	-1.172786
C	2.020280	-1.692737	1.318137
H	1.721186	3.942321	1.204158
H	1.154559	2.560120	2.150146
H	3.384943	2.130154	1.237996
H	2.844293	2.506860	-0.383803
H	2.396590	-2.210617	2.205442
H	2.540290	-2.163261	0.483077
H	0.043454	-1.682483	2.185901
H	0.430635	-3.126969	1.245891
H	-0.829022	3.121984	2.183249
H	-0.838959	4.521039	1.110629
H	-2.550566	3.239341	-0.342918
H	-3.048416	3.811539	1.219671
H	-2.537321	1.499653	2.176600
H	-3.982254	1.682710	1.180243
H	-2.902429	-0.235281	-1.604641
H	-4.272918	0.455972	-0.713151
H	-3.065528	1.505331	-1.492832
H	-2.217924	-0.586406	2.023624
H	-3.600617	-1.043616	1.020632
H	-2.154686	-2.036937	-0.660196
H	-1.816595	-2.740494	0.904312
H	2.855974	-0.835983	-1.087107
H	2.737280	0.788731	-1.738237
H	4.072463	0.362927	-0.632281
H	1.056864	3.107919	-1.546265
H	-0.655208	3.512668	-1.493545
H	0.529667	4.600544	-0.737259

H	3.556908	-0.231923	1.641819
H	1.994062	0.211652	2.339688
S	-0.101683	0.556908	-2.151321
C	-0.341950	-1.267719	-2.362369
H	0.199454	-1.577279	-3.256790
H	-1.397178	-1.473168	-2.543346
H	1.272269	-2.019999	-1.180048
H	-0.111833	-3.100443	-1.236703

^{3}[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.114746	0.647423	0.223717
O	-0.167121	0.611931	1.881183
N	-2.231971	0.584692	0.264240
C	-2.848568	1.665395	1.090821
C	-2.489880	-0.709818	0.962703
C	-2.869874	0.582319	-1.076806
N	0.084605	2.746231	0.372763
C	1.359956	2.879278	1.139643
C	-0.991201	3.393758	1.182191
C	0.194417	3.452276	-0.930344
C	-2.411997	3.079337	0.737350
N	2.036904	0.625924	0.270093
C	2.453683	2.050276	0.512175
C	2.453125	-0.235821	1.422846
C	2.763109	0.197913	-0.955981
N	-0.247250	-1.504565	0.162578
C	-1.706775	-1.832832	0.327158
C	0.529096	-2.025628	1.335855
C	0.189448	-2.220144	-1.066554
C	2.025102	-1.702221	1.329049
H	1.668555	3.929719	1.167335
H	1.160475	2.548821	2.154312
H	3.344783	2.069902	1.144392
H	2.737661	2.476151	-0.447636
H	2.437820	-2.189527	2.217137
H	2.517114	-2.190325	0.486649
H	0.067038	-1.618243	2.230510
H	0.413391	-3.115311	1.350473
H	-0.863509	3.060703	2.210599
H	-0.820871	4.474984	1.153781
H	-2.568204	3.302651	-0.319538
H	-3.072019	3.759523	1.281901
H	-2.583832	1.466134	2.127433
H	-3.935933	1.574901	0.996441
H	-2.443274	-0.192245	-1.702523
H	-3.946664	0.421823	-0.963750
H	-2.692715	1.531361	-1.572150
H	-2.198823	-0.578030	2.000309
H	-3.558625	-0.945875	0.925832
H	-2.107227	-2.052648	-0.660145
H	-1.813683	-2.743434	0.921749
H	1.248963	-2.092827	-1.248939
H	-0.010301	-3.290161	-0.955525
H	-0.365666	-1.852578	-1.925680
H	2.609852	-0.853475	-1.163171
H	2.413051	0.778766	-1.804056
H	3.835982	0.362897	-0.818238

H	0.957112	2.994983	-1.547901
H	-0.744044	3.379497	-1.470772
H	0.432186	4.504774	-0.749355
H	3.546854	-0.200290	1.486630
H	2.041366	0.212396	2.322771
O	-0.100737	0.782979	-1.669230
H	0.315113	0.047033	-2.125887

^{5}[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.129321	0.678750	0.192953
O	-0.182732	0.643135	1.845660
N	-2.325703	0.546540	0.253995
C	-2.879158	1.666575	1.073264
C	-2.518337	-0.741221	0.976114
C	-2.986873	0.517160	-1.068801
N	0.128980	2.854068	0.372468
C	1.391827	2.914911	1.161739
C	-0.991783	3.437697	1.168483
C	0.270986	3.583260	-0.907646
C	-2.397506	3.067901	0.686864
N	2.117139	0.638293	0.276398
C	2.498043	2.063151	0.549997
C	2.484050	-0.249422	1.421371
C	2.834651	0.223408	-0.953023
N	-0.263912	-1.583832	0.151057
C	-1.721430	-1.879223	0.350106
C	0.539174	-2.052920	1.325500
C	0.165823	-2.300870	-1.073415
C	2.036559	-1.713099	1.296612
H	1.747390	3.950093	1.219502
H	1.162036	2.575445	2.167333
H	3.367880	2.089989	1.212547
H	2.810682	2.501148	-0.395804
H	2.462991	-2.220302	2.167134
H	2.515717	-2.184747	0.437646
H	0.084645	-1.627055	2.216360
H	0.442158	-3.144310	1.381734
H	-0.870095	3.099045	2.196071
H	-0.879929	4.527907	1.161131
H	-2.512079	3.247896	-0.384348
H	-3.081576	3.769553	1.171098
H	-2.606706	1.473625	2.109247
H	-3.972271	1.626766	1.002218
H	-2.571418	-0.271839	-1.687491
H	-4.062745	0.353177	-0.942841
H	-2.822277	1.457404	-1.586990
H	-2.211039	-0.583562	2.005859
H	-3.578181	-1.019940	0.971385
H	-2.139358	-2.122801	-0.624800
H	-1.835192	-2.772034	0.971625
H	1.216663	-2.131644	-1.280837
H	0.007830	-3.378682	-0.957775
H	-0.417471	-1.960941	-1.927350
H	2.660270	-0.823898	-1.172890
H	2.479322	0.814119	-1.793098
H	3.912877	0.371317	-0.828107
H	1.035955	3.123372	-1.523642

H	-0.661398	3.541421	-1.463893
H	0.528860	4.629337	-0.710531
H	3.576546	-0.236853	1.524321
H	2.055315	0.188510	2.319522
O	-0.095400	0.842228	-1.678703
H	0.110771	0.032748	-2.156892

^{3}[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.120485	0.641148	0.284475
O	-0.165097	0.609621	1.926816
N	-2.220523	0.586554	0.286496
C	-2.856686	1.673267	1.090834
C	-2.498558	-0.705276	0.982672
C	-2.814349	0.579792	-1.076304
N	0.076666	2.729817	0.386628
C	1.350830	2.886647	1.150537
C	-1.000190	3.404593	1.172537
C	0.187727	3.381709	-0.945046
C	-2.420247	3.085266	0.730313
N	2.013625	0.629345	0.285279
C	2.445802	2.049925	0.535720
C	2.462541	-0.248183	1.414370
C	2.686228	0.216423	-0.978030
N	-0.251993	-1.488345	0.187650
C	-1.709526	-1.828573	0.355389
C	0.540132	-2.044442	1.332127
C	0.172029	-2.138287	-1.084157
C	2.034923	-1.714397	1.317081
H	1.652559	3.939068	1.159137
H	1.152556	2.574291	2.171477
H	3.328041	2.057547	1.179328
H	2.747348	2.475299	-0.418745
H	2.456612	-2.205366	2.198824
H	2.521713	-2.195404	0.468058
H	0.086555	-1.670081	2.245958
H	0.430117	-3.134460	1.313410
H	-0.877408	3.099793	2.210470
H	-0.823933	4.483476	1.114683
H	-2.578295	3.304467	-0.327044
H	-3.080313	3.767376	1.272179
H	-2.610697	1.484371	2.134234
H	-3.941308	1.576343	0.976710
H	-2.361553	-0.191193	-1.688165
H	-3.892304	0.409110	-0.999734
H	-2.632731	1.532364	-1.563414
H	-2.222257	-0.573581	2.024725
H	-3.567916	-0.933808	0.930394
H	-2.108758	-2.057409	-0.630124
H	-1.808290	-2.735676	0.955719
H	1.246537	-2.106644	-1.204770
H	-0.137101	-3.187327	-1.072646
H	-0.285943	-1.622144	-1.921746
H	2.565755	-0.842321	-1.161967
H	2.253059	0.762187	-1.810141
H	3.756120	0.430920	-0.902619
H	0.951250	2.901064	-1.544786
H	-0.752058	3.292803	-1.480578

H	0.431332	4.439418	-0.809338
H	3.557340	-0.212501	1.447101
H	2.078334	0.190942	2.331256
F	-0.093489	0.695948	-1.590039

^{5}[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.138002	0.660960	0.255312
O	-0.182021	0.629194	1.891742
N	-2.322360	0.553691	0.275208
C	-2.895068	1.679522	1.073336
C	-2.534200	-0.730830	0.999500
C	-2.942099	0.516510	-1.068754
N	0.117369	2.830596	0.382029
C	1.379015	2.920568	1.169686
C	-1.002249	3.443463	1.158495
C	0.257747	3.506324	-0.928195
C	-2.409651	3.077174	0.681569
N	2.095376	0.645616	0.285045
C	2.490491	2.064993	0.573573
C	2.493958	-0.262600	1.405659
C	2.765837	0.248534	-0.977776
N	-0.273375	-1.569471	0.182995
C	-1.729009	-1.873414	0.391241
C	0.553529	-2.077419	1.322136
C	0.132712	-2.216538	-1.089401
C	2.048432	-1.726540	1.273134
H	1.724069	3.959829	1.207979
H	1.151172	2.599436	2.182055
H	3.347211	2.078295	1.252169
H	2.825743	2.505806	-0.362956
H	2.492598	-2.240220	2.130823
H	2.515883	-2.185444	0.401347
H	0.114371	-1.687197	2.237323
H	0.464779	-3.170481	1.342773
H	-0.886839	3.129123	2.194746
H	-0.878629	4.531665	1.125065
H	-2.528911	3.256929	-0.388965
H	-3.088983	3.782089	1.167662
H	-2.642085	1.497098	2.116499
H	-3.986206	1.635070	0.982221
H	-2.491732	-0.262233	-1.675686
H	-4.017851	0.333582	-0.976426
H	-2.780992	1.462700	-1.577730
H	-2.246450	-0.569353	2.034534
H	-3.594764	-1.004379	0.975756
H	-2.147245	-2.135932	-0.578395
H	-1.833677	-2.755773	1.027975
H	1.199700	-2.121425	-1.252539
H	-0.117124	-3.282450	-1.063818
H	-0.381089	-1.738199	-1.918665
H	2.586294	-0.795761	-1.202908
H	2.373490	0.843797	-1.797783
H	3.846701	0.402628	-0.892292
H	1.032321	3.031477	-1.521534
H	-0.672107	3.433371	-1.485455
H	0.506954	4.561654	-0.776235
H	3.588473	-0.249151	1.477758

H	2.091600	0.162707	2.322244
F	-0.119385	0.725884	-1.600887

$^{3}[Fe^{IV}=O(TMC)(CF_3CO_2)]^{+}$

Fe	-0.145333	0.672253	0.212487
O	-0.169561	0.618120	1.836086
N	-2.258257	0.585339	0.300036
C	-2.859650	1.676766	1.128657
C	-2.490366	-0.706152	1.018792
C	-2.953783	0.554064	-1.014689
N	0.080183	2.767144	0.405189
C	1.349571	2.877132	1.189651
C	-1.005214	3.406010	1.212894
C	0.220486	3.516150	-0.873341
C	-2.420400	3.084943	0.756661
N	2.010257	0.657212	0.244325
C	2.442094	2.070117	0.535551
C	2.440119	-0.231929	1.375999
C	2.733071	0.253894	-0.994099
N	-0.276078	-1.479935	0.145364
C	-1.727681	-1.823373	0.352704
C	0.528052	-2.018332	1.293901
C	0.136188	-2.178029	-1.104153
C	2.020612	-1.695619	1.258895
H	1.652572	3.926754	1.251229
H	1.146460	2.518364	2.194026
H	3.329609	2.057695	1.171360
H	2.735404	2.527442	-0.406520
H	2.454556	-2.199204	2.127304
H	2.494375	-2.162500	0.395003
H	0.085006	-1.634750	2.208813
H	0.410773	-3.106949	1.288013
H	-0.880593	3.074470	2.242251
H	-0.837472	4.486722	1.186751
H	-2.563136	3.289967	-0.306058
H	-3.086733	3.773627	1.281610
H	-2.588011	1.483180	2.164609
H	-3.946904	1.587486	1.044860
H	-2.548842	-0.230890	-1.644459
H	-4.018039	0.364367	-0.852246
H	-2.824380	1.499844	-1.528053
H	-2.167899	-0.571851	2.046837
H	-3.559400	-0.939038	1.018384
H	-2.157713	-2.043780	-0.621722
H	-1.806760	-2.736123	0.946810
H	1.189881	-2.039602	-1.306487
H	-0.058323	-3.248662	-0.994230
H	-0.429117	-1.792279	-1.943470
H	2.531071	-0.776614	-1.253309
H	2.424471	0.883489	-1.819883
H	3.808544	0.367051	-0.831002
H	1.001171	3.081812	-1.488281
H	-0.707477	3.478731	-1.431977
H	0.478541	4.555223	-0.652648
O	-0.067929	0.681318	-1.838165
C	-0.462593	1.151335	-2.950767
O	-1.259115	2.044004	-3.202060

C	0.202295	0.427816	-4.174573
F	-0.176384	0.958905	-5.347001
F	1.552103	0.495455	-4.120724
F	-0.130826	-0.884405	-4.203855
H	3.533398	-0.189751	1.422553
H	2.045495	0.196924	2.293088

$^{5}[Fe^{IV}=O(TMC)(CF_3CO_2)]^{+}$

Fe	-0.163284	0.693047	0.163031
O	-0.195137	0.647831	1.786644
N	-2.357397	0.542366	0.270639
C	-2.891120	1.675432	1.092021
C	-2.520096	-0.740344	1.016593
C	-3.090844	0.479599	-1.017029
N	0.131578	2.864591	0.381755
C	1.387034	2.903655	1.188754
C	-0.999047	3.437656	1.179170
C	0.302908	3.649633	-0.865924
C	-2.400111	3.067437	0.685294
N	2.097992	0.658242	0.247535
C	2.492078	2.073586	0.552625
C	2.465153	-0.240876	1.388619
C	2.829894	0.248554	-0.977404
N	-0.285167	-1.568014	0.145685
C	-1.737265	-1.873312	0.369043
C	0.533259	-2.045936	1.306002
C	0.130302	-2.274918	-1.091659
C	2.027032	-1.703996	1.258403
H	1.735287	3.937808	1.279329
H	1.152045	2.536997	2.183607
H	3.363132	2.078108	1.212967
H	2.805264	2.534198	-0.382039
H	2.467550	-2.214239	2.119807
H	2.496360	-2.166257	0.389516
H	0.089776	-1.635299	2.209989
H	0.436628	-3.137102	1.350628
H	-0.880750	3.095744	2.206021
H	-0.886495	4.526581	1.177913
H	-2.498772	3.227016	-0.390831
H	-3.086524	3.780693	1.147886
H	-2.612014	1.487535	2.127181
H	-3.983820	1.641334	1.031831
H	-2.683599	-0.302109	-1.652310
H	-4.146755	0.265069	-0.826671
H	-3.000334	1.423892	-1.543340
H	-2.186785	-0.574115	2.036769
H	-3.578391	-1.019509	1.043995
H	-2.172805	-2.113642	-0.598807
H	-1.833602	-2.769301	0.987862
H	1.181707	-2.113604	-1.299110
H	-0.041764	-3.350480	-0.979613
H	-0.442001	-1.904705	-1.935663
H	2.604832	-0.778077	-1.241311
H	2.539419	0.883645	-1.808002
H	3.908488	0.337894	-0.811878
H	1.082221	3.216329	-1.486266
H	-0.620154	3.649326	-1.435754

H	0.580443	4.678095	-0.615692
O	-0.056316	0.669771	-1.830311
C	-0.496408	1.182579	-2.913592
O	-1.302516	2.078236	-3.092571
C	0.137615	0.502479	-4.174508
F	-0.302773	1.047751	-5.316745
F	1.485007	0.611562	-4.165956
F	-0.158876	-0.816524	-4.215972
H	3.557128	-0.221510	1.485616
H	2.043184	0.190949	2.293148

TS_H

$^{3\delta}TS_H$–[Fe^{IV}=O(TMC)(SR)]$^+$

Fe	-0.207662	0.665847	0.321103
O	-0.576976	0.590865	2.074948
C	0.302309	0.976997	4.395255
H	-0.061039	0.799489	3.147032
N	-2.581235	0.579583	0.291894
C	-3.081216	1.706118	1.117738
C	-2.731250	-0.733321	0.960329
C	-3.288539	0.580898	-1.000684
N	0.065126	2.751042	0.480642
C	1.293975	2.865345	1.331191
C	-1.083843	3.373425	1.229663
C	0.263427	3.492304	-0.791362
C	-2.495585	3.067881	0.719851
N	2.171403	0.631309	0.503942
C	2.476397	2.056228	0.809790
C	2.391210	-0.266292	1.668962
C	3.051569	0.223717	-0.612528
N	-0.361104	-1.432651	0.225244
C	-1.825425	-1.795015	0.333196
C	0.396388	-2.020478	1.383559
C	0.170509	-1.989201	-1.061379
C	1.900770	-1.711259	1.480219
H	1.595186	3.917056	1.391762
H	1.020498	2.546508	2.330450
H	3.291365	2.132175	1.539381
H	2.844036	2.512366	-0.107918
H	2.235329	-2.255132	2.369097
H	2.436901	-2.180566	0.654738
H	-0.109839	-1.682985	2.283368
H	0.289441	-3.109730	1.323149
H	-1.006696	3.045666	2.262841
H	-0.923686	4.456628	1.208976
H	-2.570204	3.227052	-0.358379
H	-3.139707	3.830172	1.167311
H	-2.829611	1.500575	2.155438
H	-4.175860	1.753142	1.039703
H	-2.935255	-0.221843	-1.640074
H	-4.367520	0.454074	-0.840661
H	-3.115978	1.516005	-1.527149
H	-2.489604	-0.603277	2.010142
H	-3.764127	-1.100034	0.886697
H	-2.178462	-2.018059	-0.670525
H	-1.916251	-2.720303	0.907192

H	2.908672	-0.822731	-0.861588
H	2.816229	0.810169	-1.497041
H	4.105750	0.370297	-0.344158
H	1.081723	3.061101	-1.360297
H	-0.637889	3.438763	-1.396293
H	0.489548	4.540540	-0.573892
H	3.467012	-0.306565	1.891940
H	1.903363	0.175132	2.531624
S	-0.105518	0.601502	-2.007330
C	-0.317435	-1.215038	-2.268375
H	0.269286	-1.504804	-3.140952
H	-1.360918	-1.428440	-2.499177
H	1.252887	-1.940345	-1.024404
H	-0.108884	-3.047310	-1.132791
H	1.275233	1.459651	4.401881
H	-0.497794	1.599095	4.786960
H	0.310332	-0.032991	4.795058

$^{3\pi}TS_{H}$–[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.121331	0.637922	0.272932
O	-0.247355	0.434835	2.068105
C	0.282028	1.521227	4.303351
H	0.065234	1.005775	3.003613
N	-2.282868	0.589848	0.376690
C	-2.807789	1.664131	1.272852
C	-2.520743	-0.730499	1.033791
C	-3.055895	0.646481	-0.892944
N	0.109066	2.730613	0.440412
C	1.389903	2.867826	1.198486
C	-0.955010	3.413492	1.246995
C	0.224208	3.445274	-0.859504
C	-2.390573	3.074573	0.873313
N	2.069693	0.603581	0.338225
C	2.488021	2.021993	0.600605
C	2.442506	-0.288635	1.486614
C	2.877787	0.179109	-0.843169
N	-0.277790	-1.464651	0.165661
C	-1.731464	-1.819312	0.340274
C	0.516856	-2.089606	1.276469
C	0.166210	-2.032279	-1.148338
C	2.010976	-1.750270	1.327284
H	1.706851	3.916474	1.205832
H	1.197139	2.575353	2.223017
H	3.362423	2.037076	1.256920
H	2.802321	2.448080	-0.349715
H	2.395556	-2.271830	2.208927
H	2.533920	-2.205026	0.485497
H	0.043741	-1.783692	2.204291
H	0.421177	-3.177093	1.179334
H	-0.798453	3.147233	2.288583
H	-0.793516	4.492694	1.158001
H	-2.593705	3.276042	-0.180001
H	-3.026367	3.767125	1.431330
H	-2.447569	1.453146	2.276396
H	-3.900383	1.588812	1.281256
H	-2.784785	-0.171565	-1.548630
H	-4.124144	0.580615	-0.663380

H	-2.854503	1.572804	-1.419682
H	-2.210999	-0.636468	2.068797
H	-3.587287	-0.977535	1.003269
H	-2.150779	-2.012110	-0.644188
H	-1.814852	-2.752098	0.902696
H	2.709429	-0.861283	-1.087617
H	2.606665	0.775926	-1.706443
H	3.939175	0.313089	-0.610952
H	0.992561	2.994333	-1.479490
H	-0.718743	3.390287	-1.396574
H	0.475782	4.494917	-0.680904
H	3.534410	-0.266355	1.582251
H	2.015309	0.129787	2.390416
S	-0.089387	0.574958	-2.057043
C	-0.349942	-1.231679	-2.329611
H	0.196362	-1.529705	-3.225195
H	-1.404912	-1.431722	-2.523038
H	1.249630	-2.044749	-1.165776
H	-0.167039	-3.075105	-1.209702
H	1.356006	1.647689	4.409231
H	-0.284584	2.444558	4.371026
H	-0.127819	0.704785	4.890726

$^{5\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.146106	0.677027	0.273380
O	-0.219206	0.639677	2.065167
C	-0.275292	0.598177	4.594134
H	-0.247621	0.610302	3.206184
N	-2.414908	0.575545	0.387310
C	-2.886881	1.699184	1.248727
C	-2.556452	-0.734063	1.084629
C	-3.204646	0.572812	-0.864156
N	0.141710	2.861022	0.459915
C	1.394944	2.924069	1.274052
C	-0.978976	3.466749	1.248607
C	0.305174	3.594439	-0.817052
C	-2.397276	3.086529	0.810916
N	2.173328	0.656222	0.396952
C	2.527250	2.080434	0.701132
C	2.477872	-0.254649	1.542885
C	2.989039	0.255365	-0.775883
N	-0.288887	-1.523700	0.203493
C	-1.744888	-1.840251	0.408434
C	0.532171	-2.079265	1.328361
C	0.158460	-2.078041	-1.106079
C	2.027293	-1.714225	1.358528
H	1.741076	3.962278	1.338789
H	1.142142	2.586196	2.273296
H	3.370867	2.115650	1.397818
H	2.874031	2.528614	-0.228264
H	2.425240	-2.251235	2.224996
H	2.539179	-2.156685	0.503463
H	0.058448	-1.750354	2.248982
H	0.462619	-3.173206	1.286216
H	-0.842042	3.166360	2.285122
H	-0.868838	4.555955	1.201205
H	-2.532912	3.233693	-0.263192

H	-3.061423	3.813395	1.285766
H	-2.547500	1.504170	2.263039
H	-3.983186	1.691158	1.254535
H	-2.893772	-0.236252	-1.515925
H	-4.268691	0.454288	-0.629828
H	-3.057795	1.503610	-1.404575
H	-2.226237	-0.597481	2.109145
H	-3.607688	-1.045118	1.100543
H	-2.174547	-2.060846	-0.566151
H	-1.837361	-2.753511	1.002239
H	2.810853	-0.780765	-1.040622
H	2.722315	0.866329	-1.633113
H	4.054463	0.378202	-0.548813
H	1.085992	3.139611	-1.420932
H	-0.622046	3.558466	-1.384920
H	0.564631	4.640429	-0.622608
H	3.565149	-0.261003	1.694532
H	2.017241	0.167116	2.430633
S	-0.105734	0.532464	-2.131751
C	-0.368333	-1.294827	-2.300245
H	0.156202	-1.635045	-3.193414
H	-1.428984	-1.486124	-2.467611
H	1.243702	-2.062523	-1.123844
H	-0.150904	-3.128456	-1.179334
H	0.622629	1.143017	4.869337
H	-1.205144	1.105425	4.832304
H	-0.258687	-0.459028	4.840306

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.122954	0.650037	0.261302
O	-0.156239	0.416251	2.057579
C	-0.100785	1.591996	4.303323
H	-0.119373	1.072328	2.989402
N	-2.413037	0.573798	0.413669
C	-2.834800	1.693197	1.300099
C	-2.539922	-0.740347	1.096255
C	-3.240688	0.594892	-0.811023
N	0.198855	2.764046	0.433133
C	1.483165	2.834958	1.200007
C	-0.885929	3.414927	1.243600
C	0.334347	3.499194	-0.849591
C	-2.327224	3.071532	0.856088
N	2.245263	0.583153	0.293216
C	2.603714	2.000843	0.590287
C	2.562289	-0.333347	1.427212
C	3.027332	0.183120	-0.899559
N	-0.271705	-1.494701	0.168274
C	-1.725033	-1.827040	0.394261
C	0.571567	-2.104017	1.252458
C	0.141426	-2.034006	-1.165905
C	2.076137	-1.780776	1.244154
H	1.819352	3.876695	1.250202
H	1.276179	2.505161	2.210543
H	3.466443	2.043475	1.264125
H	2.921128	2.457028	-0.345809
H	2.480713	-2.335484	2.096560
H	2.555261	-2.228582	0.372905

H	0.138912	-1.783762	2.195410
H	0.466106	-3.192820	1.175520
H	-0.726927	3.143136	2.283173
H	-0.744095	4.498221	1.168239
H	-2.497399	3.229198	-0.211166
H	-2.952723	3.813530	1.359449
H	-2.470485	1.477783	2.301916
H	-3.930573	1.712412	1.344940
H	-2.968762	-0.218574	-1.475675
H	-4.300100	0.496219	-0.546562
H	-3.092495	1.524869	-1.352829
H	-2.195888	-0.616935	2.117389
H	-3.587452	-1.064654	1.117095
H	-2.167525	-2.040795	-0.576000
H	-1.793159	-2.748543	0.977298
H	2.846418	-0.854526	-1.157565
H	2.735318	0.792270	-1.750568
H	4.100128	0.307801	-0.707591
H	1.094380	3.040558	-1.475142
H	-0.608557	3.476466	-1.390489
H	0.609552	4.540017	-0.652498
H	3.653014	-0.360634	1.557507
H	2.124396	0.085241	2.328242
S	-0.148591	0.587504	-2.039583
C	-0.416807	-1.221175	-2.317231
H	0.096968	-1.503486	-3.236747
H	-1.478940	-1.410395	-2.473807
H	1.224875	-2.018777	-1.212351
H	-0.173150	-3.082141	-1.240949
H	0.779596	2.222016	4.385406
H	-1.043185	2.118710	4.419324
H	-0.037974	0.662133	4.860652

$^{3\delta}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.258578	0.809600	0.183259
O	-0.346492	1.254095	1.910841
C	-1.395294	0.555116	4.085967
H	-0.897160	0.825844	2.904634
N	-2.519569	0.730384	0.032453
C	-3.105257	1.993102	0.556169
C	-2.791942	-0.403242	0.944961
C	-3.045038	0.450886	-1.317818
N	0.040895	2.963952	-0.024134
C	1.227205	3.214242	0.844671
C	-1.140208	3.700681	0.520488
C	0.310872	3.419694	-1.406046
C	-2.506224	3.276271	-0.031148
N	2.094675	0.850431	0.427825
C	2.414944	2.305696	0.523479
C	2.326469	0.138322	1.715347
C	2.948702	0.268600	-0.628473
N	-0.426135	-1.317710	0.522033
C	-1.894582	-1.616097	0.680350
C	0.345831	-1.652114	1.764716
C	0.072639	-2.160261	-0.596202
C	1.848702	-1.323364	1.756149
H	1.554877	4.254971	0.735956

H	0.907808	3.064513	1.871475
H	3.188223	2.476625	1.280870
H	2.847581	2.607134	-0.429025
H	2.225655	-1.726829	2.700746
H	2.355011	-1.908207	0.986714
H	-0.133303	-1.148857	2.596489
H	0.245930	-2.731117	1.934439
H	-1.136627	3.559809	1.599367
H	-0.990441	4.768763	0.321829
H	-2.499144	3.241378	-1.122750
H	-3.198982	4.083061	0.225351
H	-2.959934	2.003644	1.635630
H	-4.188067	1.986126	0.372213
H	-2.584330	-0.443339	-1.727444
H	-4.133713	0.315786	-1.283507
H	-2.809386	1.273358	-1.988576
H	-2.656334	-0.047182	1.959697
H	-3.833327	-0.739601	0.855649
H	-2.222245	-2.105291	-0.234372
H	-2.036690	-2.338129	1.488758
H	1.131414	-1.995424	-0.761912
H	-0.082799	-3.218046	-0.359756
H	-0.457625	-1.905208	-1.508006
H	2.750137	-0.791618	-0.757171
H	2.763550	0.769439	-1.578509
H	4.012262	0.386443	-0.384796
H	1.168811	2.899722	-1.820121
H	-0.541062	3.205107	-2.044122
H	0.507195	4.497973	-1.408892
H	3.404963	0.141380	1.928953
H	1.828286	0.705821	2.496685
O	-0.125722	0.575689	-1.623747
H	0.749979	0.306233	-1.922635
H	-0.522326	0.657923	4.725539
H	-2.137802	1.335136	4.229453
H	-1.810071	-0.448376	4.071678

$^{3\pi}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.226284	0.780138	0.186737
O	-0.330263	1.192116	1.947834
C	-1.543020	0.579639	4.098235
H	-0.932326	0.832353	2.844814
N	-2.330363	0.713776	0.031423
C	-3.012891	1.926594	0.578620
C	-2.692044	-0.445994	0.896140
C	-2.831745	0.478367	-1.349223
N	0.010007	2.899256	-0.007311
C	1.206489	3.178832	0.842994
C	-1.142302	3.659164	0.566314
C	0.251379	3.388917	-1.388463
C	-2.509560	3.255474	0.031556
N	1.924525	0.802634	0.425894
C	2.346637	2.245569	0.501007
C	2.241601	0.110362	1.718330
C	2.743925	0.191270	-0.655456
N	-0.380774	-1.333011	0.464726
C	-1.847554	-1.653696	0.561928

C	0.316649	-1.690154	1.742991
C	0.143852	-2.198793	-0.628847
C	1.810585	-1.356410	1.798337
H	1.531006	4.215776	0.703548
H	0.900840	3.039590	1.874059
H	3.146963	2.359363	1.236439
H	2.770680	2.514698	-0.464151
H	2.156458	-1.714283	2.772316
H	2.359843	-1.955187	1.070167
H	-0.202284	-1.187428	2.551563
H	0.204888	-2.770321	1.892659
H	-1.124477	3.499404	1.641714
H	-0.968386	4.723551	0.375451
H	-2.543555	3.282467	-1.059546
H	-3.217487	4.019350	0.364430
H	-2.876775	1.920189	1.657827
H	-4.084477	1.824339	0.375951
H	-2.353950	-0.389553	-1.786856
H	-3.916226	0.332642	-1.317002
H	-2.597119	1.329486	-1.979892
H	-2.545873	-0.145310	1.926578
H	-3.750399	-0.696864	0.766144
H	-2.156845	-2.061302	-0.397478
H	-2.008453	-2.438708	1.305347
H	1.223738	-2.152942	-0.683816
H	-0.143439	-3.236818	-0.435010
H	-0.259773	-1.861806	-1.577005
H	2.518407	-0.859309	-0.778326
H	2.552042	0.690127	-1.600466
H	3.805983	0.296138	-0.411761
H	1.156630	2.953234	-1.802668
H	-0.581652	3.127300	-2.034007
H	0.373623	4.476338	-1.378957
H	3.327815	0.153769	1.860362
H	1.763739	0.680045	2.508959
O	-0.076787	0.486604	-1.653605
H	0.561541	1.048227	-2.101822
H	-0.752181	0.912916	4.764400
H	-2.423422	1.215909	4.105359
H	-1.762725	-0.481862	4.170025

$^{5\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.136523	0.673295	0.257339
O	-0.213276	0.639882	2.055530
C	-0.236064	0.581730	4.583002
H	-0.219502	0.608976	3.195138
N	-2.362874	0.535891	0.344650
C	-2.905816	1.666136	1.154691
C	-2.541330	-0.752056	1.071578
C	-3.034852	0.494620	-0.971327
N	0.131310	2.872527	0.473305
C	1.387351	2.920219	1.276110
C	-1.003742	3.445012	1.256287
C	0.291488	3.616098	-0.795686
C	-2.404008	3.061584	0.759388
N	2.132870	0.644649	0.374064
C	2.503627	2.067893	0.676139

C	2.497643	-0.268656	1.498718
C	2.855333	0.251956	-0.859010
N	-0.278046	-1.604505	0.237648
C	-1.736394	-1.893291	0.452968
C	0.545617	-2.083552	1.391969
C	0.135942	-2.306595	-1.000068
C	2.042043	-1.730175	1.348723
H	1.749723	3.953172	1.345763
H	1.144459	2.574914	2.275468
H	3.360806	2.090243	1.355891
H	2.835538	2.517611	-0.257756
H	2.484145	-2.256651	2.200083
H	2.509170	-2.181311	0.472338
H	0.098462	-1.678357	2.294629
H	0.464091	-3.177450	1.432468
H	-0.890659	3.109653	2.285209
H	-0.907925	4.537255	1.248394
H	-2.498622	3.224647	-0.316827
H	-3.095025	3.773423	1.218613
H	-2.641122	1.477632	2.192930
H	-3.999743	1.645996	1.078952
H	-2.609712	-0.287603	-1.592643
H	-4.108246	0.314741	-0.840498
H	-2.888250	1.436988	-1.492070
H	-2.233961	-0.587274	2.098947
H	-3.598551	-1.044074	1.069078
H	-2.160092	-2.147851	-0.516858
H	-1.848439	-2.780150	1.083975
H	1.183656	-2.128057	-1.219440
H	-0.014245	-3.387262	-0.897018
H	-0.457987	-1.953969	-1.840846
H	2.660209	-0.785206	-1.110765
H	2.519552	0.871731	-1.686353
H	3.936029	0.374383	-0.723744
H	1.062479	3.159361	-1.407363
H	-0.634254	3.582327	-1.364164
H	0.550831	4.660482	-0.588088
H	3.591187	-0.269519	1.597224
H	2.078539	0.155432	2.406526
O	-0.108468	0.830727	-1.644634
H	0.178320	0.081946	-2.175735
H	-0.789385	1.478294	4.845841
H	-0.746139	-0.348014	4.816277
H	0.813989	0.602212	4.858327

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.252551	0.791981	0.166212
O	-0.433129	1.251617	1.893914
C	-1.359883	0.444149	4.120143
H	-0.884119	0.767616	2.813772
N	-2.461076	0.697370	-0.009387
C	-3.078775	1.950876	0.513645
C	-2.754739	-0.443581	0.896167
C	-2.968672	0.419978	-1.371308
N	0.039856	2.983135	-0.043595
C	1.207412	3.213636	0.856161
C	-1.158451	3.700706	0.494055

C	0.335563	3.483934	-1.404403
C	-2.509949	3.248946	-0.068934
N	2.008932	0.822084	0.467949
C	2.373208	2.272484	0.561334
C	2.250265	0.113272	1.760393
C	2.840405	0.223025	-0.602040
N	-0.408752	-1.389153	0.489563
C	-1.881499	-1.665140	0.609846
C	0.315112	-1.715721	1.758400
C	0.104719	-2.244901	-0.610020
C	1.809497	-1.358605	1.802181
H	1.563933	4.244668	0.749614
H	0.857759	3.069786	1.872468
H	3.135954	2.416568	1.332592
H	2.834415	2.552475	-0.384128
H	2.164606	-1.740351	2.763865
H	2.356181	-1.937906	1.056740
H	-0.202709	-1.216709	2.570324
H	0.226611	-2.795968	1.929382
H	-1.161179	3.556282	1.571588
H	-1.025567	4.770463	0.295248
H	-2.498053	3.220681	-1.161005
H	-3.223754	4.036362	0.188510
H	-2.938644	1.960801	1.592883
H	-4.157083	1.909891	0.317441
H	-2.481882	-0.455661	-1.788011
H	-4.052610	0.259616	-1.339009
H	-2.749585	1.256668	-2.028918
H	-2.608765	-0.099136	1.913583
H	-3.802993	-0.749676	0.796773
H	-2.200609	-2.117606	-0.326407
H	-2.055594	-2.409383	1.392151
H	1.178939	-2.141767	-0.711257
H	-0.126044	-3.295345	-0.401896
H	-0.348989	-1.940235	-1.547539
H	2.623949	-0.832340	-0.720961
H	2.630611	0.712431	-1.549157
H	3.904785	0.336398	-0.364948
H	1.227493	3.008389	-1.807940
H	-0.499210	3.283288	-2.072848
H	0.511439	4.564649	-1.380270
H	3.327016	0.144740	1.972676
H	1.735558	0.675059	2.535236
O	-0.056276	0.469329	-1.650905
H	0.317372	1.208015	-2.142004
H	-0.437661	0.442320	4.694244
H	-2.012585	1.287435	4.324882
H	-1.865769	-0.515770	4.082465

$^{3\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.140448	0.647361	0.358741
O	-0.246978	0.654706	2.172248
C	-0.298323	0.720365	4.742642
H	-0.268066	0.679492	3.258555
N	-2.270970	0.589918	0.332254
C	-2.904693	1.700024	1.102150
C	-2.549002	-0.691731	1.047628

C	-2.839421	0.556075	-1.039015
N	0.068324	2.771482	0.453942
C	1.324888	2.914981	1.248639
C	-1.035083	3.442271	1.200815
C	0.219126	3.408785	-0.878799
C	-2.442412	3.102539	0.723846
N	2.016205	0.641871	0.408557
C	2.435254	2.065347	0.671769
C	2.436276	-0.244698	1.540632
C	2.705047	0.228656	-0.843913
N	-0.286642	-1.507616	0.291447
C	-1.749142	-1.831618	0.456510
C	0.504664	-2.045564	1.443629
C	0.145187	-2.165145	-0.971669
C	2.000305	-1.709777	1.431704
H	1.640282	3.964356	1.260451
H	1.095679	2.607643	2.263312
H	3.295027	2.075865	1.345704
H	2.771009	2.486160	-0.273328
H	2.420542	-2.206782	2.310968
H	2.488692	-2.186763	0.581340
H	0.045017	-1.662804	2.349721
H	0.403137	-3.137109	1.435583
H	-0.937064	3.152340	2.244918
H	-0.874609	4.523800	1.131930
H	-2.565984	3.295829	-0.343417
H	-3.118880	3.799368	1.225472
H	-2.682230	1.527109	2.152844
H	-3.989053	1.621664	0.966173
H	-2.370485	-0.223071	-1.628317
H	-3.918639	0.381083	-0.981632
H	-2.652268	1.500650	-1.539917
H	-2.283726	-0.537699	2.088245
H	-3.616946	-0.928259	0.985231
H	-2.138489	-2.086929	-0.526577
H	-1.859682	-2.721676	1.080661
H	1.218448	-2.106007	-1.098688
H	-0.138067	-3.221930	-0.946458
H	-0.327441	-1.670166	-1.813952
H	2.558112	-0.824436	-1.044096
H	2.302068	0.794211	-1.678062
H	3.779150	0.413850	-0.745400
H	0.991585	2.912824	-1.454621
H	-0.707979	3.323476	-1.437106
H	0.471199	4.466225	-0.750212
H	3.531224	-0.220895	1.591384
H	2.040056	0.194521	2.450983
F	-0.080677	0.687691	-1.573151
H	0.598926	1.281722	4.982195
H	-1.233504	1.232210	4.944058
H	-0.275308	-0.329069	5.016822

$^{3\pi}$TS$_{H}$–[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.085225	0.657632	0.373969
O	-0.246755	0.541108	2.147676
C	0.753608	1.462629	4.302165
H	0.283510	1.019698	3.027102

N	-2.199835	0.594222	0.392180
C	-2.826378	1.703083	1.172463
C	-2.487468	-0.681137	1.111925
C	-2.801629	0.560656	-0.965387
N	0.118411	2.738639	0.428787
C	1.403493	2.939680	1.157580
C	-0.957254	3.435957	1.200452
C	0.208392	3.351518	-0.923690
C	-2.380728	3.103599	0.774439
N	2.034326	0.648440	0.338408
C	2.494897	2.061774	0.588020
C	2.522303	-0.257404	1.430700
C	2.662106	0.241230	-0.951634
N	-0.246223	-1.484301	0.296267
C	-1.698293	-1.823619	0.515017
C	0.589627	-2.051814	1.403251
C	0.127755	-2.135629	-0.990643
C	2.083262	-1.720851	1.327722
H	1.710529	3.989129	1.094406
H	1.226128	2.709956	2.201486
H	3.357193	2.059062	1.258021
H	2.836609	2.469188	-0.360493
H	2.543597	-2.225716	2.182212
H	2.533036	-2.187442	0.450995
H	0.174384	-1.682232	2.336183
H	0.481079	-3.142255	1.380426
H	-0.832942	3.166677	2.247246
H	-0.784389	4.513383	1.109615
H	-2.541418	3.295841	-0.287821
H	-3.035455	3.803994	1.299567
H	-2.576286	1.537706	2.218338
H	-3.913009	1.615187	1.065259
H	-2.361463	-0.231640	-1.559154
H	-3.881735	0.404234	-0.880931
H	-2.612168	1.496996	-1.480461
H	-2.213316	-0.528866	2.150465
H	-3.557530	-0.909058	1.056166
H	-2.119169	-2.099138	-0.449479
H	-1.778202	-2.704125	1.156547
H	1.194731	-2.088641	-1.163184
H	-0.164326	-3.189609	-0.961577
H	-0.374342	-1.631057	-1.809535
H	2.482881	-0.803429	-1.164446
H	2.240999	0.829958	-1.759634
H	3.742719	0.401106	-0.892163
H	0.990753	2.878414	-1.505336
H	-0.725070	3.213547	-1.459018
H	0.417715	4.420555	-0.820917
H	3.617963	-0.230833	1.418935
H	2.190854	0.162307	2.374591
F	-0.100733	0.676292	-1.492370
H	1.826217	1.617271	4.232553
H	0.182898	2.365888	4.497564
H	0.463262	0.611014	4.910416

$^{5\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.137976	0.650427	0.343112

O	-0.215251	0.619409	2.123295
C	-0.245410	0.624027	4.645758
H	-0.231238	0.619932	3.272320
N	-2.349777	0.539701	0.353690
C	-2.916448	1.671680	1.145527
C	-2.557083	-0.747790	1.075532
C	-2.971385	0.499446	-0.988121
N	0.123830	2.846135	0.491817
C	1.377866	2.920667	1.294490
C	-1.011310	3.445119	1.254579
C	0.285011	3.539960	-0.805403
C	-2.411798	3.066936	0.756761
N	2.110648	0.646080	0.387140
C	2.498079	2.062495	0.710036
C	2.506984	-0.291387	1.484062
C	2.787586	0.276857	-0.880258
N	-0.284879	-1.590641	0.255820
C	-1.741701	-1.892423	0.475969
C	0.558113	-2.112197	1.376769
C	0.110440	-2.223824	-1.026604
C	2.052734	-1.751825	1.319113
H	1.732330	3.957099	1.345965
H	1.135937	2.593008	2.300357
H	3.339836	2.065576	1.407762
H	2.856261	2.516629	-0.211699
H	2.508502	-2.288272	2.156829
H	2.509460	-2.187757	0.430065
H	0.125222	-1.741626	2.301875
H	0.480305	-3.206689	1.379681
H	-0.907484	3.129563	2.291158
H	-0.903999	4.535770	1.225978
H	-2.508953	3.237581	-0.317817
H	-3.100262	3.777236	1.222001
H	-2.675709	1.487705	2.190779
H	-4.007884	1.645762	1.044510
H	-2.520393	-0.280467	-1.593749
H	-4.048063	0.316478	-0.898323
H	-2.809593	1.444195	-1.500129
H	-2.275421	-0.584869	2.110927
H	-3.615750	-1.031249	1.045724
H	-2.162354	-2.166900	-0.489509
H	-1.843857	-2.768836	1.121748
H	1.171610	-2.099152	-1.210707
H	-0.112245	-3.296272	-1.003789
H	-0.429554	-1.753176	-1.843515
H	2.592653	-0.758019	-1.136985
H	2.409308	0.899688	-1.686413
H	3.870579	0.411789	-0.784436
H	1.067026	3.070271	-1.393697
H	-0.636412	3.475581	-1.378069
H	0.534574	4.593806	-0.639269
H	3.602207	-0.290214	1.553030
H	2.111824	0.114945	2.411116
F	-0.117909	0.739972	-1.554175
H	0.668267	1.149265	4.907000
H	-1.160022	1.157571	4.885701
H	-0.253346	-0.429644	4.906759

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.102874	0.691440	0.363138
O	-0.304958	0.653037	2.123398
C	0.871080	1.271237	4.289354
H	0.344690	0.971648	2.990754
N	-2.275513	0.580496	0.373990
C	-2.861537	1.732204	1.126270
C	-2.516311	-0.682184	1.128279
C	-2.880387	0.505724	-0.975292
N	0.135668	2.892274	0.400551
C	1.400240	3.015600	1.168834
C	-0.988168	3.530760	1.145571
C	0.273837	3.508123	-0.937235
C	-2.389817	3.121008	0.683685
N	2.078220	0.677810	0.364064
C	2.504683	2.095010	0.646332
C	2.540380	-0.258166	1.440103
C	2.688580	0.286252	-0.934473
N	-0.269160	-1.582685	0.313872
C	-1.721040	-1.860161	0.568001
C	0.591301	-2.073031	1.431363
C	0.091159	-2.258914	-0.955083
C	2.083563	-1.720392	1.317698
H	1.774060	4.045815	1.130185
H	1.174051	2.790565	2.205351
H	3.327745	2.095446	1.364580
H	2.900828	2.503785	-0.280457
H	2.569914	-2.238239	2.149860
H	2.511276	-2.172009	0.422398
H	0.184311	-1.665168	2.353371
H	0.508939	-3.166633	1.478790
H	-0.874851	3.269003	2.196330
H	-0.883538	4.619096	1.061692
H	-2.507743	3.257810	-0.393400
H	-3.081298	3.834479	1.139654
H	-2.611414	1.590728	2.175481
H	-3.951897	1.675799	1.028629
H	-2.435812	-0.301007	-1.548225
H	-3.959946	0.341709	-0.887764
H	-2.700162	1.429383	-1.517644
H	-2.239991	-0.494362	2.160371
H	-3.581058	-0.940165	1.093156
H	-2.160695	-2.174061	-0.376819
H	-1.823870	-2.705182	1.254757
H	1.152835	-2.173999	-1.157111
H	-0.162131	-3.324022	-0.903926
H	-0.445375	-1.794049	-1.777971
H	2.445932	-0.739670	-1.182574
H	2.302194	0.922204	-1.724706
H	3.777525	0.384573	-0.875532
H	1.064567	3.021328	-1.499837
H	-0.647781	3.389866	-1.500459
H	0.502368	4.575186	-0.836854
H	3.637192	-0.251984	1.441383
H	2.213959	0.148939	2.391373
F	-0.118671	0.686999	-1.487158

H	1.864032	1.690745	4.163579
H	0.126860	1.967910	4.662685
H	0.847909	0.290865	4.754878

$^{3\sigma}TS_{H}$–[Fe^{IV}=O(TMC)(CF_3CO_2)]$^+$

Fe	-0.157595	0.673238	0.340495
O	-0.225740	0.646907	2.134804
C	-0.272202	0.633517	4.674544
H	-0.245689	0.642376	3.247696
N	-2.295222	0.589222	0.374431
C	-2.899715	1.692568	1.181160
C	-2.534249	-0.702137	1.091061
C	-2.953968	0.555114	-0.957280
N	0.066185	2.795843	0.490356
C	1.332155	2.911158	1.279442
C	-1.034206	3.434558	1.273802
C	0.213076	3.514497	-0.802844
C	-2.443729	3.096867	0.803129
N	2.008289	0.672328	0.351241
C	2.432507	2.088597	0.650928
C	2.439262	-0.232053	1.469987
C	2.719668	0.279502	-0.896656
N	-0.296673	-1.487344	0.244072
C	-1.752352	-1.825480	0.450416
C	0.519149	-2.028967	1.382329
C	0.113886	-2.170119	-1.014131
C	2.011730	-1.695075	1.341519
H	1.642707	3.960248	1.324994
H	1.119283	2.568311	2.285827
H	3.306035	2.076672	1.306187
H	2.748829	2.540371	-0.286362
H	2.452221	-2.206824	2.202031
H	2.481600	-2.153795	0.471280
H	0.076886	-1.656656	2.300626
H	0.414178	-3.119174	1.365650
H	-0.919766	3.118266	2.308210
H	-0.880795	4.517651	1.232904
H	-2.571734	3.291176	-0.263578
H	-3.118032	3.791646	1.309862
H	-2.647734	1.505997	2.222496
H	-3.986983	1.617406	1.077222
H	-2.546430	-0.245424	-1.565402
H	-4.026985	0.389804	-0.823989
H	-2.789811	1.490320	-1.481303
H	-2.232405	-0.560377	2.122862
H	-3.601898	-0.943628	1.067284
H	-2.172234	-2.065179	-0.523872
H	-1.834437	-2.728093	1.059812
H	1.169449	-2.034000	-1.210441
H	-0.086374	-3.241648	-0.921338
H	-0.444309	-1.765753	-1.849754
H	2.521812	-0.752380	-1.155207
H	2.392363	0.906880	-1.717554
H	3.796681	0.400560	-0.747843
H	1.012375	3.079668	-1.393269
H	-0.702912	3.442891	-1.378929
H	0.446020	4.564917	-0.605985

O	-0.092563	0.702562	-1.843065
C	-0.461840	1.151816	-2.965611
O	-1.249889	2.049575	-3.245747
C	0.216446	0.407499	-4.170606
F	-0.155968	0.902220	-5.362701
F	1.566689	0.491074	-4.108532
F	-0.099657	-0.910453	-4.171994
H	3.533620	-0.199932	1.508639
H	2.052796	0.191770	2.391199
H	0.780033	0.638963	4.939020
H	-0.811944	1.546002	4.905729
H	-0.800945	-0.287099	4.898554

$^{3\pi}TS_{H}$–[Fe^{IV}=O(TMC)(CF_3CO_2)]$^+$

Fe	-0.063219	0.719480	0.257308
O	-0.157053	0.591674	2.017063
C	0.795135	1.447946	4.202650
H	0.380871	1.056156	2.912026
N	-2.188691	0.623859	0.412014
C	-2.758791	1.740508	1.227943
C	-2.415318	-0.650632	1.160548
C	-2.923683	0.566139	-0.879090
N	0.172341	2.806311	0.383051
C	1.471844	2.968359	1.101201
C	-0.892353	3.475286	1.198241
C	0.260621	3.508100	-0.927138
C	-2.322239	3.135358	0.800212
N	2.076732	0.705948	0.203030
C	2.543908	2.114082	0.468074
C	2.572367	-0.202744	1.293286
C	2.724875	0.298622	-1.076846
N	-0.221567	-1.447477	0.224188
C	-1.661654	-1.787415	0.511805
C	0.649789	-1.990642	1.319839
C	0.115435	-2.155887	-1.042645
C	2.137832	-1.664533	1.191619
H	1.779968	4.018293	1.075233
H	1.317691	2.698946	2.138256
H	3.431504	2.096926	1.103613
H	2.847980	2.545661	-0.482472
H	2.628043	-2.175210	2.025614
H	2.555841	-2.123229	0.295416
H	0.263342	-1.608786	2.259414
H	0.537029	-3.080103	1.317788
H	-0.738989	3.190824	2.236604
H	-0.731191	4.554981	1.123261
H	-2.498543	3.308603	-0.263130
H	-2.969151	3.843795	1.323688
H	-2.455752	1.574037	2.259219
H	-3.849494	1.661152	1.180521
H	-2.549257	-0.243884	-1.496402
H	-3.986071	0.396940	-0.682214
H	-2.797569	1.493312	-1.426392
H	-2.079448	-0.494525	2.179319
H	-3.484861	-0.884128	1.174186
H	-2.130572	-2.053497	-0.432817
H	-1.709531	-2.674272	1.147317

H	1.152408	-2.010948	-1.315170
H	-0.061702	-3.227475	-0.912211
H	-0.506869	-1.785841	-1.848545
H	2.468039	-0.716920	-1.345117
H	2.402257	0.954409	-1.875949
H	3.810640	0.368159	-0.964571
H	1.034681	3.065524	-1.545323
H	-0.679843	3.431399	-1.459751
H	0.503457	4.559828	-0.753049
O	-0.087825	0.669824	-1.783415
C	-0.508654	1.099923	-2.899438
O	-1.301556	1.994039	-3.165046
C	0.081358	0.304559	-4.117833
F	-0.124901	0.938361	-5.283536
F	1.409324	0.092923	-4.007835
F	-0.509181	-0.913378	-4.215335
H	3.666871	-0.170683	1.267786
H	2.253999	0.214103	2.242359
H	1.868815	1.604131	4.162218
H	0.214065	2.343542	4.399868
H	0.486059	0.575262	4.769571

$^{5\sigma}TS_{H}$–$[Fe^{IV}=O(TMC)(CF_3CO_2)]^+$

Fe	-0.155459	0.674535	0.292432
O	-0.211360	0.636760	2.056115
C	-0.259195	0.627513	4.572756
H	-0.237504	0.632960	3.221995
N	-2.371745	0.528239	0.360282
C	-2.905677	1.666869	1.171860
C	-2.540084	-0.758813	1.098617
C	-3.091133	0.468931	-0.933672
N	0.137641	2.870032	0.482472
C	1.394475	2.911676	1.287986
C	-1.001538	3.440802	1.267272
C	0.310451	3.646937	-0.768328
C	-2.399433	3.056871	0.765485
N	2.106026	0.655016	0.335197
C	2.501185	2.068950	0.663912
C	2.495225	-0.273066	1.446566
C	2.822416	0.273387	-0.908304
N	-0.288148	-1.582654	0.223543
C	-1.741077	-1.891858	0.463226
C	0.554605	-2.086612	1.356422
C	0.107383	-2.268053	-1.032998
C	2.047548	-1.733475	1.292272
H	1.752003	3.944319	1.368506
H	1.158419	2.556318	2.285326
H	3.362026	2.062958	1.337633
H	2.833297	2.534371	-0.261792
H	2.504897	-2.263789	2.132826
H	2.501738	-2.175170	0.404954
H	0.122098	-1.705103	2.276793
H	0.470158	-3.179794	1.372644
H	-0.888387	3.109360	2.297524
H	-0.903628	4.531650	1.257685
H	-2.486116	3.208392	-0.313022
H	-3.091108	3.774276	1.213971

H	-2.641059	1.480543	2.210486
H	-3.998503	1.647860	1.099186
H	-2.690889	-0.326041	-1.557221
H	-4.154645	0.277670	-0.757911
H	-2.974272	1.405871	-1.469191
H	-2.223384	-0.594561	2.123085
H	-3.596813	-1.047828	1.108454
H	-2.178527	-2.148215	-0.499641
H	-1.828895	-2.781119	1.093027
H	1.155375	-2.100103	-1.254181
H	-0.060446	-3.346268	-0.939674
H	-0.477757	-1.882059	-1.861066
H	2.597484	-0.749591	-1.187658
H	2.513461	0.921156	-1.722550
H	3.903591	0.364627	-0.760263
H	1.105107	3.221346	-1.374832
H	-0.604006	3.622823	-1.352543
H	0.565475	4.684110	-0.527663
O	-0.099601	0.718693	-1.779311
C	-0.513755	1.206070	-2.877488
O	-1.312189	2.106301	-3.090161
C	0.128159	0.499666	-4.121091
F	-0.283651	1.032356	-5.281896
F	1.477938	0.585568	-4.095244
F	-0.188284	-0.816344	-4.149859
H	3.589499	-0.264908	1.518690
H	2.097772	0.141160	2.368767
H	0.640782	1.173356	4.838737
H	-1.188303	1.137391	4.807831
H	-0.242939	-0.428579	4.822816

$^{5\pi}TS_{H}$–[Fe^{IV}=O(TMC)(CF_3CO_2)]$^+$

Fe	-0.081428	0.757750	0.223785
O	-0.230696	0.730108	1.980154
C	0.902408	1.215783	4.179885
H	0.435505	0.993504	2.859925
N	-2.257223	0.602134	0.381203
C	-2.790583	1.767422	1.159381
C	-2.434406	-0.655612	1.167795
C	-3.000059	0.496104	-0.898471
N	0.199678	2.971907	0.333942
C	1.475272	3.040810	1.096129
C	-0.918515	3.568549	1.127912
C	0.342865	3.707428	-0.944465
C	-2.323456	3.147705	0.683163
N	2.121202	0.725695	0.224706
C	2.555205	2.141590	0.501327
C	2.586913	-0.194278	1.315726
C	2.760633	0.313986	-1.054290
N	-0.233220	-1.552012	0.249926
C	-1.674856	-1.827857	0.555054
C	0.646190	-2.001193	1.372107
C	0.107439	-2.301640	-0.983199
C	2.133984	-1.656487	1.220472
H	1.857078	4.068118	1.103180
H	1.266017	2.767733	2.123772
H	3.418434	2.136539	1.170854

H	2.894894	2.565197	-0.441062
H	2.638931	-2.163399	2.048022
H	2.541347	-2.118450	0.321060
H	0.254402	-1.566361	2.287992
H	0.560973	-3.091897	1.455654
H	-0.776320	3.281670	2.167904
H	-0.831536	4.659225	1.071640
H	-2.443920	3.257699	-0.397024
H	-3.014009	3.869917	1.125896
H	-2.495731	1.627858	2.196539
H	-3.883733	1.721083	1.112051
H	-2.605763	-0.315412	-1.503134
H	-4.056428	0.298880	-0.691618
H	-2.907471	1.417497	-1.463371
H	-2.093157	-0.460816	2.178164
H	-3.497732	-0.916125	1.204860
H	-2.153098	-2.122219	-0.377259
H	-1.755176	-2.685172	1.229689
H	1.148052	-2.159977	-1.252622
H	-0.068457	-3.373048	-0.834858
H	-0.504837	-1.950209	-1.807927
H	2.469985	-0.693171	-1.327337
H	2.453558	0.981298	-1.851526
H	3.849428	0.351816	-0.947869
H	1.119178	3.257250	-1.558033
H	-0.586205	3.671499	-1.503267
H	0.612278	4.749713	-0.743508
O	-0.069517	0.652276	-1.768578
C	-0.519037	1.131857	-2.858559
O	-1.284528	2.059846	-3.064424
C	0.012455	0.345812	-4.106746
F	-0.254457	0.987311	-5.254718
F	1.345573	0.146237	-4.057360
F	-0.573268	-0.874281	-4.181478
H	3.683085	-0.183658	1.306110
H	2.272339	0.227912	2.263514
H	1.890093	1.656910	4.095328
H	0.132610	1.878688	4.561077
H	0.880412	0.208031	4.580884

IN

$^{3\delta}$I−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.255839	0.679478	0.232953
O	-0.583238	0.697482	2.049438
C	0.734082	0.811700	5.321142
H	0.125383	0.532035	2.677031
N	-2.613451	0.591613	0.206466
C	-3.114533	1.733780	1.011196
C	-2.760498	-0.702867	0.909381
C	-3.326202	0.562561	-1.083491
N	0.027864	2.780269	0.392617
C	1.231086	2.898953	1.277690
C	-1.135701	3.413692	1.108802
C	0.261002	3.507061	-0.881230
C	-2.536033	3.088872	0.581156
N	2.136799	0.660275	0.500001

C	2.430252	2.090700	0.794354
C	2.364538	-0.227771	1.669797
C	3.025727	0.244323	-0.607749
N	-0.394677	-1.419439	0.201240
C	-1.859205	-1.779613	0.302255
C	0.347835	-1.979824	1.383405
C	0.154871	-2.002603	-1.066422
C	1.851766	-1.668704	1.503873
H	1.529150	3.951016	1.345845
H	0.926309	2.578868	2.269316
H	3.227610	2.179009	1.541467
H	2.817509	2.536874	-0.119994
H	2.170292	-2.203204	2.404095
H	2.396756	-2.152475	0.692916
H	-0.181648	-1.641123	2.270053
H	0.249630	-3.070539	1.340535
H	-1.075692	3.100168	2.147824
H	-0.978754	4.496968	1.071842
H	-2.592057	3.215025	-0.502720
H	-3.192780	3.859438	0.994782
H	-2.853768	1.551325	2.051242
H	-4.210045	1.771922	0.940918
H	-2.972160	-0.253115	-1.706509
H	-4.404685	0.437212	-0.919749
H	-3.156476	1.486653	-1.630381
H	-2.507767	-0.546383	1.952896
H	-3.794363	-1.069743	0.855031
H	-2.204893	-2.014908	-0.701194
H	-1.956475	-2.696425	0.888633
H	2.886886	-0.805238	-0.846778
H	2.792680	0.820633	-1.499167
H	4.077532	0.397299	-0.334595
H	1.087772	3.063532	-1.428373
H	-0.627875	3.453702	-1.504866
H	0.490574	4.556497	-0.672533
H	3.443554	-0.286091	1.871188
H	1.930723	0.239329	2.554475
S	-0.091483	0.573483	-2.065788
C	-0.312461	-1.248512	-2.293885
H	0.283115	-1.557647	-3.153461
H	-1.354950	-1.456631	-2.532801
H	1.236993	-1.956933	-1.014010
H	-0.127928	-3.060570	-1.122740
H	1.567526	0.155312	5.524848
H	0.891153	1.879030	5.263139
H	-0.267883	0.412058	5.267965

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.124578	0.573509	0.190467
O	-0.206629	0.397981	2.055372
C	0.269219	2.207234	5.237854
H	0.018969	1.171012	2.579135
N	-2.273657	0.539575	0.333608
C	-2.790878	1.595934	1.257849
C	-2.505800	-0.790016	0.974040
C	-3.062484	0.621653	-0.925319
N	0.118808	2.679544	0.442661

C	1.413829	2.800362	1.178422
C	-0.934158	3.345980	1.275736
C	0.217033	3.426095	-0.841222
C	-2.371646	3.016904	0.899951
N	2.069993	0.541564	0.267386
C	2.494538	1.953708	0.548825
C	2.442534	-0.364602	1.405359
C	2.878129	0.131487	-0.919036
N	-0.283616	-1.511152	0.071877
C	-1.735488	-1.867762	0.245806
C	0.507614	-2.146136	1.179464
C	0.158243	-2.059724	-1.250367
C	2.004599	-1.821605	1.228821
H	1.740884	3.845768	1.190635
H	1.251641	2.514391	2.214549
H	3.381760	1.955371	1.187965
H	2.791505	2.397050	-0.399206
H	2.386956	-2.355682	2.103970
H	2.521725	-2.271098	0.380536
H	0.040931	-1.836696	2.109417
H	0.400416	-3.232406	1.081094
H	-0.774064	3.061384	2.315360
H	-0.771565	4.427112	1.217738
H	-2.576695	3.249032	-0.146546
H	-3.006146	3.693090	1.479143
H	-2.434556	1.354431	2.255941
H	-3.883688	1.525438	1.264563
H	-2.790484	-0.175343	-1.606170
H	-4.127468	0.539939	-0.686421
H	-2.874862	1.564363	-1.428027
H	-2.170916	-0.713402	2.002987
H	-3.574172	-1.030054	0.964644
H	-2.163997	-2.032615	-0.739916
H	-1.819276	-2.814188	0.785131
H	2.711101	-0.906642	-1.173796
H	2.604880	0.737443	-1.775483
H	3.939774	0.264241	-0.687477
H	0.984171	2.994984	-1.476662
H	-0.729208	3.372363	-1.372238
H	0.460204	4.474517	-0.643659
H	3.534380	-0.344696	1.501354
H	2.010186	0.040251	2.313535
S	-0.094950	0.568785	-2.112518
C	-0.355143	-1.235026	-2.417310
H	0.191207	-1.515978	-3.318321
H	-1.410420	-1.429040	-2.615151
H	1.241576	-2.076330	-1.268275
H	-0.179256	-3.099801	-1.330921
H	1.283316	2.579361	5.237036
H	-0.557707	2.900899	5.283307
H	0.082981	1.144221	5.284065

$^{5\sigma}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.109461	0.760764	0.221318
O	-0.121752	0.897062	2.107834
C	-0.696384	-0.380887	5.212283
H	-0.320186	0.376333	2.892220

N	-2.385839	0.635883	0.405863
C	-2.843560	1.806059	1.212429
C	-2.500082	-0.632146	1.179940
C	-3.208751	0.552621	-0.821464
N	0.158631	2.956081	0.293454
C	1.426485	3.071160	1.081015
C	-0.954999	3.592298	1.068206
C	0.291456	3.616024	-1.025599
C	-2.376527	3.168676	0.679749
N	2.210812	0.767560	0.306871
C	2.556331	2.210359	0.527750
C	2.542808	-0.075287	1.496384
C	3.006072	0.308348	-0.857945
N	-0.238887	-1.462697	0.302757
C	-1.686240	-1.774753	0.566200
C	0.624244	-1.947244	1.427238
C	0.177948	-2.093623	-0.981668
C	2.111905	-1.549864	1.399853
H	1.762759	4.114601	1.088472
H	1.191662	2.773254	2.097307
H	3.414043	2.289782	1.203486
H	2.879640	2.610829	-0.431498
H	2.543230	-2.035588	2.280411
H	2.607411	-2.027876	0.554471
H	0.169925	-1.601054	2.352302
H	0.579600	-3.043276	1.440440
H	-0.793968	3.349223	2.115918
H	-0.861651	4.678357	0.955121
H	-2.532804	3.246713	-0.399001
H	-3.041376	3.916544	1.119729
H	-2.471912	1.676921	2.226141
H	-3.939159	1.791649	1.249851
H	-2.909243	-0.293632	-1.430195
H	-4.265924	0.443146	-0.553565
H	-3.082508	1.449502	-1.421506
H	-2.174425	-0.430198	2.195528
H	-3.546709	-0.955581	1.230649
H	-2.137232	-2.067926	-0.378981
H	-1.757688	-2.645471	1.223827
H	2.820311	-0.738849	-1.070224
H	2.726456	0.877813	-1.739461
H	4.075794	0.438994	-0.656340
H	1.062287	3.131810	-1.619943
H	-0.647303	3.544223	-1.571110
H	0.549098	4.672654	-0.897342
H	3.632138	-0.060628	1.631925
H	2.086590	0.391620	2.364274
S	-0.135488	0.443253	-2.161014
C	-0.387296	-1.391485	-2.208100
H	0.116081	-1.783051	-3.092062
H	-1.450649	-1.598054	-2.334538
H	1.262345	-2.070160	-1.030374
H	-0.122934	-3.149054	-0.982489
H	0.368072	-0.482040	5.367584
H	-1.171264	0.578470	5.357933
H	-1.300882	-1.260835	5.044447

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(SR)]$^{+}$

Fe	-0.114837	0.584487	0.179263
O	-0.133731	0.386709	2.048089
C	-0.201192	2.260823	5.176084
H	-0.163524	1.184629	2.583517
N	-2.412613	0.527540	0.379270
C	-2.829917	1.622885	1.296075
C	-2.525236	-0.802021	1.033103
C	-3.251212	0.574836	-0.836940
N	0.208145	2.695099	0.439142
C	1.503567	2.759766	1.190465
C	-0.866662	3.333728	1.274371
C	0.327571	3.462886	-0.827816
C	-2.313948	3.010238	0.892994
N	2.261611	0.529854	0.229521
C	2.617254	1.942066	0.547993
C	2.571861	-0.399140	1.354317
C	3.048954	0.146352	-0.964530
N	-0.266136	-1.528646	0.071952
C	-1.719816	-1.866672	0.290431
C	0.568972	-2.147300	1.157773
C	0.151194	-2.053563	-1.267784
C	2.076596	-1.840613	1.153942
H	1.834096	3.802302	1.253333
H	1.323982	2.417984	2.205294
H	3.491027	1.977766	1.208110
H	2.916080	2.418404	-0.384357
H	2.473943	-2.408144	2.001311
H	2.552671	-2.283809	0.278628
H	0.136994	-1.823949	2.099927
H	0.450956	-3.234359	1.079269
H	-0.701514	3.053584	2.315019
H	-0.717608	4.417193	1.224030
H	-2.490435	3.201352	-0.167543
H	-2.929266	3.741942	1.423270
H	-2.473971	1.376724	2.294559
H	-3.925628	1.649213	1.339729
H	-2.971702	-0.211770	-1.530428
H	-4.307415	0.452616	-0.568997
H	-3.120586	1.524138	-1.349405
H	-2.160931	-0.701203	2.050031
H	-3.571205	-1.130583	1.066178
H	-2.165785	-2.044943	-0.685314
H	-1.786475	-2.808131	0.840929
H	2.873638	-0.889763	-1.233028
H	2.756022	0.763084	-1.810130
H	4.121063	0.273598	-0.769910
H	1.083541	3.021786	-1.470361
H	-0.620280	3.446871	-1.359771
H	0.599610	4.500112	-0.609512
H	3.661998	-0.433277	1.488608
H	2.129541	0.011581	2.256864
S	-0.152239	0.581976	-2.104558
C	-0.405118	-1.226013	-2.410177
H	0.114610	-1.492093	-3.331122
H	-1.465645	-1.417787	-2.574776
H	1.234719	-2.036442	-1.310879

H	-0.162429	-3.100784	-1.355275
H	0.711155	2.839681	5.177960
H	-1.157769	2.762571	5.196138
H	-0.156189	1.183830	5.246698

$^{3\delta}$I–[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.218736	0.858268	0.086695
O	-0.379660	1.280085	1.860402
C	-1.746373	0.131691	4.921055
H	-0.851357	0.685180	2.449956
N	-2.493654	0.771438	0.002329
C	-3.070258	2.043640	0.515191
C	-2.764136	-0.348755	0.932709
C	-3.038484	0.474197	-1.337551
N	0.075340	2.995755	-0.107571
C	1.268250	3.245526	0.753236
C	-1.099640	3.739789	0.442637
C	0.337856	3.445221	-1.494027
C	-2.471230	3.315648	-0.094442
N	2.112041	0.874064	0.364918
C	2.445537	2.327789	0.425239
C	2.328046	0.202066	1.677582
C	2.971337	0.256586	-0.667109
N	-0.407974	-1.280519	0.511495
C	-1.877062	-1.568374	0.669032
C	0.351025	-1.593816	1.765636
C	0.092456	-2.155679	-0.581356
C	1.852039	-1.257876	1.764086
H	1.600901	4.283090	0.633621
H	0.954708	3.104360	1.782254
H	3.235427	2.507183	1.163408
H	2.859677	2.607258	-0.542020
H	2.222880	-1.629548	2.723840
H	2.364901	-1.866998	1.018155
H	-0.139121	-1.092600	2.597556
H	0.254254	-2.670219	1.952337
H	-1.087068	3.605135	1.521929
H	-0.946724	4.805379	0.234221
H	-2.472917	3.266469	-1.185583
H	-3.158368	4.128887	0.156550
H	-2.913030	2.068989	1.592805
H	-4.154560	2.037125	0.341619
H	-2.582875	-0.424520	-1.742860
H	-4.126388	0.340232	-1.287388
H	-2.811856	1.289124	-2.020599
H	-2.631293	0.015669	1.949312
H	-3.807994	-0.679535	0.857484
H	-2.209753	-2.050743	-0.247238
H	-2.026662	-2.292408	1.474546
H	1.153628	-2.002489	-0.744037
H	-0.071074	-3.206812	-0.321939
H	-0.431075	-1.920021	-1.502464
H	2.768912	-0.806282	-0.764537
H	2.792806	0.729085	-1.632639
H	4.033390	0.377438	-0.419130
H	1.184072	2.912097	-1.915459
H	-0.523853	3.240647	-2.122508

H	0.547439	4.520706	-1.501361
H	3.404049	0.213053	1.901785
H	1.821869	0.795857	2.433760
O	-0.109923	0.575807	-1.702455
H	0.741912	0.232667	-1.996415
H	-0.714669	0.307483	5.189371
H	-2.423301	0.967669	4.817683
H	-2.127478	-0.878220	4.877925

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.179034	0.814890	0.109810
O	-0.326529	1.229331	1.940094
C	-2.042487	0.212778	4.979080
H	-0.943967	0.723160	2.474272
N	-2.300046	0.751605	0.005982
C	-2.970986	1.976395	0.541469
C	-2.663247	-0.394829	0.887091
C	-2.821582	0.497173	-1.364467
N	0.057279	2.918148	-0.088871
C	1.256932	3.198909	0.755658
C	-1.087115	3.691221	0.485613
C	0.293349	3.396401	-1.475122
C	-2.462059	3.291571	-0.032123
N	1.959555	0.826717	0.349336
C	2.392764	2.266154	0.403783
C	2.273863	0.157289	1.655570
C	2.772910	0.191212	-0.722523
N	-0.355327	-1.298915	0.450724
C	-1.822220	-1.609821	0.567709
C	0.349536	-1.641580	1.728371
C	0.154045	-2.190492	-0.629859
C	1.843453	-1.307385	1.766917
H	1.578684	4.236867	0.618232
H	0.956529	3.057338	1.787965
H	3.204893	2.383259	1.125757
H	2.802029	2.525548	-0.570399
H	2.197607	-1.646901	2.744431
H	2.385242	-1.920708	1.045323
H	-0.160229	-1.132962	2.542150
H	0.236966	-2.719099	1.894538
H	-1.061678	3.542010	1.562233
H	-0.907344	4.752134	0.281382
H	-2.505100	3.300329	-1.123219
H	-3.160441	4.067224	0.293699
H	-2.823221	1.989230	1.619782
H	-4.045538	1.878389	0.352831
H	-2.353871	-0.380228	-1.794090
H	-3.906583	0.359465	-1.318142
H	-2.588447	1.336823	-2.010830
H	-2.537735	-0.084255	1.921436
H	-3.721735	-0.646983	0.762118
H	-2.144100	-2.028743	-0.382464
H	-1.981275	-2.384155	1.322787
H	1.233885	-2.153125	-0.693900
H	-0.138677	-3.222951	-0.415488
H	-0.254191	-1.866883	-1.580711
H	2.535951	-0.858684	-0.830252

H	2.585025	0.678548	-1.674603
H	3.836254	0.288538	-0.481260
H	1.186300	2.942767	-1.896635
H	-0.550650	3.143619	-2.110044
H	0.432697	4.481841	-1.474139
H	3.359943	0.203095	1.797258
H	1.793779	0.741120	2.434203
O	-0.067999	0.477411	-1.718059
H	0.576412	1.024580	-2.176457
H	-1.111276	0.717968	5.189829
H	-2.937754	0.787967	4.792244
H	-2.099003	-0.864151	5.043489

$^{5\sigma}$IN−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.207622	0.652760	0.207065
O	-0.490386	0.564867	2.088948
C	0.745742	0.858641	5.279469
H	0.059795	0.652485	2.871866
N	-2.442357	0.533804	0.170464
C	-3.022327	1.660677	0.959743
C	-2.675239	-0.762997	0.868626
C	-3.032728	0.515281	-1.184752
N	0.069438	2.856145	0.490062
C	1.268177	2.877924	1.376118
C	-1.113729	3.421847	1.205825
C	0.323710	3.624861	-0.748868
C	-2.480591	3.054754	0.611225
N	2.056260	0.605973	0.486573
C	2.418496	2.018110	0.851446
C	2.360373	-0.350894	1.592337
C	2.841892	0.242160	-0.718046
N	-0.375572	-1.631495	0.150223
C	-1.848090	-1.905404	0.280077
C	0.376106	-2.127769	1.345039
C	0.101758	-2.323544	-1.069490
C	1.879110	-1.798127	1.385514
H	1.639354	3.904564	1.484183
H	0.951910	2.541266	2.358471
H	3.219060	2.015843	1.597202
H	2.829905	2.483991	-0.041571
H	2.270515	-2.353224	2.243482
H	2.383093	-2.235281	0.522629
H	-0.116314	-1.719064	2.222996
H	0.279144	-3.220815	1.374739
H	-1.073443	3.065731	2.233237
H	-1.013088	4.513513	1.223656
H	-2.500249	3.228425	-0.467427
H	-3.194451	3.769883	1.028825
H	-2.819391	1.456707	2.008552
H	-4.109645	1.655349	0.815232
H	-2.575493	-0.261415	-1.790368
H	-4.113461	0.340545	-1.123799
H	-2.850191	1.464097	-1.682137
H	-2.418542	-0.612349	1.911940
H	-3.733759	-1.042859	0.801070
H	-2.217951	-2.144303	-0.715467
H	-2.005275	-2.799046	0.892211

H	1.161184	-2.148106	-1.229638
H	-0.058932	-3.404785	-0.988174
H	-0.441959	-1.957397	-1.937990
H	2.641117	-0.781635	-1.016279
H	2.564736	0.896339	-1.540184
H	3.914780	0.338074	-0.517366
H	1.132730	3.173930	-1.314332
H	-0.560578	3.610737	-1.380802
H	0.575925	4.662921	-0.503402
H	3.449255	-0.382218	1.728131
H	1.941437	0.053112	2.510645
O	-0.040764	0.836442	-1.676002
H	0.274002	0.107225	-2.218674
H	-0.326986	0.944103	5.374225
H	1.217855	-0.108935	5.369738
H	1.353412	1.750633	5.226272

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(OH)]$^{+}$

Fe	-0.178570	0.829863	0.070543
O	-0.402193	1.254728	1.835180
C	-1.668237	0.120725	4.957351
H	-0.770043	0.599171	2.433562
N	-2.353710	0.717502	-0.053662
C	-2.980129	1.975784	0.462726
C	-2.679510	-0.414284	0.861253
C	-2.879064	0.427092	-1.408942
N	0.087239	3.087666	-0.118054
C	1.249642	3.279060	0.785427
C	-1.114228	3.786870	0.413255
C	0.395603	3.579926	-1.475137
C	-2.452156	3.282326	-0.139426
N	1.999461	0.860692	0.414964
C	2.391059	2.308004	0.485453
C	2.252505	0.168740	1.717871
C	2.813659	0.235444	-0.655031
N	-0.371342	-1.432950	0.488092
C	-1.842599	-1.666853	0.595822
C	0.342259	-1.707301	1.766199
C	0.146297	-2.323221	-0.576382
C	1.827899	-1.308312	1.803944
H	1.645073	4.299097	0.695131
H	0.897427	3.139451	1.802195
H	3.169351	2.442381	1.242553
H	2.839887	2.566672	-0.471756
H	2.194679	-1.653354	2.775189
H	2.384088	-1.899782	1.075305
H	-0.194713	-1.212483	2.575354
H	0.283164	-2.783584	1.978893
H	-1.114219	3.660702	1.494290
H	-1.020120	4.860378	0.203196
H	-2.439590	3.240405	-1.231399
H	-3.195179	4.046763	0.105332
H	-2.819612	1.999453	1.538538
H	-4.060397	1.908239	0.287204
H	-2.394784	-0.450296	-1.826371
H	-3.960479	0.259312	-1.363117
H	-2.689098	1.267178	-2.073388

H	-2.547432	-0.063588	1.881590
H	-3.736044	-0.686304	0.757492
H	-2.170149	-2.115438	-0.339910
H	-2.058815	-2.398692	1.381565
H	1.224937	-2.242840	-0.659309
H	-0.103988	-3.368496	-0.358298
H	-0.282991	-2.031714	-1.530895
H	2.592414	-0.822208	-0.743264
H	2.579103	0.703476	-1.605909
H	3.880327	0.352531	-0.432997
H	1.221715	3.022268	-1.908860
H	-0.469181	3.457396	-2.125678
H	0.657752	4.644880	-1.449735
H	3.331644	0.208701	1.914641
H	1.749754	0.745392	2.489130
O	0.081840	0.508966	-1.697994
H	-0.401884	1.103715	-2.282261
H	-0.633140	0.259865	5.233663
H	-2.302023	0.981657	4.800368
H	-2.094119	-0.871957	4.944145

$^{3\sigma}$IN−[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.084339	0.579724	0.312099
O	-0.062207	0.391205	2.113046
C	-1.006364	1.797600	5.170079
H	-0.484536	1.065772	2.655997
N	-2.196689	0.500227	0.396951
C	-2.780578	1.606056	1.222888
C	-2.465959	-0.810634	1.066138
C	-2.818539	0.524821	-0.951316
N	0.192574	2.843358	0.579386
C	1.457089	2.842811	1.351383
C	-0.922774	3.436433	1.358376
C	0.352309	3.569728	-0.696278
C	-2.321189	3.028161	0.881397
N	2.055685	0.562696	0.342613
C	2.520831	1.946668	0.717758
C	2.496512	-0.441878	1.369742
C	2.660720	0.231347	-0.974613
N	-0.289065	-1.739697	0.142549
C	-1.738759	-1.977244	0.399637
C	0.569422	-2.277698	1.233707
C	0.052122	-2.371818	-1.149386
C	2.057560	-1.898544	1.144013
H	1.874811	3.855689	1.426097
H	1.236919	2.504363	2.360104
H	3.367742	1.871658	1.403489
H	2.893488	2.418602	-0.188921
H	2.552033	-2.463294	1.940575
H	2.491417	-2.283860	0.220609
H	0.162983	-1.920025	2.176312
H	0.501483	-3.374913	1.229651
H	-0.800194	3.150179	2.405313
H	-0.842940	4.530872	1.332337
H	-2.440785	3.231257	-0.184556
H	-3.027416	3.696611	1.381052
H	-2.560600	1.390828	2.268444

H	-3.869718	1.552755	1.118659
H	-2.391290	-0.247563	-1.581347
H	-3.897490	0.367176	-0.857539
H	-2.632891	1.481778	-1.429160
H	-2.154339	-0.713248	2.101364
H	-3.541926	-1.015197	1.046825
H	-2.211296	-2.194454	-0.557295
H	-1.879930	-2.867892	1.021463
H	1.114763	-2.290389	-1.354778
H	-0.211290	-3.437292	-1.145564
H	-0.483487	-1.872463	-1.954149
H	2.364392	-0.759741	-1.295245
H	2.321795	0.942939	-1.721155
H	3.752126	0.268046	-0.899015
H	1.110018	3.096341	-1.314003
H	-0.580033	3.550798	-1.255789
H	0.636591	4.613180	-0.511815
H	3.592504	-0.424455	1.389897
H	2.131511	-0.093255	2.331085
F	-0.091291	0.736816	-1.484937
H	-1.140037	2.869584	5.160767
H	-1.869738	1.148139	5.168112
H	-0.018496	1.378066	5.292324

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.133616	0.612176	0.301658
O	-0.294704	0.501843	2.142928
C	1.310852	1.987559	5.092220
H	0.303068	1.042549	2.667769
N	-2.236621	0.548906	0.303137
C	-2.878466	1.644337	1.091940
C	-2.529318	-0.735249	1.003727
C	-2.822576	0.534415	-1.061958
N	0.075980	2.699053	0.434526
C	1.345537	2.890550	1.192042
C	-1.017526	3.381084	1.195238
C	0.197150	3.344712	-0.901372
C	-2.428859	3.052975	0.728787
N	1.993506	0.614866	0.339182
C	2.448232	2.021995	0.629055
C	2.461413	-0.310465	1.424007
C	2.654723	0.234116	-0.942636
N	-0.286776	-1.518195	0.201651
C	-1.739775	-1.866840	0.389896
C	0.525535	-2.097357	1.321339
C	0.116852	-2.152223	-1.084728
C	2.021020	-1.770130	1.284940
H	1.653971	3.940580	1.151745
H	1.155517	2.663599	2.238802
H	3.297933	2.005948	1.314708
H	2.807142	2.451663	-0.302928
H	2.460773	-2.292435	2.139737
H	2.489388	-2.220636	0.409523
H	0.091859	-1.735342	2.248561
H	0.415389	-3.187185	1.284581
H	-0.919855	3.091885	2.240315
H	-0.844544	4.460332	1.131044

H	-2.563663	3.263306	-0.333660
H	-3.098731	3.742145	1.249646
H	-2.646817	1.460795	2.138846
H	-3.962700	1.556452	0.963106
H	-2.365013	-0.239632	-1.666703
H	-3.901677	0.363447	-0.994669
H	-2.638369	1.483691	-1.555134
H	-2.256546	-0.598519	2.044877
H	-3.599814	-0.959663	0.944775
H	-2.147859	-2.118350	-0.586672
H	-1.828391	-2.762569	1.008912
H	1.186232	-2.090770	-1.238184
H	-0.164247	-3.209543	-1.072623
H	-0.376193	-1.644409	-1.907258
H	2.482502	-0.806568	-1.179508
H	2.250756	0.837377	-1.748786
H	3.733237	0.394714	-0.854926
H	0.990961	2.883447	-1.476874
H	-0.724656	3.219615	-1.459609
H	0.404612	4.410911	-0.770229
H	3.556954	-0.284701	1.433903
H	2.118317	0.088205	2.375042
F	-0.098113	0.680230	-1.555455
H	2.383199	1.960089	4.962953
H	0.791103	2.934332	5.068682
H	0.775614	1.085658	5.351352

$^{5\sigma}$IN−[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	-0.186393	0.577783	0.312300
O	-0.386893	0.389666	2.172638
C	0.383216	1.494611	5.278395
H	-0.092450	0.849625	2.965306
N	-2.401378	0.447390	0.226383
C	-3.004659	1.536899	1.050461
C	-2.624767	-0.875142	0.879736
C	-2.971144	0.466828	-1.138639
N	0.049396	2.777682	0.585558
C	1.273475	2.832407	1.433757
C	-1.127134	3.330742	1.320873
C	0.256074	3.533515	-0.671707
C	-2.499586	2.953961	0.746973
N	2.063808	0.598901	0.453067
C	2.424913	1.998493	0.869210
C	2.427543	-0.401318	1.505931
C	2.794187	0.307670	-0.805682
N	-0.313829	-1.655580	0.107909
C	-1.775444	-1.983855	0.259967
C	0.497429	-2.226005	1.230020
C	0.135426	-2.215555	-1.190918
C	1.990072	-1.852475	1.238423
H	1.621419	3.867579	1.531920
H	1.004670	2.490207	2.428826
H	3.229145	1.970157	1.609339
H	2.829276	2.500347	-0.007121
H	2.424023	-2.434076	2.057312
H	2.479437	-2.231069	0.340407
H	0.034017	-1.899638	2.156955

H	0.429567	-3.319644	1.174223
H	-1.068540	2.982484	2.351021
H	-1.037087	4.422928	1.340238
H	-2.551999	3.171848	-0.321961
H	-3.216444	3.635317	1.212601
H	-2.798120	1.303016	2.092900
H	-4.091585	1.509790	0.908895
H	-2.493730	-0.283704	-1.761504
H	-4.049583	0.275545	-1.100290
H	-2.795173	1.434458	-1.600718
H	-2.379904	-0.756590	1.930381
H	-3.678977	-1.164174	0.795825
H	-2.156222	-2.220356	-0.731861
H	-1.889646	-2.889355	0.862155
H	1.197913	-2.054857	-1.336739
H	-0.059596	-3.293015	-1.226692
H	-0.392699	-1.720702	-2.001296
H	2.612824	-0.709788	-1.131803
H	2.447379	0.977708	-1.587705
H	3.871607	0.437332	-0.657145
H	1.072455	3.103814	-1.243389
H	-0.637256	3.479997	-1.287975
H	0.478430	4.582340	-0.446243
H	3.519175	-0.398427	1.615454
H	1.999341	-0.059019	2.444450
F	-0.073552	0.789066	-1.565294
H	0.937594	0.575273	5.400082
H	0.911444	2.431511	5.175347
H	-0.690034	1.494619	5.404029

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(F)]$^{+}$

Fe	0.011934	0.622624	0.258078
O	0.201096	0.515773	2.058024
C	-0.605716	2.022860	5.132871
H	-0.197757	1.207476	2.596482
N	-2.083988	0.599864	0.550808
C	-2.561896	1.753378	1.379864
C	-2.314686	-0.675795	1.298351
C	-2.834106	0.584351	-0.731002
N	0.361718	2.887614	0.398903
C	1.694920	2.884827	1.044224
C	-0.659173	3.538140	1.257617
C	0.410605	3.557661	-0.915257
C	-2.106473	3.148115	0.934852
N	2.143433	0.549535	0.086746
C	2.671483	1.936776	0.349340
C	2.659618	-0.419356	1.112591
C	2.613091	0.143749	-1.264996
N	-0.256607	-1.696111	0.211929
C	-1.679624	-1.885782	0.615063
C	0.689261	-2.208967	1.241446
C	-0.053570	-2.391333	-1.076128
C	2.170697	-1.872286	0.997366
H	2.140470	3.888496	1.035279
H	1.566256	2.591520	2.082508
H	3.582027	1.871421	0.949325
H	2.959723	2.359272	-0.611190

H	2.724926	-2.413814	1.770366
H	2.508364	-2.309156	0.056831
H	0.379616	-1.802486	2.200981
H	0.597669	-3.303003	1.293217
H	-0.441100	3.286697	2.297666
H	-0.558121	4.628407	1.180984
H	-2.323910	3.310474	-0.122440
H	-2.746150	3.854784	1.470309
H	-2.245765	1.575731	2.408092
H	-3.656752	1.723811	1.384409
H	-2.482237	-0.220306	-1.367391
H	-3.900843	0.451891	-0.526745
H	-2.680492	1.518191	-1.263178
H	-1.903186	-0.545325	2.294347
H	-3.391465	-0.854210	1.391277
H	-2.246270	-2.127714	-0.283048
H	-1.779767	-2.747164	1.284106
H	0.985357	-2.343658	-1.385520
H	-0.335120	-3.449199	-0.998792
H	-0.655239	-1.915105	-1.847869
H	2.266469	-0.852451	-1.511191
H	2.221110	0.830590	-2.008458
H	3.707321	0.154426	-1.293263
H	1.100001	3.045551	-1.580540
H	-0.570394	3.532485	-1.383669
H	0.725877	4.602505	-0.803207
H	3.752554	-0.429030	1.026675
H	2.397581	-0.018924	2.087156
F	-0.163869	0.715491	-1.533331
H	-0.644680	3.102415	5.114771
H	-1.519213	1.453785	5.227225
H	0.348892	1.519264	5.178378

$^{3\sigma}$IN−[Fe^{IV}=O(TMC)(CF$_3$CO$_2$)]$^+$

Fe	-0.197222	0.567138	0.315981
O	-0.325859	0.372578	2.200085
C	0.067484	1.652389	5.294384
H	-0.211451	0.908143	2.992427
N	-2.336786	0.481565	0.309139
C	-2.947905	1.547273	1.159764
C	-2.585566	-0.842426	0.963286
C	-2.973154	0.511600	-1.033135
N	0.023993	2.694736	0.572985
C	1.281877	2.773686	1.377864
C	-1.092981	3.302512	1.357283
C	0.192264	3.468797	-0.686565
C	-2.492396	2.969710	0.851951
N	1.967979	0.567173	0.360345
C	2.388957	1.966596	0.737518
C	2.380303	-0.398258	1.435715
C	2.697546	0.237380	-0.895673
N	-0.339313	-1.589922	0.106274
C	-1.798675	-1.935820	0.278757
C	0.464786	-2.186438	1.226705
C	0.085525	-2.203189	-1.182243
C	1.958016	-1.852473	1.216228
H	1.600776	3.817760	1.463940

H	1.064774	2.413661	2.377897
H	3.247881	1.920197	1.410246
H	2.728292	2.460435	-0.169690
H	2.389649	-2.410836	2.051901
H	2.438627	-2.260528	0.326791
H	0.017495	-1.848473	2.156049
H	0.357949	-3.274265	1.155730
H	-0.998170	2.967251	2.388539
H	-0.949210	4.387561	1.352886
H	-2.603857	3.209302	-0.207123
H	-3.179486	3.637902	1.376814
H	-2.707448	1.309598	2.193383
H	-4.034090	1.478183	1.040848
H	-2.554734	-0.258896	-1.672143
H	-4.048175	0.340224	-0.925217
H	-2.800305	1.469920	-1.510080
H	-2.286643	-0.747057	2.001507
H	-3.653646	-1.078439	0.917236
H	-2.206430	-2.130413	-0.710780
H	-1.887716	-2.865542	0.845022
H	1.144061	-2.060322	-1.357585
H	-0.118889	-3.277616	-1.151509
H	-0.460248	-1.750894	-2.001650
H	2.494292	-0.776593	-1.213311
H	2.391006	0.913111	-1.685548
H	3.772699	0.339269	-0.722273
H	1.003621	3.061177	-1.279794
H	-0.713748	3.420158	-1.280788
H	0.418478	4.510449	-0.441314
O	-0.090574	0.724330	-1.867747
C	-0.427777	1.233676	-2.974759
O	-1.246792	2.110588	-3.231100
C	0.368063	0.637750	-4.190436
F	-0.099105	1.065207	-5.375033
F	1.675870	0.993243	-4.127705
F	0.326096	-0.714196	-4.210062
H	3.473433	-0.365358	1.496800
H	1.971447	-0.033992	2.372723
H	1.142153	1.760489	5.258728
H	-0.560168	2.531693	5.271253
H	-0.367919	0.686504	5.506078

$^{3\pi}$IN−[Fe^{IV}=O(TMC)(CF$_3$CO$_2$)]$^+$

Fe	-0.116531	0.677483	0.190544
O	-0.204972	0.567398	2.006518
C	1.359818	1.886992	4.944696
H	0.416940	1.105479	2.506353
N	-2.229505	0.578972	0.333514
C	-2.814194	1.687143	1.152877
C	-2.458876	-0.699184	1.073955
C	-2.953648	0.528767	-0.964296
N	0.126400	2.769067	0.381564
C	1.412979	2.930236	1.122732
C	-0.955470	3.427098	1.183869
C	0.240636	3.492009	-0.916711
C	-2.374284	3.087874	0.749125
N	2.032794	0.674365	0.210076

C	2.495765	2.078122	0.503612
C	2.511002	-0.247022	1.297908
C	2.709762	0.283749	-1.060837
N	-0.266252	-1.480028	0.151903
C	-1.707867	-1.828830	0.413240
C	0.582588	-2.027209	1.264397
C	0.099000	-2.178292	-1.112511
C	2.073698	-1.705510	1.171418
H	1.722048	3.979810	1.104560
H	1.250809	2.680607	2.169055
H	3.371443	2.052639	1.155013
H	2.817429	2.523444	-0.434465
H	2.544191	-2.227402	2.009747
H	2.509729	-2.154550	0.278942
H	0.177800	-1.646807	2.196637
H	0.467568	-3.116312	1.255272
H	-0.826136	3.129240	2.222754
H	-0.794129	4.507777	1.127800
H	-2.525752	3.271456	-0.316388
H	-3.035912	3.788696	1.264291
H	-2.527220	1.509864	2.186724
H	-3.903635	1.605588	1.086207
H	-2.563089	-0.266590	-1.590608
H	-4.015233	0.342633	-0.779215
H	-2.835420	1.465707	-1.496730
H	-2.119158	-0.551415	2.092784
H	-3.529000	-0.928878	1.090171
H	-2.166646	-2.077421	-0.541324
H	-1.763239	-2.726698	1.032465
H	1.140562	-2.026349	-1.363727
H	-0.075725	-3.251593	-0.993836
H	-0.508930	-1.804670	-1.927879
H	2.460905	-0.729406	-1.345297
H	2.400651	0.947681	-1.858745
H	3.792724	0.354896	-0.926317
H	1.027014	3.058715	-1.525789
H	-0.689488	3.421359	-1.467934
H	0.478129	4.541436	-0.723389
O	-0.086718	0.666182	-1.820681
C	-0.501007	1.115023	-2.932819
O	-1.296659	2.008690	-3.188040
C	0.107956	0.344491	-4.156667
F	-0.094507	0.994579	-5.313547
F	1.436753	0.145436	-4.036263
F	-0.468886	-0.877440	-4.277856
H	3.605616	-0.216156	1.290398
H	2.185631	0.154820	2.253578
H	2.433604	1.870549	4.824800
H	0.835835	2.831778	4.957916
H	0.829900	0.974986	5.178534

$^{5\sigma}$IN−[Fe^{IV}=O(TMC)(CF$_3$CO$_2$)]$^+$

Fe	-0.154879	0.576416	0.273641
O	-0.194574	0.413547	2.110553
C	-0.349316	1.543722	5.140780
H	-0.283164	0.889660	2.946915
N	-2.378984	0.432017	0.346075

C	-2.901997	1.543771	1.199881
C	-2.539035	-0.879920	1.043533
C	-3.112046	0.415148	-0.941166
N	0.141689	2.773844	0.541876
C	1.405886	2.784915	1.337643
C	-0.996568	3.327278	1.340266
C	0.313145	3.592345	-0.683523
C	-2.396238	2.947389	0.837701
N	2.109943	0.559576	0.294597
C	2.507163	1.959443	0.679393
C	2.506186	-0.416288	1.363438
C	2.820223	0.230527	-0.967259
N	-0.294074	-1.668132	0.116157
C	-1.745665	-1.988828	0.360663
C	0.563608	-2.221246	1.217014
C	0.085219	-2.296489	-1.175393
C	2.056619	-1.868635	1.145894
H	1.768627	3.812789	1.449121
H	1.184627	2.404392	2.329190
H	3.368894	1.926055	1.351088
H	2.839127	2.460713	-0.227405
H	2.523212	-2.436132	1.956579
H	2.499247	-2.270186	0.233917
H	0.148230	-1.869887	2.157011
H	0.474842	-3.313654	1.187446
H	-0.879775	2.995059	2.370931
H	-0.905451	4.418514	1.347281
H	-2.487624	3.131396	-0.235143
H	-3.087117	3.649609	1.310620
H	-2.636969	1.318503	2.231094
H	-3.995391	1.533444	1.134840
H	-2.714682	-0.355782	-1.596319
H	-4.173021	0.213436	-0.761625
H	-3.003313	1.369874	-1.445745
H	-2.206562	-0.750511	2.067959
H	-3.595478	-1.169999	1.055069
H	-2.192416	-2.213169	-0.606071
H	-1.824027	-2.899440	0.960240
H	1.129861	-2.117104	-1.403355
H	-0.080649	-3.377897	-1.127991
H	-0.511476	-1.874873	-1.977765
H	2.590353	-0.778635	-1.289620
H	2.511589	0.914943	-1.751057
H	3.902351	0.310936	-0.820528
H	1.100743	3.182056	-1.309248
H	-0.606096	3.597035	-1.260684
H	0.577982	4.618399	-0.408890
O	-0.109617	0.732224	-1.784620
C	-0.523130	1.265831	-2.862997
O	-1.366715	2.131073	-3.038561
C	0.213324	0.705145	-4.127947
F	-0.305470	1.177394	-5.271432
F	1.523229	1.049812	-4.108839
F	0.155405	-0.643523	-4.186300
H	3.600765	-0.409898	1.429422
H	2.108199	-0.047299	2.304307
H	0.534081	2.166483	5.123609

H	-1.327603	2.002003	5.109975
H	-0.258525	0.494502	5.383547

$^{5\pi}$IN−[Fe^{IV}=O(TMC)(CF$_3$CO$_2$)]$^+$

Fe	-0.132123	0.745841	0.154754
O	-0.268077	0.750545	1.970107
C	1.480797	1.398340	4.903070
H	0.548067	0.872015	2.466437
N	-2.257752	0.589788	0.286246
C	-2.815293	1.742758	1.072896
C	-2.455182	-0.675325	1.062781
C	-2.983789	0.498726	-1.006216
N	0.153891	2.998592	0.329778
C	1.405192	3.047614	1.128636
C	-0.985819	3.577502	1.101155
C	0.334113	3.756531	-0.930176
C	-2.370791	3.136939	0.618357
N	2.043135	0.732951	0.246144
C	2.486866	2.146585	0.543628
C	2.509178	-0.196390	1.332643
C	2.704752	0.330121	-1.028322
N	-0.261979	-1.587947	0.176714
C	-1.710832	-1.851038	0.443177
C	0.579598	-2.020053	1.331760
C	0.114028	-2.353922	-1.034621
C	2.067452	-1.660862	1.227426
H	1.800659	4.069473	1.162004
H	1.167572	2.770116	2.151994
H	3.341057	2.122685	1.223342
H	2.842644	2.574972	-0.390062
H	2.555691	-2.164098	2.067007
H	2.505384	-2.114805	0.338487
H	0.151801	-1.584534	2.231456
H	0.504814	-3.111188	1.421900
H	-0.866456	3.282064	2.141845
H	-0.914222	4.670090	1.056197
H	-2.467792	3.256078	-0.463215
H	-3.087950	3.838172	1.052425
H	-2.526915	1.595561	2.110356
H	-3.905994	1.672605	1.013199
H	-2.584422	-0.307373	-1.614428
H	-4.042297	0.301919	-0.814023
H	-2.883415	1.427586	-1.557475
H	-2.113899	-0.492427	2.075347
H	-3.522993	-0.914660	1.094685
H	-2.173690	-2.119404	-0.504709
H	-1.821633	-2.719762	1.099450
H	1.163510	-2.219258	-1.273607
H	-0.069801	-3.423469	-0.880921
H	-0.471287	-2.010527	-1.882450
H	2.411709	-0.671443	-1.317300
H	2.416842	1.009822	-1.822080
H	3.790180	0.361574	-0.897597
H	1.121589	3.312475	-1.534233
H	-0.580824	3.733474	-1.512760
H	0.603211	4.794748	-0.706866
O	-0.048772	0.639528	-1.815512

C	-0.490532	1.128576	-2.906395
O	-1.193449	2.102700	-3.114235
C	-0.050949	0.274129	-4.143787
F	-0.253160	0.923528	-5.300017
F	1.249974	-0.073931	-4.097260
F	-0.773362	-0.872574	-4.192820
H	3.604318	-0.178165	1.323073
H	2.215527	0.218371	2.296053
H	2.425465	1.899397	4.747511
H	0.573679	1.977103	4.999720
H	1.462347	0.336632	5.103405