Electronic Structure of the Ferryl Intermediate in the α-Ketoglutarate Dependent Non-Heme Iron Halogenase SyrB2: Contributions to H-atom Abstraction Reactivity

Supporting Information

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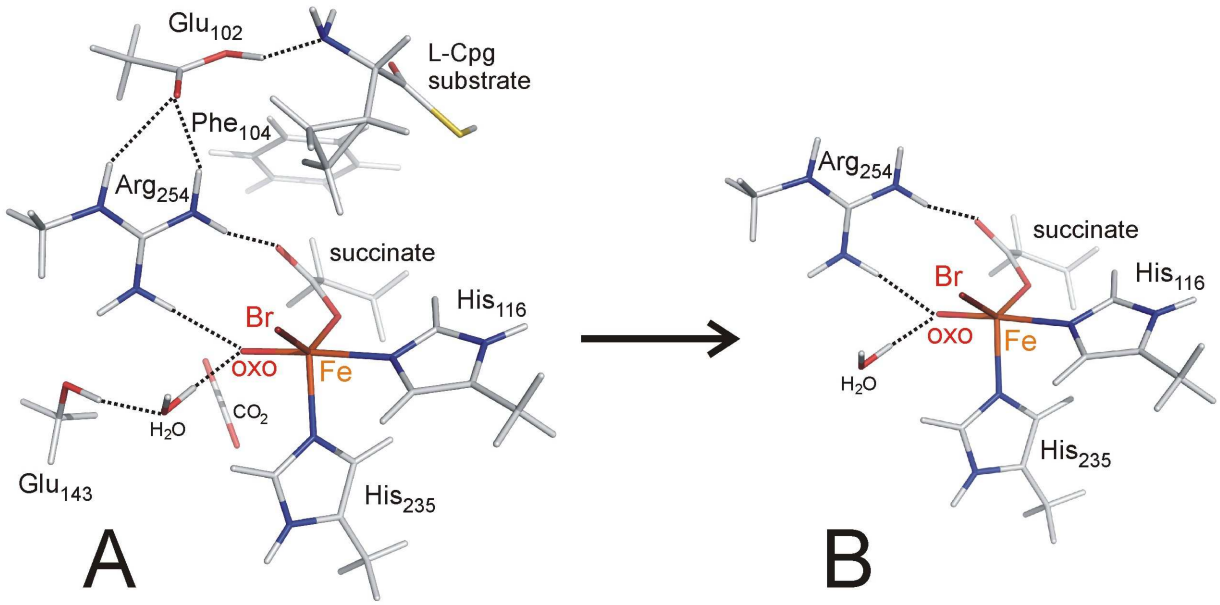


Figure S1. **A**. DFT cluster model of the enzymatic Br—Fe^{IV}=O intermediate (taken from Ref. 20 in the main text). **B**. Truncated model of the Br—Fe^{IV}=O structure used in multiconfigurational and multireference calculations.

Technical details on CASSCF calculations (section 2.6 in the main text)

To prevent Fe 3s and three Fe 3p orbitals from mixing with the other orbitals in CASSCF calculations the SUPSYMMETRY keyword of MOLCAS was used.

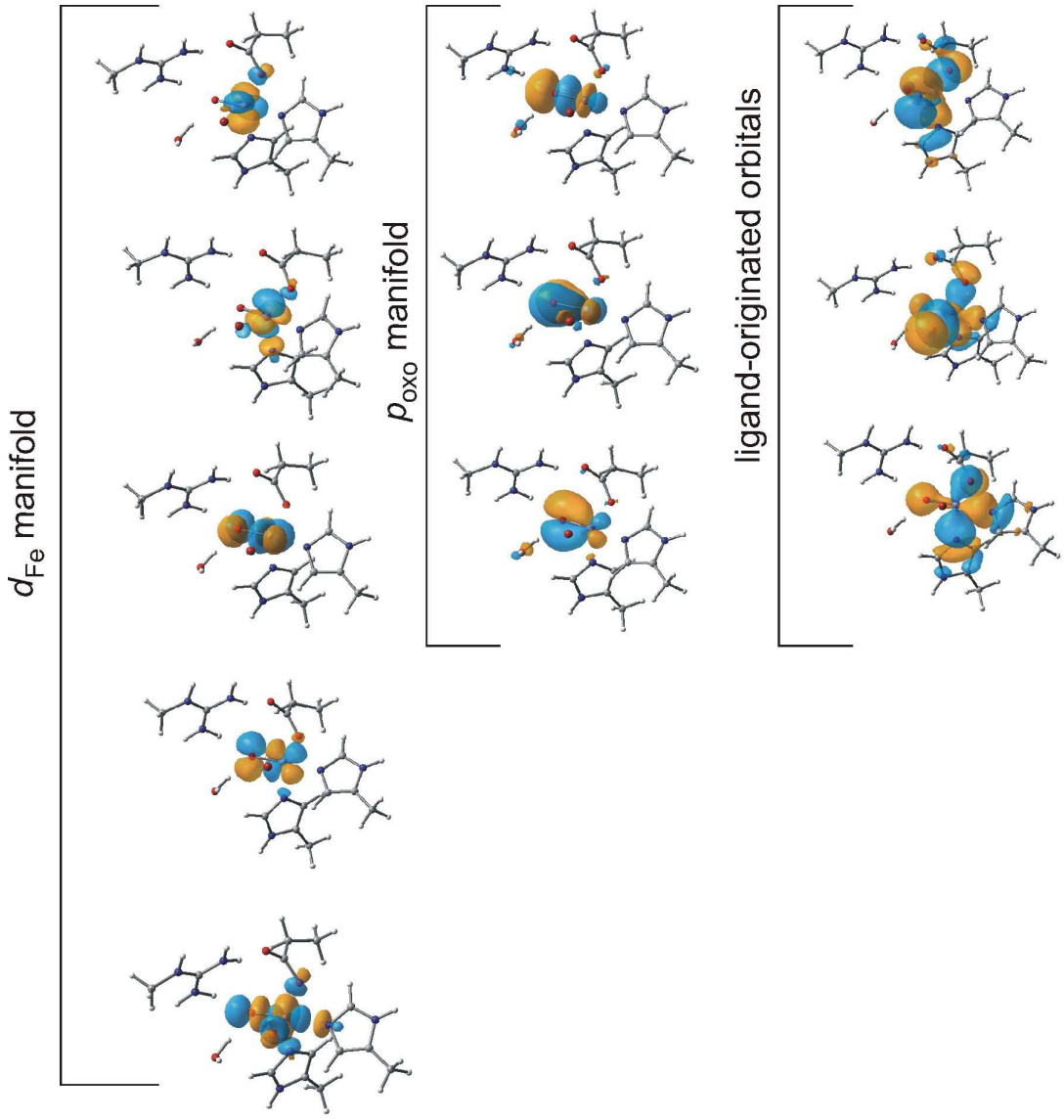


Figure S2. Molecular orbitals of the 16-in-11 active space used in CASSCF/CASPT2 calculations.

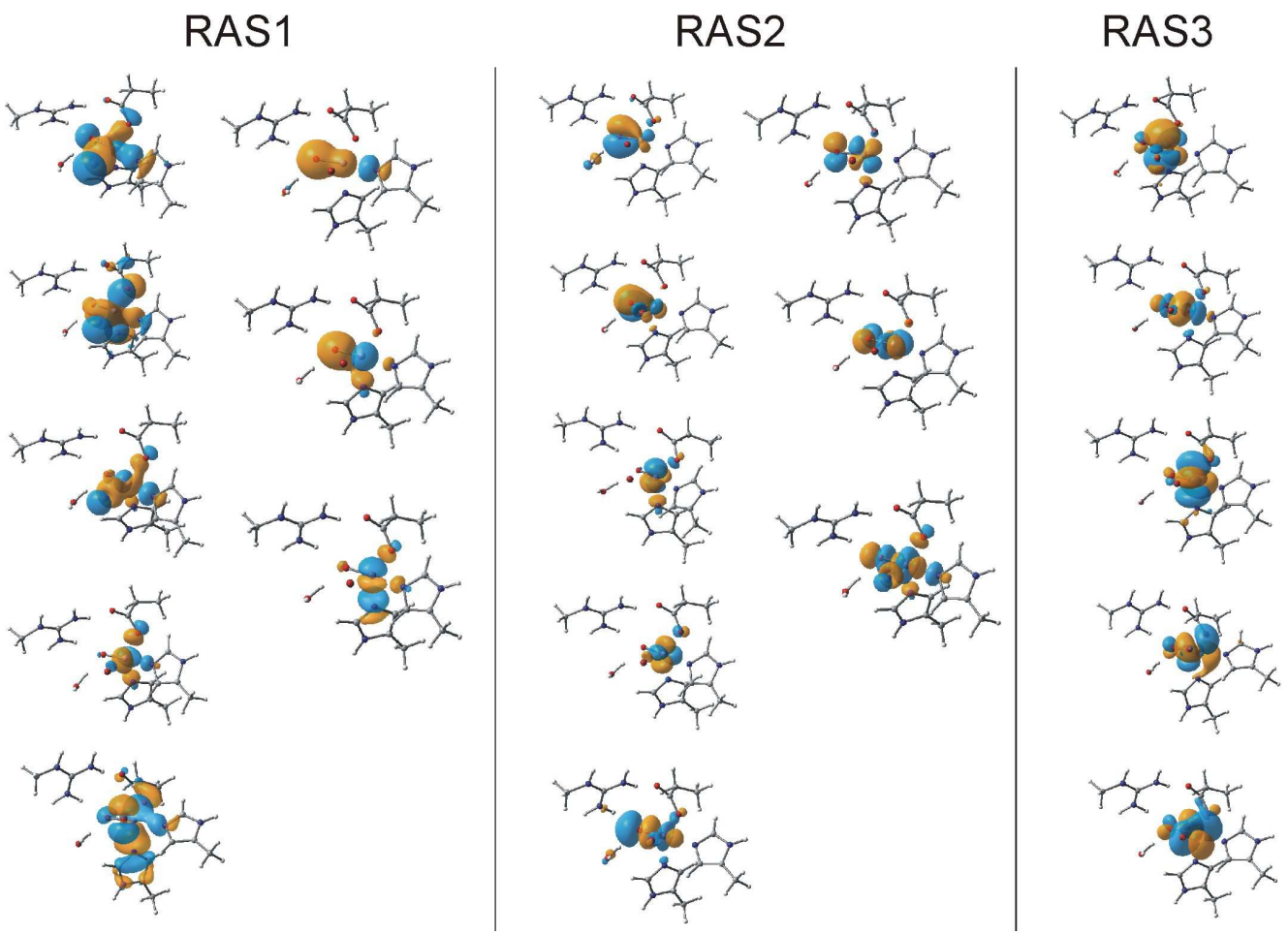
Technical details on RASSCF calculations

(section 2.6 in the main text)

Technical details on RASSCF calculations (section 2.6 in the main text)

The RASSCF active space 26-in-21 used in the study was divided into three subspaces: RAS1 space comprises 16 electrons in 8 orbitals allowing only single and double excitations from this subset of active orbitals; RAS2 space comprises 10 electrons in 8 orbitals with all possible occupations (FCI within RAS2); RAS3 space with 0 electrons in 5 orbitals allowing only single excitations to this subset of active orbitals. The state-average RASSCF were performed over the lowest eleven $S = 2$ states. The active space orbitals are shown in **Figure S2**.

(SyrB2)Fe^{IV}=O:



(TMG$_3$tren)Fe^{IV}=O:

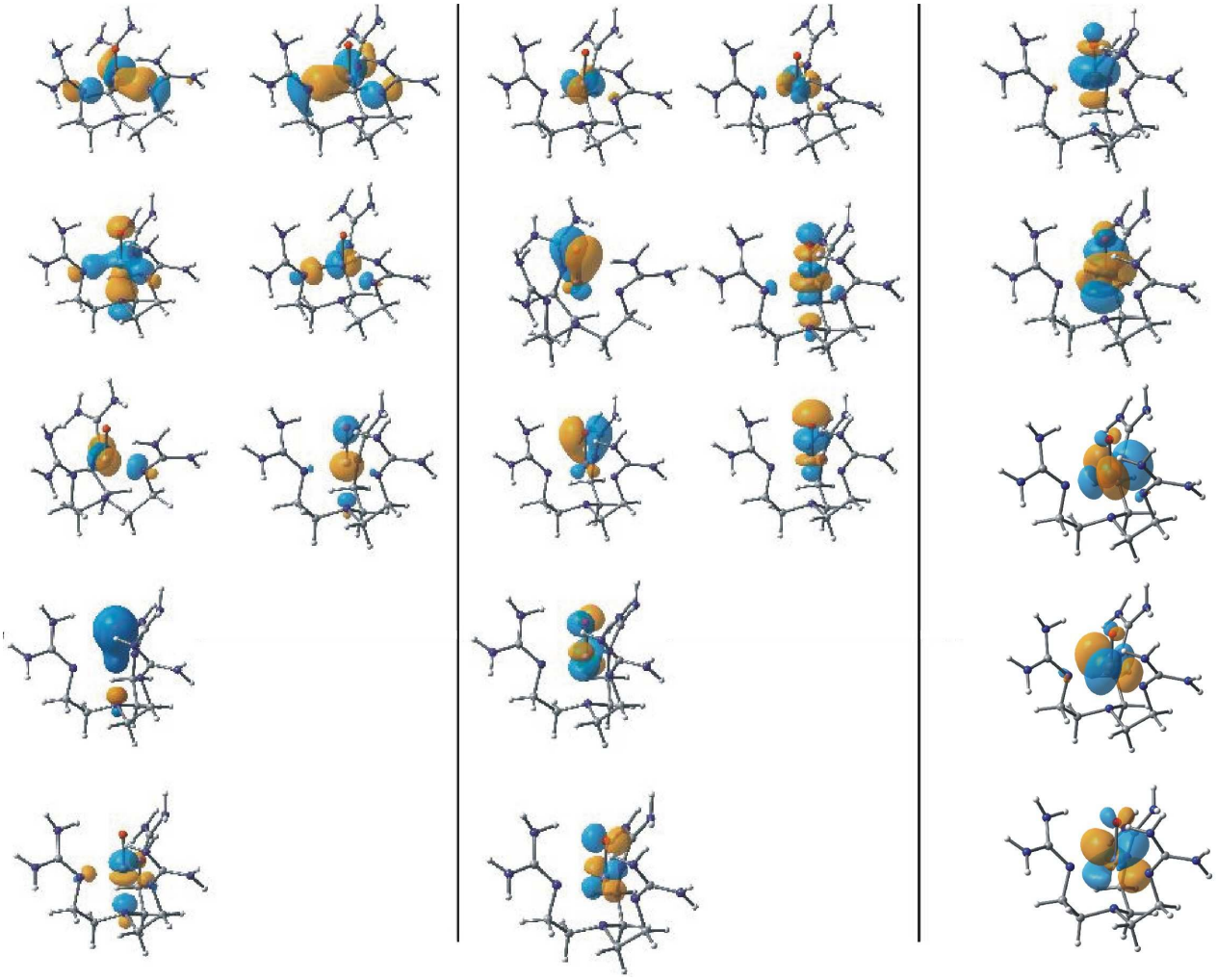


Figure S3. Molecular orbitals of the 26-in-21 active space used in RASSCF calculations.

NOTE: 4*d* orbitals were included in RAS3 to account for double-shell effect (see Ref. 32 in the main text).

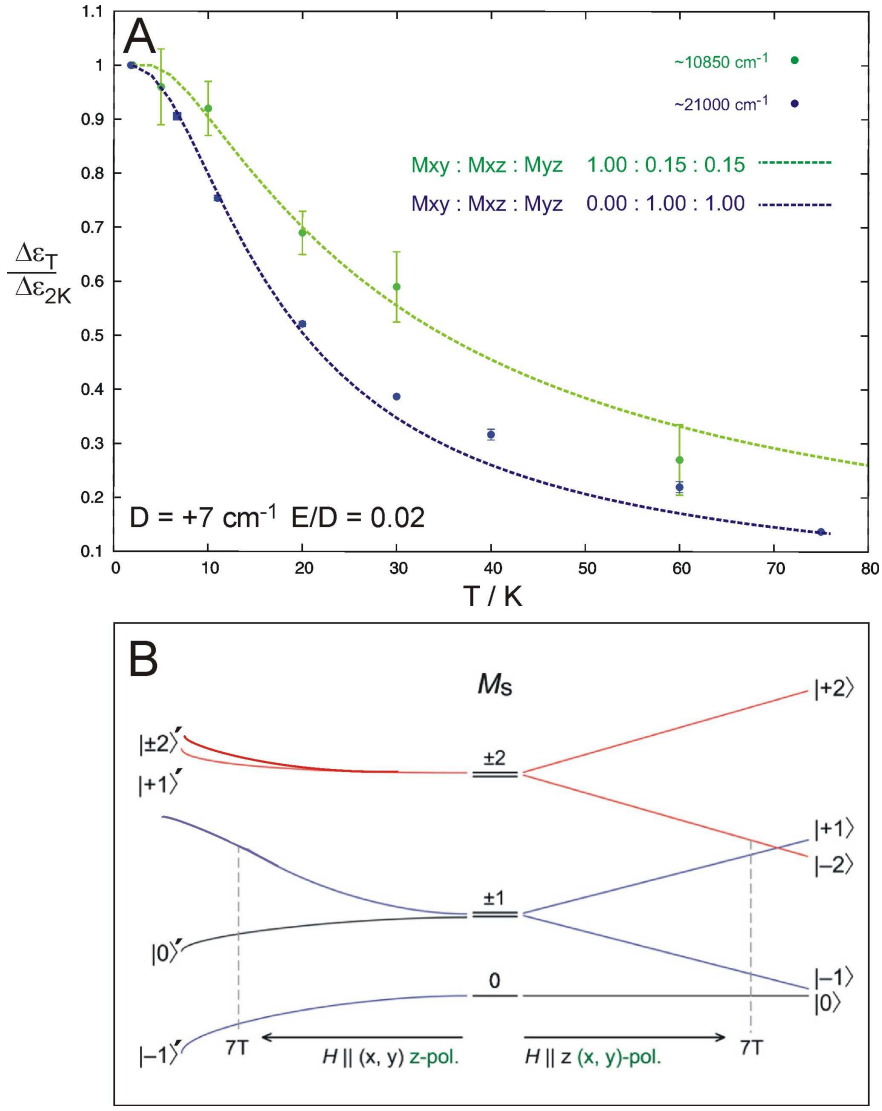


Figure S4. **A.** Temperature dependence of MCD spectral features (I, II and III in **Figure 2**) measured at ~12100, ~17600 and ~21000 cm^{-1} and fitted according to Ref. 36 (from the main text) with ZFS D = +7 cm^{-1} and E/D = 0.01. **B.** Schematic depiction of splitting of M_s sublevels of an $S = 2$ species with positive ZFS D parameter in an applied field H. The z axis of the molecule is defined along the Fe–oxo bond axis. For z-polarized transitions in MCD, H has a non-vanishing component parallel to the (x,y) plane; at 7 T, the MCD-active $M_s = -1$ sublevel is lowest in energy, so there is MCD intensity at low temperature (temp), but with increasing temp, the population of the $M_s = -1$ sublevel decreases, whereas the populations of the $M_s = 0, +1$ sublevels increase. Because $M_s = 0$ is MCD inactive and $M_s = +1$ produces MCD intensity of the opposite sign, the overall MCD intensity decreases as temp increases. For (x,y)-polarized transitions, H has a non-vanishing component parallel to the z axis; at 7 T, the MCD-inactive $M_s = 0$ sublevel is lowest in energy; as temp increases, the MCD-active $M_s = -1$ sublevel is populated, causing no decrease in MCD intensity, but further increasing temp populates the $M_s = +1$ sublevel and produces MCD intensity of the opposite sign, thereby decreasing overall MCD intensity. Thus, z-pol. transitions start with high MCD intensity at low temp, and decrease with increasing temp, whereas (x;y)-pol. transitions first do not decrease (may even increase) in MCD intensity with increasing temp, then decrease at higher temp.

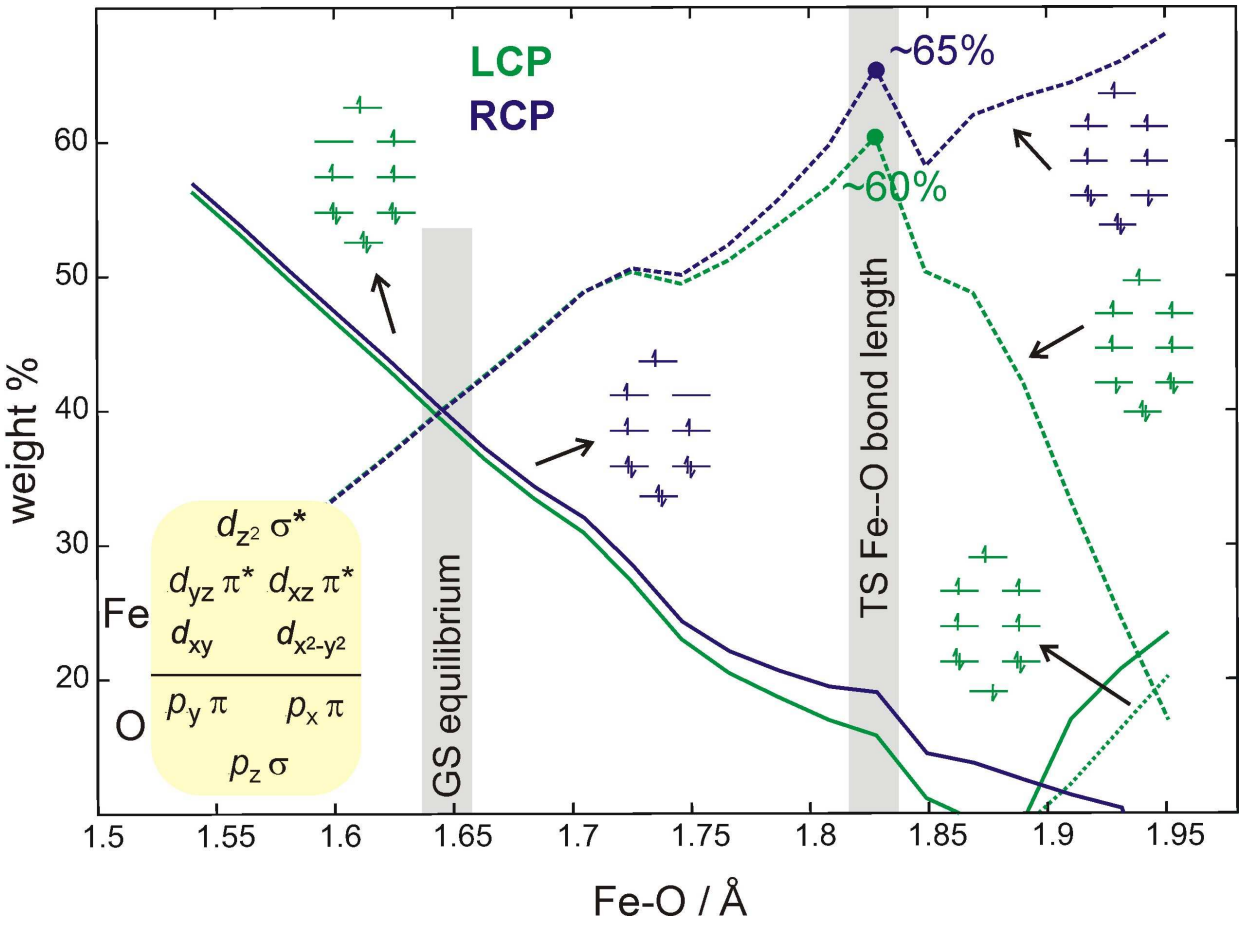
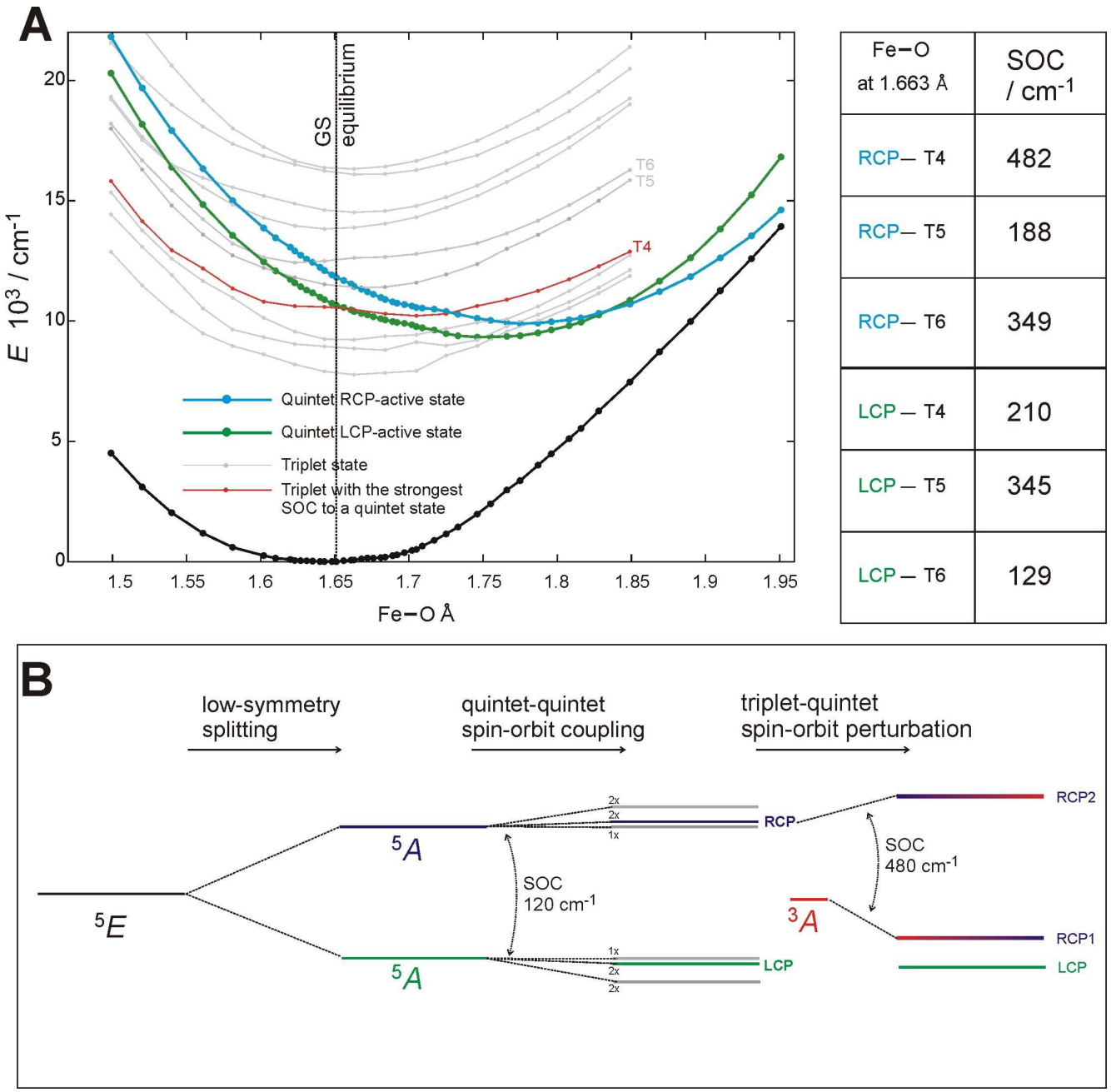


Figure S5. Evolution of the two dominant electronic configurations contributing to the CASPT2 wave function characters of the two lowest-energy, low-symmetry split ^{5}E LF excited states in SyrB2 Br—Fe^{IV}=O (the state that is RCP-active in MCD is π-reactive in H-atom abstraction due to the orientation of the π^* FMO into the substrate). Other electronic configurations with <10% of weight are not shown. Orbitals associated with the configurations are displayed in **Figure 8** (left panel therein). The GS equilibrium and TS Fe—O lengths are indicated by a grey bars.



Fe–O at 1.663 Å	SOC / cm^{-1}
RCP— T4	482
RCP— T5	188
RCP— T6	349
LCP — T4	210
LCP — T5	345
LCP — T6	129

Figure S6. **A**. Potential-energy curves (PECs) of the three lowest quintet (S = 2) and ten lowest triplet (S = 1) states along the Fe–oxo stretching coordinate. In the vicinity of the ground-state equilibrium, three triplet PECs (denoted as T4, T5 and T6) cross two lowest excited quintet (LCP- and RCP-active) states. In right table, the SOC interactions between these triplets and quintets, calculated as $|a| = \sqrt{\left|\left\langle {}^5E \mid H_x^{SOC} \mid {}^3A \right\rangle\right|^2 + \left|\left\langle {}^5E \mid H_y^{SOC} \mid {}^3A \right\rangle\right|^2 + \left|\left\langle {}^5E \mid H_z^{SOC} \mid {}^3A \right\rangle\right|^2}$, are shown. Note, SOC is strongest between the RCP-active quintet state and the triplet T4 that cross at the ground-state equilibrium. **B.** Sequence of effects perturbing the LF ^{5}E state from trigonal-bipyramidal (TBP) C_3 symmetry giving rise to three NIR MCD-active states in the low-symmetry TBP structure of the enzymatic Fe^{IV}=O intermediate.

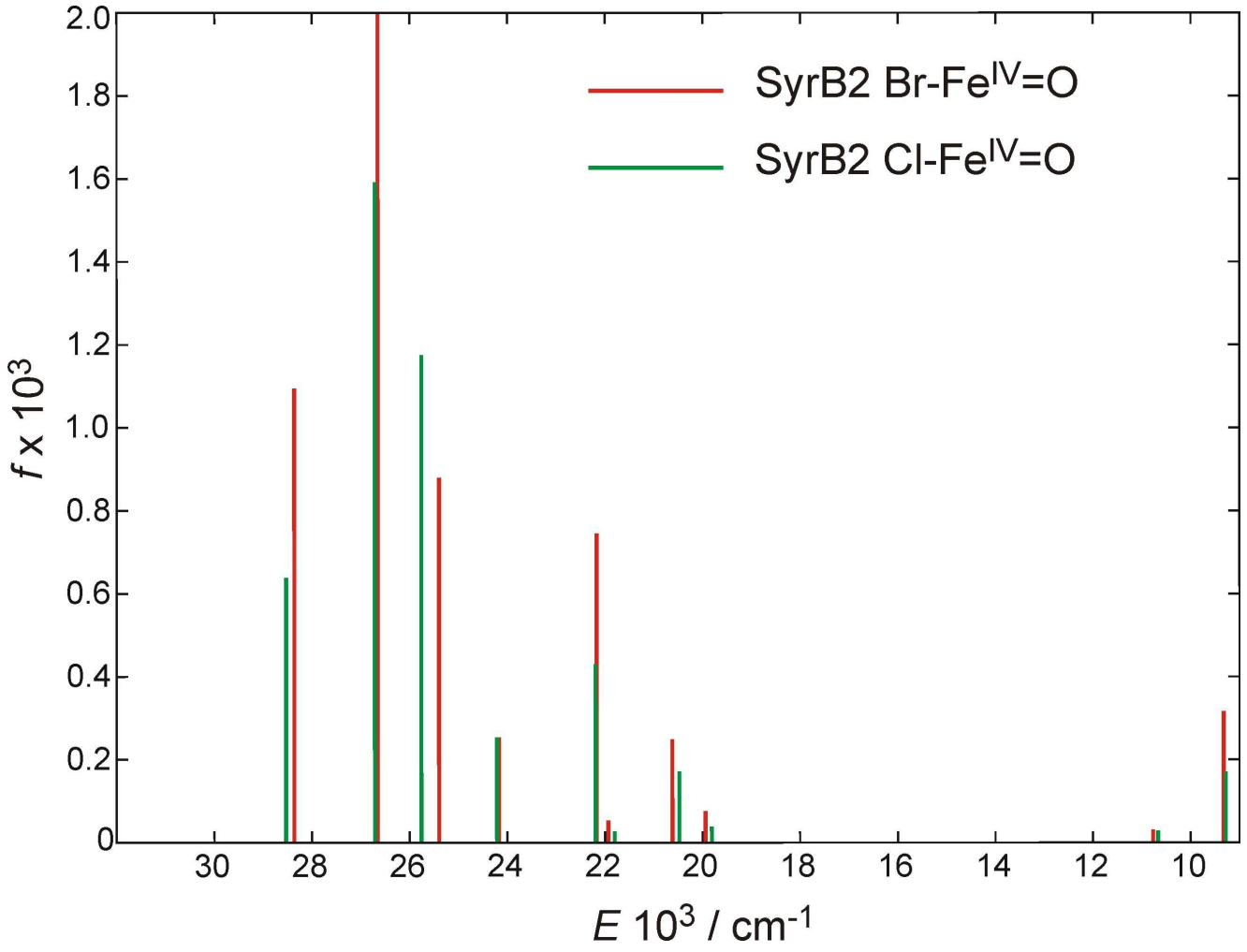


Figure S7. Calculated electronic spectra of the SyrB2 Br—Fe^{IV}=O (red) and Cl—Fe^{IV}=O species (green) using the same level of theory as in **Figure 6**. Polarization and assignment of transitions are also shown in **Figure 6**. Orbitals from the active space of RASSCF(26-in-8,5,5) calculations are shown for SyrB2 Br—Fe^{IV}=O in **Figure S3**. The same type of active-space orbitals was used for the SyrB2 Cl—Fe^{IV}=O model corresponding to the structure from **Figure S1B** (the Br ligand is replaced by Cl).

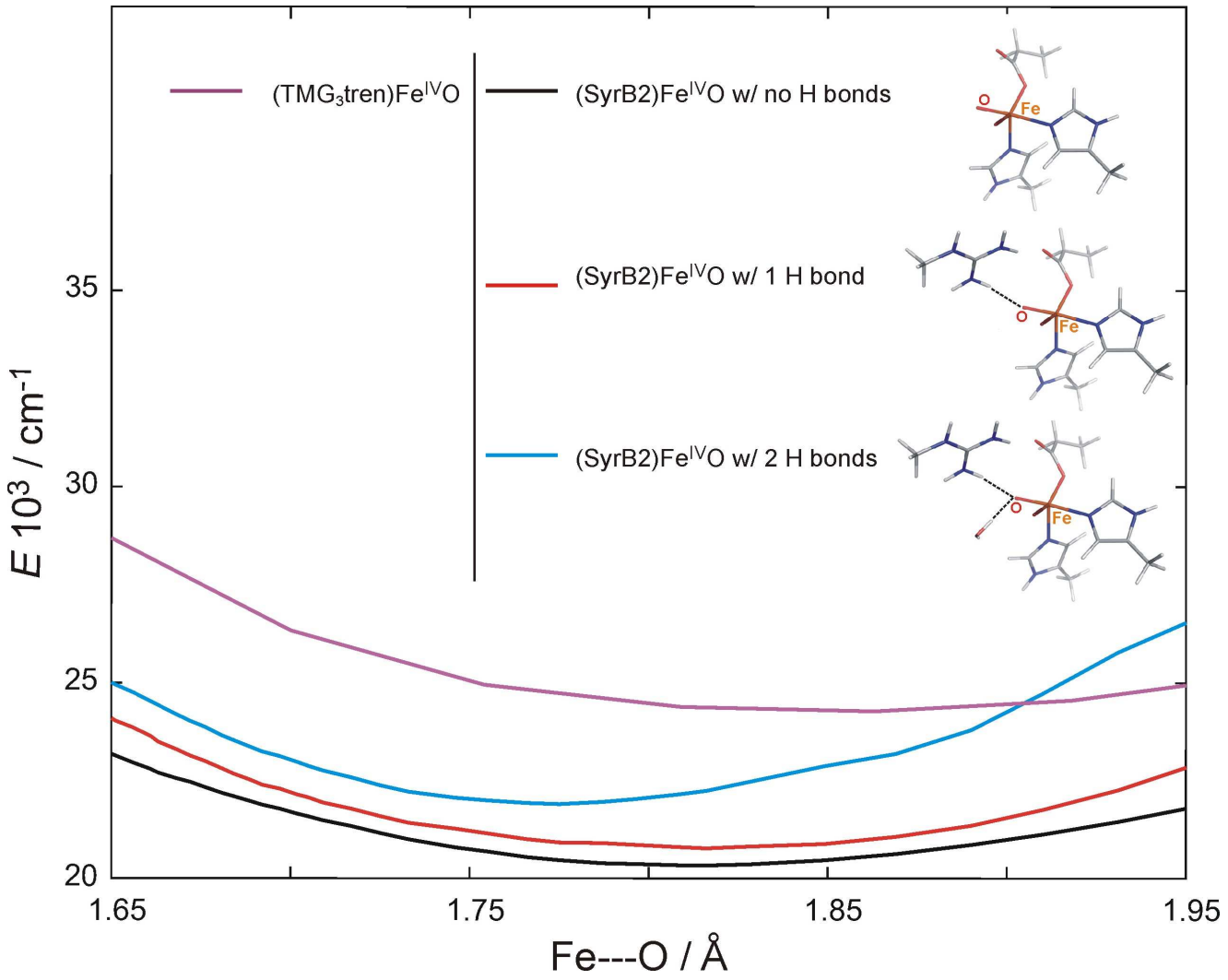


Figure S8. The potential energy surface of the CT state (root #4 in SA-CASSCF/MS-CASPT2 calculations) of the $S = 2$ (TMG3tren)Fe^{IV}=O system and SyrB2 Br—Fe^{IV}=O intermediate with the oxo group having 0,1 or 2 hydrogen bonds with the second-shell environment.

Note: The SA-CASSCF/MS-CASPT2 potential energy surfaces of the three structural models of Fe^{IV}=O were calculated along the Fe—O vibration mode of the Br–Fe^{IV}=O structure from **Figure S1A** that was obtained from the BP86/def2-SVP frequency analysis using the G09 program package.

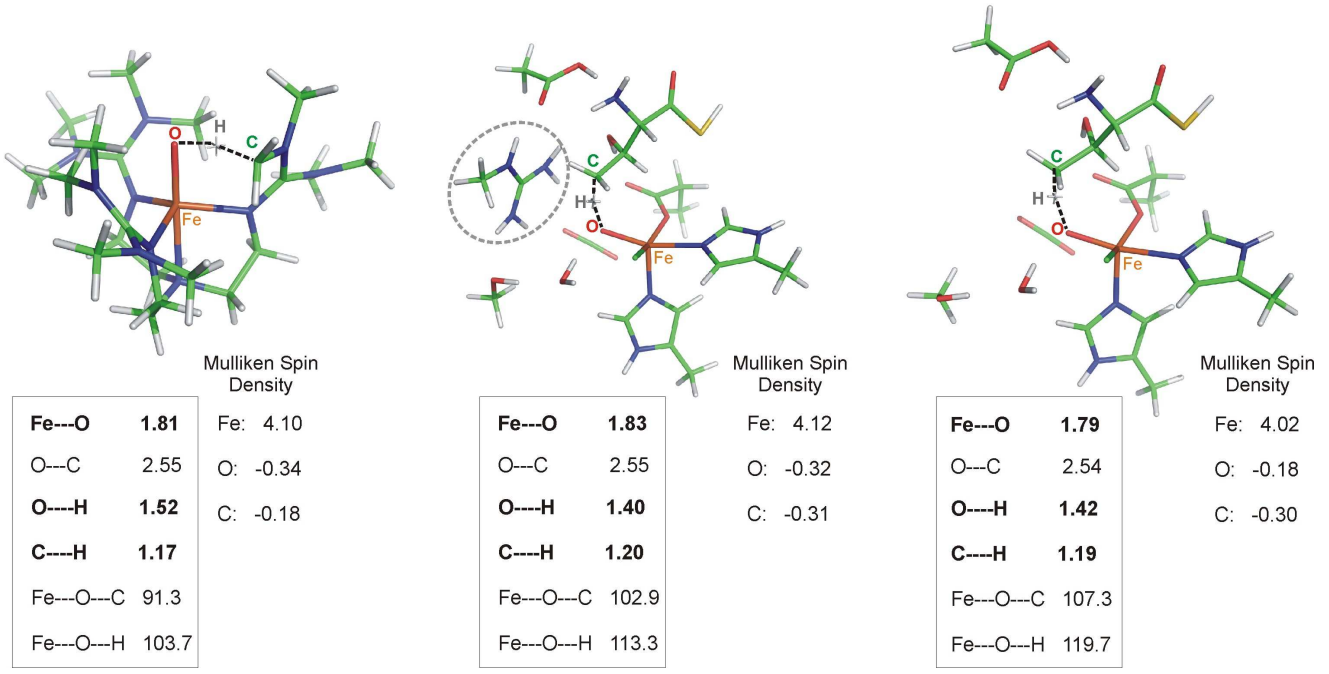


Figure S9. Geometric and electronic structure parameters for transition states of the π(S_{Fe}=5/2)-controlled H-atom abstraction pathway in both the TMG_3tren (*left*) and SyrB2 systems (*middle*, *right*). Here, two cluster models for SyrB2 (with and without the second-shell Arginine residue) are presented. Distances are in Å.

Table S1. The (activation/reaction) potential energies, enthalpies and free energies of the π(S_{Fe}=5/2)-controlled H-atom abstraction from the native substrate by the (SyrB2)Fe^{IV}=O and (TMG_3tren)Fe^{IV}=O species. The intrinsic reaction barriers are also presented. All values are in kcal mol^{-1}.

System	$\Delta E^{\neq}$ / $\Delta H^{\neq}$ / $\Delta G^{\neq}$	ΔE^{0} / ΔH^{0} / ΔG^{0}	$\Delta E^{\neq}_{intr}$ /$\Delta H^{\neq}_{intr}$ / $\Delta G^{\neq}_{intr}$
(SyrB2)Fe^{IV}=O[a]	23.1 / 18.9 / 19.8	3.9 / 0.6 / 2.3	21.1 /18.6 / 18.6
(SyrB2)Fe^{IV}=O[b]	26.5 / 22.5 / 24.2	7.4 / 5.3 / 4.2	22.6 / 19.8 / 22.0
(TMG_3tren)Fe^{IV}=O[c]	25.3 / 21.6 / 21.4	5.9 / 3.2 / 0.5	22.3 / 20.3 / 21.6

[a]Within the cluster model from **Figure 1D**, the second-shell residue Arg_{254} appears to destabilize sterically the transition state/product relative to the reactant by ~3-4 kcal mol^{-1}. Here, the DFT results are presented for the cluster model in the absence of the Arg_{254} residue.
[b]the Arg-including cluster model of the active site from **Figure 1D**.
[c]Calculated at the same level of theory as SyrB2 (described in Computational Details) but with a dielectric constant of ε = 35.7 mimicking the solvation effect of acetonitrile (no frznuclei option for vibrational analysis was used).

XYZ coordinates:

Br-Fe^{IV}=O system from Figure S1A

O	2.42500	39.29800	13.30200
C	4.49800	35.62100	14.45200
O	4.09100	34.87300	13.64300
O	4.90000	36.34900	15.28200
C	6.28800	35.85600	10.91300
O	6.82300	36.94900	11.43500
C	6.86900	34.49900	11.35000
H	6.19900	34.19100	12.18600
H	6.63600	33.80200	10.52100
Br	4.59400	40.34900	10.67800
Fe	5.83100	38.57500	11.81800
C	-0.72500	37.74000	9.52600
N	0.59400	37.35300	9.03000
C	1.72300	37.12500	9.74700
N	2.87900	36.96800	9.07900
N	1.74200	37.04400	11.08800
H	-1.11400	38.59200	8.93300
H	-0.65700	38.06200	10.58300
H	3.74900	36.67200	9.56100
H	2.87700	37.04700	8.05200
H	2.67500	37.05000	11.52600
H	0.93600	37.13000	11.73700
C	7.98600	38.98100	16.99200
C	7.09300	39.12300	15.81400
N	5.77700	39.56000	15.89100
C	7.30200	38.85100	14.47500
C	5.22100	39.52500	14.65600
N	6.13500	39.10300	13.77600
H	8.98600	38.63500	16.67000
H	7.58900	38.24000	17.71900
H	8.11700	39.94100	17.53500
H	8.20900	38.48100	13.98600
H	4.16900	39.75700	14.42900
C	0.28900	36.82300	14.63500
O	0.26500	37.61200	13.44800
H	0.14100	37.44000	15.55100
H	0.99000	38.29700	13.50500
C	9.79800	42.69300	11.33300
C	9.05600	41.38500	11.26300
N	9.57100	40.23600	10.66300
C	7.80200	41.00000	11.71500
C	8.66400	39.22900	10.76100
N	7.57200	39.66400	11.39900
H	9.17800	43.44600	11.85400
H	10.03200	43.08200	10.32000
H	10.75500	42.59100	11.88600
H	7.05000	41.60400	12.23200
H	8.81100	38.21600	10.37200
C	1.26700	34.41100	6.09500
C	2.36400	35.45000	6.00700
O	2.18800	36.63400	6.33500
O	3.52000	34.96400	5.58500
H	1.48700	33.52700	5.46900
H	0.29900	34.86300	5.80600
H	1.18000	34.08100	7.15200

H	3.13500	38.72300	12.88500
H	2.33500	40.01400	12.63800
H	0.71600	37.25300	8.01300
H	5.28900	39.84300	16.74500
H	10.48600	40.15700	10.21200
H	-1.45300	36.90200	9.46600
H	-0.54400	36.09300	14.58200
H	1.23600	36.24500	14.75600
C	8.33600	34.35200	11.78400
H	8.52900	33.30700	12.09700
H	8.58500	35.01800	12.63600
H	9.03300	34.58800	10.95300
C	8.05600	31.64500	8.97200
C	7.45500	30.68500	9.80600
C	7.25700	32.49500	8.18500
C	6.05200	30.57100	9.85000
C	5.85400	32.37600	8.22300
C	5.25300	31.41600	9.05800
H	8.08100	30.01900	10.42200
H	7.72000	33.24000	7.51800
H	5.58100	29.81800	10.50300
H	5.23000	33.03700	7.60100
H	4.15500	31.32400	9.09100
H	9.15500	31.73000	8.93400
O	4.41600	37.79200	12.20800
O	5.32100	35.87200	10.13900
N	5.53200	36.43500	4.63700
C	6.71600	37.19200	5.08600
C	7.74100	36.18400	5.64500
S	9.10900	36.94900	6.55600
C	6.39900	38.32400	6.06600
O	7.66300	34.98500	5.44700
H	5.05100	36.97400	3.90200
H	7.24200	37.64800	4.20900
H	4.26200	35.68400	5.44400
H	5.87200	35.57000	4.18600
C	4.97900	38.80500	6.30400
C	5.71100	38.04200	7.38400
H	7.17300	39.11000	6.07400
H	4.83000	39.88800	6.43800
H	4.14900	38.28300	5.80100
H	5.40500	37.00100	7.57700
H	6.05300	38.58200	8.28000
H	9.79700	35.77600	6.65400

Truncated Br-Fe^{IV}=O system from Figure S1B

O	1.811177	1.614236	2.905669
C	-2.199012	-1.768483	0.678534
O	-1.215121	-1.506092	-0.168011
C	-2.552488	-3.245916	0.925606
H	-1.963636	-3.501764	1.836252
H	-3.609939	-3.240640	1.257669
Br	0.000000	2.444216	-0.048505
Fe	0.000000	0.000000	0.000000
C	-2.066151	3.890650	5.434311
N	-2.755534	3.152640	4.378400
C	-2.315838	2.067669	3.693101

N	-3.025558	1.658752	2.626500
N	-1.211310	1.380125	4.028472
H	-2.114913	4.978154	5.225987
H	-0.999293	3.597237	5.472392
H	-2.808746	0.769548	2.138717
H	-3.862899	2.190998	2.350707
H	-0.878976	0.693971	3.334418
H	-0.571969	1.563420	4.825419
C	4.528402	-3.226191	-0.812680
C	3.638666	-2.113100	-0.395852
N	3.994568	-1.147557	0.537059
C	2.342019	-1.799035	-0.758915
C	2.947741	-0.310394	0.736989
N	1.932265	-0.685098	-0.047661
H	4.024860	-3.848291	-1.576189
H	4.787963	-3.884299	0.043983
H	5.481487	-2.857971	-1.248659
H	1.687766	-2.312441	-1.470904
H	2.925724	0.510670	1.469625
C	1.510610	1.098033	-5.425657
C	0.813040	0.582016	-4.195409
N	-0.317798	-0.232743	-4.233463
C	1.063937	0.752775	-2.841350
C	-0.707573	-0.525497	-2.964937
N	0.116455	0.063186	-2.091615
H	2.375368	1.721200	-5.130773
H	0.833087	1.722381	-6.045106
H	1.884062	0.268628	-6.062318
H	1.855037	1.340491	-2.364554
H	-1.570069	-1.148451	-2.704730
H	1.122546	1.024065	2.474318
H	1.616623	2.480582	2.489648
H	-3.682491	3.486994	4.083167
H	4.895538	-1.083573	1.018671
H	-0.789962	-0.560648	-5.080433
H	-2.513251	3.699320	6.433304
C	-2.330260	-4.319261	-0.151903
H	-2.610634	-5.313452	0.249014
H	-1.270745	-4.365966	-0.478207
H	-2.953949	-4.131133	-1.050417
O	0.000000	0.000000	1.664009
O	-2.804810	-0.893776	1.312630

Truncated Cl-Fe^{IV}=O system (in analogy to the Br-Fe^{IV}=O system)

O	-1.75616322	1.69164550	2.97552601
C	2.01477068	-1.97552959	0.63457381
O	1.65181960	-0.98176900	-0.16698852
C	3.52070957	-2.20376413	0.84507616
H	3.76549376	-1.59167424	1.73406711
H	3.61739384	-3.24832497	1.17683177
Cl	-2.28311935	-0.23631989	-0.04132987
Fe	0.00000000	0.00000000	0.00000000
C	-3.46780724	-2.44306397	5.58973704
N	-2.72993249	-3.07471039	4.49122588
C	-1.73357369	-2.50650892	3.77587535
N	-1.28356082	-3.13705852	2.67758583
N	-1.17495434	-1.33576553	4.11983056
H	-4.33017382	-3.07750634	5.82608329

H	-3.83867883	-1.44911014	5.29540919
H	-0.45180334	-2.81334721	2.16743593
H	-1.71302812	-4.01884534	2.39262626
H	-0.53900520	-0.91152974	3.43932895
H	-1.42501299	-0.74505163	4.92578491
C	2.73892362	4.80801900	-0.89570191
C	1.73118030	3.81548728	-0.44499896
N	0.78485295	4.07285393	0.54025062
C	1.51857232	2.50664517	-0.80753223
C	0.05957602	2.95271107	0.76708137
N	0.48447653	1.98160622	-0.04707917
H	3.36099507	4.37809246	-1.69282306
H	3.40943393	5.10824188	-0.07294408
H	2.27119326	5.72430861	-1.29341638
H	2.04871904	1.90913827	-1.54260597
H	-0.72104303	2.85809211	1.52288683
C	-1.41588316	1.35793819	-5.35890010
C	-0.76589159	0.73976303	-4.15128349
N	0.23440300	-0.23097722	-4.22431118
C	-0.95595486	0.93031563	-2.79864112
C	0.60926145	-0.58711832	-2.96944927
N	-0.10148475	0.10288791	-2.07237518
H	-2.16775505	2.09261369	-5.04062701
H	-1.92340833	0.59991938	-5.97734628
H	-0.68038006	1.87647711	-5.99544578
H	-1.65666550	1.59162820	-2.29894062
H	1.37368831	-1.32166475	-2.73702311
H	-1.19243142	1.01556099	2.51105614
H	-2.66568919	1.52648364	2.66826562
H	-2.97861756	-4.02569619	4.21226935
H	0.66282795	4.95583804	1.03198938
H	0.62059493	-0.62403268	-5.08030658
H	-2.84927016	-2.34081747	6.49664067
C	4.53350871	-1.90496018	-0.27262855
H	5.55208017	-2.10797863	0.09050209
H	4.48900949	-0.85369558	-0.59764153
H	4.36024691	-2.54097963	-1.15534197
O	0.00000000	0.00000000	1.66398564
O	1.20752636	-2.68201414	1.25257289

Cl-bound (SyrB2)Fe^{IV}=O (this includes the second-shell Arg residue) : – HAA via $\pi(S_{FeIII}=5/2)$ channel:

Reactant:

O	2.4612061	38.8708961	12.9847683
C	4.5257187	35.1597681	12.9962230
O	3.4299112	35.0073747	12.6258241
O	5.6031101	35.2665526	13.4117404
C	6.6665190	35.8510029	10.5426793
O	7.0069105	37.0334187	10.9832857
C	7.8250950	34.8688887	10.4274486
H	7.4801666	34.0327368	9.8007478
H	8.6419430	35.3839206	9.8934825
Cl	4.7706780	40.3407448	11.1130337
Fe	5.9433673	38.4683342	11.6909761
C	-0.7249998	37.7398794	9.5259973
N	0.4557399	36.9682757	9.1831607
C	1.2396417	36.3411636	10.0586365

N	2.3159313	35.6672796	9.6024920
N	0.9754403	36.3261632	11.3680435
H	-1.0746267	38.2530135	8.6199157
H	-0.4963913	38.4993903	10.2946511
H	3.0142981	35.3871844	10.2866691
H	2.7377198	35.9723156	8.7179659
H	1.6646133	35.9011560	11.9785176
H	0.2686525	36.8916265	11.8528418
H	0.7114172	36.8677019	8.1850541
H	-1.5406990	37.0983686	9.9066399
C	7.9859868	38.9808601	16.9919242
C	7.1137727	38.8863936	15.7855513
N	5.7308848	38.9494734	15.8455108
C	7.3986720	38.7266474	14.4503596
C	5.2250168	38.8243475	14.5998138
N	6.2197065	38.6896324	13.7352827
H	9.0424920	38.9129795	16.6939774
H	7.7794898	38.1627581	17.7040659
H	7.8409256	39.9382020	17.5227906
H	8.3669120	38.6368679	13.9646843
H	4.1639986	38.8551682	14.3413517
C	0.2889999	36.8228997	14.6349059
O	0.0397206	37.7028974	13.5547439
H	0.5088452	37.3707433	15.5721307
H	0.8471747	38.2430384	13.4122572
C	9.7979882	42.6928270	11.3329858
C	9.1016327	41.3676044	11.2816357
N	9.6573809	40.2426065	10.6884304
C	7.8689039	40.9502015	11.7240220
C	8.7828804	39.2170695	10.7785490
N	7.6843772	39.6170352	11.4020306
H	9.1607529	43.4253609	11.8493863
H	10.0057201	43.0751999	10.3182314
H	10.7569526	42.6270676	11.8762248
H	7.0909743	41.5245335	12.2191657
H	8.9459238	38.2162374	10.3880261
C	1.2670006	34.4108703	6.0949983
C	1.9293302	35.7669099	6.0518322
O	1.4597482	36.7435635	6.6420439
O	3.0474171	35.8105368	5.3842337
H	1.6020849	33.7717038	5.2660120
H	0.1734026	34.5280784	6.0888987
H	1.5539026	33.9329483	7.0490389
H	3.0978901	38.2871955	12.5113727
H	2.6468541	39.7339107	12.5797449
H	5.1818384	39.0776766	16.6893357
H	10.5664857	40.1982965	10.2399448
H	-0.6133118	36.2126334	14.8016154
H	1.1369594	36.1328190	14.4345983
C	8.3359977	34.3519294	11.7839777
H	9.1828797	33.6644130	11.6307383
H	7.5425610	33.8138383	12.3254807
H	8.6706891	35.1884773	12.4189851
O	4.5756333	37.6003180	11.8901973
O	5.5210575	35.5320197	10.2231278
N	4.1052997	38.2625944	5.6964812
C	5.1120965	38.4459874	6.7398252
C	6.3956493	37.7433211	6.2826801
S	7.6859169	37.6075809	7.5627713

C	4.6067649	37.9252405	8.0977612
O	6.5735743	37.3631825	5.1601270
H	3.2765123	38.8235516	5.8919313
H	5.3923839	39.5111636	6.8805953
H	3.5017825	36.7212171	5.5211483
H	4.4794473	38.5296595	4.7849478
C	3.3441271	38.6501953	8.5558850
H	8.5786707	37.0681782	6.7001938
H	5.3992863	38.1284610	8.8412295
O	4.4011221	36.5273634	7.9796937
H	4.8590744	36.0884349	8.7268266
H	3.1143022	38.3575523	9.5901981
H	2.5005373	38.3792017	7.9067073
H	3.4994605	39.7399685	8.5518574

Transition State:

O	2.3902330	38.9087405	13.1575422
C	4.4123016	35.2691905	12.9037301
O	3.3901912	34.8786016	12.4978436
O	5.4106371	35.6218649	13.3761229
C	6.7313479	35.9213613	10.6385097
O	6.8882533	37.1171042	11.1180729
C	8.0164617	35.1207136	10.4921704
H	7.8810944	34.4179073	9.6556430
H	8.8437496	35.8064183	10.2467888
Cl	4.6228435	40.6533980	11.5519803
Fe	5.7424481	38.5858139	11.7915815
C	-0.7249998	37.7398994	9.5259973
N	0.3959915	36.8674770	9.2285403
C	1.1319410	36.2054199	10.1204028
N	2.1706000	35.4631198	9.6741078
N	0.8658220	36.2238931	11.4274112
H	-0.9752183	38.2980109	8.6133661
H	-0.4686300	38.4615975	10.3217232
H	2.8303751	35.1334335	10.3732563
H	2.6276008	35.7509627	8.8044711
H	1.5447094	35.7878594	12.0420044
H	0.1970632	36.8409791	11.9091780
H	0.6717189	36.7471607	8.2365116
H	-1.6165860	37.1724105	9.8493178
C	7.9859948	38.9808961	16.9919322
C	7.0482565	38.8570001	15.8306164
N	5.6717194	38.9875211	15.9533193
C	7.2553823	38.6313046	14.4901762
C	5.0969016	38.8518090	14.7403726
N	6.0387016	38.6345129	13.8316192
H	9.0214210	38.8390471	16.6496628
H	7.7733758	38.2215726	17.7645116
H	7.9123242	39.9773042	17.4617384
H	8.1907847	38.4790691	13.9577577
H	4.0261579	38.9190573	14.5254864
C	0.2889999	36.8229187	14.6349259
O	-0.0020071	37.6978882	13.5617701
H	0.5123423	37.3751285	15.5682349
H	0.7854782	38.2759467	13.4368967
C	9.7979992	42.6928500	11.3329918
C	9.0527953	41.4027888	11.2662393

N	9.5730896	40.2496423	10.6987515
C	7.7937753	41.0487454	11.6831038
C	8.6506754	39.2661473	10.7842560
N	7.5557581	39.7220681	11.3759916
H	9.1724711	43.4558071	11.8190073
H	10.0616373	43.0603347	10.3253925
H	10.7329958	42.5962075	11.9129276
H	7.0351671	41.6643488	12.1579242
H	8.7833219	38.2533496	10.4153180
C	1.2669996	34.4108913	6.0949983
C	1.9568785	35.7524495	6.1324555
O	1.5055303	36.7007003	6.7862321
O	3.0727545	35.8268394	5.4684598
H	1.6328820	33.7912725	5.2645134
H	0.1779830	34.5540439	6.0313887
H	1.4858624	33.8979555	7.0487918
H	2.9433505	38.3794308	12.5248840
H	2.5874661	39.8157842	12.8681349
H	5.1711190	39.1669034	16.8178819
H	10.4891429	40.1601284	10.2719954
H	-0.5921415	36.1864618	14.8169877
H	1.1531802	36.1571331	14.4189767
C	8.3359987	34.3519494	11.7839937
H	9.2637541	33.7686969	11.6694556
H	7.5179920	33.6553873	12.0296655
H	8.4596064	35.0464914	12.6314243
O	4.1548077	37.6934788	11.5331981
O	5.6438264	35.4166984	10.3370004
N	3.9340441	38.2752535	6.1021362
C	5.0092708	38.3847758	7.0773286
C	6.2766762	37.7982532	6.4329012
S	7.6859169	37.6075809	7.5627713
C	4.6646868	37.6786942	8.4057006
O	6.3518558	37.5417005	5.2648456
H	3.0484439	38.6217514	6.4710094
H	5.2614729	39.4358604	7.3309104
H	3.5129869	36.7335822	5.6739761
H	4.1679339	38.7729521	5.2428449
C	3.5175330	38.3408612	9.1466567
H	8.5137298	37.1933008	6.5754990
H	5.5595988	37.7895283	9.0449243
O	4.4248014	36.3134325	8.1502404
H	4.8599251	35.8163523	8.8801977
H	3.5932070	37.9186311	10.2721210
H	2.5275309	38.0709980	8.7546300
H	3.6458785	39.4248780	9.2769916

Product:

O	2.4854240	38.6431362	12.9598287
C	4.3966793	34.9339827	13.0406479
O	3.3381372	34.7176172	12.5991378
O	5.4428343	35.1072445	13.5099195
C	6.6956148	35.7926980	10.5208648
O	7.0006942	36.9766390	10.9236994
C	7.8444177	34.8114707	10.4003084
H	7.5001485	33.9529328	9.8045747
H	8.6635567	35.3105437	9.8559566
Cl	4.7089323	40.3317777	11.1210209

Fe	5.8947027	38.4621592	11.7092808
C	-0.7249998	37.7398794	9.5259973
N	0.4728764	36.9744986	9.2171559
C	1.1408613	36.1994706	10.0692435
N	2.1979794	35.4970966	9.6048366
N	0.7841464	36.0582623	11.3513018
H	-0.8797671	38.4744640	8.7237956
H	-0.6109277	38.2838861	10.4795559
H	2.7901112	35.0358098	10.2883656
H	2.7042828	35.8524368	8.7826917
H	1.4354899	35.5648050	11.9528357
H	0.1655668	36.7008578	11.8674908
H	0.7786103	36.9167608	8.2283879
H	-1.6199219	37.0950743	9.5980808
C	7.9859878	38.9808591	16.9919152
C	7.0910774	38.8366499	15.8024199
N	5.7066204	38.7944939	15.8882150
C	7.3579217	38.7264162	14.4588991
C	5.1847184	38.6635852	14.6495530
N	6.1693868	38.6202197	13.7619162
H	9.0356148	39.0036587	16.6646500
H	7.8641398	38.1373259	17.6937232
H	7.7776252	39.9148874	17.5425926
H	8.3191230	38.7242923	13.9512906
H	4.1191385	38.6286448	14.4025720
C	0.2889999	36.8228997	14.6349059
O	0.0478501	37.6201160	13.4913762
H	0.5518093	37.4379496	15.5176817
H	0.8775920	38.1210677	13.3083400
C	9.7979972	42.6928180	11.3329868
C	9.1297470	41.3581673	11.2767267
N	9.7233255	40.2265933	10.7362950
C	7.8848518	40.9382370	11.6772194
C	8.8532759	39.1937312	10.8191398
N	7.7278896	39.5968397	11.3862447
H	9.1235470	43.4230618	11.8033390
H	10.0489491	43.0615975	10.3227367
H	10.7311811	42.6577944	11.9224164
H	7.0813295	41.5174062	12.1247336
H	9.0418599	38.1846415	10.4610836
C	1.2669996	34.4108703	6.0949983
C	1.9745748	35.7463642	6.0779876
O	1.5574702	36.7251643	6.7031512
O	3.0777196	35.7675736	5.3824201
H	1.5881448	33.7743816	5.2587979
H	0.1778989	34.5659270	6.0787037
H	1.5236750	33.9106837	7.0460213
H	3.0761965	38.0353281	12.4330730
H	2.6868567	39.5090878	12.5694334
H	5.1660803	38.8622010	16.7446034
H	10.6507724	40.1835083	10.3271208
H	-0.6295046	36.2616437	14.8722673
H	1.1082189	36.0883572	14.4753520
C	8.3359977	34.3519304	11.7839767
H	9.1744341	33.6454627	11.6779695
H	7.5279739	33.8530879	12.3423569
H	8.6758238	35.2151702	12.3794114
O	4.3708973	37.3526238	11.7033259
O	5.5275534	35.4281693	10.2601433

N	4.0389321	38.2271176	5.8130333
C	5.0571423	38.3914031	6.8418900
C	6.3490246	37.7381475	6.3310544
S	7.6859169	37.6075809	7.5627713
C	4.5758560	37.8202950	8.1895270
O	6.5004247	37.3957038	5.1928150
H	3.1469910	38.6246182	6.1102657
H	5.3172605	39.4550446	7.0295507
H	3.5462433	36.6689565	5.5268679
H	4.3342750	38.6451856	4.9309751
C	3.3822934	38.5470132	8.7124742
H	8.5618600	37.1188355	6.6537353
H	5.4048038	37.9675633	8.9163015
O	4.3421084	36.4219388	8.0460777
H	4.8625773	35.9521157	8.7298949
H	4.4955717	36.5954133	11.0883467
H	2.9510471	38.2170062	9.6572619
H	3.1030046	39.5294779	8.3242112

Cl-bound (SyrB2)Fe^{IV}=O (this model does not include the second-shell Arg residue) : – HAA via $\pi(S_{FeIII}=5/2)$ channel:

Reactant:

O	2.5263138	38.8639641	13.0772981
C	4.3380922	35.1339713	13.0228619
O	3.2382278	35.1160936	12.6503238
O	5.4210671	35.1175081	13.4553061
C	6.6829439	35.8168120	10.5941648
O	7.0205259	37.0367488	10.9540769
C	7.8779591	34.8910624	10.4210707
H	7.5651504	34.0662279	9.7630677
H	8.6954659	35.4426536	9.9283337
Cl	4.7806190	40.3201084	11.0417440
Fe	5.9654761	38.4591277	11.6708662
C	7.9859858	38.9808521	16.9919152
C	7.1252278	38.9112185	15.7771246
N	5.7410256	38.9512042	15.8255135
C	7.4252604	38.7881135	14.4418711
C	5.2499386	38.8455161	14.5708853
N	6.2555898	38.7478287	13.7155590
H	9.0460117	38.9597899	16.6983556
H	7.8036096	38.1261188	17.6675216
H	7.8088042	39.9082838	17.5653512
H	8.3991681	38.7223127	13.9630853
H	4.1891651	38.8610111	14.2962731
C	0.2890009	36.8228887	14.6349019
O	0.0438772	38.1251056	14.1839784
H	0.9650836	36.7815684	15.5224159
H	0.8591982	38.4434996	13.7544747
C	9.7979882	42.6928100	11.3329738
C	9.1078900	41.3683048	11.2548474
N	9.6494453	40.2657548	10.6075841
C	7.8914088	40.9327491	11.7211267
C	8.7774169	39.2347659	10.6939686
N	7.7032939	39.6121487	11.3647432

H	9.1684550	43.4035373	11.8883696
H	9.9796624	43.1128637	10.3276307
H	10.7708712	42.6183550	11.8510657
H	7.1223270	41.4852833	12.2541974
H	8.9200385	38.2480176	10.2611667
C	1.2669996	34.4108603	6.0949963
C	1.8877190	35.7860190	5.9991939
O	1.3477191	36.7909600	6.4333129
O	3.0795158	35.7637361	5.4301414
H	1.4085899	33.8533340	5.1553265
H	0.2011212	34.4929132	6.3491474
H	1.7937268	33.8555180	6.8904779
H	3.0360491	38.1774643	12.5977290
H	2.7285676	39.6534644	12.5476124
H	5.1775728	39.0416611	16.6639525
H	10.5386436	40.2403467	10.1213899
H	-0.6697088	36.3662804	14.9410924
H	0.7387383	36.1664517	13.8587568
C	8.3359947	34.3519164	11.7839757
H	9.1753920	33.6467805	11.6648258
H	7.5075667	33.8337375	12.2926103
H	8.6616415	35.1792097	12.4365904
O	4.6292855	37.5845551	11.9519755
O	5.5398861	35.4185153	10.4341335
N	3.9298591	38.2376621	6.0817375
C	4.9551668	38.3355404	7.1095999
C	6.2981080	38.0045351	6.4421623
S	7.6859148	37.6075704	7.5627689
C	4.6426266	37.4493121	8.3237955
O	6.4677457	38.0622743	5.2547390
H	2.9991065	38.4526583	6.4425244
H	5.0795976	39.3670213	7.5075201
H	3.5260724	36.6588579	5.5966565
H	4.1439693	38.8324341	5.2831008
C	3.3024162	37.7707229	8.9811199
H	8.5651062	37.5409151	6.5360036
H	5.4372281	37.6677128	9.0645572
O	4.7162980	36.1062736	7.9061052
H	4.8065505	35.5806255	8.7196969
H	3.2199728	37.1587020	9.8923303
H	2.4701703	37.5199373	8.3062555
H	3.2505269	38.8289781	9.2800217

Transition State:

O	2.5307726	38.9719975	13.1518904
C	4.3311466	35.1881156	12.9202908
O	3.3091889	34.8734411	12.4680338
O	5.3387632	35.4584271	13.4440528
C	6.7622583	35.8439964	10.6177515
O	6.9881876	37.0571460	11.0429562
C	8.0193241	35.0128528	10.4397601
H	7.8257955	34.2528596	9.6674210
H	8.8548800	35.6526418	10.1121423
Cl	4.7787860	40.4802368	11.0859827
Fe	5.8326889	38.4797994	11.7470312
C	7.9859928	38.9808851	16.9919272
C	7.0659698	38.8583119	15.8165002

N	5.6848598	38.9575183	15.9173634
C	7.3006681	38.6611389	14.4769162
C	5.1349964	38.8259360	14.6903220
N	6.0974808	38.6473702	13.7970211
H	9.0282838	38.8698568	16.6583184
H	7.7840406	38.2012034	17.7475423
H	7.8853875	39.9652054	17.4829252
H	8.2472441	38.5392370	13.9568133
H	4.0659168	38.8874349	14.4485741
C	0.2889999	36.8229087	14.6349219
O	0.0661707	38.1472178	14.2406924
H	0.9758158	36.7304042	15.5100830
H	0.8846122	38.4767170	13.8233036
C	9.7979952	42.6928380	11.3329888
C	9.1134364	41.3691094	11.2991260
N	9.6532749	40.2455350	10.6906003
C	7.8948009	40.9552717	11.7765237
C	8.7722711	39.2233080	10.8115364
N	7.6989007	39.6269301	11.4661881
H	9.1632927	43.4219600	11.8580565
H	9.9858327	43.0789592	10.3148762
H	10.7684629	42.6431399	11.8592528
H	7.1267955	41.5349217	12.2819998
H	8.9127402	38.2232548	10.4099488
C	1.2669996	34.4108813	6.0949973
C	1.8949274	35.7792855	6.2459708
O	1.4282733	36.6537666	6.9587367
O	3.0015360	35.9061223	5.5362650
H	1.2434904	34.1139858	5.0341156
H	0.2567285	34.4094710	6.5267949
H	1.8980156	33.6788687	6.6283190
H	3.0286769	38.3306505	12.5857431
H	2.7034327	39.8080044	12.6879738
H	5.1606093	39.1064304	16.7727085
H	10.5424879	40.2013117	10.2062419
H	-0.6754183	36.3746849	14.9356636
H	0.7128252	36.1876031	13.8262782
C	8.3359967	34.3519404	11.7839897
H	9.2289948	33.7078738	11.7155326
H	7.4851836	33.7346543	12.1146570
H	8.5143535	35.1174316	12.5573462
O	4.3020366	37.5860699	11.6889435
O	5.6578150	35.3467079	10.4253404
N	3.8295912	38.3353970	6.3730977
C	4.9214992	38.3783446	7.3314916
C	6.2216743	38.0681192	6.5649952
S	7.6859148	37.6075694	7.5627709
C	4.6829515	37.4262920	8.5149504
O	6.3045521	38.1824107	5.3729581
H	2.9233257	38.4837950	6.8205576
H	5.0785529	39.3842899	7.7785291
H	3.4410548	36.7829483	5.7887875
H	3.9689938	39.0001001	5.6141151
C	3.4222890	37.7573360	9.3051599
H	8.4824676	37.5720640	6.4695647
H	5.5443157	37.6053508	9.1862888
O	4.6895116	36.1099089	8.0343456
H	4.8876824	35.5484320	8.8079967
H	3.6399815	37.3982933	10.4186108

H	2.5384887	37.2120919	8.9401884
H	3.2476357	38.8364275	9.4236465

Product:

O	2.5240372	38.8118777	13.1511778
C	4.7280570	35.2443650	13.5630300
O	3.6203591	34.9400332	13.3949211
O	5.8418789	35.5173242	13.7761767
C	6.6223946	35.7885232	10.6394241
O	6.9400924	37.0080851	10.9434628
C	7.7965342	34.8473845	10.4312586
H	7.4497770	33.9994261	9.8209779
H	8.5839978	35.3829429	9.8762762
Cl	4.7241092	40.4115471	11.1128969
Fe	5.8427116	38.4870485	11.7227364
C	7.9859858	38.9808521	16.9919052
C	7.0809824	38.8865912	15.8090168
N	5.6970297	38.9053921	15.9009896
C	7.3388472	38.7715311	14.4651789
C	5.1669956	38.8023015	14.6615220
N	6.1472360	38.7220782	13.7740637
H	9.0340173	38.9689535	16.6578147
H	7.8398303	38.1327116	17.6843869
H	7.8184508	39.9134438	17.5598178
H	8.2970162	38.7238830	13.9537673
H	4.0973939	38.8076734	14.4098036
C	0.2889999	36.8228897	14.6349019
O	-0.0225873	37.9603051	13.8847329
H	0.7584414	37.0559905	15.6209924
H	0.8232962	38.3391438	13.5752079
C	9.7979982	42.6928010	11.3329738
C	9.1234264	41.3617233	11.2716304
N	9.6724614	40.2484617	10.6502241
C	7.9054967	40.9321996	11.7383837
C	8.7974072	39.2179754	10.7545224
N	7.7199659	39.6059615	11.4102487
H	9.1536715	43.4050418	11.8691907
H	9.9866491	43.0994877	10.3232012
H	10.7661787	42.6405993	11.8628833
H	7.1333271	41.4972240	12.2544346
H	8.9451000	38.2229441	10.3415659
C	1.2669996	34.4108603	6.0949963
C	1.8935173	35.7859711	6.0603823
O	1.3805692	36.7628894	6.5820667
O	3.0571058	35.7965178	5.4354069
H	1.3683932	33.9121625	5.1178885
H	0.2122909	34.4833286	6.3942178
H	1.8173828	33.8028002	6.8339664
H	3.0237675	38.1415644	12.6135637
H	2.6847807	39.6255787	12.6465441
H	5.1590241	38.9874485	16.7567653
H	10.5646267	40.2157856	10.1701097
H	-0.6435992	36.2688338	14.8482506
H	0.9770421	36.1237026	14.1102031
C	8.3359947	34.3519174	11.7839747
H	9.1862661	33.6657184	11.6368644
H	7.5495768	33.8212116	12.3440285
H	8.6695912	35.2017924	12.4018938

O	4.3309920	37.4177326	11.8386476
O	5.4605912	35.3637026	10.5555041
N	3.9144983	38.2571498	6.1138813
C	4.9601530	38.3296294	7.1203465
C	6.2753978	37.9116853	6.4470318
S	7.6859148	37.6075704	7.5627699
C	4.6128229	37.4697516	8.3641622
O	6.4063955	37.8472922	5.2554075
H	2.9956540	38.4740523	6.5053742
H	5.1336688	39.3580814	7.5041731
H	3.5026878	36.6899980	5.6138579
H	4.1168144	38.8580610	5.3171166
C	3.2996241	37.8407668	8.9701054
H	8.5349746	37.4151475	6.5270283
H	5.4121516	37.6966289	9.1002330
O	4.6703524	36.1169081	7.9692759
H	4.7292466	35.5952499	8.7883379
H	4.3908668	36.5866089	11.3119499
H	2.3973087	37.3509785	8.5948826
H	3.2409689	38.6654047	9.6817503

(TMG$_3$tren)Fe^{IV}=O – self-decay via π(S_{FeIII}=5/2) channel for HAA:

Reactant

Fe	0.0015693	-0.0000372	0.3662862
N	-0.0000785	-0.0018133	2.5297535
C	-0.7995873	-1.1792512	2.9652558
H	-1.1268880	-1.0520752	4.0123642
H	-0.1554256	-2.0685242	2.9129822
C	-1.9779356	-1.3655026	2.0197986
H	-2.5004172	-2.3085866	2.2518602
H	-2.7112889	-0.5536466	2.1714546
N	-1.4452920	-1.3728086	0.6535828
C	-2.0194181	-2.1384343	-0.2868185
N	-3.3431977	-2.4478840	-0.2629071
C	-4.3577305	-1.5338471	0.2509669
H	-3.9394399	-0.5288927	0.3674308
H	-4.7590995	-1.8756273	1.2203749
H	-5.1920448	-1.4845583	-0.4688094
C	-3.8594399	-3.7344758	-0.7347471
H	-3.0353809	-4.4468474	-0.8677948
H	-4.4046859	-3.6298778	-1.6882994
H	-4.5559285	-4.1331805	0.0216688
N	-1.2642070	-2.6596208	-1.2822520
C	-1.7656543	-2.8281072	-2.6430119
H	-2.7487428	-2.3518387	-2.7475032
H	-1.8500768	-3.8936256	-2.9165741
H	-1.0626738	-2.3394850	-3.3382810
C	0.1430414	-2.9808734	-1.1035006
H	0.3930471	-2.9253203	-0.0377188
H	0.7821779	-2.2719732	-1.6541629
H	0.3282383	-4.0040800	-1.4742517
C	1.4184036	-0.1056538	2.9679924
H	1.4699462	-0.4525143	4.0153810
H	1.8663751	0.8966829	2.9156876
C	2.1703183	-1.0335258	2.0235473

H	3.2476193	-1.0156517	2.2574841
H	1.8324920	-2.0744900	2.1733143
N	1.9134075	-0.5662031	0.6576937
C	2.8642377	-0.6784377	-0.2820228
N	3.7939328	-1.6699803	-0.2597607
C	3.5095803	-3.0064176	0.2516469
H	2.4299460	-3.1463376	0.3683896
H	4.0068039	-3.1857833	1.2206228
H	3.8830770	-3.7523694	-0.4698511
C	5.1654272	-1.4735228	-0.7334352
H	5.3703169	-0.4034377	-0.8653487
H	5.3455373	-1.9968901	-1.6880278
H	5.8602808	-1.8784820	0.0210746
N	2.9383425	0.2385899	-1.2753225
C	3.3306503	-0.1096690	-2.6380031
H	3.4113484	-1.1989383	-2.7436430
H	4.2939685	0.3514620	-2.9151721
H	2.5527067	0.2539195	-3.3303965
C	2.5127152	1.6174115	-1.0935446
H	2.3415204	1.8046603	-0.0268900
H	1.5778408	1.8167572	-1.6414185
H	3.3052802	2.2901223	-1.4652327
C	-0.6203556	1.2779216	2.9678388
H	-0.3480814	1.4946057	4.0158861
H	-1.7126099	1.1648577	2.9136636
C	-0.1919620	2.3941865	2.0254906
H	-0.7486606	3.3168906	2.2595476
H	0.8775953	2.6241516	2.1775415
N	-0.4638085	1.9388708	0.6584055
C	-0.8425679	2.8198598	-0.2800885
N	-0.4501259	4.1212701	-0.2539857
C	0.8496958	4.5425327	0.2580265
H	1.5111684	3.6776469	0.3728820
H	0.7565513	5.0607716	1.2280029
H	1.3083501	5.2409728	-0.4622221
C	-1.3073569	5.2115641	-0.7233957
H	-2.3359388	4.8531158	-0.8558961
H	-0.9449379	5.6329349	-1.6763973
H	-1.3050280	6.0131556	0.0341316
N	-1.6713238	2.4267221	-1.2759051
C	-1.5679363	2.9487094	-2.6355959
H	-0.6640382	3.5620389	-2.7397461
H	-2.4485873	3.5555876	-2.9071776
H	-1.4973640	2.0971101	-3.3332390
C	-2.6517016	1.3670058	-1.0993254
H	-2.7210669	1.1131844	-0.0352574
H	-2.3598195	0.4635070	-1.6582694
H	-3.6328446	1.7204579	-1.4616726
O	0.0023692	0.0016860	-1.2567297

Transition State:

Fe	-0.0465525	-0.0702939	0.2413175
N	-0.0303507	-0.0332306	2.5714672
C	-0.7914024	-1.2181777	3.0151898
H	-1.1176747	-1.1076338	4.0660020
H	-0.1301109	-2.0953522	2.9587244
C	-1.9813701	-1.4416165	2.0885712

H	-2.4798141	-2.3915653	2.3452258
H	-2.7300717	-0.6448563	2.2439498
N	-1.4804609	-1.4616593	0.7122152
C	-2.0762343	-2.2521388	-0.1935192
N	-3.4102771	-2.5121418	-0.1591245
C	-4.3737607	-1.5310596	0.3272290
H	-3.9117080	-0.5358630	0.3618575
H	-4.7516376	-1.7879070	1.3319559
H	-5.2312236	-1.4984815	-0.3654617
C	-3.9820906	-3.7909244	-0.5838450
H	-3.1861199	-4.5364708	-0.7064962
H	-4.5363555	-3.6949083	-1.5332690
H	-4.6817134	-4.1413451	0.1933422
N	-1.3383553	-2.8378156	-1.1663788
C	-1.8369317	-3.0212037	-2.5270009
H	-2.8300385	-2.5675636	-2.6332187
H	-1.8977202	-4.0896193	-2.7942396
H	-1.1451023	-2.5160997	-3.2219820
C	0.0779020	-3.1159989	-0.9992528
H	0.3390384	-3.0669750	0.0652209
H	0.6866776	-2.3817340	-1.5548378
H	0.2948120	-4.1267310	-1.3852734
C	1.3959418	-0.0963171	2.9506257
H	1.5145750	-0.4434354	3.9939245
H	1.8195312	0.9161914	2.8846725
C	2.1521304	-1.0067034	1.9849817
H	3.2320318	-0.9630940	2.2019056
H	1.8399460	-2.0543633	2.1415828
N	1.8736007	-0.5633452	0.6149958
C	2.8192538	-0.6455936	-0.3340998
N	3.7876226	-1.5959873	-0.3150918
C	3.5566111	-2.9363273	0.2153974
H	2.4818940	-3.1165491	0.3299249
H	4.0567963	-3.0828069	1.1880151
H	3.9625722	-3.6745915	-0.4961751
C	5.1396350	-1.3561578	-0.8235002
H	5.2986654	-0.2821410	-0.9837430
H	5.3195619	-1.8947357	-1.7696022
H	5.8659343	-1.7150716	-0.0754474
N	2.8245068	0.2549481	-1.3488188
C	3.2025398	-0.1037029	-2.7139567
H	3.3378369	-1.1893837	-2.7978938
H	4.1333008	0.4010769	-3.0241355
H	2.3881031	0.2014376	-3.3922280
C	2.3390125	1.6185044	-1.1892192
H	2.1920492	1.8326229	-0.1233202
H	1.3788584	1.7499478	-1.7140328
H	3.0845179	2.3170993	-1.6069852
C	-0.6820742	1.2304866	2.9618285
H	-0.4402410	1.4961913	4.0078287
H	-1.7710529	1.0917646	2.8965349
C	-0.2732473	2.3530770	2.0182449
H	-0.8445102	3.2634801	2.2640579
H	0.7897825	2.5983530	2.1823989
N	-0.5157684	1.9414580	0.6300798
C	-0.7973526	2.8812582	-0.2699027
N	-0.4661041	4.1939086	-0.1124293
C	0.7953032	4.6192358	0.4873884
H	1.4989539	3.7790801	0.5283696

H	0.6569656	5.0280207	1.5029684
H	1.2366220	5.4083375	-0.1445677
C	-1.3334540	5.2836605	-0.5656147
H	-2.3244713	4.8934822	-0.8308825
H	-0.9054363	5.8092566	-1.4365905
H	-1.4472970	6.0102702	0.2564751
N	-1.4842901	2.5598899	-1.4129969
C	-1.1715259	3.1992598	-2.6959110
H	-0.3261383	3.8879449	-2.5817675
H	-2.0398697	3.7551293	-3.0859733
H	-0.8925396	2.4166675	-3.4211998
C	-2.2508546	1.3595322	-1.5128426
H	-2.6717173	1.0703825	-0.5400643
H	-1.5383102	0.4963818	-1.8377024
H	-3.0291105	1.4574137	-2.2863965
O	-0.1855142	-0.1342536	-1.5590532

Product

Fe	-0.0194483	-0.0036829	0.2125430
N	-0.0208577	-0.0065987	2.5686215
C	-0.8613843	-1.1509187	2.9698507
H	-1.2147997	-1.0380525	4.0117782
H	-0.2494653	-2.0637344	2.9207404
C	-2.0350977	-1.2980077	2.0067368
H	-2.6038963	-2.2093831	2.2546611
H	-2.7302125	-0.4489425	2.1347361
N	-1.5047906	-1.3575965	0.6417920
C	-2.0764173	-2.1730652	-0.2538955
N	-3.3990483	-2.4876803	-0.2195627
C	-4.4138954	-1.5513392	0.2520537
H	-3.9995642	-0.5382406	0.3001206
H	-4.7989893	-1.8318627	1.2472823
H	-5.2587821	-1.5525683	-0.4570359
C	-3.9074203	-3.8022347	-0.6159821
H	-3.0777816	-4.5132095	-0.7184835
H	-4.4632262	-3.7549686	-1.5679778
H	-4.5919442	-4.1673114	0.1678300
N	-1.3166799	-2.7363842	-1.2276699
C	-1.8204274	-2.9826623	-2.5752108
H	-2.8090071	-2.5226162	-2.7023040
H	-1.8982501	-4.0616598	-2.7920388
H	-1.1211659	-2.5333399	-3.3015318
C	0.0940574	-3.0408257	-1.0361535
H	0.3397064	-2.9622050	0.0300238
H	0.7243400	-2.3343778	-1.5998154
H	0.2911132	-4.0699224	-1.3826432
C	1.3914170	-0.1656875	2.9703840
H	1.4677003	-0.5515244	4.0040514
H	1.8728897	0.8225807	2.9452450
C	2.1125297	-1.0842720	1.9880622
H	3.1875358	-1.1159712	2.2300371
H	1.7335563	-2.1163447	2.0992132
N	1.8903924	-0.5715659	0.6342403
C	2.8609991	-0.6490191	-0.2872769
N	3.7945643	-1.6358066	-0.2907320
C	3.5133500	-2.9865925	0.1837140
H	2.4341130	-3.1314347	0.2964215

H	4.0096185	-3.1909632	1.1479961
H	3.8889464	-3.7116647	-0.5577949
C	5.1599076	-1.4265351	-0.7752088
H	5.3608148	-0.3534132	-0.8874230
H	5.3297405	-1.9293169	-1.7428569
H	5.8641368	-1.8469129	-0.0380605
N	2.9429816	0.3040413	-1.2483180
C	3.2747651	-0.0101229	-2.6346995
H	3.4236497	-1.0901726	-2.7557057
H	4.1860759	0.5188869	-2.9608735
H	2.4281220	0.2989559	-3.2712481
C	2.4870338	1.6665960	-1.0284939
H	2.3609958	1.8391591	0.0480405
H	1.5257139	1.8422088	-1.5387133
H	3.2425833	2.3666524	-1.4247120
C	-0.5882939	1.2913660	2.9777543
H	-0.3011193	1.5413177	4.0158709
H	-1.6855012	1.2201412	2.9422087
C	-0.1396893	2.3838686	2.0126122
H	-0.6349809	3.3343276	2.2712035
H	0.9461827	2.5534560	2.1226369
N	-0.4805309	1.9644787	0.6510106
C	-0.8403495	2.8793999	-0.2473560
N	-0.4652144	4.1847237	-0.1997344
C	0.8388528	4.6065766	0.3033992
H	1.5124457	3.7466804	0.3785810
H	0.7585657	5.0933947	1.2903203
H	1.2747209	5.3320708	-0.4043187
C	-1.3461091	5.2771741	-0.6184943
H	-2.3693196	4.9081151	-0.7643147
H	-0.9916849	5.7475400	-1.5515690
H	-1.3597378	6.0454408	0.1731337
N	-1.6790501	2.5044722	-1.2773777
C	-1.5221872	3.0787405	-2.6215438
H	-0.5996158	3.6689864	-2.6660374
H	-2.3790071	3.7184829	-2.8844081
H	-1.4483105	2.2538133	-3.3473565
C	-2.6051215	1.4986182	-1.1232730
H	-2.8014456	1.1410348	-0.1157363
H	-0.8280272	-0.0770814	-2.1470139
H	-3.2502851	1.2697396	-1.9704812
O	-0.0108557	-0.0134249	-1.6350450