Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

Mechanistic study on a dinuclear iron water oxidation catalyst with high catalytic activity

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Computational details

All Density Function Theory (DFT) calculations were performed with Jaguar 10.3 program package[1] by Schrödinger, LLC, New York, NY, 2019. All geometrical optimizations were performed with the B3LYP-D3 functional (Becke's three-parameter hybrid functional and the LYP correlation functional[2] with adding the D3 version of Grimme's dispersion with the original D3[3] damping function) and the LACVP** basis set that applies effective core potentials on heavy atoms to save computational cost.[4] Single-point calculations using the B3LYP-D3 functional with a larger basis set LACV3P**++[5] were first performed on the optimized geometries and then compared to the performance of three other functionals, ωB97M-V[6], M06-L-D4[7, 8] and PBE0-D4[8, 9]. As indicated in Table S1, the B3LYP-D3,ωB97M-V and M06-L-D4 functionals favor the same spin multiplicity and degeneracies for all species while the PBE0-D4 functional shows differences of favored spin multiplicity for $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$ from 5 (calculated with the B3LYP-D3,ωB97M-V and M06-L-D4 functionals) to 11, for $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$ from 2 to 10. For the calculated reduction potentials of two PCET processes proposed in our mechanism, the B3LYP-D3 functional produces similar results to the more accurate ωB97M-V[10] functional as indicated in Table S2. Consequently, all calculations were performed with B3LYP-D3. Frequency calculations with LACVP** were performed on optimized geometries to verify that the geometries correspond to the minima and to acquire the thermal corrections to Gibbs free energy. The solvation free energies were computed by adapting the Poisson Boltzmann Finite element method (PBF) implemented in Jaguar 10.3.[11, 12] The Gibbs free energies (G) are calculated at standard state of 1M(aq) (and 1 atm for gaseous species) and the G of each species is defined as the following equation $G = E(\text{B3LYP-D3/LACV3P}^{**++}) + G_{solv} + ZPE + H_{298} - T*S_{298}$ + 1.90 kcal/mol (a concentration correction to the solvation free energy when changing from 1 M(g) to 1 M(aq) that by default is calculated at 1M(g) to 1M(aq) in Jaguar). The water oxidation reaction for this dinuclear includes three steps, oxidations to high-valent species $[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}$, decomposition into two identical mononuclear moieties ($[Cl\text{-}Fe^{IV}\text{=}O]^{+}$, $[O\text{-}Fe^{IV}\text{=}Cl]^{+}$) by Cl^- attacking, radical coupling between these two mononuclear moieties ($[Cl\text{-}Fe^{IV}\text{=}O\bullet\bullet\bullet O\text{=}Fe^{IV}\text{-}Cl]^{2+}$, triplet-tripet) in an open-shell antiferromagnetic fashion.

Transition metals have different possibilities in spin states. Consequently, different spin multiplicities from low to high have been tested when optimizing different species at their different oxidation states. The structures with lowest Gibbs free energies were used to calculate redox potentials. The energy differences of each species with different spin multiplicities are shown in Table S1.

After obtaining the Gibbs free energy of all species, the standard reduction potentials were calculated based on the Nernst equation under standard conditions (at 1atm and 25 °C):

$$E^0 = -\frac{\Delta G^0}{nF}$$

where ΔG^0 is the reactive Gibbs free energy under standard conditions; n is the number of electrons transferred in each sub-reaction; F is the Faraday constant, 96485 C/mol; E^0 is the standard reduction potentials for the corresponding reaction. Standard hydrogen electrode (SHE) is used as the reference with an absolute electrode potential of 4.28 V.[13, 14] The experimental value of -270.28 kcal/mol is used as the Gibbs free energy of proton at 1M, determined by Tissandier et al.[15] As the cyclic voltammetry was carried out at pH 1 against Ag/AgCl reference electrode, the Gibbs free energy of proton is calibrated based on the following equation:

$$G = G^0 - 2.303RT * pH$$

All the potentials in this study were reported against Ag/AgCl reference electrode by the conversion equation shown below:

$$E_{SHE} = E_{Ag/AgCl} + 0.059 * pH + E_{Ag/AgCl}^{0}$$

where $E_{Ag/AgCl}^{0}$ =0.1976 V at 25 °C.[16]

To identify the transition states of Fe-O-Fe bond breakage by Cl^- attacking and O-O bond formation by radical coupling, the potential energy surfaces were searched by carrying out relaxed coordinate scans of the Cl^--Fe distance (from 4.888 Å to 2.188 Å) and the terminal O-O bond distance (from 4.093 Å to 1.200 Å) of the dimer at the antiferromagnetic open shell singlet state ([Cl-Fe^{IV}=O•••O=Fe^{IV}-Cl]$^{2+}$,

triplet-tripet), respectively. Frequencies calculations were conducted to ensure that there was only one imaginary frequency for each obtained transition state and to acquire the thermal corrections for calculating Gibbs free energy.

Table S1. The energy differences in kcal/mol of $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$, $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$, $[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}$ among different multiplicity with B3LYP-D3, ωB97M-V, M06-L-D4 and PBE0-D4 functionals

	Spin multiplicity	B3LYP-D3	ωB97M-V	M06-L-D4	PBE0-D4
$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$	1, unrestricted	18.09	12.28	13.85	25.50
	3	15.88	12.04	4.50	24.60
	5	0.00*	0.00*	0.00*	2.90
	7	0.95	1.37	0.45	3.82
	9	10.15	13.89	8.77	8.38
	11	2.88	6.16	3.51	0.00*
	Spin multiplicity	B3LYP-D3	ωB97M-V	M06-L-D4	PBE0-D4
$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$	2	0.00*	0.00*	0.78	2.34
	4	0.70	0.35	0.00*	3.22
	6	10.07	12.70	6.45	8.89
	8	20.39	26.33	16.15	14.79
	10	7.12	14.67	6.46	0.00*
	Spin multiplicity	B3LYP-D3	ωB97M-V	M06-L-D4	PBE0-D4
$[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}$	1, unrestricted	0.00*	0.00*	0.00*	0.00*
	3	9.34	6.26	13.33	9.83
	5	0.84	0.31	2.10	0.83
	7	33.17	13.71	8.51	5.55
	9	22.01	21.98	31.68	16.08
	11	31.73	34.73	37.30	22.48

* indicates the spin states of the lowest free energies with different functionals

Table S2. The calculated potentials in V with B3LYP-D3, ωB97M-V, M06-L-D4 and PBE0-D4 functionals for two PCET processes proposed in our mechanism

Functional	$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}+e^{-}+H^{+}\rightarrow$ $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$	$[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}+e^{-}+H^{+}\rightarrow$ $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$
B3LYP-D3	1.66	1.44
ωB97M-V	1.65	1.62
M06-L-D4	1.06	0.96
PBE0-D4	1.68	1.52

Table S3. The spin density distributions on the axial atoms of $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$, $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$, $[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}$ among different multiplicity with B3LYP-D3 functional

	Spin multiplicity	O1	Fe1	O2	Fe2	Cl
$[Cl\text{-}Fe^{III}\text{-}O\text{-}$	1, unrestricted	-0.00230	0.51426	0.40153	-0.91995	-0.02800

Fe^{III}-OH_2]$^{3+}$	3	-0.00069	0.38232	0.72776	0.93855	0.02016
	5*	0.02003	3.88713	0.62818	-0.92133	-0.02616
	7	0.01976	3.88708	0.69906	1.03712	0.06548
	9	0.02156	3.90463	0.63670	2.81526	0.08494
	11	0.01911	3.92662	0.84686	3.98160	0.40457
	Spin multiplicity	O1	Fe1	O2	Fe2	Cl
[Cl-Fe^{III}-O-Fe^{IV}-OH]$^{3+}$	2*	0.13932	1.24577	0.60902	-0.94259	-0.02958
	4	0.15308	0.92846	0.74989	1.25409	0.04526
	6	0.15248	0.92227	0.67650	3.06887	-0.03407
	8	0.01390	2.80609	0.63151	3.09807	-0.02822
	10	0.47518	3.97793	0.60417	3.16761	0.05989
	Spin multiplicity	O1	Fe1	O2	Fe2	Cl
[Cl-Fe^{IV}-O-Fe^{IV}=O]$^{3+}$	1, unrestricted*	-0.99249	-1.04192	0.68599	1.31371	0.05619
	3	1.00122	1.03265	-0.44354	0.49775	0.01531
	5	0.99499	1.03357	0.72691	1.31021	0.05191
	7	0.75264	2.93891	0.67263	1.37050	0.06916
	9	1.46490	3.92622	0.65887	1.44708	0.10874
	11	1.46718	3.89893	0.56141	3.19644	0.07992

* indicates the spin states of the lowest free energies

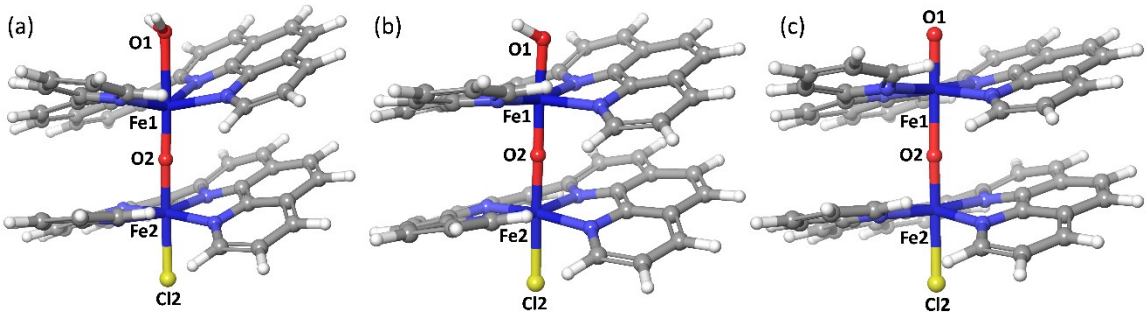

Figure S1. The numbering of the axial atoms of (a) [Cl-Fe^{III}-O-Fe^{III}-OH_2]$^{3+}$ (complex 1), (b) [Cl-Fe^{III}-O-Fe^{IV}-OH]$^{3+}$ (complex 2) and (c) [Cl-Fe^{IV}-O-Fe^{IV}=O]$^{3+}$ (complex 3)

Table S4. The absolute energies of reactant, transition state (TS) and product of the nitrate attack and water attack

Nitrate attack	E (B3LYP-D3/LACV3P^{**++}) (a.u.)	G_{solv} (kcal/mol)	ZPE (kcal/mol)	ΔH_{298} (kcal/mol)	ΔS_{298} (cal/(k•mol))	Energy barrier (kcal/mol)	Reaction energy (kcal/mol)
Reactant (Quintet)	-3577.363988	-140.295	472.438	32.193	266.202	-	-
TS (Quintet)	-3577.334373	-136.702	472.429	31.835	264.174	22.4	-
Product (Quintet)	-3577.365197	-126.947	472.321	32.399	269.009	-	11.8
Water attack	E (B3LYP-D3/LACV3P^{**++}) (a.u.)	G_{solv} (kcal/mol)	ZPE (kcal/mol)	ΔH_{298} (kcal/mol)	ΔS_{298} (cal/(k•mol))	Energy barrier (kcal/mol)	Reaction energy (kcal/mol)

Reactant (Quintet)	-3373.085846	-260.261	476.98	31.885	264.105	-	-
TS (Quintet)	-3373.056097	-257.342	477.513	30.994	257.579	23.2	-
Product (Quintet)	-3373.080799	-254.714	478.715	30.769	256.145	-	11.7

Table S5. The absolute energies of reactant, transition state (TS) and product of the chloride attack and radical coupling processes

Chloride attack	E (B3LYP-D3/LACV3P^{**++}) (a.u.)	G_{solv} (kcal/mol)	ZPE (kcal/mol)	ΔH_{298} (kcal/mol)	ΔS_{298} (cal/(k•mol))	Energy barrier (kcal/mol)	Reaction energy (kcal/mol)
Reactant (Quintet)	-3757.217386	-141.518	461.566	31.500	271.036	-	-
TS (Quintet)	-3757.182808	-142.616	461.089	31.103	270.389	19.9	-
Product (Quintet)	-3757.227903	-128.356	462.193	31.629	276.925	-	5.6
Radical coupling	E (B3LYP-D3/LACV3P^{**++}) (a.u.)	G_{solv} (kcal/mol)	ZPE (kcal/mol)	ΔH_{298} (kcal/mol)	ΔS_{298} (cal/(k•mol))	Energy barrier (kcal/mol)	Reaction energy (kcal/mol)
Reactant (open shell singlet)	-3757.224326	-131.214	461.026	31.850	275.754	-	-
TS (open shell singlet)	-3757.201018	-135.500	461.704	31.118	269.804	12.1	-
Product (open shell singlet)	-3757.234786	-136.390	463.042	31.070	269.211	-	-8.6

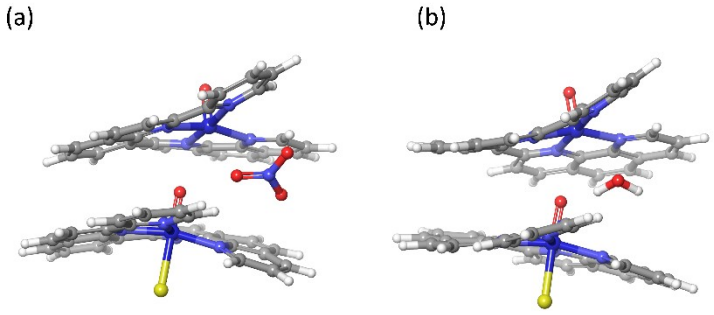

Figure S2. The transition state structures of (a) nitrate and (b) water attack

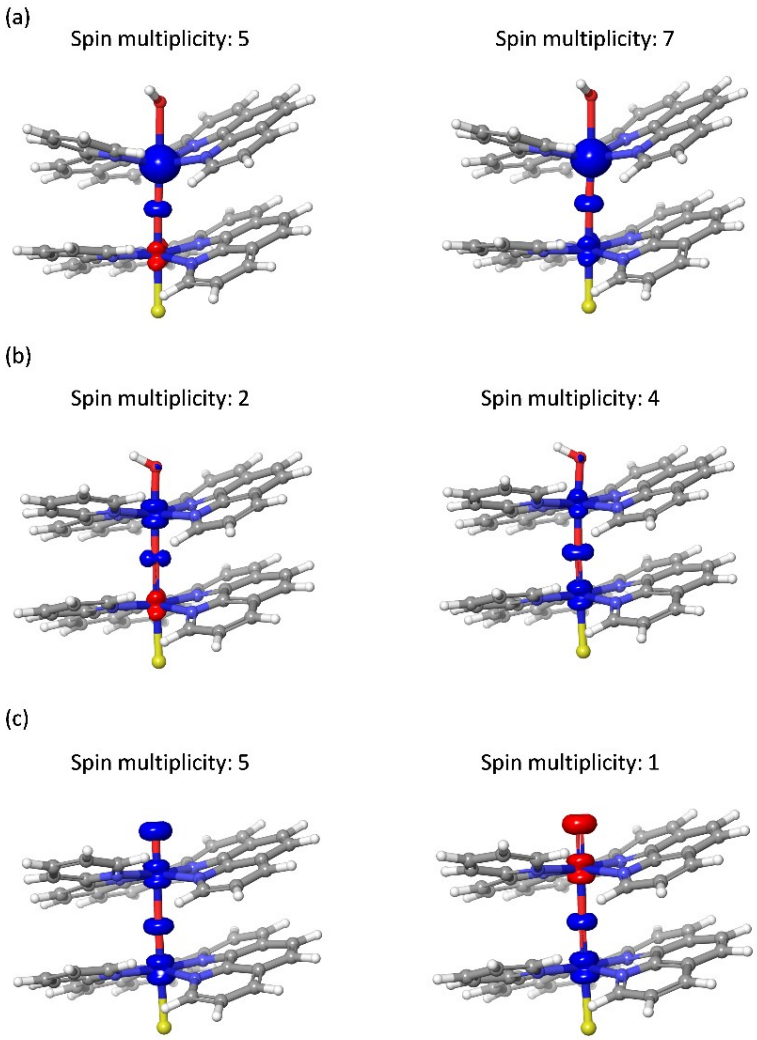

Figure S3. The spin density distributions of optimized structures with favored spin states and degenerate states of (a) $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$ (complex 1), (b) $[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$ (complex 2) and (c) $[Cl\text{-}Fe^{IV}\text{-}O\text{-}Fe^{IV}\text{=}O]^{3+}$ (complex 3) at an isovalue of 0.05 electrons/bohr^3

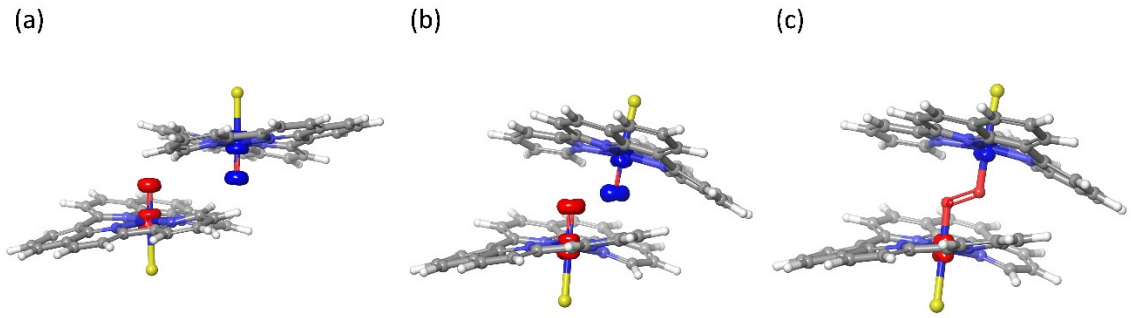

Figure S4. The spin density distributions of (a) reactant (complex 5), (b) transition state (5TS) and (c) product (5IM) at an isovalue of 0.05 electrons/bohr^3 in the radical coupling process

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Cartesian coordinates

$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{III}\text{-}OH_2]^{3+}$—Quintet

E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3297.935662

G_{solv} (kcal/mol) = -258.959

ZPE (kcal/mol) = 472.251

ΔH_{298} (kcal/mol) = 32.394

ΔS_{298} (cal/(k•mol)) = 282.875

Fe1	5.9531436565	10.9019425398	3.7206900943
Cl2	6.9083857773	12.9308268420	3.6097599343
N3	7.0624209738	10.5890208782	5.3660532020
C4	8.3786182766	10.4928011991	5.5321801191
H5	8.9934631425	10.6935144258	4.6623789574
N6	4.5793818198	11.3584164715	5.0414291351
C7	8.9472935572	10.1823392867	6.7819969803
H8	10.0265204536	10.1178959250	6.8705444918
N9	4.8420242890	11.4794867882	2.1797092460
C10	8.1266970425	9.9763879184	7.8776428555
H11	8.5489504184	9.7262106541	8.8470040001
N12	7.0926865131	10.1479180115	2.2836071933
C13	6.7294952855	10.1456950580	7.7377703053
C14	6.2569065832	10.4892832947	6.4541411817
C15	5.7751317608	10.0315850128	8.8067602381
H16	6.1299387681	9.7414246959	9.7913301737
C17	4.4524179422	10.3132381415	8.6049492924
H18	3.7447045955	10.2376251019	9.4246623504
C19	3.9802230781	10.7711016485	7.3291431029
C20	4.8940661113	10.8579651907	6.2638702369
C21	2.6539036640	11.1669593579	7.0392699185
H22	1.8822850248	11.0805280653	7.7992115503
C23	2.3509601104	11.6804156013	5.7971677910
H24	1.3330822005	11.9774792634	5.5802520739
C25	3.3527917582	11.8255190236	4.7935185888
C26	3.0574741797	12.5211308952	3.5221697034
C27	2.0458855267	13.4801221056	3.5493933339
H28	1.5623714739	13.7129638886	4.4911542485
C29	1.6414063225	14.2076917658	2.4159065641
H30	0.8562901932	14.9510180829	2.5067584071
C31	2.2567985507	13.9742393267	1.2110743062
H32	1.9621299893	14.5163706246	0.3172494254
C33	3.3186766547	13.0396298026	1.1263979920
C34	3.7583118932	12.3142308681	2.2848919472
C35	3.9853092314	12.8316474847	-0.1028164907
H36	3.6648803412	13.3867173076	-0.9799208536
C37	5.0436174000	11.9618855150	-0.1748855932
H38	5.5841353211	11.8258956541	-1.1030524962
C39	5.4669418156	11.3169476368	1.0032013871
C40	6.6574270969	10.4521478496	1.0413934852
C41	7.2822573614	9.9231190376	-0.0911361480
H42	6.9308650840	10.1770347317	-1.0838984646
C43	8.3582232737	9.0533060947	0.0698169555
H44	8.8651985959	8.6440034006	-0.7985208810
C45	8.7635543205	8.7093208678	1.3595737116
H46	9.5849335288	8.0216165567	1.5290649155
C47	8.0953683762	9.2744261004	2.4411724021
H48	8.3504602831	9.0190909672	3.4604340445
O49	5.3265832382	9.1794853325	3.8724022841

O50	3.5048758413	5.4385303642	4.1724677237
H51	3.9938383632	4.6248985275	3.9910699888
H52	2.7041504948	5.3922543398	3.6328772404
Fe53	4.5650563853	7.6229044086	4.0321586136
N54	5.0123280216	7.0842532981	6.0564760941
N55	2.6712445761	7.9646042270	4.9667187968
N56	3.4993449042	7.7738575610	2.1564183527
N57	5.7755908814	6.4018339106	2.7407987852
C58	6.1815604370	6.7438959323	6.5952816252
H59	7.0583981613	6.8813643271	5.9692282271
C60	6.2928739304	6.2416015986	7.9012896750
H61	7.2655186946	5.9620512901	8.2917989042
C62	5.1463459350	6.1022355833	8.6621589304
H63	5.1969764595	5.6988438493	9.6693501534
C64	3.8962097493	6.4949230076	8.1302711407
C65	3.8804082000	6.9981351241	6.8070066668
C66	2.6676184316	6.4018796293	8.8655381276
H67	2.6918351613	5.9985673037	9.8735738476
C68	1.4897236038	6.8043789967	8.3076667952
H69	0.5605505964	6.7227219944	8.8630597370
C70	1.4508031357	7.3409017601	6.9787191071
C71	2.6416585619	7.4462629703	6.2262228928
C72	0.2605243331	7.7594637350	6.3394042830
H73	-0.6905869499	7.6544134984	6.8535531081
C74	0.3067628058	8.2786890434	5.0645543540
H75	-0.6135516183	8.5553374523	4.5652299958
C76	1.5500320713	8.4059207679	4.3834922790
C77	1.5856698461	9.0354171325	3.0358933498
C78	0.6385572848	10.0225450709	2.7745500595
H79	-0.0112693770	10.3538397291	3.5773122039
C80	0.4799827344	10.6263719359	1.5127928702
H81	-0.2768281896	11.3917557826	1.3779395868
C82	1.2681151127	10.2231014496	0.4619897857
H83	1.1360357309	10.6418780950	-0.5312022890
C84	2.2647864471	9.2368574427	0.6680628993
C85	2.4752958799	8.6631335022	1.9668825864
C86	3.0824810364	8.7943969585	-0.3995929376
H87	2.9230087674	9.2064574578	-1.3920687424
C88	4.0658195392	7.8595276767	-0.1835980545
H89	4.7008191843	7.5297561736	-0.9961485713
C90	4.2647371076	7.3806403536	1.1308752928
C91	5.3766227428	6.4449042805	1.4481730633
C92	5.9764239664	5.6275143486	0.4852591985
H93	5.6275962872	5.6345976836	-0.5407958560
C94	7.0032114774	4.7633968582	0.8648056792
H95	7.4671283025	4.1119749531	0.1303574337
C96	7.4124418392	4.7353465097	2.1984683891
H97	8.2033005172	4.0726279960	2.5337698141
C98	6.7659019097	5.5716362593	3.1044257487
H99	7.0302609617	5.5743391802	4.1565231031

$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{IV}\text{-}OH]^{3+}$—Doublet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3297.269864
G_{solv} (kcal/mol) = -260.759
ZPE (kcal/mol) = 467.214
ΔH_{298} (kcal/mol) = 30.784
ΔS_{298} (cal/(k•mol)) = 265.306

Fe1	5.8589436729	10.6744887968	3.7783649365
Cl2	6.8744518636	12.6761268801	3.7582008009
N3	6.9030749377	10.3332316330	5.4673491079
C4	8.2125227885	10.2069657247	5.6716832634
H5	8.8545441081	10.3262023997	4.8075275404
N6	4.4635026627	11.2031480895	5.0427720498
C7	8.7483082821	9.9828501408	6.9524213866
H8	9.8231278205	9.8922131847	7.0674915823
N9	4.8678474027	11.3298961765	2.1888652250
C10	7.9024329377	9.9042160651	8.0448224123
H11	8.2986785352	9.7306093905	9.0414118805
N12	7.0666192538	9.9253789252	2.3979561596
C13	6.5154576495	10.1094206948	7.8625588324
C14	6.0746826454	10.3506477538	6.5432991123
C15	5.5489084100	10.1401483442	8.9246279293
H16	5.8819392309	9.9310920172	9.9369011005
C17	4.2427159864	10.4594845105	8.6783892427
H18	3.5234651814	10.4948209312	9.4904240252
C19	3.8088609919	10.8180831458	7.3591709845
C20	4.7344604327	10.7655523797	6.3008748444
C21	2.5092869449	11.2598139800	7.0207993911
H22	1.7249472070	11.2702044009	7.7723588085
C23	2.2519154310	11.7027364393	5.7431076636
H24	1.2543629101	12.0380466740	5.4944560402
C25	3.2744493137	11.7382066765	4.7498064611
C26	3.0457278062	12.4136566714	3.4531054947
C27	2.0654589806	13.4067445747	3.4314789256
H28	1.5539686972	13.6669688811	4.3502569104
C29	1.7271006777	14.1392226676	2.2808283970
H30	0.9602527170	14.9046792920	2.3373965208
C31	2.3884399417	13.8863314547	1.1052676135
H32	2.1507657012	14.4352145969	0.1987299852
C33	3.4307361502	12.9271393756	1.0717956547
C34	3.7947541489	12.1845265007	2.2470063634
C35	4.1605196023	12.7235313440	-0.1207532004
H36	3.8925713827	13.2879900822	-1.0094387481
C37	5.2186154633	11.8511312854	-0.1402870372
H38	5.8074304756	11.7217839136	-1.0392172750
C39	5.5686422997	11.1880180022	1.0508103223
C40	6.7584670810	10.3247570439	1.1442447900
C41	7.5188112109	9.9008629230	0.0504267119
H42	7.2830338336	10.2382668426	-0.9513693173
C43	8.5901676865	9.0351800741	0.2595424997
H44	9.2038279626	8.7136620382	-0.5763161805
C45	8.8507228629	8.5779270020	1.5517389086
H46	9.6581809348	7.8826326608	1.7537330391
C47	8.0545601012	9.0420599350	2.5934210830
H48	8.1981270326	8.7057300703	3.6108365609
O49	5.1239959374	8.9796281818	3.8471683104
O50	3.4407056749	5.8738795493	4.0018140618
H51	3.6081850229	5.2543979876	3.2782321503

Fe53	4.3161654706	7.4637693708	3.8844895206
N54	5.0964044083	7.1209258043	5.7247474787
N55	2.7508834728	8.0410373486	4.9298259678
N56	3.5143379886	7.9427410308	2.1402821638
N57	5.6190016647	6.4936902179	2.7327963296
C58	6.3394745298	6.8718329837	6.1232680591
H59	7.1193327360	6.9778834522	5.3785195686
C60	6.6341233906	6.4882003730	7.4427736096
H61	7.6611269284	6.2742824768	7.7182004338
C62	5.6068695074	6.3687310919	8.3633929405
H63	5.8086548789	6.0378300680	9.3777903960
C64	4.2874701843	6.7003344543	7.9802932976
C65	4.0957799944	7.1037140838	6.6409168919
C66	3.1485357984	6.6617582723	8.8546044844
H67	3.2871304363	6.3232365306	9.8770546682
C68	1.9104728058	7.0313962919	8.4100252781
H69	1.0521402731	6.9790879304	9.0725156776
C70	1.7147603327	7.5014655989	7.0678666476
C71	2.8194325754	7.5557931157	6.1976752325
C72	0.4741863761	7.8962932191	6.5175940342
H73	-0.4329106764	7.8118836952	7.1088113566
C74	0.4173118863	8.3655630990	5.2230049333
H75	-0.5441686570	8.6189846452	4.7952835559
C76	1.5922854159	8.4742335344	4.4268067641
C77	1.5282696158	9.0655868211	3.0699854123
C78	0.5058015979	9.9791024956	2.8220184271
H79	-0.1460140552	10.2745625277	3.6359857886
C80	0.2696855273	10.5541268180	1.5603110325
H81	-0.5514338778	11.2516921316	1.4339887945
C82	1.0692682380	10.2063970751	0.4999152908
H83	0.8880877309	10.6059255434	-0.4934059075
C84	2.1531036909	9.3142518666	0.6928635177
C85	2.4224486366	8.7533553198	1.9880796935
C86	2.9943004094	8.9658649451	-0.3894589996
H87	2.7841458617	9.3733806732	-1.3740678386
C88	4.0615553740	8.1246184837	-0.1958515461
H89	4.7089946857	7.8541182958	-1.0193216849
C90	4.3056264069	7.6344435579	1.1022777755
C91	5.4288023691	6.7307483630	1.4124045255
C92	6.1888705665	6.0643392545	0.4484551653
H93	6.0233454946	6.2442419706	-0.6067616200
C94	7.1295047578	5.1183264818	0.8545467036
H95	7.7154325310	4.5787428158	0.1168107678
C96	7.2715627028	4.8438095215	2.2142421461
H97	7.9572794673	4.0821312636	2.5697986377
C98	6.4882253314	5.5488695238	3.1234737415
H99	6.5214337290	5.3328946405	4.1820402813

[Cl-Fe^{IV}-O-Fe^{IV}=O]$^{3+}$—Unrestricted singlet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3296.609083
G_{solv} (kcal/mol) = -260.078
ZPE (kcal/mol) = 460.935
ΔH_{298} (kcal/mol) = 30.368
ΔS_{298} (cal/(k•mol)) = 262.406

Fe1	5.8542864870000	10.6217399303000	3.8003493448000
Cl2	6.8807592912000	12.6445151559000	3.8443896704000
N3	6.9017961271000	10.2862589092000	5.4899745636000
C4	8.2084750802000	10.1378406805000	5.6939130931000
H5	8.8531610104000	10.2294832160000	4.8293045417000
N6	4.4672294695000	11.2047866368000	5.0575814704000
C7	8.7420236217000	9.9270911971000	6.9774557531000
H8	9.8150212502000	9.8158979332000	7.0911023878000
N9	4.9156538946000	11.3560378815000	2.2150426932000
C10	7.8969307825000	9.8868421991000	8.0720154964000
H11	8.2911185901000	9.7233407505000	9.0710501385000
N12	7.1196971734000	9.9338213313000	2.4345293064000
C13	6.5139875827000	10.1170629243000	7.8880018855000
C14	6.0732809424000	10.3423447949000	6.5652031777000
C15	5.5526430698000	10.1855386032000	8.9523166048000
H16	5.8861529828000	9.9907619140000	9.9672066753000
C17	4.2507353086000	10.5193257731000	8.7033738698000
H18	3.5342819074000	10.5796750496000	9.5161565856000
C19	3.8182945189000	10.8591450097000	7.3791130940000
C20	4.7406200016000	10.7788093979000	6.3194232033000
C21	2.5204046000000	11.3030416756000	7.0366042267000
H22	1.7379293736000	11.3272899015000	7.7895109833000
C23	2.2622544155000	11.7278853714000	5.7536162180000
H24	1.2649542595000	12.0614037373000	5.5006989438000
C25	3.2842237835000	11.7469159806000	4.7584593574000
C26	3.0613394517000	12.4141214572000	3.4575024075000
C27	2.0672213032000	13.3927554995000	3.4203852338000
H28	1.5375057438000	13.6455915318000	4.3304709332000
C29	1.7362469036000	14.1215911374000	2.2657228048000
H30	0.9566124813000	14.8745670560000	2.3109032930000
C31	2.4223200389000	13.8825103755000	1.1020833295000
H32	2.1931803290000	14.4305482997000	0.1930546724000
C33	3.4800635837000	12.9400246590000	1.0844197084000
C34	3.8328914144000	12.1974086211000	2.2636094274000
C35	4.2363712133000	12.7572981455000	-0.0941313296000
H36	3.9780541054000	13.3249031665000	-0.9834019786000
C37	5.3065784710000	11.9002555631000	-0.0996383135000
H38	5.9138224509000	11.7853464405000	-0.9879242408000
C39	5.6394587184000	11.2266697761000	1.0897698296000
C40	6.8258497555000	10.3590089623000	1.1861220136000
C41	7.5910843588000	9.9432691626000	0.0927016037000
H42	7.3675440004000	10.2982245053000	-0.9056211164000
C43	8.6468027413000	9.0571640670000	0.2951873930000
H44	9.2607955229000	8.7388209260000	-0.5414661063000
C45	8.8870425458000	8.5718754452000	1.5805776205000
H46	9.6768379241000	7.8552992738000	1.7774914582000
C47	8.0880090810000	9.0292589498000	2.6230947798000
H48	8.2091522012000	8.6615053676000	3.6322373365000
O49	5.1498331676000	9.1027439719000	3.8077874040000
O50	3.5244102336000	5.8856563517000	3.8796829387000
Fe53	4.2457386168000	7.3418075055000	3.8499049844000

N54	5.0740003347000	7.0983404685000	5.6889933322000
N55	2.7162882296000	8.0089404237000	4.9115724064000
N56	3.4842833466000	7.9324163067000	2.1270194939000
N57	5.6272975102000	6.4960772838000	2.6832083403000
C58	6.3206323586000	6.8449444676000	6.0763888179000
H59	7.0873404457000	6.8996356284000	5.3131842975000
C60	6.6393929446000	6.5143437441000	7.4050378863000
H61	7.6693499774000	6.2970934690000	7.6664254940000
C62	5.6306299025000	6.4428052590000	8.3504074580000
H63	5.8487546953000	6.1475605435000	9.3729221118000
C64	4.3069702551000	6.7726731963000	7.9790623890000
C65	4.0921222850000	7.1285082915000	6.6290417763000
C66	3.1856528242000	6.7722467170000	8.8762200073000
H67	3.3429490637000	6.4687314815000	9.9069033260000
C68	1.9401552974000	7.1308132784000	8.4428214466000
H69	1.0948750789000	7.1044011938000	9.1232477307000
C70	1.7205096351000	7.5533850073000	7.0889116499000
C71	2.8075709587000	7.5716411470000	6.1963987774000
C72	0.4697014846000	7.9333847456000	6.5497340904000
H73	-0.4258434919000	7.8683308688000	7.1604470401000
C74	0.3902725206000	8.3660771514000	5.2444903964000
H75	-0.5781443899000	8.6127075393000	4.8293144810000
C76	1.5523179098000	8.4470881034000	4.4243383199000
C77	1.4805811790000	9.0299649926000	3.0643604400000
C78	0.4505587166000	9.9369748670000	2.8219831311000
H79	-0.2081414859000	10.2165427517000	3.6356578764000
C80	0.2160333405000	10.5290561732000	1.5686176363000
H81	-0.6125268277000	11.2184680083000	1.4473156110000
C82	1.0296615534000	10.2087937634000	0.5110341723000
H83	0.8546265970000	10.6239355828000	-0.4768567158000
C84	2.1215654238000	9.3254320660000	0.6988578703000
C85	2.3869322746000	8.7404603134000	1.9841174355000
C86	2.9766915440000	9.0135180291000	-0.3832094877000
H87	2.7699576638000	9.4409006676000	-1.3599160986000
C88	4.0523242128000	8.1825020810000	-0.1985590002000
H89	4.7121920591000	7.9409932719000	-1.0210014824000
C90	4.2866395490000	7.6562883989000	1.0872693504000
C91	5.4140917103000	6.7479475559000	1.3709577696000
C92	6.1506283553000	6.0898424455000	0.3836466996000
H93	5.9617936739000	6.2784903035000	-0.6660177419000
C94	7.0924254124000	5.1324688777000	0.7594864127000
H95	7.6570397548000	4.5950456634000	0.0039800064000
C96	7.2578689635000	4.8409204913000	2.1122201344000
H97	7.9407994104000	4.0671101675000	2.4460532792000
C98	6.4942216840000	5.5398697069000	3.0431811615000
H99	6.5390230064000	5.3002161134000	4.0963592944000

Cl^- attack:
Reactant—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.217386
G_{solv} (kcal/mol) = -141.518
ZPE (kcal/mol) = 461.566
ΔH_{298} (kcal/mol) = 31.500
ΔS_{298} (cal/(k•mol)) = 271.036

Fe1	5.7998021287	10.6106241027	3.8069898264
Cl2	6.8037878779	12.6559715943	3.8409900887
N3	6.9625840916	10.2038273127	5.3975383744
C4	8.2607450301	9.9461407740	5.4886584297
H5	8.8467335039	10.0019154459	4.5850614166
N6	4.4992424757	11.1445516493	5.1899540917
C7	8.8805569216	9.6512873877	6.7217619402
H8	9.9379660142	9.4179118601	6.7213915909
N9	4.7165201207	11.3829909205	2.3188740695
C10	8.1322278081	9.6311265215	7.8760237468
H11	8.5894628110	9.3957963561	8.8326079572
N12	6.9529687275	10.0017766602	2.3153424549
C13	6.7497690027	9.9379031010	7.8096384816
C14	6.2198201087	10.2392150482	6.5395755926
C15	5.8761565290	9.9893493162	8.9452784835
H16	6.2841990524	9.7457736229	9.9212403371
C17	4.5627941418	10.3462677981	8.8155838957
H18	3.9097967658	10.3768604104	9.6818654164
C19	4.0322874547	10.7249728192	7.5422804800
C20	4.8790190842	10.6942603293	6.4149762164
C21	2.6996997182	11.1263131823	7.3050973913
H22	1.9733148840	11.0964532557	8.1120403763
C23	2.3299068073	11.5636091536	6.0539914888
H24	1.3018595598	11.8486193383	5.8778231145
C25	3.2773196985	11.6449799530	4.9931102623
C26	2.9277831338	12.3335142313	3.7296541055
C27	1.8861628322	13.2595402835	3.7929228310
H28	1.4184737141	13.4648694336	4.7473292005
C29	1.4282853920	13.9925622407	2.6858617836
H30	0.6143339618	14.6992167478	2.8085122340
C31	2.0353850654	13.8175103397	1.4685948700
H32	1.7091453211	14.3694459570	0.5921036434
C33	3.1325395090	12.9322923587	1.3477123856
C34	3.6115604343	12.1808395507	2.4739346009
C35	3.7939856706	12.8001294183	0.1062708005
H36	3.4373203652	13.3697499733	-0.7468817051
C37	4.8869151926	11.9849744605	-0.0063789890
H38	5.4190244468	11.9032874299	-0.9442568773
C39	5.3451111284	11.2987776304	1.1358078043
C40	6.5572032086	10.4677667087	1.1079137004
C41	7.2474330815	10.1205822113	-0.0552452344
H42	6.9348399508	10.5010073615	-1.0194569225
C43	8.3512670994	9.2709298156	0.0383373134
H44	8.9131655616	9.0077572990	-0.8525366088
C45	8.6925489032	8.7444720552	1.2797858065
H46	9.5024240241	8.0357454252	1.4137356717
C47	7.9536685606	9.1204165707	2.4010764384
H48	8.1512327199	8.6370584108	3.3575686641
O49	5.0961787066	9.0954749722	3.8155898144
O50	3.3190833686	5.9265021209	3.7763467838

Fe53	4.1021569593	7.3521665722	3.8028643504
N54	4.7409184466	7.1141308561	5.7109374724
N55	2.5142927765	8.1290998118	4.7109311609
N56	3.5214804195	7.9548607701	2.0036890752
N57	5.5801330365	6.5035410328	2.7880962406
C58	5.9370436866	6.8173791096	6.2095054391
H59	6.8074132935	6.8528725422	5.5506925358
C60	6.1154245697	6.5101377561	7.5733562905
H61	7.1156651347	6.2608145064	7.9106229301
C62	5.0349067139	6.5239690994	8.4302783247
H63	5.1451418802	6.2613474557	9.4782598042
C64	3.7690188138	6.9197303689	7.9356013313
C65	3.6855386177	7.2301700063	6.5629402510
C66	2.5892020963	7.0456024917	8.7426005371
H67	2.6494820542	6.7828017038	9.7946397775
C68	1.4103246858	7.4812044413	8.2053400027
H69	0.5193514844	7.5586614495	8.8214183221
C70	1.3264138929	7.8525936480	6.8236273000
C71	2.4746292723	7.7422249578	6.0147047727
C72	0.1572364046	8.3124894525	6.1781539324
H73	-0.7816734462	8.3516599721	6.7223785509
C74	0.2098047043	8.6927392465	4.8563443133
H75	-0.7013818288	8.9992721910	4.3604488936
C76	1.4311370095	8.6432108222	4.1232107506
C77	1.4939422647	9.1665065956	2.7385142539
C78	0.5369060388	10.1197063673	2.3850624065
H79	-0.1392092135	10.4920954006	3.1445216231
C80	0.4054818149	10.6468373952	1.0907302194
H81	-0.3688189927	11.3767102693	0.8824398167
C82	1.2538691422	10.2090887335	0.1038888785
H83	1.1601180728	10.5676107163	-0.9168747473
C84	2.2894032886	9.2954185967	0.4115897086
C85	2.4554634654	8.7785796899	1.7401324441
C86	3.2050940873	8.8977973609	-0.5931172327
H87	3.0678942330	9.2654260668	-1.6058699527
C88	4.2550388412	8.0769598577	-0.2868109154
H89	4.9662580967	7.7823993837	-1.0463909273
C90	4.4011399146	7.6255476826	1.0446832634
C91	5.5217948743	6.7699880347	1.4560904146
C92	6.4346492002	6.2017657636	0.5717754689
H93	6.3814341194	6.4063473838	-0.4897177003
C94	7.4081741161	5.3258228360	1.0647652596
H95	8.1241207115	4.8688076744	0.3894842388
C96	7.4341387210	5.0407425424	2.4207909247
H97	8.1707296249	4.3790882751	2.8597046679
C98	6.4879688039	5.6462085735	3.2537203624
H99	6.4502313398	5.4081146124	4.3033000544
Cl98	8.8912136039	6.9998959768	4.7137608629

Cl^- attack:
Transition state—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.182808
G_{solv} (kcal/mol) = -142.616
ZPE (kcal/mol) = 461.089
ΔH_{298} (kcal/mol) = 31.103
ΔS_{298} (cal/(k•mol)) = 270.389

Cl98	0.0000000000000	0.0000000000000	0.0000000000000
Fe53	0.0000000000000	0.0000000000000	3.7138605317000
O49	2.9030140301120	0.0000000000000	2.5189703050402
Fe1	4.2658065548816	-0.1814923730094	1.6394928854911
Cl2	6.2821882637158	-0.4950616727155	0.2862207646550
N3	3.4121377693359	-1.3646668988888	0.2506465335861
C4	3.0563843590064	-1.1276921302703	-1.0076724312521
H5	3.3019555846498	-0.1571908182252	-1.4207573857534
N6	4.5755168522162	-1.8967016707760	2.5776758178410
C7	2.4052300446989	-2.0958675819088	-1.7968160616655
H8	2.1313961004415	-1.8415902909931	-2.8167162352904
N9	5.4863582237534	0.8382284274750	2.8188400377474
C10	2.1091388537789	-3.3318032281592	-1.2562253533303
H11	1.5825663544875	-4.0875299335623	-1.8362268009743
N12	3.9319469496539	1.5971764017037	0.8412050599084
C13	2.5297400829306	-3.6256413051357	0.0638465892027
C14	3.2100592338059	-2.6070640496790	0.7662783592808
C15	2.3465559448228	-4.8996139171450	0.7018521187629
H16	1.7902014857163	-5.6676463034189	0.1698314727610
C17	2.8699920281409	-5.1478606412227	1.9410587724915
H18	2.7340723191533	-6.1156934325880	2.4180341996455
C19	3.6360742665034	-4.1483614557917	2.6284519840821
C20	3.8065959761412	-2.8822275965939	2.0335106444005
C21	4.2449781399770	-4.3276009093165	3.8915084805011
H22	4.1149630582067	-5.2633073482951	4.4305300402810
C23	4.9975264991527	-3.3133259993200	4.4391594656925
H24	5.4203904765880	-3.4664209206289	5.4237115712256
C25	5.2079778097770	-2.0837265457167	3.7425989203257
C26	6.1407394459889	-1.0573792922206	4.2811626397491
C27	7.0225037405082	-1.4759937063490	5.2815557119207
H28	7.0171091253694	-2.5096039501669	5.6054200557706
C29	7.9696588284479	-0.6358999391604	5.8933403895702
H30	8.6130623113237	-1.0362505227119	6.6718941217627
C31	8.0809255797849	0.6685298617844	5.4811162711511
H32	8.8108330512352	1.3439757149287	5.9218201479604
C33	7.2504968948749	1.1503465346792	4.4388184935102
C34	6.2564210558629	0.3094655843924	3.8242485065956
C35	7.4216901423368	2.4756073591887	3.9724234623034
H36	8.1835280903135	3.1037250646858	4.4298083398077
C37	6.6413840327987	2.9538756605425	2.9517587383932
H38	6.7760688665316	3.9634391171772	2.5795768384272
C39	5.6675009957903	2.1019633443000	2.3928508690217
C40	4.7614544580028	2.5543203323141	1.3198592456843
C41	4.6651944107758	3.8753002353975	0.8727699125358
H42	5.3368453085312	4.6419890149906	1.2449231917766
C43	3.6647364016030	4.2089298846084	-0.0435992564592
H44	3.5748599367922	5.2311827002215	-0.4026976338242
C45	2.7603649857188	3.2275991835132	-0.4476120481325
H46	1.9305866847441	3.4546654433756	-1.1112218436097
C47	2.9181482741926	1.9251731165638	0.0281492585533

H48	2.1899160298420	1.1497016433895	-0.1922337099172
O50	-0.9540834231280	0.0422253908443	5.0094342357591
N54	-0.3019697406812	-1.9274829864554	3.1761018577561
N55	1.4269585161146	-0.8104919342111	4.8339720250114
N56	0.8046042433142	1.7848092610123	3.7639067245454
N57	-1.4091650620784	0.9015379929268	2.6665508873616
C58	-1.0109129934749	-2.4632804704081	2.1799105783364
H59	-1.3787274398403	-1.7788178864834	1.4244535497626
C60	-1.2183457682189	-3.8536110251234	2.0883032373649
H61	-1.7984929620488	-4.2420943253258	1.2559464900551
C62	-0.6949259097715	-4.6943215258006	3.0555318210071
H63	-0.8689754150430	-5.7674831303732	3.0155766336423
C64	0.1023427140983	-4.1504162408762	4.0932804940389
C65	0.2966963291986	-2.7538087074456	4.0824829264746
C66	0.7378532721743	-4.9222974810023	5.1268257463459
H67	0.5709769055789	-5.9971488899573	5.1464135036691
C68	1.5372956450599	-4.3235164972747	6.0639004080504
H69	2.0090861831194	-4.9122858229521	6.8475372798419
C70	1.7980513508852	-2.9122363685067	6.0184734964103
C71	1.1899968372470	-2.1416263668089	5.0108555956956
C72	2.6288672929317	-2.2047314171543	6.9210833249502
H73	3.0835622758596	-2.7230957692514	7.7632079749694
C74	2.8606093870818	-0.8600028935816	6.7294401426347
H75	3.4776759166243	-0.3372892579217	7.4503443731024
C76	2.2841658868641	-0.1549509427806	5.6278314493148
C77	2.6550151764164	1.2513683452839	5.3350301334159
C78	3.8132794893544	1.7383735156962	5.9468997022864
H79	4.3871668114562	1.0945736149855	6.6022467964963
C80	4.3164623970025	3.0348126588419	5.7444007345480
H81	5.2199717056677	3.3432356966180	6.2622154430568
C82	3.6659481980165	3.8844390748159	4.8836134126552
H83	4.0332836705752	4.8908533422353	4.6944180541294
C84	2.4934083086615	3.4501327414244	4.2149365348621
C85	1.9599697290296	2.1324894184581	4.4276985315464
C86	1.8392837235475	4.3262472645964	3.3162266365022
H87	2.2563085627016	5.3165275274687	3.1456571898488
C88	0.6893403269165	3.9357952292527	2.6750620308543
H89	0.1848113930305	4.6040383405670	1.9857101333875
C90	0.1756079616114	2.6531693928191	2.9393786360475
C91	-1.1034758855785	2.1862523748502	2.3719621108071
C92	-1.9921941330864	2.9848155480744	1.6512900147442
H93	-1.7493065609964	4.0143970415084	1.4088827248889
C94	-3.2210962476744	2.4448166468401	1.2628088327041
H95	-3.9270046559879	3.0512094010341	0.7006588755070
C96	-3.5418171833165	1.1382948071602	1.6298718771007
H97	-4.5000911889063	0.6931046111105	1.3774415104454
C98	-2.6049109647350	0.3941172980568	2.3455326375806
H99	-2.8159304610310	-0.6146844994611	2.6802463679779

Cl^- attack:
Product—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.227903
G_{solv} (kcal/mol) = -128.356
ZPE (kcal/mol) = 462.193
ΔH_{298} (kcal/mol) = 31.629
ΔS_{298} (cal/(k•mol)) = 276.925

Fe1	6.7015930000	12.3090900000	4.3334810000
Cl2	8.5709510000	13.6533340000	4.7723760000
N3	7.6211810000	11.0243750000	5.6205010000
C4	8.5972730000	10.1449960000	5.4254750000
H5	8.9865670000	10.0305870000	4.4283660000
N6	5.8771980000	12.9986460000	5.9884490000
C7	9.1479100000	9.3761980000	6.4653030000
H8	9.9174780000	8.6550550000	6.2150150000
N9	6.0835530000	13.8324910000	3.2388940000
C10	8.6984730000	9.5592700000	7.7555080000
H11	9.1096250000	8.9843800000	8.5798560000
N12	7.5338350000	11.7611550000	2.6027110000
C13	7.7081740000	10.5345550000	8.0068750000
C14	7.2011290000	11.2469920000	6.8957540000
C15	7.2263280000	10.8546550000	9.3182160000
H16	7.6097320000	10.2914800000	10.1633490000
C17	6.3326380000	11.8674510000	9.5075400000
H18	5.9907020000	12.1248350000	10.5052650000
C19	5.8512790000	12.6356210000	8.3990130000
C20	6.2728620000	12.3110780000	7.0934330000
C21	5.0075680000	13.7597930000	8.5221920000
H22	4.6931950000	14.0985140000	9.5052000000
C23	4.6141110000	14.4390020000	7.3957400000
H24	4.0156370000	15.3312230000	7.5099590000
C25	5.0188530000	14.0183840000	6.0946710000
C26	4.5175470000	14.7472460000	4.9066500000
C27	3.3896460000	15.5507480000	5.0713710000
H28	2.8262350000	15.4937180000	5.9939930000
C29	2.9313100000	16.4547620000	4.0978140000
H30	2.0504320000	17.0552460000	4.2977150000
C31	3.6325250000	16.5954740000	2.9268880000
H32	3.3441810000	17.3313460000	2.1822650000
C33	4.7348960000	15.7481150000	2.6613490000
C34	5.1438920000	14.7512510000	3.6110500000
C35	5.4411680000	15.8539820000	1.4415200000
H36	5.1749680000	16.6423750000	0.7440580000
C37	6.4307170000	14.9558410000	1.1375490000
H38	6.9686810000	15.0216780000	0.2013280000
C39	6.6902140000	13.9084450000	2.0442070000
C40	7.5416840000	12.7613210000	1.6911850000
C41	8.2183550000	12.6238210000	0.4771610000
H42	8.2512100000	13.4396870000	-0.2336830000
C43	8.8490240000	11.4146110000	0.1858570000
H44	9.3973290000	11.2975720000	-0.7434480000
C45	8.7378360000	10.3591740000	1.0867000000
H46	9.1708290000	9.3818720000	0.9053620000
C47	8.0575890000	10.5749580000	2.2814960000
H48	7.9233520000	9.7662060000	2.9827970000
O49	5.3959880000	11.3513630000	4.0610090000
O50	6.3246860000	4.8932770000	3.7957610000

Fe53	7.5204010000	5.9808930000	3.5658310000
N54	8.2008550000	5.8450530000	5.4688190000
N55	6.3249530000	7.3378270000	4.3668470000
N56	7.0449320000	6.4553470000	1.7089680000
N57	8.5581720000	4.5392810000	2.6810560000
C58	9.3075390000	5.3069970000	5.9722660000
H59	10.0438780000	4.9557510000	5.2604920000
C60	9.5254810000	5.2112670000	7.3584210000
H61	10.4358340000	4.7455340000	7.7196250000
C62	8.5709490000	5.6953370000	8.2357990000
H63	8.7039040000	5.5971890000	9.3096360000
C64	7.4295560000	6.3521600000	7.7238960000
C65	7.3147260000	6.4269760000	6.3174440000
C66	6.4097940000	6.9634500000	8.5286190000
H67	6.4755540000	6.8722780000	9.6089120000
C68	5.3779250000	7.6486040000	7.9528890000
H69	4.6081990000	8.1032820000	8.5692190000
C70	5.2956920000	7.8025690000	6.5292540000
C71	6.2762040000	7.1993030000	5.7193370000
C72	4.2809730000	8.5087520000	5.8465100000
H73	3.4592400000	8.9517200000	6.4012070000
C74	4.3351710000	8.6292880000	4.4779300000
H75	3.5431120000	9.1545960000	3.9661530000
C76	5.4077330000	8.0676940000	3.7269450000
C77	5.5168700000	8.3164480000	2.2703600000
C78	4.8591960000	9.4459220000	1.7833030000
H79	4.3880830000	10.1210750000	2.4841640000
C80	4.8371680000	9.8027950000	0.4247850000
H81	4.2989170000	10.6928720000	0.1157970000
C82	5.4934090000	9.0200070000	-0.4897130000
H83	5.4811040000	9.2575460000	-1.5491610000
C84	6.2225780000	7.8869660000	-0.0548240000
C85	6.2692970000	7.5214150000	1.3341480000
C86	6.9409850000	7.1120160000	-0.9922630000
H87	6.8973660000	7.3794720000	-2.0438170000
C88	7.6929150000	6.0476190000	-0.5738860000
H89	8.2582620000	5.4593170000	-1.2836330000
C90	7.7377890000	5.7491920000	0.8025420000
C91	8.5415610000	4.6339500000	1.3327770000
C92	9.1823990000	3.6806740000	0.5370560000
H93	9.1748130000	3.7613470000	-0.5423990000
C94	9.8089390000	2.5969060000	1.1487360000
H95	10.3106570000	1.8459130000	0.5472430000
C96	9.7473240000	2.4729790000	2.5350140000
H97	10.1787420000	1.6207470000	3.0478630000
C98	9.0991420000	3.4647860000	3.2657530000
H99	8.9818330000	3.3908180000	4.3379210000
Cl98	9.3427950000	7.5067480000	3.2658510000

Radical coupling of two subunits after Cl^- attack:
Reactant—Antiferromagnetic open shell singlet state (Triplet-triplet)
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.224326
G_{solv} (kcal/mol) = -131.214
ZPE (kcal/mol) = 461.026
ΔH_{298} (kcal/mol) = 31.850
ΔS_{298} (cal/(k•mol)) = 275.754

Fe1	3.2101309221	10.6045669346	5.0607279529
Cl2	3.1687959345	12.4889863989	6.4218377289
N3	1.6975558483	9.9601600573	6.2473463623
C4	1.6945778158	9.4919255576	7.4894650837
H5	2.6405257179	9.4661381290	8.0080164755
N6	1.7301242754	11.3024907630	3.9569293422
C7	0.5171359273	9.0711668416	8.1326694119
H8	0.5818354121	8.6809310364	9.1419728010
N9	4.6034147422	11.5902589811	4.0425530876
C10	-0.6903517571	9.1647314853	7.4719193057
H11	-1.6126317873	8.8360148299	7.9405693115
N12	4.7847256559	9.9012740430	6.0508720520
C13	-0.7244128667	9.7217308011	6.1742036980
C14	0.5078720840	10.1189309943	5.6101829844
C15	-1.9263347064	9.9122227897	5.4154077961
H16	-2.8692299481	9.5988254793	5.8520438928
C17	-1.8897407734	10.4772401637	4.1730244520
H18	-2.8020457234	10.6132321910	3.6003225968
C19	-0.6549851937	10.9413711985	3.6143799631
C20	0.5350363623	10.7902085731	4.3522393431
C21	-0.5245121316	11.5477441687	2.3466579839
H22	-1.3859589899	11.6260818378	1.6903665663
C23	0.6958138263	12.0397542445	1.9510951034
H24	0.7886334519	12.4700146597	0.9640239632
C25	1.8330578017	11.9830847133	2.8110165570
C26	3.0770054173	12.7017796318	2.4475135485
C27	2.9568845741	13.7180561857	1.4981245586
H28	1.9774694010	13.9724129056	1.1148471073
C29	4.0383634755	14.4773532262	1.0200347241
H30	3.8663080386	15.2450089810	0.2734865150
C31	5.2928451320	14.2417030489	1.5200802295
H32	6.1520297307	14.8085097812	1.1760408628
C33	5.4769148256	13.2716585864	2.5357347977
C34	4.3772131806	12.4835863596	3.0277284568
C35	6.7551405536	13.0968132344	3.1084846963
H36	7.5860602080	13.6916977070	2.7412828298
C37	6.9310408585	12.2068538106	4.1332253374
H38	7.9011906695	12.0889298677	4.5956647071
C39	5.8226455746	11.4701144852	4.5916454295
C40	5.9392099713	10.5108973197	5.7029824987
C41	7.1416201202	10.1842349443	6.3375810434
H42	8.0618313489	10.6902535054	6.0777621282
C43	7.1486619654	9.1891365645	7.3135965957
H44	8.0712516100	8.9367339188	7.8271733461
C45	5.9660690270	8.5084970656	7.5895493296
H46	5.9249091470	7.6889400642	8.2986096186
C47	4.8035873807	8.8877101672	6.9237173257
H48	3.8891405945	8.3242789709	7.0552363126
O49	3.1932343532	9.2476557181	4.1292797354
Fe50	2.8961030748	5.2432357178	6.2402850670

Cl51	2.8184860728	3.4168608889	4.8084378941
N52	1.5798706852	6.0827287538	4.9388448917
C53	1.7467265690	6.5734575751	3.7175819674
H54	2.7341759483	6.5005248337	3.2892379488
N55	1.2406079218	4.6685443276	7.1537500406
C56	0.6892069027	7.1378570716	2.9820820874
H57	0.8929620046	7.5361550510	1.9949851980
N58	4.0668986386	4.0876796924	7.3625772494
C59	-0.5783794579	7.1697359304	3.5247519578
H60	-1.4102526403	7.6068094526	2.9809640132
N61	4.6393320427	5.8067907454	5.4539477055
C62	-0.7984255345	6.5962580909	4.7975103834
C63	0.3235732809	6.0482658649	5.4582039088
C64	-2.0832630069	6.5116903073	5.4283918362
H65	-2.9395769212	6.9394024405	4.9170193133
C66	-2.2334361986	5.8960922697	6.6380052850
H67	-3.2104031782	5.8324409199	7.1085614293
C68	-1.1172435103	5.2755999498	7.2875026267
C69	0.1528020945	5.3318570564	6.6792873338
C70	-1.1853810948	4.5822413727	8.5154723856
H71	-2.1148304427	4.5597765862	9.0764784377
C72	-0.0729727308	3.9297849979	8.9897762785
H73	-0.1291530779	3.4278684375	9.9455703749
C74	1.1475527132	3.9116114035	8.2509860041
C75	2.2610066403	3.0357623425	8.6815996727
C76	1.9269874959	1.9657787504	9.5125089677
H77	0.8867107901	1.7823843470	9.7482329197
C78	2.8659685775	1.0692890611	10.0489057963
H79	2.5309861772	0.2643400359	10.6942491466
C80	4.1924129392	1.2250557364	9.7402898300
H81	4.9473719265	0.5572034913	10.1435838229
C82	4.5914758667	2.2467842408	8.8443032657
C83	3.6373608049	3.1637087069	8.2802768328
C84	5.9472743861	2.3484306686	8.4647569971
H85	6.6701332771	1.6636354212	8.8969687656
C86	6.3329151629	3.2797891893	7.5392676396
H87	7.3641178170	3.3417541235	7.2210137929
C88	5.3541533231	4.1263708784	6.9828767056
C89	5.6885726435	5.1032198658	5.9344332703
C90	6.9868040061	5.3424257264	5.4730964683
H91	7.8225441452	4.7643562645	5.8441158373
C92	7.2007315510	6.3418384278	4.5262601688
H93	8.2008702126	6.5281289670	4.1477647027
C94	6.1192525632	7.1091654364	4.1041014022
H95	6.2342316810	7.9321127772	3.4077177960
C96	4.8533717810	6.8178572638	4.6047323872
H97	4.0129467200	7.4540901040	4.3635510528
O98	2.9186872748	6.5707773724	7.2138090554

Radical coupling of two subunits after Cl^- attack:
Transition state—Antiferromagnetic open shell singlet state (Triplet-triplet)
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.201018
G_{solv} (kcal/mol) = -135.500
ZPE (kcal/mol) = 461.704
ΔH_{298} (kcal/mol) = 31.118
ΔS_{298} (cal/(k•mol)) = 269.804

Fe1	2.4574610000	10.9379410000	5.4459910000
Cl2	2.8508240000	13.0511860000	6.3103040000
N3	0.5158880000	11.3251200000	5.8615030000
C4	-0.1247190000	11.4645250000	7.0174030000
H5	0.4822390000	11.4366490000	7.9135640000
N6	1.9488920000	11.6389690000	3.6750190000
C7	-1.5141410000	11.6740770000	7.0804620000
H8	-1.9891000000	11.7742970000	8.0491630000
N9	4.3828770000	10.9099940000	5.0431160000
C10	-2.2477900000	11.7570490000	5.9115360000
H11	-3.3242610000	11.9055120000	5.9380830000
N12	3.0218770000	10.0585140000	7.1122690000
C13	-1.5747020000	11.7008640000	4.6695100000
C14	-0.1753910000	11.5154910000	4.7097060000
C15	-2.2091130000	11.8594670000	3.3906020000
H16	-3.2889600000	11.9705720000	3.3559240000
C17	-1.4728260000	11.9014440000	2.2399680000
H18	-1.9614880000	12.0352050000	1.2797470000
C19	-0.0403110000	11.8269270000	2.2783870000
C20	0.5997520000	11.6371290000	3.5174920000
C21	0.8097830000	11.9460680000	1.1558260000
H22	0.3860400000	12.0416770000	0.1601900000
C23	2.1749170000	11.9537380000	1.3330760000
H24	2.8136510000	12.0368110000	0.4635720000
C25	2.7551210000	11.8465260000	2.6324100000
C26	4.2198480000	11.9767950000	2.8183300000
C27	4.9180970000	12.6599450000	1.8229590000
H28	4.3665870000	13.1276030000	1.0166060000
C29	6.3150560000	12.8150770000	1.8174560000
H30	6.7919770000	13.3614470000	1.0109660000
C31	7.0513260000	12.2797360000	2.8438730000
H32	8.1329690000	12.3756060000	2.8691000000
C33	6.3991520000	11.6274190000	3.9183900000
C34	4.9706040000	11.4802180000	3.9441420000
C35	7.1554590000	11.1446600000	5.0112790000
H36	8.2368090000	11.2559650000	4.9970250000
C37	6.5259840000	10.5763920000	6.0865150000
H38	7.0958130000	10.2349730000	6.9405970000
C39	5.1193810000	10.4906050000	6.0812580000
C40	4.3615740000	9.9472110000	7.2211140000
C41	4.9412110000	9.2984010000	8.3136280000
H42	6.0175810000	9.2283020000	8.4085830000
C43	4.1177650000	8.7200460000	9.2759180000
H44	4.5512060000	8.2210320000	10.1372220000
C45	2.7365130000	8.7686480000	9.1001530000
H46	2.0586880000	8.2927260000	9.7991600000
C47	2.2297800000	9.4398200000	7.9924370000
H48	1.1693950000	9.4620730000	7.7847920000
O49	2.0875290000	9.4247640000	4.8020680000
Fe50	2.8872200000	6.4945080000	4.5540930000

Cl51	2.3999080000	4.5645610000	3.3769430000
N52	0.9855680000	7.0337200000	4.1751000000
C53	0.3746210000	7.3935500000	3.0546070000
H54	0.9281290000	7.2499510000	2.1350490000
N55	2.0956940000	5.8206700000	6.2299220000
C56	-0.9288150000	7.9227340000	3.0545680000
H57	-1.3807800000	8.2196560000	2.1145270000
N58	4.6398580000	5.6353510000	4.8865170000
C59	-1.6126950000	8.0552240000	4.2484330000
H60	-2.6118990000	8.4787200000	4.2723180000
N61	3.8290670000	7.2921810000	3.0040290000
C62	-1.0193550000	7.5810440000	5.4402080000
C63	0.2836760000	7.0515300000	5.3346120000
C64	-1.6632640000	7.5659120000	6.7239800000
H65	-2.6554070000	7.9991130000	6.8132780000
C66	-1.0621160000	6.9866120000	7.8070070000
H67	-1.5690070000	6.9580120000	8.7671540000
C68	0.2261350000	6.3656480000	7.6920380000
C69	0.8948350000	6.4132140000	6.4552160000
C70	0.9036240000	5.6975460000	8.7372180000
H71	0.4640290000	5.6551180000	9.7298700000
C72	2.1205510000	5.1043590000	8.4927360000
H73	2.6450170000	4.6245430000	9.3081210000
C74	2.7096450000	5.1333880000	7.1929660000
C75	3.9648890000	4.3987470000	6.9153650000
C76	4.2588710000	3.3243940000	7.7520020000
H77	3.5407610000	3.0296170000	8.5075420000
C78	5.4351310000	2.5621000000	7.6522040000
H79	5.5996060000	1.7380220000	8.3376240000
C80	6.3561500000	2.8715760000	6.6848840000
H81	7.2795750000	2.3090150000	6.5891130000
C82	6.0937660000	3.9163650000	5.7654450000
C83	4.8846420000	4.6875570000	5.8441360000
C84	7.0123950000	4.1887510000	4.7260540000
H85	7.9280250000	3.6082410000	4.6658470000
C86	6.7317830000	5.1506020000	3.7918670000
H87	7.4141420000	5.3387070000	2.9741060000
C88	5.5106990000	5.8485700000	3.8886020000
C89	5.0970160000	6.8432770000	2.8800070000
C90	5.9411880000	7.3533170000	1.8904700000
H91	6.9554850000	6.9900930000	1.7878900000
C92	5.4714030000	8.3520610000	1.0416540000
H93	6.1122360000	8.7503840000	0.2623280000
C94	4.1828510000	8.8461520000	1.2290210000
H95	3.7871380000	9.6485940000	0.6178430000
C96	3.3964890000	8.2984470000	2.2375560000
H97	2.4223220000	8.6950790000	2.4822000000
O98	3.2720790000	7.8892850000	5.3907300000

Radical coupling of two subunits after Cl^- attack:
Product—Antiferromagnetic open shell singlet state (Triplet-triplet)
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3757.234786
G_{solv} (kcal/mol) = -136.390
ZPE (kcal/mol) = 463.042
ΔH_{298} (kcal/mol) = 31.070
ΔS_{298} (cal/(k•mol)) = 269.211

Fe1	2.5036960000	11.0208240000	5.4986480000
Cl2	2.9149360000	13.0820760000	6.4122320000
N3	0.5483480000	11.3702380000	5.9210470000
C4	-0.0960800000	11.4827950000	7.0783010000
H5	0.5092930000	11.4458970000	7.9751070000
N6	1.9737330000	11.7407520000	3.7423180000
C7	-1.4875280000	11.6763900000	7.1479390000
H8	-1.9631130000	11.7532030000	8.1194240000
N9	4.4234090000	10.9518880000	5.0549460000
C10	-2.2226870000	11.7766000000	5.9816460000
H11	-3.2996910000	11.9169900000	6.0113830000
N12	3.0969690000	10.0882420000	7.1365870000
C13	-1.5497650000	11.7519010000	4.7392410000
C14	-0.1488620000	11.5732530000	4.7741720000
C15	-2.1882740000	11.9450540000	3.4678510000
H16	-3.2687080000	12.0519040000	3.4389470000
C17	-1.4541490000	12.0309610000	2.3192740000
H18	-1.9433380000	12.1972560000	1.3641150000
C19	-0.0222840000	11.9648120000	2.3553850000
C20	0.6234590000	11.7307820000	3.5847250000
C21	0.8219580000	12.1535650000	1.2389310000
H22	0.3942400000	12.2978410000	0.2509220000
C23	2.1860830000	12.1695470000	1.4147800000
H24	2.8216180000	12.3043020000	0.5503030000
C25	2.7723360000	11.9988790000	2.7044620000
C26	4.2392960000	12.1110700000	2.8783850000
C27	4.9304790000	12.8371200000	1.9084710000
H28	4.3721880000	13.3596190000	1.1416360000
C29	6.3295830000	12.9651750000	1.8799380000
H30	6.8006870000	13.5472210000	1.0953200000
C31	7.0763210000	12.3531970000	2.8545890000
H32	8.1601320000	12.4207820000	2.8570000000
C33	6.4328810000	11.6593330000	3.9082800000
C34	5.0019700000	11.5464830000	3.9630530000
C35	7.2035630000	11.1016930000	4.9546610000
H36	8.2858070000	11.1785360000	4.9110690000
C37	6.5873340000	10.5101000000	6.0243040000
H38	7.1696920000	10.1144600000	6.8455720000
C39	5.1777320000	10.4812980000	6.0589120000
C40	4.4384750000	9.9543650000	7.2166150000
C41	5.0382810000	9.3195270000	8.3078890000
H42	6.1150680000	9.2377610000	8.3799120000
C43	4.2305930000	8.7830460000	9.3072050000
H44	4.6772870000	8.3001990000	10.1705390000
C45	2.8460690000	8.8550300000	9.1675030000
H46	2.1788200000	8.4146560000	9.8990350000
C47	2.3208800000	9.5068640000	8.0565220000
H48	1.2558450000	9.5443650000	7.8789300000
O49	2.0626350000	9.4292680000	4.7694400000
Fe50	2.4572490000	6.8265170000	4.2815560000

Cl51	2.0217950000	4.8681530000	3.1904270000
N52	0.5533570000	7.3581780000	3.8922380000
C53	-0.0769710000	7.6309050000	2.7572740000
H54	0.4758020000	7.4503020000	1.8435190000
N55	1.6866190000	6.2570750000	6.0019560000
C56	-1.4019510000	8.1049190000	2.7311960000
H57	-1.8685130000	8.3240310000	1.7769920000
N58	4.2351110000	6.0618030000	4.6978280000
C59	-2.0881270000	8.2773830000	3.9183690000
H60	-3.1058620000	8.6565170000	3.9235080000
N61	3.4041450000	7.6104200000	2.7277450000
C62	-1.4711170000	7.9016060000	5.1329530000
C63	-0.1483560000	7.4170510000	5.0520920000
C64	-2.1135850000	7.9370250000	6.4163810000
H65	-3.1191840000	8.3408660000	6.4832070000
C66	-1.4952300000	7.4355890000	7.5269170000
H67	-2.0003670000	7.4410280000	8.4883460000
C68	-0.1924930000	6.8413310000	7.4394760000
C69	0.4791100000	6.8481710000	6.2022000000
C70	0.4860740000	6.2175220000	8.5109010000
H71	0.0403210000	6.2047060000	9.5019320000
C72	1.7076380000	5.6237110000	8.2916910000
H73	2.2320890000	5.1747340000	9.1246460000
C74	2.3009690000	5.6102650000	6.9947700000
C75	3.5651250000	4.8799860000	6.7549940000
C76	3.8664180000	3.8380480000	7.6291620000
H77	3.1425980000	3.5524160000	8.3827670000
C78	5.0603070000	3.0985720000	7.5702970000
H79	5.2305220000	2.2977050000	8.2816560000
C80	5.9928410000	3.4015580000	6.6109650000
H81	6.9311720000	2.8584820000	6.5489050000
C82	5.7236560000	4.4129080000	5.6568090000
C83	4.4939710000	5.1535140000	5.6885160000
C84	6.6544640000	4.6820120000	4.6280750000
H85	7.5867900000	4.1259500000	4.5998570000
C86	6.3643770000	5.6106680000	3.6635770000
H87	7.0569470000	5.7949830000	2.8527950000
C88	5.1212960000	6.2733260000	3.7145700000
C89	4.6978750000	7.2202890000	2.6636770000
C90	5.5540230000	7.7352750000	1.6879340000
H91	6.5882780000	7.4190590000	1.6381970000
C92	5.0683560000	8.6745840000	0.7812270000
H93	5.7167060000	9.0733680000	0.0076730000
C94	3.7502050000	9.1061690000	0.8992410000
H95	3.3359480000	9.8541660000	0.2343800000
C96	2.9539370000	8.5598810000	1.9013860000
H97	1.9445260000	8.9027740000	2.0726510000
O98	2.9046640000	8.3590160000	5.1219440000

$[Cl\text{-}Fe^{III}\text{-}O\text{-}Fe^{V}\text{-}OH_2]^{5+}$—Nonet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3296.798859
G_{solv} (kcal/mol) = -660.784
ZPE (kcal/mol) = 470.56
ΔH_{298} (kcal/mol) = 32.514
ΔS_{298} (cal/(k•mol)) = 283.971

Fe1	6.0442117162000	10.8076519573000	3.8989049603000
Cl2	7.0834063857000	12.7448878648000	3.6908485086000
N3	6.8332502136000	10.8171457778000	5.7622267356000
C4	8.1051270729000	10.7377048489000	6.1753854375000
H5	8.8680140482000	10.6351247546000	5.4144828246000
N6	4.4976116037000	11.6112480600000	4.7962057859000
C7	8.4562686664000	10.8398872862000	7.5295187830000
H8	9.5022440009000	10.7690953837000	7.8119388596000
N9	5.3519314348000	11.1727132384000	2.0800276299000
C10	7.4686058570000	11.0622672057000	8.4803778061000
H11	7.7230534367000	11.1517296517000	9.5336980378000
N12	7.4477533837000	9.8203216227000	2.9232744714000
C13	6.1319055066000	11.2371347583000	8.0521785707000
C14	5.8709041563000	11.1257976188000	6.6677763977000
C15	5.0516349257000	11.5961726529000	8.9293408740000
H16	5.2439240112000	11.6628219259000	9.9971869110000
C17	3.7991951803000	11.8930703771000	8.4326788523000
H18	3.0013903519000	12.1873057345000	9.1088438785000
C19	3.5543502795000	11.8875517392000	7.0311358598000
C20	4.5969529241000	11.5076120821000	6.1440827704000
C21	2.3353314952000	12.2800206994000	6.4238048004000
H22	1.4786263350000	12.5323447437000	7.0424498425000
C23	2.2561233897000	12.3805114208000	5.0555604027000
H24	1.3197718108000	12.6868327332000	4.6111368319000
C25	3.3854356093000	12.1178845880000	4.2157078484000
C26	3.3594707441000	12.4639850688000	2.7910612294000
C27	2.3798445855000	13.3944666840000	2.3782372578000
H28	1.7243981871000	13.8383970969000	3.1166245109000
C29	2.2401250682000	13.8503434604000	1.0622438278000
H30	1.4804250355000	14.5876957947000	0.8220986470000
C31	3.1020357513000	13.3772049204000	0.0949235509000
H32	3.0269545800000	13.7212100703000	-0.9335061272000
C33	4.1374915776000	12.4653859679000	0.4428913262000
C34	4.2997320113000	12.0016398908000	1.7936607757000
C35	5.0538171987000	12.0454737114000	-0.5466371945000
H36	4.9482047832000	12.4123758051000	-1.5644190372000
C37	6.0932377012000	11.2081947162000	-0.2139268403000
H38	6.8187132052000	10.9160579655000	-0.9626109774000
C39	6.2346627118000	10.8033336565000	1.1225275318000
C40	7.3783628976000	9.9985752982000	1.5815178764000
C41	8.3435657698000	9.4379215966000	0.7405811917000
H42	8.3101736203000	9.5997260237000	-0.3301233110000
C43	9.3740631994000	8.6749737300000	1.2914475365000
H44	10.1511519623000	8.2634599768000	0.6533863846000
C45	9.3824634134000	8.4404042529000	2.6681539676000
H46	10.1524239064000	7.8328033358000	3.1334764587000
C47	8.3884403998000	9.0218949450000	3.4499568027000
H48	8.3359257164000	8.8540334421000	4.5167703224000
O49	5.2272632647000	9.2421070119000	4.0998723763000
O50	3.5267289037000	5.4632391732000	3.6231336097000
H51	4.0318012695000	4.6852316027000	3.3457555586000

H52	2.6325674039000	5.3414065144000	3.2733193561000
Fe53	4.4087638252000	7.6130401438000	3.9072895559000
N54	5.2198523472000	6.6439829647000	5.6291494851000
N55	2.6976955155000	7.5755927355000	5.2022765244000
N56	3.0322865778000	8.1577390694000	2.3574010838000
N57	5.4393154613000	6.9032440326000	2.1852323339000
C58	6.4823930018000	6.2572343199000	5.8605543242000
H59	7.2294371738000	6.6158723828000	5.1594110538000
C60	6.8374077957000	5.4355203462000	6.9377384317000
H61	7.8711945767000	5.1344171249000	7.0751671502000
C62	5.8450599299000	5.0061027011000	7.8093680587000
H63	6.0858691031000	4.3502811057000	8.6428573668000
C64	4.5114976220000	5.4331548881000	7.6090780294000
C65	4.2458000117000	6.2695183534000	6.4979707875000
C66	3.4328142717000	5.0473763510000	8.4738169184000
H67	3.6402591962000	4.3935847236000	9.3165971038000
C68	2.1485529032000	5.4899083727000	8.2408000232000
H69	1.3383976187000	5.1822897975000	8.8959034520000
C70	1.8632466242000	6.3501563361000	7.1437062276000
C71	2.9060248255000	6.7543125446000	6.2628399577000
C72	0.5598625294000	6.8221589604000	6.8488094949000
H73	-0.2816053347000	6.5075303756000	7.4607342551000
C74	0.3638948816000	7.6567044624000	5.7732828797000
H75	-0.6442380645000	7.9654264079000	5.5264995217000
C76	1.4565498290000	8.0561088454000	4.9492976689000
C77	1.2023353702000	8.9523605621000	3.8069887891000
C78	0.1032686220000	9.8245972633000	3.9142109179000
H79	-0.4027819066000	9.9196224791000	4.8687044454000
C80	-0.3898084621000	10.5782400548000	2.8414340659000
H81	-1.2548127389000	11.2196173561000	2.9828263151000
C82	0.1963962841000	10.4451446763000	1.5968606503000
H83	-0.2122701630000	10.9632544502000	0.7330378573000
C84	1.3318332444000	9.6081101493000	1.4276640859000
C85	1.8974586000000	8.9010084585000	2.5400732040000
C86	1.9118173804000	9.4350068886000	0.1490905702000
H87	1.4709016163000	9.9373561871000	-0.7081711135000
C88	3.0100131611000	8.6198714522000	-0.0096988720000
H89	3.4479091657000	8.4773244692000	-0.9897100461000
C90	3.5639245437000	7.9991883158000	1.1285056517000
C91	4.7691261764000	7.1382074920000	1.0281160639000
C92	5.1760185919000	6.5440567576000	-0.1693635831000
H93	4.6170222372000	6.6949689621000	-1.0854488537000
C94	6.2856511555000	5.6946586286000	-0.1739860264000
H95	6.5945055625000	5.2042074638000	-1.0933148996000
C96	6.9732302991000	5.4698239794000	1.0197033175000
H97	7.8330895526000	4.8080430752000	1.0600683846000
C98	6.5132796601000	6.0937398961000	2.1776365602000
H99	7.0002074420000	5.9285753111000	3.1316657880000

NO_3^- attack:
Transition state—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3577.334373
G_{solv} (kcal/mol) = -136.702
ZPE (kcal/mol) = 472.429
ΔH_{298} (kcal/mol) = 31.835
ΔS_{298} (cal/(k•mol)) = 264.174

Fe1	10.2439910000000	7.0867170000000	2.3028160000000
Cl2	11.9148000000000	8.7113110000000	2.0831570000000
N3	11.5508220000000	6.2406980000000	3.5596490000000
C4	12.7330530000000	5.6792780000000	3.3383350000000
H5	13.0740710000000	5.6493380000000	2.3126010000000
N6	9.5634920000000	7.9220910000000	3.9462760000000
C7	13.5324480000000	5.1862060000000	4.3826210000000
H8	14.4909780000000	4.7383760000000	4.1460590000000
N9	9.2424450000000	8.3112990000000	1.0971790000000
C10	13.0798000000000	5.2598770000000	5.6844200000000
H11	13.6676950000000	4.8561320000000	6.5024280000000
N12	10.7862840000000	6.2470900000000	0.5916320000000
C13	11.8470090000000	5.8941810000000	5.9471000000000
C14	11.1422190000000	6.4069420000000	4.8399440000000
C15	11.2974790000000	6.0944340000000	7.2579340000000
H16	11.8156130000000	5.6579710000000	8.1062130000000
C17	10.1656380000000	6.8367400000000	7.4473230000000
H18	9.7660140000000	6.9905680000000	8.4452090000000
C19	9.5231670000000	7.4843600000000	6.3417060000000
C20	10.0243570000000	7.2671850000000	5.0434720000000
C21	8.4183260000000	8.3580520000000	6.4348370000000
H22	7.9378850000000	8.5224850000000	7.3947680000000
C23	7.9605560000000	9.0079520000000	5.3104680000000
H24	7.1021320000000	9.6596140000000	5.3964440000000
C25	8.5937480000000	8.8323020000000	4.0457270000000
C26	8.2333370000000	9.6868520000000	2.8865680000000
C27	7.6068170000000	10.8977780000000	3.1810480000000
H28	7.4438890000000	11.1709900000000	4.2155620000000
C29	7.2131780000000	11.8320170000000	2.2084160000000
H30	6.7325030000000	12.7550620000000	2.5146810000000
C31	7.4719310000000	11.5742820000000	0.8867660000000
H32	7.1953580000000	12.2819360000000	0.1108440000000
C33	8.1501730000000	10.3872730000000	0.5194130000000
C34	8.5472310000000	9.4193570000000	1.5046240000000
C35	8.4759250000000	10.1599160000000	-0.8374120000000
H36	8.1835540000000	10.8960500000000	-1.5805940000000
C37	9.1727950000000	9.0395430000000	-1.2002020000000
H38	9.4554540000000	8.8759860000000	-2.2316780000000
C39	9.5700830000000	8.1367790000000	-0.1926180000000
C40	10.4018570000000	6.9582500000000	-0.4909960000000
C41	10.7645700000000	6.5533700000000	-1.7777090000000
H42	10.4828810000000	7.1390890000000	-2.6438050000000
C43	11.5036970000000	5.3825100000000	-1.9401500000000
H44	11.8133130000000	5.0661950000000	-2.9314570000000
C45	11.8120990000000	4.6188920000000	-0.8176130000000
H46	12.3473790000000	3.6789950000000	-0.8981750000000
C47	11.4230920000000	5.0802300000000	0.4391850000000
H48	11.5584480000000	4.4940580000000	1.3388550000000
O49	9.0736660000000	5.9430720000000	2.5008960000000
O50	5.9867220000000	2.9639940000000	3.3275200000000

Fe51	7.4480400000000	3.6084800000000	3.1459330000000
N52	8.0776770000000	3.2719060000000	5.0580040000000
N53	6.7369100000000	5.2800590000000	3.9428400000000
N54	7.2867960000000	4.2513600000000	1.2989880000000
N55	8.0396380000000	1.9435980000000	2.2563040000000
C56	8.8653790000000	2.3325580000000	5.5820970000000
H57	9.3497520000000	1.6399560000000	4.9062880000000
C58	9.0767910000000	2.2211670000000	6.9701450000000
H59	9.7420290000000	1.4450260000000	7.3307870000000
C60	8.4306720000000	3.0783380000000	7.8331640000000
H61	8.5521050000000	2.9856790000000	8.9087020000000
C62	7.5924240000000	4.0895190000000	7.3049310000000
C63	7.4827830000000	4.1666740000000	5.9011900000000
C64	6.8399630000000	5.0089230000000	8.1082750000000
H65	6.9145780000000	4.9334880000000	9.1890630000000
C66	6.0174760000000	5.9366030000000	7.5334740000000
H67	5.4181700000000	6.5998100000000	8.1501690000000
C68	5.9281740000000	6.0528240000000	6.1093330000000
C69	6.7023810000000	5.1979490000000	5.3011150000000
C70	5.0802860000000	6.9489360000000	5.4224040000000
H71	4.3916930000000	7.5778050000000	5.9795850000000
C72	5.1155720000000	7.0095500000000	4.0491880000000
H73	4.4270210000000	7.6694970000000	3.5408670000000
C74	6.0107820000000	6.1970150000000	3.2937180000000
C75	6.1510480000000	6.3863520000000	1.8304770000000
C76	5.6939990000000	7.5972590000000	1.3113080000000
H77	5.2960680000000	8.3466660000000	1.9820620000000
C78	5.7581540000000	7.9384780000000	-0.0484130000000
H79	5.3665420000000	8.8938450000000	-0.3796360000000
C80	6.3419690000000	7.0671980000000	-0.9309400000000
H81	6.4216250000000	7.3047270000000	-1.9874130000000
C82	6.8764820000000	5.8427450000000	-0.4643620000000
C83	6.7768690000000	5.4660320000000	0.9156990000000
C84	7.5544950000000	4.9854660000000	-1.3619710000000
H85	7.6527270000000	5.2830380000000	-2.4018240000000
C86	8.0782360000000	3.7983200000000	-0.9268900000000
H87	8.6047790000000	3.1409000000000	-1.6056370000000
C88	7.8996850000000	3.4359370000000	0.4218680000000
C89	8.2884250000000	2.1141780000000	0.9377500000000
C90	8.7474680000000	1.0600730000000	0.1530830000000
H91	8.9558700000000	1.1985790000000	-0.9002830000000
C92	8.8978780000000	-0.2001840000000	0.7372810000000
H93	9.2517090000000	-1.0365410000000	0.1432450000000
C94	8.5526580000000	-0.3761590000000	2.0711760000000
H95	8.6176950000000	-1.3452210000000	2.5521580000000
C96	8.1279200000000	0.7313260000000	2.8039620000000
H97	7.8305870000000	0.6485290000000	3.8402720000000
O98	10.3827980000000	3.4557960000000	2.5830460000000
N100	10.8401760000000	2.6947110000000	3.5052560000000
O101	11.2445230000000	3.2035020000000	4.5725800000000
O102	10.8186470000000	1.4532650000000	3.3429370000000

H_2O attack:
Transition state—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3373.056097
G_{solv} (kcal/mol) = -257.342
ZPE (kcal/mol) = 477.513
ΔH_{298} (kcal/mol) = 30.994
ΔS_{298} (cal/(k•mol)) = 257.579

Fe1	10.3211870000000	6.8820230000000	2.4895910000000
Cl2	12.0472880000000	8.4147440000000	2.3089620000000
N3	11.5790320000000	6.0281710000000	3.8242380000000
C4	12.6744160000000	5.2960200000000	3.6314290000000
H5	12.9456880000000	5.0781720000000	2.6095300000000
N6	9.6689700000000	7.8652710000000	4.0701720000000
C7	13.4801970000000	4.8525910000000	4.6921510000000
H8	14.3594340000000	4.2562470000000	4.4738780000000
N9	9.4092790000000	8.0762600000000	1.2051230000000
C10	13.1531630000000	5.2041870000000	5.9880150000000
H11	13.7651170000000	4.8789750000000	6.8245420000000
N12	10.9428930000000	5.9848600000000	0.8060530000000
C13	12.0413160000000	6.0465190000000	6.2143330000000
C14	11.2883530000000	6.4469370000000	5.0850650000000
C15	11.6878920000000	6.5627330000000	7.5046810000000
H16	12.2570850000000	6.2361160000000	8.3692210000000
C17	10.6939630000000	7.4881180000000	7.6362100000000
H18	10.4584380000000	7.9107640000000	8.6082470000000
C19	9.9848980000000	7.9695060000000	6.4887450000000
C20	10.2625260000000	7.4280390000000	5.2171700000000
C21	9.0636280000000	9.0370620000000	6.5220770000000
H22	8.8473600000000	9.5390630000000	7.4608040000000
C23	8.4872840000000	9.4744340000000	5.3550740000000
H24	7.8507290000000	10.3454370000000	5.3985100000000
C25	8.7671710000000	8.8541420000000	4.1006140000000
C26	8.1076990000000	9.3563280000000	2.8702510000000
C27	7.0414510000000	10.2454080000000	3.0269240000000
H28	6.6290810000000	10.4137340000000	4.0122120000000
C29	6.4583270000000	10.9672140000000	1.9730030000000
H30	5.6485660000000	11.6591730000000	2.1793890000000
C31	6.9635400000000	10.8253040000000	0.7049370000000
H32	6.5856650000000	11.4184140000000	-0.1224860000000
C33	7.9868330000000	9.8793900000000	0.4600530000000
C34	8.5283550000000	9.0743190000000	1.5218160000000
C35	8.4896430000000	9.7120770000000	-0.8495510000000
H36	8.1242080000000	10.3563990000000	-1.6439010000000
C37	9.4250750000000	8.7453850000000	-1.1084340000000
H38	9.8212030000000	8.6173280000000	-2.1071770000000
C39	9.8439630000000	7.9097020000000	-0.0563810000000
C40	10.7289880000000	6.7553700000000	-0.2850320000000
C41	11.2556190000000	6.4003260000000	-1.5291000000000
H42	11.1242630000000	7.0415430000000	-2.3911050000000
C43	11.9645250000000	5.2073170000000	-1.6556070000000
H44	12.4034370000000	4.9305630000000	-2.6092210000000
C45	12.0676270000000	4.3668900000000	-0.5489360000000
H46	12.5615770000000	3.4031970000000	-0.6121330000000
C47	11.5345730000000	4.7897260000000	0.6663400000000
H48	11.5362630000000	4.1472520000000	1.5370520000000
O49	9.1253030000000	5.7438510000000	2.6833370000000
O50	5.6489520000000	3.0244310000000	2.9672060000000

Fe51	7.1327520000000	3.6263110000000	2.9174680000000
N52	7.7198470000000	3.1023510000000	4.7919050000000
N53	6.5524870000000	5.2824000000000	3.8247120000000
N54	7.1261850000000	4.4696590000000	1.1509190000000
N55	7.7918610000000	2.0670430000000	1.8829850000000
C56	8.3935790000000	2.0379420000000	5.2303610000000
H57	8.7555480000000	1.3489090000000	4.4813230000000
C58	8.6557660000000	1.8213080000000	6.5921240000000
H59	9.1914420000000	0.9272930000000	6.8925120000000
C60	8.2206640000000	2.7445630000000	7.5257110000000
H61	8.3985640000000	2.5890150000000	8.5861040000000
C62	7.5485330000000	3.9076580000000	7.0874280000000
C63	7.3266000000000	4.0406220000000	5.6970530000000
C64	7.0959810000000	4.9482070000000	7.9648070000000
H65	7.2525290000000	4.8328370000000	9.0325620000000
C66	6.4736250000000	6.0575000000000	7.4690850000000
H67	6.1224270000000	6.8373530000000	8.1372810000000
C68	6.2616140000000	6.2142370000000	6.0612030000000
C69	6.6951840000000	5.2084550000000	5.1780260000000
C70	5.6434180000000	7.3362700000000	5.4686530000000
H71	5.2878880000000	8.1516500000000	6.0919910000000
C72	5.5007970000000	7.3931890000000	4.1043160000000
H73	5.0678970000000	8.2815270000000	3.6713320000000
C74	5.9466710000000	6.3347460000000	3.2591880000000
C75	5.7941400000000	6.4465930000000	1.7911300000000
C76	4.9571840000000	7.4471550000000	1.2915070000000
H77	4.3186560000000	7.9979060000000	1.9692890000000
C78	4.8795310000000	7.7894820000000	-0.0689760000000
H79	4.1993990000000	8.5726910000000	-0.3859060000000
C80	5.6867190000000	7.1442010000000	-0.9728240000000
H81	5.6884900000000	7.4184640000000	-2.0236010000000
C82	6.4969910000000	6.0647020000000	-0.5442850000000
C83	6.5003200000000	5.6450730000000	0.8283490000000
C84	7.2946550000000	5.3581190000000	-1.4731420000000
H85	7.3334310000000	5.6992740000000	-2.5037690000000
C86	7.9739110000000	4.2296650000000	-1.0880810000000
H87	8.5629340000000	3.6682060000000	-1.8013940000000
C88	7.8038210000000	3.7608030000000	0.2276570000000
C89	8.2042270000000	2.4032180000000	0.6382320000000
C90	8.8051290000000	1.4618130000000	-0.1979630000000
H91	9.1514420000000	1.7347250000000	-1.1870750000000
C92	8.9093340000000	0.1402700000000	0.2395860000000
H93	9.3632220000000	-0.6117310000000	-0.3981540000000
C94	8.3725280000000	-0.2115240000000	1.4770340000000
H95	8.3701130000000	-1.2398880000000	1.8215640000000
C96	7.8161370000000	0.7875170000000	2.2726480000000
H97	7.3495600000000	0.5672160000000	3.2243530000000
O98	10.1055760000000	3.3060760000000	3.0302670000000
H99	10.5511810000000	3.2293990000000	3.8831010000000
H100	9.8333210000000	4.2533940000000	2.9714820000000

Stepwise dissociative pathway:
Reactant—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3296.606691
G_{solv} (kcal/mol) = -260.079
ZPE (kcal/mol) = 461.975
ΔH_{298} (kcal/mol) = 29.614
ΔS_{298} (cal/(k•mol)) = 248.667

Fe1	5.8661760000000	10.6201300000000	3.8150800000000
Cl2	6.8287230000000	12.6779210000000	3.8251420000000
N3	7.0222230000000	10.3077490000000	5.4390520000000
C4	8.3422470000000	10.1900420000000	5.5615510000000
H5	8.9299560000000	10.2939800000000	4.6587480000000
N6	4.5359620000000	11.1441950000000	5.1564460000000
C7	8.9602850000000	9.9955290000000	6.8092890000000
H8	10.0404880000000	9.9077350000000	6.8549000000000
N9	4.8183010000000	11.3420460000000	2.2948590000000
C10	8.1874800000000	9.9423760000000	7.9555230000000
H11	8.6478090000000	9.7930060000000	8.9282260000000
N12	7.0739620000000	9.9898290000000	2.3714140000000
C13	6.7906460000000	10.1396800000000	7.8577460000000
C14	6.2619540000000	10.3464260000000	6.5643050000000
C15	5.8971480000000	10.1894940000000	8.9809210000000
H16	6.3005600000000	10.0136000000000	9.9737030000000
C17	4.5718960000000	10.4796900000000	8.8128660000000
H18	3.9059610000000	10.5236710000000	9.6686300000000
C19	4.0454330000000	10.7910150000000	7.5158690000000
C20	4.9027840000000	10.7376930000000	6.4007120000000
C21	2.7099230000000	11.1713900000000	7.2497010000000
H22	1.9737730000000	11.1646350000000	8.0483610000000
C23	2.3555630000000	11.5740340000000	5.9823230000000
H24	1.3299770000000	11.8571760000000	5.7884690000000
C25	3.3154530000000	11.6369260000000	4.9295320000000
C26	2.9938200000000	12.3078160000000	3.6512760000000
C27	1.9612710000000	13.2460350000000	3.6837710000000
H28	1.4674950000000	13.4593530000000	4.6235890000000
C29	1.5474870000000	13.9870060000000	2.5637770000000
H30	0.7419320000000	14.7068130000000	2.6636490000000
C31	2.1880310000000	13.8034790000000	1.3646400000000
H32	1.8963220000000	14.3635280000000	0.4811660000000
C33	3.2769800000000	12.9015560000000	1.2743970000000
C34	3.7122910000000	12.1446820000000	2.4162900000000
C35	3.9782450000000	12.7694140000000	0.0559370000000
H36	3.6572210000000	13.3468880000000	-0.8061690000000
C37	5.0721400000000	11.9468020000000	-0.0229800000000
H38	5.6357550000000	11.8702890000000	-0.9430140000000
C39	5.4880480000000	11.2602830000000	1.1320400000000
C40	6.7066330000000	10.4329180000000	1.1494270000000
C41	7.4328340000000	10.0693350000000	0.0115120000000
H42	7.1508540000000	10.4394320000000	-0.9663020000000
C43	8.5266440000000	9.2166160000000	0.1431430000000
H44	9.1121130000000	8.9408770000000	-0.7284430000000
C45	8.8410210000000	8.7071630000000	1.4031180000000
H46	9.6614020000000	8.0121890000000	1.5449270000000
C47	8.0769970000000	9.1116560000000	2.4926820000000
H48	8.2534820000000	8.7202330000000	3.4847760000000
O49	5.2212560000000	9.0726930000000	3.8379770000000
O50	3.4619020000000	5.8854790000000	3.8539150000000

Fe53	4.2222850000000	7.3239070000000	3.8389790000000
N54	4.9544070000000	7.1152480000000	5.7162420000000
N55	2.6632450000000	8.0637070000000	4.8001900000000
N56	3.5856990000000	7.9132450000000	2.0677900000000
N57	5.6501790000000	6.4324700000000	2.7739290000000
C58	6.1768580000000	6.8494280000000	6.1680420000000
H59	6.9785120000000	6.8639280000000	5.4399040000000
C60	6.4278610000000	6.5636880000000	7.5213360000000
H61	7.4400940000000	6.3349110000000	7.8368350000000
C62	5.3771890000000	6.5537140000000	8.4224900000000
H63	5.5426960000000	6.2959920000000	9.4648380000000
C64	4.0795030000000	6.8995060000000	7.9793970000000
C65	3.9335130000000	7.2077210000000	6.6090590000000
C66	2.9200170000000	6.9632910000000	8.8244910000000
H67	3.0234770000000	6.6951020000000	9.8717460000000
C68	1.7045120000000	7.3377040000000	8.3225290000000
H69	0.8296740000000	7.3588240000000	8.9655310000000
C70	1.5571010000000	7.7150700000000	6.9450860000000
C71	2.6832520000000	7.6704140000000	6.1026800000000
C72	0.3435420000000	8.1102050000000	6.3348980000000
H73	-0.5820110000000	8.0925160000000	6.9036040000000
C74	0.3372090000000	8.4986810000000	5.0133910000000
H75	-0.6046340000000	8.7553430000000	4.5468440000000
C76	1.5367760000000	8.5189390000000	4.2440740000000
C77	1.5433940000000	9.0548970000000	2.8620000000000
C78	0.5353570000000	9.9604140000000	2.5328400000000
H79	-0.1629890000000	10.2745490000000	3.2989870000000
C80	0.3731180000000	10.5124490000000	1.2504300000000
H81	-0.4435500000000	11.2012030000000	1.0632330000000
C82	1.2440770000000	10.1589750000000	0.2501070000000
H83	1.1271230000000	10.5436190000000	-0.7584510000000
C84	2.3164320000000	9.2746940000000	0.5268270000000
C85	2.5051310000000	8.7265300000000	1.8420590000000
C86	3.2279790000000	8.9253030000000	-0.4962590000000
H87	3.0766100000000	9.3227670000000	-1.4955400000000
C88	4.2870210000000	8.0958390000000	-0.2283980000000
H89	4.9886220000000	7.8256610000000	-1.0064890000000
C90	4.4429810000000	7.6022280000000	1.0821620000000
C91	5.5373130000000	6.6833260000000	1.4491450000000
C92	6.3386640000000	6.0145230000000	0.5213690000000
H93	6.2332200000000	6.2031950000000	-0.5397310000000
C94	7.2395310000000	5.0481210000000	0.9681860000000
H95	7.8543130000000	4.5039040000000	0.2580480000000
C96	7.2994030000000	4.7571310000000	2.3295580000000
H97	7.9466010000000	3.9765530000000	2.7149010000000
C98	6.4756530000000	5.4666250000000	3.1998520000000
H99	6.4374960000000	5.2285880000000	4.2537550000000

Stepwise dissociative pathway:
Product—Quintet
E (B3LYP-D3/LACV3P^{**++}) (a.u.) = -3296.564670
G_{solv} (kcal/mol) = -254.766
ZPE (kcal/mol) = 462.746
ΔH_{298} (kcal/mol) = 29.650
ΔS_{298} (cal/(k•mol)) = 250.306

Fe1	5.2148570000000	10.5438950000000	3.2919050000000
Cl2	5.9629770000000	12.6578070000000	3.8658570000000
N3	6.7610570000000	9.9044810000000	4.4339670000000
C4	8.0766380000000	9.9934510000000	4.2675600000000
H5	8.4216430000000	10.5509320000000	3.4060500000000
N6	4.2238430000000	10.3549660000000	4.9875240000000
C7	8.9872700000000	9.4328120000000	5.1817720000000
H8	10.0509410000000	9.5311800000000	4.9950060000000
N9	3.7427280000000	11.5158950000000	2.3845370000000
C10	8.5144140000000	8.7793260000000	6.3039190000000
H11	9.2005570000000	8.3304730000000	7.0165260000000
N12	6.0767310000000	10.6757220000000	1.5089870000000
C13	7.1220920000000	8.7527440000000	6.5491960000000
C14	6.2891410000000	9.3659840000000	5.5880030000000
C15	6.5183660000000	8.2013880000000	7.7306430000000
H16	7.1574490000000	7.7066550000000	8.4564960000000
C17	5.1789980000000	8.3393030000000	7.9657850000000
H18	4.7370270000000	7.9474800000000	8.8774480000000
C19	4.3452630000000	9.0724050000000	7.0578980000000
C20	4.9054050000000	9.5736760000000	5.8669830000000
C21	2.9819780000000	9.3735660000000	7.2725200000000
H22	2.4705350000000	8.9858750000000	8.1489910000000
C23	2.3109150000000	10.1746930000000	6.3784630000000
H24	1.2644220000000	10.3865480000000	6.5473130000000
C25	2.9645290000000	10.7214820000000	5.2328640000000
C26	2.2663890000000	11.6951350000000	4.3619350000000
C27	1.2027740000000	12.3957850000000	4.9353320000000
H28	0.9828660000000	12.2554200000000	5.9865040000000
C29	0.4147090000000	13.3264460000000	4.2377330000000
H30	-0.3904020000000	13.8419750000000	4.7502220000000
C31	0.6900420000000	13.5776780000000	2.9170470000000
H32	0.0969890000000	14.2854020000000	2.3456970000000
C33	1.7936830000000	12.9482450000000	2.2899670000000
C34	2.6250000000000	12.0164100000000	3.0033640000000
C35	2.1206670000000	13.2738710000000	0.9537630000000
H36	1.4898900000000	13.9693490000000	0.4089360000000
C37	3.2444780000000	12.7489540000000	0.3722510000000
H38	3.5216410000000	13.0285700000000	-0.6352360000000
C39	4.0646160000000	11.8940770000000	1.1363110000000
C40	5.3498740000000	11.3911340000000	0.6218200000000
C41	5.8074550000000	11.5964200000000	-0.6836350000000
H42	5.2363440000000	12.1879820000000	-1.3873810000000
C43	7.0181440000000	11.0304260000000	-1.0770270000000
H44	7.3974580000000	11.1937910000000	-2.0805460000000
C45	7.7195990000000	10.2369830000000	-0.1708100000000
H46	8.6500310000000	9.7519110000000	-0.4443090000000
C47	7.2039970000000	10.0753030000000	1.1117730000000
H48	7.6906430000000	9.4406320000000	1.8386870000000
O49	4.7439850000000	9.0121640000000	2.9100700000000
O50	1.9646230000000	3.9428470000000	4.7635440000000

Fe53	3.2261620000000	4.9140240000000	4.9289920000000
N54	3.3631850000000	4.9663670000000	6.9595890000000
N55	2.0624330000000	6.4670770000000	5.2255230000000
N56	3.6456720000000	5.4337650000000	3.0960220000000
N57	4.4601500000000	3.4209460000000	4.5718060000000
C58	4.1720430000000	4.3526760000000	7.8282150000000
H59	5.0283870000000	3.8307470000000	7.4177940000000
C60	3.9323210000000	4.3709100000000	9.2126810000000
H61	4.6177540000000	3.8541750000000	9.8759210000000
C62	2.8125650000000	5.0201470000000	9.7055940000000
H63	2.5893590000000	5.0062290000000	10.7688210000000
C64	1.9604490000000	5.7148050000000	8.8135770000000
C65	2.3091430000000	5.6842860000000	7.4465080000000
C66	0.7809480000000	6.4336890000000	9.2038870000000
H67	0.4940880000000	6.4347650000000	10.2507530000000
C68	0.0208560000000	7.0920130000000	8.2755980000000
H69	-0.8838870000000	7.6111960000000	8.5771450000000
C70	0.4077190000000	7.1247060000000	6.8945760000000
C71	1.5675900000000	6.4417840000000	6.4972890000000
C72	-0.2981320000000	7.7910970000000	5.8627790000000
H73	-1.2496620000000	8.2689240000000	6.0787860000000
C74	0.2212340000000	7.8293190000000	4.5894960000000
H75	-0.3420630000000	8.3225360000000	3.8092330000000
C76	1.4603640000000	7.1952830000000	4.2737260000000
C77	2.0905960000000	7.3552820000000	2.9505620000000
C78	1.6955590000000	8.4573600000000	2.1919000000000
H79	0.9787380000000	9.1557740000000	2.6053330000000
C80	2.2104970000000	8.7494520000000	0.9199220000000
H81	1.8512660000000	9.6214580000000	0.3842210000000
C82	3.1696750000000	7.9321380000000	0.3814550000000
H83	3.5873400000000	8.1270830000000	-0.6016750000000
C84	3.6493050000000	6.8195560000000	1.1166490000000
C85	3.1284400000000	6.5143470000000	2.4192340000000
C86	4.6627490000000	6.0059680000000	0.5740000000000
H87	5.0538310000000	6.2363040000000	-0.4119930000000
C88	5.1544010000000	4.9333670000000	1.2813880000000
H89	5.9359190000000	4.3104190000000	0.8674720000000
C90	4.6151550000000	4.6609080000000	2.5453700000000
C91	5.0256270000000	3.4874890000000	3.3407090000000
C92	5.8386060000000	2.4544930000000	2.8749970000000
H93	6.2934270000000	2.5033810000000	1.8938240000000
C94	6.0296760000000	1.3244820000000	3.6718820000000
H95	6.6522150000000	0.5083430000000	3.3179220000000
C96	5.3783580000000	1.2389140000000	4.9013390000000
H97	5.4598630000000	0.3554010000000	5.5249010000000
C98	4.5897720000000	2.3087820000000	5.3141680000000
H99	4.0183420000000	2.2737610000000	6.2326680000000