Supporting Information for

Theoretical insights into the reactivity of Fe-based catalysts for water oxidation: The role of electron-withdrawing groups

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This supplemental file includes the following materials:

1. Some details on theoretical methods and computational procedures.

Molecular geometries and electronic structures are obtained by carrying out density functional theory (DFT) calculations with the ωB97XD dispersion-corrected density functional.[1] The hybrid B3LYP exchange-correlation functional[2,3] is also used to extract from the single-point calculations at the structures obtained with the ωB97XD functional for the complex **(1)** and complex **(4)** in the Supporting Information (See section 3, Supporting Information) for a comparison purpose. The geometry optimization and subsequent frequency analysis are performed with the 6-31G* basis set. The calculation involves spin densities of multiple atoms, so broken-symmetry (BS) approximation is adopted in the framework of DFT. To calculate the transition states, the QST3 and TS algorithms of the Gaussian09 suite of program is adopted. All minima and TSs were verified by no and one imaginary frequency in harmonic vibrational analysis.

The energetic data onto iron species are extracted from the single-point calculations done at the optimized geometries, with the correlation consistent cc-pVTZ basis set[4,5] for all the atoms.

To account for the solvation effects due to water environment, the polarizable continuum model (PCM) of Truhlar and co-workers[6] are adopted for geometry optimization directly using the B3LYP and the ωB97XD functional.

2. Energy profiles for O-O bond-formation for complex (1) and complex (4) with the oxyl radical mechanism calculated by B3LYP functional.

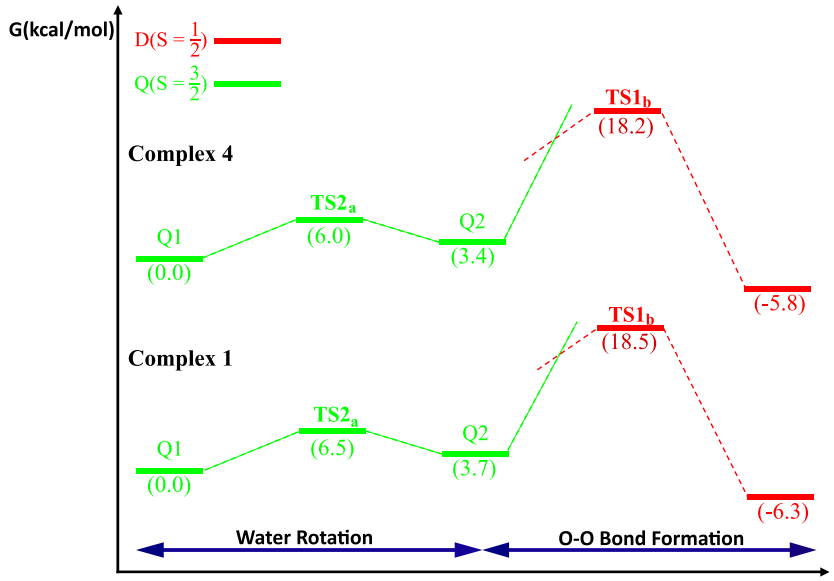

Figure S1. Energy profiles for O-O bond-formation with complex **(1)** and **(4)** (L^{N4} = Pytacn). The red and green lines represent the pathways taking D (S=1/2) and Q (S=3/2) as the reactant respectively. In order to simplify the figure, which just represents the minimum energy pathways. The TS_a represents the transition state of the water rotation step and the TS_b represents the transition state of the O-O bond formation step.

3. The bond length, bond order of Fe-O and Mulliken spin population on oxygen atom calculated by different methods.

Method	BLYP	B3LYP	ωB97	ωB97XD	MP2	[a]B3LYP-D3
Bond length of Fe-O (Å)	1.68	1.70	1.72	1.81	1.75	1.63
Bond order of Fe-O	1.20	1.15	1.18	1.07	0.97	1.73
Mulliken spin on O atom	0.74	0.80	0.89	0.79	0.77	0.84

Table S1 The bond length, bond order of Fe-O and Mulliken spin population on oxygen atom (which is directly linked to iron atom) calculated by different methods. [a]The results of B3LYP-D3[7,8] functional is calculated by the ORCA program.[9-11]

4. Optimized geometric structures of complexes (1) to (6) (And some related species).

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-

oxyl radical (S=2) in complex (**1**):

N	−2.26999800	−0.00866000	−0.30840800
C	−2.68588200	−0.98899400	0.73516200
C	−1.85364500	−0.80042600	1.98149200
N	−0.40300500	−0.66661200	1.68013300
C	0.29732000	−1.94900700	1.44513300
C	−0.02217600	−2.51241900	0.08598800
N	−0.10845200	−1.42247900	−0.93756300
C	−2.36839900	−0.61072700	−1.65548600
C	−1.26502800	−1.64845300	−1.86743300
C	1.17302600	−1.30877700	−1.68424800
C	2.16692600	−0.55069500	−0.86634000
N	1.63578200	0.39225900	−0.07390200
C	2.42213000	1.19824600	0.64530800
C	3.79787600	1.08230100	0.59968200
C	4.35962700	0.09962000	−0.20397900
C	3.53314000	−0.73093700	−0.94794600
Fe	−0.33331500	0.41820700	−0.06348600
C	−3.11622800	1.19875800	−0.24609900
C	0.24052500	−0.03164500	2.84991800
H	−2.60337700	−1.99523600	0.33062800
H	−3.74043200	−0.82857800	0.96981100
H	−2.01509600	−1.62704900	2.67956800
H	−2.15273200	0.12785800	2.47199600
H	0.02730200	−2.66944600	2.22269700
H	1.36641700	−1.74692300	1.53114300
H	−0.95999900	−3.05958100	0.09608000
H	0.75611700	−3.21905500	−0.20829300
H	−2.26745100	0.20305000	−2.37185600
H	−3.35824600	−1.06057500	−1.77525200
H	−0.90766700	−1.57568900	−2.89388000
H	−1.63032300	−2.66347200	−1.71889200
H	1.53601800	−2.30019700	−1.96147800
H	1.91922200	1.93606000	1.25925100
H	4.41122700	1.74941100	1.19208300
H	5.43559600	−0.02332700	−0.25133800
H	3.93328100	−1.50955800	−1.58652600
H	−3.12286400	1.57446600	0.77699300
H	−2.70507700	1.95397700	−0.91571000
H	−4.13329900	0.93953800	−0.55403200
H	−0.21096300	0.94215200	3.02897400
H	0.09628500	−0.67499500	3.72368300
H	1.30847400	0.08700700	2.66491200

H	0.98175300	−0.74247700	−2.59892100
O	−0.51182800	1.79253100	0.97839400
O	−0.30411200	1.06501300	−1.47638100
H	−0.60586400	2.59406500	0.39569000
O	−0.73418600	3.76024200	−0.79656400
H	−0.66815700	3.06182800	−1.46454500
H	−1.67851400	3.96846400	−0.78448200

Cartesian coordinates of transient state ($TS2_a$) associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=2) in complex (**1**):

N	−2.30558300	0.01392200	−0.17717700
C	−2.66029000	−1.18272200	0.65934800
C	−1.72818700	−1.29764200	1.84351300
N	−0.29467800	−1.12014600	1.46421700
C	0.32556800	−2.31673900	0.84517500
C	−0.11439900	−2.46149900	−0.58981900
N	−0.13026000	−1.12436100	−1.27437200
C	−2.48877500	−0.29581000	−1.63029100
C	−1.28208200	−1.04295000	−2.23749600
C	1.18595200	−0.86281400	−1.93625400
C	2.16476800	−0.29830600	−0.94872500
N	1.62724400	0.46071200	0.02901800
C	2.41136800	1.10817300	0.90191300
C	3.79092800	1.00922300	0.83471300
C	4.35984200	0.21178300	−0.15393300
C	3.53697200	−0.45212000	−1.05825800
Fe	−0.33937600	0.45687000	0.00060500
C	−3.19192400	1.15096200	0.17993400
C	0.45350300	−0.83587100	2.71421700
H	−2.64841600	−2.07267400	0.03567700
H	−3.68739900	−1.06864100	1.01487100
H	−1.86377800	−2.26215000	2.34336900
H	−1.95775800	−0.50628400	2.56018500
H	0.06426400	−3.21602000	1.41260000
H	1.40764800	−2.18639100	0.90256700
H	−1.10487200	−2.90009700	−0.65651500
H	0.56355400	−3.12558300	−1.12993200
H	−2.61500600	0.65643900	−2.14336800
H	−3.41343200	−0.86720100	−1.74471600
H	−0.94550500	−0.50067900	−3.11952800
H	−1.54418100	−2.05514900	−2.54686400
H	1.56263800	−1.77290900	−2.40628300
H	1.90532700	1.69720100	1.65709000

H	4.40055800	1.54372600	1.55303700
H	5.43709900	0.10564800	−0.22223200
H	3.94430900	−1.07852000	−1.84340800
H	−3.22735500	1.26817700	1.26532300
H	−2.82307800	2.06641800	−0.28386900
H	−4.20561700	0.93826700	−0.17248500
H	0.06835600	0.06981200	3.17746800
H	0.32962400	−1.68194000	3.39913000
H	1.51477200	−0.71388000	2.49911000
H	1.03173100	−0.11609900	−2.71918200
O	−0.42866800	1.52063400	1.40142200
O	−0.38504300	1.37628900	−1.28191500
O	−0.93436800	4.02987200	−0.33209600
H	−0.89864700	3.25967800	−0.91968600
H	−1.33714200	1.66950900	1.71023600
H	−1.15401600	3.62535400	0.51945600

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (**1**):

N	−2.28150000	0.05497300	−0.18056800
C	−2.68257900	−0.83406200	0.96029000
C	−1.72919200	−0.66465100	2.11882500
N	−0.30009600	−0.69008900	1.67828000
C	0.23533400	−2.05602400	1.44708700
C	−0.26117400	−2.60717700	0.13404500
N	−0.25122500	−1.53902400	−0.92163000
C	−2.54662000	−0.63089700	−1.47889600
C	−1.45866300	−1.67011100	−1.81526500
C	1.02803800	−1.58224400	−1.69377500
C	2.10237300	−0.84833300	−0.94810400
N	1.67332100	0.20896600	−0.22996300
C	2.54569200	1.00653200	0.39848000
C	3.90776000	0.76616300	0.33695600
C	4.36412000	−0.33483200	−0.37961700
C	3.44932000	−1.15565500	−1.03175500
Fe	−0.29603400	0.35551600	−0.17686700
C	−3.05396900	1.31966800	−0.12590000
C	0.50550300	−0.09504800	2.77476800
H	−2.72663900	−1.86275400	0.61204200
H	−3.69667100	−0.56952600	1.26934800
H	−1.90012700	−1.43504200	2.87656800
H	−1.89253000	0.31323300	2.57879400
H	−0.05074000	−2.71848400	2.26980200

H	1.32341300	−1.97856700	1.44026000
H	−1.26845100	−3.00079100	0.22557800
H	0.37420500	−3.43305300	−0.19143000
H	−2.56899000	0.14073400	−2.24735000
H	−3.53478800	−1.09556100	−1.43134600
H	−1.13870400	−1.51843100	−2.84458800
H	−1.83643700	−2.68879500	−1.73137100
H	1.30664700	−2.61585600	−1.90620300
H	2.12597000	1.83380800	0.95681400
H	4.58953000	1.42987800	0.85445500
H	5.42500000	−0.55401700	−0.43181800
H	3.76682700	−2.02178500	−1.60055100
H	−3.00120800	1.73393900	0.88256600
H	−2.64616200	2.03166900	−0.84467800
H	−4.10174800	1.11149500	−0.36145100
H	0.19382200	0.93222900	2.95089400
H	0.35475500	−0.68734000	3.68341200
H	1.56373200	−0.11117300	2.51378800
H	0.86959100	−1.06741900	−2.64477600
O	−0.16530500	1.80712200	0.81210100
O	−0.34519900	0.86458500	−1.65325100
H	−1.00497900	2.11065500	1.19602100
O	0.20223900	3.70406300	−1.23227800
H	0.52927300	3.09409600	−1.90518200
H	0.12143700	3.12996600	−0.44715500

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (**1**):

N	−2.34284300	0.19300200	−0.24040000
C	−2.83794100	−0.87884600	0.69625700
C	−1.96191000	−0.92545500	1.92982500
N	−0.50117400	−0.91679000	1.58411300
C	0.01307200	−2.22302200	1.06238800
C	−0.33865900	−2.43320900	−0.40186300
N	−0.21566800	−1.14999100	−1.20558100
C	−2.52039700	−0.21890000	−1.67512400
C	−1.33611800	−1.05749500	−2.21202100
C	1.12833400	−1.06168400	−1.86862700
C	2.14961000	−0.53491500	−0.90180900
N	1.66329100	0.29239900	0.05326300
C	2.50658000	0.91102900	0.90099900
C	3.87958400	0.71620100	0.83073600
C	4.38914600	−0.15073400	−0.13610300

C	3.51253100	−0.78559600	−1.01427400
Fe	−0.31920100	0.44814900	−0.01133800
C	−3.11938100	1.44265200	−0.00153000
C	0.23601300	−0.60506400	2.84291100
H	−2.86184800	−1.83239400	0.17510100
H	−3.86982700	−0.65481600	0.98237600
H	−2.19687000	−1.80582500	2.53888100
H	−2.13926600	−0.03370000	2.53571100
H	−0.38344400	−3.04993500	1.66229800
H	1.09655800	−2.21088500	1.18885800
H	−1.35333400	−2.80320700	−0.51656700
H	0.32296100	−3.18662100	−0.83665300
H	−2.59705100	0.69715200	−2.25948300
H	−3.46816100	−0.75662000	−1.76931700
H	−0.94419100	−0.57515800	−3.10610400
H	−1.64186700	−2.06863700	−2.48743900
H	1.41592000	−2.02946200	−2.28697400
H	2.05645600	1.56599700	1.63622500
H	4.52879600	1.23299200	1.52823000
H	5.45713900	−0.33044800	−0.20690700
H	3.87089800	−1.46199700	−1.78241000
H	−3.13080900	1.66889700	1.06621300
H	−2.66446400	2.26745400	−0.55062600
H	−4.15157900	1.29987000	−0.33915200
H	−0.07818300	0.36568000	3.22506500
H	0.01466100	−1.37559100	3.59051600
H	1.30974000	−0.59323200	2.65884100
H	1.04615200	−0.34740200	−2.69249200
O	−0.28438400	1.93597200	1.28594700
O	−0.28608500	1.47767400	−1.30462400
H	−1.11920600	2.08209600	1.76712700
O	−0.14888735	3.33091539	−0.88239790
H	−1.02845635	3.59088639	−1.21895190
H	−0.11628405	2.77619965	0.33182785

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (**1**):

N	−2.34106400	−0.43432000	0.06566900
C	−2.89807800	0.95942500	0.08351700
C	−2.12749000	1.83097500	−0.89081000
N	−0.64053100	1.65511700	−0.76066700
C	−0.04225600	2.40200800	0.39111900
C	−0.30581700	1.71816900	1.72676000

N	-0.25563300	0.20200900	1.61913300
C	-2.42125900	-1.05917000	1.42011400
C	-1.39911600	-0.43238300	2.38322300
C	1.07288000	-0.30390500	2.09246000
C	2.11281700	-0.09102400	1.02644500
N	1.65382500	-0.13428500	-0.24841100
C	2.52639800	-0.05083000	-1.27024000
C	3.89227100	0.08714400	-1.06034000
C	4.36934900	0.15214100	0.24879100
C	3.46645400	0.06298200	1.30662400
Fe	-0.32890600	-0.33302600	-0.31400100
C	-3.10197500	-1.26743200	-0.90344800
C	-0.02313600	2.18440800	-2.00937100
H	-2.85674500	1.34749400	1.09901500
H	-3.95585800	0.93730000	-0.19693700
H	-2.39123300	2.88676100	-0.76135600
H	-2.38302300	1.54195600	-1.91280100
H	-0.43269600	3.42604400	0.41639700
H	1.02998300	2.46225400	0.20065100
H	-1.27854400	2.00500700	2.11671600
H	0.43665000	2.04955600	2.45740300
H	-2.21214500	-2.11989100	1.28703800
H	-3.43838000	-0.95858200	1.81539100
H	-1.00338400	-1.20735100	3.04058300
H	-1.85854200	0.32421300	3.01967900
H	1.35270000	0.17210300	3.03638000
H	2.10752200	-0.10000000	-2.26765000
H	4.56122500	0.14805100	-1.91131700
H	5.43037000	0.27125400	0.44433000
H	3.79819900	0.10666000	2.33823800
H	-3.14793000	-0.75750700	-1.86796200
H	-2.60755500	-2.23248300	-1.02212400
H	-4.12368800	-1.42253800	-0.53832400
H	-0.40285500	1.63662400	-2.87136400
H	-0.27299900	3.24645400	-2.11936900
H	1.06119800	2.08177400	-1.96445700
H	0.97830700	-1.37841100	2.26810000
O	-0.21525300	-0.79756700	-2.26023000
O	-0.20622600	-2.09746700	0.11570700
H	-1.06349600	-0.77116400	-2.73798200
O	0.60515100	-2.83324800	-0.85828500
H	0.06087100	-3.63624200	-0.97050900
H	0.05178600	-1.74911200	-2.21040400

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (**1**):

N	−2.29314700	−0.06539500	−0.30081800
C	−2.68860500	−1.09439800	0.72884500
C	−1.86237000	−0.93058100	1.98870000
N	−0.39967000	−0.77260200	1.69789200
C	0.30443700	−2.05094700	1.37242100
C	0.00892700	−2.53709300	−0.03862300
N	−0.07437800	−1.39161300	−1.03091500
C	−2.38603100	−0.62294700	−1.69020200
C	−1.22708000	−1.58785700	−1.99407100
C	1.22568700	−1.22876700	−1.76196300
C	2.21046000	−0.50918400	−0.88965400
N	1.66316000	0.38643100	−0.03442800
C	2.44436200	1.17198500	0.73006100
C	3.82848000	1.07727700	0.67422300
C	4.40797700	0.14443900	−0.18553800
C	3.58910800	−0.66012500	−0.97660800
Fe	−0.33450300	0.43502500	−0.06548000
C	−3.18309000	1.12805400	−0.19131000
C	0.23338100	−0.20723700	2.92236200
H	−2.58836100	−2.08595400	0.29438600
H	−3.74810900	−0.95829400	0.96309100
H	−2.02097900	−1.78307400	2.65881200
H	−2.17406500	−0.02505900	2.51262000
H	0.02274000	−2.82598200	2.09435800
H	1.37203600	−1.86245700	1.49118200
H	−0.92569200	−3.08954100	−0.07291100
H	0.79444400	−3.22670600	−0.35852800
H	−2.35963300	0.22742800	−2.37007500
H	−3.35514700	−1.12026600	−1.79921000
H	−0.87436100	−1.40550400	−3.00869700
H	−1.54507200	−2.62916500	−1.94207400
H	1.59989700	−2.19974100	−2.09555300
H	1.93706500	1.87366200	1.38038000
H	4.43184300	1.72421200	1.30053900
H	5.48698500	0.04326500	−0.24097900
H	4.00323500	−1.39439400	−1.65860900
H	−3.20628400	1.46583200	0.84415500
H	−2.80636300	1.92407800	−0.83290600
H	−4.19069500	0.83915300	−0.50765100
H	−0.21230900	0.75925300	3.15236100
H	0.07180300	−0.89331500	3.76203800

H	1.30565300	-0.08853700	2.76763400
H	1.03945300	-0.61283500	-2.64588700
O	-0.56396700	1.81426000	0.99323100
O	-0.32203000	1.23912000	-1.49597500
H	-0.66187800	2.65185000	0.44838800
O	-0.84386700	3.96790600	-0.61294500
H	-0.76756100	3.40861700	-1.40806100
H	-1.79826500	4.14909100	-0.55478200

Cartesian coordinates of transient state ($TS2_a$) associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (**1**):

N	-2.29150400	-0.11007400	-0.23400800
C	-2.59375400	-1.35255500	0.56346600
C	-1.74536900	-1.38961900	1.81654600
N	-0.29854300	-1.11699400	1.53100500
C	0.44104600	-2.26816800	0.92884200
C	0.11835500	-2.45949100	-0.54314600
N	-0.04254400	-1.13666200	-1.27197200
C	-2.40024400	-0.35908600	-1.70934300
C	-1.21370200	-1.18179500	-2.23283300
C	1.22765800	-0.77029800	-1.98485700
C	2.21392000	-0.22111600	-1.00055800
N	1.66299700	0.46689500	0.02721200
C	2.43578600	1.09343000	0.93209700
C	3.82090800	1.03962200	0.84662900
C	4.40660800	0.31697400	-0.19229100
C	3.59347100	-0.32163900	-1.12792600
Fe	-0.33984700	0.44996800	0.06746600
C	-3.24369700	0.98058300	0.14433400
C	0.35268000	-0.79500000	2.83137000
H	-2.43812100	-2.22334500	-0.06688500
H	-3.65353000	-1.33785800	0.83185500
H	-1.85021000	-2.35845800	2.31707000
H	-2.07661000	-0.61065400	2.50652700
H	0.20906500	-3.18767200	1.47821500
H	1.50407400	-2.06346300	1.06153700
H	-0.79406500	-3.03434400	-0.67279300
H	0.92066600	-3.02583400	-1.02194900
H	-2.43074300	0.61747000	-2.19036600
H	-3.35181200	-0.86638500	-1.89843800
H	-0.89870000	-0.77662700	-3.19349100
H	-1.48353700	-2.22635800	-2.38887300
H	1.61689700	-1.63598700	-2.52631700

H	1.92289300	1.63422700	1.71793400
H	4.41862400	1.55317000	1.59076100
H	5.48650800	0.24931600	-0.27413900
H	4.01187400	-0.89175100	-1.94980500
H	-3.30417100	1.05248600	1.23114000
H	-2.90946900	1.92747600	-0.27982700
H	-4.23185000	0.72221900	-0.24927700
H	-0.11158900	0.08861500	3.26529800
H	0.23269200	-1.64674000	3.51081700
H	1.41701500	-0.61338300	2.68073300
H	0.99391200	0.01377700	-2.70945000
O	-0.44292300	1.61441900	1.41258100
O	-0.41250300	1.49753800	-1.21557700
O	-1.41960800	4.06780200	-0.44489300
H	-1.02636500	3.24229700	-0.79131100
H	-1.34137400	1.79341900	1.74647200
H	-1.49062300	3.87395100	0.50391800

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (**1**):

N	-2.27829600	0.07117700	-0.18466100
C	-2.69691200	-0.85212800	0.93167300
C	-1.79970500	-0.66360700	2.13724700
N	-0.34439900	-0.64103000	1.76565300
C	0.24097300	-1.99360100	1.49283700
C	-0.18589000	-2.55770500	0.14851000
N	-0.24200500	-1.48981000	-0.93204400
C	-2.50800800	-0.56110400	-1.52420200
C	-1.47261300	-1.65930800	-1.80552000
C	1.01221100	-1.51014800	-1.76060400
C	2.11826900	-0.84121400	-1.00315300
N	1.71357900	0.15984700	-0.18635300
C	2.61210400	0.91232100	0.47552000
C	3.97400300	0.67044300	0.35592600
C	4.40664300	-0.37281600	-0.46193200
C	3.46710200	-1.13904300	-1.15062200
Fe	-0.26993600	0.40110200	-0.10607700
C	-3.04626600	1.34872100	-0.10258200
C	0.39596300	-0.08303000	2.93490900
H	-2.68870600	-1.87566600	0.56693000
H	-3.73076000	-0.61819800	1.20000300
H	-1.98444600	-1.45035700	2.87653400
H	-2.01513500	0.30005600	2.60279600

H	−0.05052100	−2.68745300	2.28934100
H	1.32501100	−1.88189300	1.53255200
H	−1.16129800	−3.03020300	0.21413500
H	0.51983400	−3.33303600	−0.15918000
H	−2.43475900	0.23452400	−2.26411100
H	−3.52704100	−0.96015100	−1.54772600
H	−1.17157800	−1.60581400	−2.85110200
H	−1.87894000	−2.65568400	−1.63221500
H	1.25936900	−2.53560300	−2.04573400
H	2.21782600	1.70993400	1.09252800
H	4.67345800	1.29354000	0.90121200
H	5.46522600	−0.58835900	−0.56444200
H	3.76457100	−1.95594700	−1.79847800
H	−2.97631200	1.74674600	0.90934400
H	−2.63914500	2.06988500	−0.80974600
H	−4.09336800	1.13577900	−0.34205400
H	−0.02239200	0.88048800	3.23275100
H	0.29227400	−0.76780500	3.78406400
H	1.45307900	0.02993900	2.69625200
H	0.82151100	−0.93681900	−2.67151200
O	−0.25916200	1.98322500	0.71119000
O	−0.27927000	1.07574900	−1.60032500
H	−0.24959900	1.93292200	1.68449100
O	−0.87879100	3.98423100	−1.22453600
H	−0.69723100	3.33850300	−1.92728200
H	−0.71768100	3.44722100	−0.42322700

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (**1**):

N	−2.39407900	−0.01904000	−0.39251500
C	−2.81791100	−0.97045100	0.68433500
C	−2.05327000	−0.68905000	1.96563900
N	−0.57055800	−0.54756100	1.74889700
C	0.15060200	−1.84759400	1.56358900
C	−0.06402600	−2.48041100	0.19237300
N	−0.12949900	−1.47236000	−0.92289700
C	−2.38041200	−0.65568100	−1.73490700
C	−1.28139800	−1.73176600	−1.84868600
C	1.16193300	−1.38673200	−1.64885300
C	2.19665000	−0.67296500	−0.81723000
N	1.73302700	0.29848400	−0.00406500
C	2.59360100	1.04101800	0.71772100
C	3.96527500	0.82882300	0.66400900
C	4.45407300	−0.18608700	−0.15879900

C	3.55852000	−0.94723700	−0.90772600
Fe	−0.36199600	0.58507600	−0.02731800
C	−3.25831300	1.18907500	−0.39693300
C	−0.00376500	0.10603500	2.96465300
H	−2.67444100	−1.99115100	0.33760000
H	−3.89054400	−0.85288600	0.87138600
H	−2.24043900	−1.47417400	2.70701800
H	−2.39206800	0.26089500	2.38532200
H	−0.16967400	−2.54826600	2.34375800
H	1.20849800	−1.64040200	1.72558300
H	−0.97917400	−3.06768400	0.18795500
H	0.75469700	−3.18274100	0.00354900
H	−2.20763000	0.14200800	−2.45766800
H	−3.36130100	−1.09965800	−1.94328500
H	−0.92256900	−1.74995900	−2.87925600
H	−1.68694000	−2.72275600	−1.63905700
H	1.51625800	−2.38154900	−1.94049600
H	2.16077200	1.81287900	1.34330200
H	4.62757500	1.44430700	1.26228700
H	5.51965300	−0.38524500	−0.21422000
H	3.90080800	−1.74595600	−1.55700000
H	−3.27406200	1.63042200	0.60171700
H	−2.86370200	1.91624800	−1.10867900
H	−4.28008200	0.91440700	−0.68506200
H	−0.49849400	1.06062800	3.14117700
H	−0.16047500	−0.54630300	3.83181100
H	1.06588700	0.26929900	2.83267100
H	0.99749500	−0.80745200	−2.56266800
O	−0.34297400	2.41098200	0.98665100
O	−0.28497500	1.30010600	−1.52218600
H	−1.21244500	2.55064800	1.40569000
O	−0.11777620	3.19208366	−1.47978373
H	−1.03251220	3.27921366	−1.81373773
H	−0.28652926	3.06867624	−0.17337663

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (**1**):

N	−2.38370200	0.01846900	−0.49602400
C	−2.91234400	−0.67358100	0.72290300
C	−2.21017000	−0.14696800	1.96236500
N	−0.71502500	−0.09753700	1.80050700
C	−0.04591700	−1.43570500	1.93699700
C	−0.21681600	−2.36196800	0.72932400

N	-0.19776200	-1.63901000	-0.58425900
C	-2.33063500	-0.87963800	-1.67858100
C	-1.33265000	-2.03418700	-1.47683200
C	1.11538800	-1.75587900	-1.25557800
C	2.15063400	-0.90257200	-0.56578500
N	1.70066100	0.22825700	0.01635600
C	2.57552100	1.07923100	0.58632000
C	3.94121700	0.82852500	0.60666300
C	4.41361400	-0.34547000	0.01893600
C	3.50671400	-1.22209900	-0.57185800
Fe	-0.37427600	0.58824200	-0.11547300
C	-3.20086000	1.22057100	-0.80094100
C	-0.17512700	0.78066100	2.87716200
H	-2.78101500	-1.74745300	0.61238600
H	-3.98983900	-0.49684600	0.80961700
H	-2.46448300	-0.75139400	2.84048700
H	-2.53254600	0.87942300	2.15402400
H	-0.43144800	-1.93253100	2.83499200
H	1.01175500	-1.22920900	2.10359300
H	-1.14782200	-2.91956300	0.81092400
H	0.58912500	-3.10354000	0.75638700
H	-2.03170400	-0.26050500	-2.52618200
H	-3.33041800	-1.27960600	-1.88898300
H	-0.94819500	-2.33168600	-2.45489200
H	-1.83117200	-2.91062200	-1.05863900
H	1.44951800	-2.79906100	-1.30550100
H	2.15845500	1.97522800	1.03180400
H	4.61187600	1.53792300	1.07830600
H	5.47413400	-0.57693000	0.02389400
H	3.83562500	-2.14528900	-1.03706300
H	-3.24853800	1.86322100	0.08126000
H	-2.74552600	1.77020400	-1.62554400
H	-4.21864700	0.92277400	-1.08058700
H	-0.63519400	1.76604300	2.81321900
H	-0.39697700	0.33828700	3.85568200
H	0.90564200	0.87693600	2.76862200
H	1.00511700	-1.39244800	-2.28217200
O	-0.29868600	2.66420500	0.44296700
O	-0.20747600	1.07652800	-1.85517600
H	-1.20434200	3.02304700	0.43136600
O	0.73129400	2.18099100	-2.02332800
H	0.20101600	2.77997800	-2.58432800
H	0.12510600	2.99876300	-0.37872000

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (**2**):

N	−2.93062100	−0.09075300	−0.37243000
C	−3.37693300	−1.00860000	0.74062300
C	−2.59847800	−0.72736200	2.01060900
N	−1.12412400	−0.59999900	1.76580100
C	−0.41515900	−1.90524200	1.59794900
C	−0.67439200	−2.52832700	0.23708500
N	−0.69442400	−1.49145200	−0.87162300
C	−2.96918000	−0.78649700	−1.70234700
C	−1.80618800	−1.78116200	−1.85912800
C	0.63539900	−1.41741600	−1.55968500
C	1.58864000	−0.59843200	−0.74244600
N	1.02064000	0.37628400	0.00198400
C	1.77379200	1.24454400	0.69809200
C	3.16062400	1.16697100	0.68966600
C	3.73393400	0.15055600	−0.06172200
C	2.96992100	−0.75027100	−0.78914200
Fe	−0.98818300	0.42456000	−0.10394600
C	−3.81504100	1.11229500	−0.42341100
C	−0.53810200	0.08433000	2.95243900
H	−3.27639100	−2.03856100	0.40849600
H	−4.44234500	−0.83733000	0.91774000
H	−2.78799600	−1.51227700	2.75103900
H	−2.92631500	0.22423600	2.43246800
H	−0.72336300	−2.60328300	2.38482300
H	0.64963600	−1.70952400	1.73156200
H	−1.62395800	−3.05484700	0.22690600
H	0.09928100	−3.26873300	0.01881600
H	−2.90789200	−0.00947500	−2.46272200
H	−3.93716300	−1.28797600	−1.80016600
H	−1.41041800	−1.70307300	−2.87123100
H	−2.13325800	−2.81106900	−1.71616800
H	1.02269500	−2.41983000	−1.75895400
H	1.24926400	2.00765200	1.25850800
H	3.75693200	1.87342500	1.25130200
H	3.42121700	−1.53989400	−1.37581100
H	−3.86535300	1.56410100	0.56681500
H	−3.41501200	1.82847400	−1.14032600
H	−4.81485800	0.79292300	−0.73475300
H	−0.98146500	1.07261000	3.06294200
H	−0.74324200	−0.51185500	3.84915700
H	0.54146800	0.17998000	2.83550900

H	0.49505500	−0.90821000	−2.51736000
O	−1.23677400	1.89565800	0.81231800
O	−0.91027600	1.09842800	−1.59883100
H	−1.31846200	2.67995900	0.18835700
O	−1.49490200	3.88676800	−0.98479600
H	−1.37734000	3.26745800	−1.72861700
H	−2.45609000	4.03911000	−0.96687200
Cl	5.18833381	0.02540158	−0.08736500

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (**2**):

N	−2.28709900	0.05189400	−0.18047800
C	−2.68536500	−0.83059500	0.96515900
C	−1.72595200	−0.65707700	2.11960000
N	−0.29954900	−0.69142600	1.67851100
C	0.23419000	−2.05655400	1.44547900
C	−0.26164300	−2.60672500	0.13198800
N	−0.25264900	−1.53727700	−0.92215600
C	−2.55037000	−0.63985500	−1.47665000
C	−1.45805800	−1.67367000	−1.81592100
C	1.02650000	−1.58187000	−1.69374400
C	2.10047500	−0.84707300	−0.94880700
N	1.67135100	0.20883800	−0.22896100
C	2.54452100	1.00634900	0.39850400
C	3.90673900	0.76712000	0.33542400
C	4.36273600	−0.33253600	−0.38334000
C	3.44763400	−1.15329700	−1.03477300
Fe	−0.29784700	0.35765000	−0.17881100
C	−3.06863100	1.31133400	−0.13398200
C	0.50761400	−0.09327000	2.77144600
H	−2.73281600	−1.85998700	0.62070100
H	−3.69711100	−0.56268900	1.27942900
H	−1.89841100	−1.42255700	2.88220900
H	−1.88374500	0.32339200	2.57498200
H	−0.05080700	−2.72124700	2.26708900
H	1.32245100	−1.97946200	1.43814200
H	−1.26882200	−3.00052600	0.22421500
H	0.37253300	−3.43321800	−0.19473300
H	−2.57847700	0.13037900	−2.24642700
H	−3.53650100	−1.10902000	−1.42730600
H	−1.13928800	−1.51846700	−2.84524400
H	−1.83107300	−2.69445300	−1.73570500
H	1.30634800	−2.61545200	−1.90509300

H	2.12401800	1.83308100	0.95730500
H	4.58918800	1.43027600	0.85273700
H	3.76540900	−2.01781000	−1.60592600
H	−3.01650900	1.73881400	0.86887200
H	−2.67069500	2.01841800	−0.86264700
H	−4.11577700	1.09332100	−0.36364000
H	0.18980800	0.93215300	2.94766800
H	0.36404300	−0.68628500	3.68105800
H	1.56509700	−0.10420300	2.50751800
H	0.86807400	−1.06866500	−2.64564300
O	−0.16902600	1.80608500	0.82145400
O	−0.34645700	0.86546000	−1.66021100
H	−1.00914700	2.10624300	1.20648100
O	0.58300400	3.63041800	−0.83118200
H	0.67023500	3.04743600	−1.59663400
H	0.20456100	3.04189000	−0.15028200
Cl	5.96783790	−1.01298694	−0.62465806

Cartesian coordinates of transient state ($TS1_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (**2**):

N	−2.39214500	−0.03647800	−0.39509500
C	−2.80363600	−0.98477500	0.67399600
C	−2.04429600	−0.67945600	1.94753800
N	−0.57624400	−0.50833500	1.71718500
C	0.16297800	−1.79234500	1.54961700
C	−0.04485500	−2.43652000	0.18821000
N	−0.13090600	−1.43694100	−0.92378300
C	−2.38652700	−0.66982600	−1.72838500
C	−1.27205600	−1.72210100	−1.84392300
C	1.14672400	−1.35690200	−1.65916800
C	2.18672600	−0.67063300	−0.81844600
N	1.72904100	0.29367800	−0.00615900
C	2.58827800	1.01103100	0.72873100
C	3.95305300	0.78358200	0.69894900
C	4.41746900	−0.23016200	−0.13026000
C	3.53639600	−0.97447000	−0.90398100
Fe	−0.38571800	0.58188400	−0.04471100
C	−3.25555900	1.16265000	−0.38952100
C	−0.01970100	0.16042200	2.92068500
H	−2.64098800	−2.00559600	0.33578000
H	−3.87763000	−0.88555300	0.85879400
H	−2.20904200	−1.46172700	2.69573500
H	−2.40307700	0.26609500	2.36071900

H	−0.14550800	−2.48975200	2.33590600
H	1.21887200	−1.56889400	1.70631500
H	−0.94938900	−3.03940200	0.19317600
H	0.78348700	−3.12616700	−0.00054900
H	−2.23425300	0.12533500	−2.45863500
H	−3.36028800	−1.13258300	−1.92397300
H	−0.91360400	−1.73450900	−2.87390600
H	−1.65683600	−2.72058600	−1.63339000
H	1.48521800	−2.34978800	−1.97168100
H	2.16421900	1.78643100	1.35563800
H	4.62014400	1.37896800	1.30952100
H	3.87681200	−1.76918500	−1.55713500
H	−3.24334400	1.61700400	0.60307400
H	−2.88000500	1.88358700	−1.11737800
H	−4.28360100	0.88539900	−0.64845700
H	−0.52566600	1.10977400	3.09071000
H	−0.16757500	−0.48788600	3.79127200
H	1.04739900	0.33760100	2.78872600
H	0.98904900	−0.75352100	−2.55786800
O	−0.26931400	2.34118200	0.85381000
O	−0.30563900	1.30533500	−1.51333100
H	−1.09485300	2.52698600	1.33056800
O	−0.14990300	3.20898900	−1.47315100
H	−1.11001000	3.28931500	−1.61862600
H	−0.18777104	3.01483186	−0.17820000
Cl	6.11758600	−0.57626900	−0.19607800

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (2):

N	3.00556400	0.12972400	−0.33652300
C	3.49559400	0.27631100	1.07593000
C	2.70984300	−0.64790200	1.98610400
N	1.23031300	−0.56632700	1.73666200
C	0.57866400	0.64339300	2.33561900
C	0.82139400	1.90192100	1.51303600
N	0.80617000	1.62271600	0.01882300
C	3.06817100	1.42980300	−1.07324500
C	1.92052400	2.37772900	−0.67331500
C	−0.53148800	1.96281100	−0.56317300
C	−1.51359900	0.85878200	−0.28549300
N	−0.98675300	−0.38404500	−0.19206700
C	−1.79425600	−1.44825000	−0.03756100
C	−3.17488200	−1.32101400	0.04362600

C	-3.69681600	-0.03677300	-0.03585900
C	-2.88587600	1.07629400	-0.20156100
Fe	1.01246600	-0.34577400	-0.30066600
C	3.84299800	-0.86980300	-1.05450700
C	0.61294800	-1.76821500	2.36549400
H	3.41022700	1.31694700	1.38012600
H	4.55990500	0.02488000	1.12136000
H	2.92254300	-0.43164500	3.03927600
H	2.99772700	-1.68293200	1.78661700
H	0.94189500	0.79542700	3.35838000
H	-0.48925600	0.42740600	2.39298400
H	1.77810800	2.34945300	1.76723700
H	0.05440400	2.64469300	1.74638600
H	2.99202800	1.19002400	-2.13287200
H	4.04214700	1.90088700	-0.90217200
H	1.52189900	2.84983400	-1.57113700
H	2.26497100	3.17674500	-0.01575300
H	-0.88954900	2.92529300	-0.18814600
H	-1.31703200	-2.41777000	0.02099600
H	-3.80639700	-2.19001300	0.17010900
H	-3.29422000	2.07657600	-0.26335300
H	3.90181000	-1.78980600	-0.46910000
H	3.40103000	-1.08212100	-2.02856800
H	4.85630000	-0.47485500	-1.18998900
H	1.02995700	-2.67281800	1.92365300
H	0.81933400	-1.76353900	3.44224800
H	-0.46645600	-1.75493100	2.21586300
H	-0.41830500	2.04121000	-1.64743500
O	1.01378900	-2.33326500	-0.57814600
O	0.95979800	-0.09214700	-2.09892100
H	1.87797400	-2.76734300	-0.46118500
O	0.26304800	-1.18202300	-2.78485100
H	0.87534000	-1.34209400	-3.52894900
H	0.79922500	-2.38428800	-1.54304100
Cl	-5.10251862	0.14241843	0.05519353

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (2):

N	-2.77019300	-0.09227200	-0.44489100
C	-3.26879400	-0.98568800	0.65123300
C	-2.52638500	-0.70637100	1.93824800
N	-1.05250100	-0.59549200	1.72712900
C	-0.36162800	-1.90887000	1.60585400

C	-0.61985100	-2.56549500	0.26878100
N	-0.60926900	-1.56233300	-0.85832000
C	-2.81350800	-0.79209500	-1.76117700
C	-1.70868900	-1.84872900	-1.84990700
C	0.72388700	-1.55546200	-1.52831700
C	1.68515300	-0.78383500	-0.68248900
N	1.14042100	0.23334300	0.00513400
C	1.89850400	1.06880300	0.72499800
C	3.27144000	0.90532800	0.80237200
C	3.81905200	-0.15938200	0.11072200
C	3.05060200	-1.02558700	-0.64528100
Fe	-0.82554600	0.34815900	-0.14848700
C	-3.60729300	1.13414200	-0.51084700
C	-0.47988300	0.06374000	2.92824800
H	-3.17920000	-2.02055100	0.33290800
H	-4.33468500	-0.79261000	0.79323000
H	-2.74271100	-1.48181900	2.67938500
H	-2.85755600	0.25389700	2.33928100
H	-0.68820800	-2.57587700	2.41031200
H	0.70523900	-1.72487400	1.74386300
H	-1.57624900	-3.07881500	0.26985500
H	0.14313500	-3.32338400	0.08052000
H	-2.68415000	-0.03167300	-2.53029400
H	-3.80292600	-1.24216600	-1.88361400
H	-1.29073000	-1.84470600	-2.85542700
H	-2.09077800	-2.85067900	-1.65885100
H	1.06155500	-2.57555800	-1.72155000
H	1.39076300	1.87614500	1.23738400
H	3.87520500	1.58495800	1.38827300
H	3.48247000	-1.85707400	-1.18693600
H	-3.66612200	1.58336700	0.48014100
H	-3.16695200	1.84392800	-1.20992300
H	-4.60800100	0.84807200	-0.84779600
H	-0.98441500	1.00756400	3.14028800
H	-0.62163700	-0.59043900	3.79469100
H	0.58645200	0.24080600	2.79190600
H	0.62775000	-1.03457400	-2.48448900
O	-1.01002400	1.94120300	0.57753600
O	-0.67605500	0.94779000	-1.65402600
H	-1.18145100	1.93805400	1.53170200
O	-1.51033400	3.77944100	-1.51055000
H	-1.30083000	3.08724100	-2.15259700
H	-1.41249800	3.30211500	-0.66713000
Cl	5.22151577	-0.37105670	0.17919967

Cartesian coordinates of transient state (TS2b) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (2):

N	−2.38922700	−0.03406400	−0.39473200
C	−2.80189000	−0.98164900	0.67445000
C	−2.04070300	−0.67850200	1.94740400
N	−0.57244000	−0.51121000	1.71646300
C	0.16342900	−1.79679100	1.54805900
C	−0.04793500	−2.44102800	0.18703500
N	−0.13383200	−1.44244300	−0.92462200
C	−2.38585100	−0.66746100	−1.72806700
C	−1.27585800	−1.72448100	−1.84306700
C	1.14485600	−1.36035400	−1.65865600
C	2.18483700	−0.67355400	−0.81805100
N	1.72395600	0.29199700	−0.00685900
C	2.57967700	1.01421100	0.73031700
C	3.94480000	0.78394400	0.69600900
C	4.42975500	−0.22686200	−0.12773700
C	3.53804300	−0.96720200	−0.89574600
Fe	−0.37881400	0.58018700	−0.04507600
C	−3.25158900	1.16560500	−0.38944800
C	−0.01392500	0.15612000	2.91964500
H	−2.64191100	−2.00284600	0.33611700
H	−3.87549800	−0.88011100	0.86046500
H	−2.20725900	−1.46033800	2.69572900
H	−2.39685100	0.26799500	2.36077400
H	−0.14500400	−2.49310400	2.33541500
H	1.22001100	−1.57500400	1.70199300
H	−0.95350200	−3.04251300	0.19414400
H	0.77906900	−3.13223500	−0.00234100
H	−2.22978800	0.12730200	−2.45802300
H	−3.36167700	−1.12578600	−1.92414400
H	−0.91841700	−1.73993100	−2.87343900
H	−1.66540600	−2.72094200	−1.63127400
H	1.48400800	−2.35358600	−1.97022300
H	2.14621700	1.78749500	1.35370800
H	4.60630100	1.38502400	1.30821900
H	3.87809900	−1.76251600	−1.54938000
H	−3.24148300	1.61867000	0.60375400
H	−2.87397500	1.88717500	−1.11564400
H	−4.27939600	0.88968200	−0.65093500
H	−0.51646300	1.10755600	3.08845800
H	−0.16440800	−0.49086100	3.79081100

H	1.05376800	0.32925200	2.78729000
H	0.98398000	−0.76002900	−2.55887900
O	−0.27657600	2.34398700	0.85555200
O	−0.29906800	1.30475500	−1.51317700
H	−1.10583100	2.52662200	1.32676000
O	−0.17552400	3.19439100	−1.36038500
H	−1.08049200	3.30462000	−1.70391000
H	−0.28187200	2.91499600	−0.07157300
Cl	6.12696463	−0.56388836	−0.19663452

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (2):

N	3.00556400	0.12972400	−0.33652300
C	3.49559400	0.27631100	1.07593000
C	2.70984300	−0.64790200	1.98610400
N	1.23031300	−0.56632700	1.73666200
C	0.57866400	0.64339300	2.33561900
C	0.82139400	1.90192100	1.51303600
N	0.80617000	1.62271600	0.01882300
C	3.06817100	1.42980300	−1.07324500
C	1.92052400	2.37772900	−0.67331500
C	−0.53148800	1.96281100	−0.56317300
C	−1.51359900	0.85878200	−0.28549300
N	−0.98675300	−0.38404500	−0.19206700
C	−1.79425600	−1.44825000	−0.03756100
C	−3.17488200	−1.32101400	0.04362600
C	−3.69681600	−0.03677300	−0.03585900
C	−2.88587600	1.07629400	−0.20156100
Fe	1.01246600	−0.34577400	−0.30066600
C	3.84299800	−0.86980300	−1.05450700
C	0.61294800	−1.76821500	2.36549400
H	3.41022700	1.31694700	1.38012600
H	4.55990500	0.02488000	1.12136000
H	2.92254300	−0.43164500	3.03927600
H	2.99772700	−1.68293200	1.78661700
H	0.94189500	0.79542700	3.35838000
H	−0.48925600	0.42740600	2.39298400
H	1.77810800	2.34945300	1.76723700
H	0.05440400	2.64469300	1.74638600
H	2.99202800	1.19002400	−2.13287200
H	4.04214700	1.90088700	−0.90217200
H	1.52189900	2.84983400	−1.57113700
H	2.26497100	3.17674500	−0.01575300

H	−0.88954900	2.92529300	−0.18814600
H	−1.31703200	−2.41777000	0.02099600
H	−3.80639700	−2.19001300	0.17010900
H	−3.29422000	2.07657600	−0.26335300
H	3.90181000	−1.78980600	−0.46910000
H	3.40103000	−1.08212100	−2.02856800
H	4.85630000	−0.47485500	−1.18998900
H	1.02995700	−2.67281800	1.92365300
H	0.81933400	−1.76353900	3.44224800
H	−0.46645600	−1.75493100	2.21586300
H	−0.41830500	2.04121000	−1.64743500
O	1.01378900	−2.33326500	−0.57814600
O	0.95979800	−0.09214700	−2.09892100
H	1.87797400	−2.76734300	−0.46118500
O	0.26304800	−1.18202300	−2.78485100
H	0.87534000	−1.34209400	−3.52894900
H	0.79922500	−2.38428800	−1.54304100
Cl	−5.10251862	0.14241843	0.05519353

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (**3**):

N	−2.26653800	−0.11722300	−0.26197200
C	−2.61330700	−1.14288400	0.77295100
C	−1.76887500	−0.94114900	2.01067500
N	−0.32856000	−0.73637500	1.68538300
C	0.40835900	−1.98806700	1.37428200
C	0.08653500	−2.51002100	−0.01235000
N	−0.06052800	−1.39028700	−1.01029500
C	−2.38250300	−0.68566600	−1.63435800
C	−1.21869000	−1.63638900	−1.93774800
C	1.20907700	−1.20516500	−1.76861600
C	2.18858400	−0.46681300	−0.91162500
N	1.63108500	0.42749500	−0.07071700
C	2.39736900	1.22449900	0.68780900
C	3.77791700	1.13693400	0.64543100
C	4.36730300	0.20144800	−0.19859000
C	3.56254400	−0.61142500	−0.98948900
Fe	−0.34571600	0.42456700	−0.07476000
C	−3.17787400	1.04891900	−0.14047600
C	0.30520300	−0.13138700	2.88067600
H	−2.49227700	−2.13477300	0.34435000
H	−3.67123500	−1.03778000	1.02591100
H	−1.88341800	−1.78929900	2.69373800

H	−2.10196100	−0.03959100	2.52861700
H	0.17686600	−2.75520000	2.12051300
H	1.47256900	−1.76083200	1.45395700
H	−0.83007100	−3.09269800	−0.00216700
H	0.88057700	−3.18295800	−0.34347600
H	−2.37688700	0.15545700	−2.32664700
H	−3.34579700	−1.19648800	−1.72100800
H	−0.89281600	−1.47794100	−2.96481500
H	−1.51800700	−2.68039700	−1.85014000
H	1.59834500	−2.16674000	−2.11009300
H	1.87858300	1.92934300	1.32576700
H	4.37322400	1.79109600	1.27043900
H	−3.17108700	1.40695500	0.88834000
H	−2.84226300	1.84131300	−0.80898900
H	−4.18822800	0.73288800	−0.41657700
H	−0.15887300	0.82968200	3.09541500
H	0.17335000	−0.80337000	3.73578400
H	1.37218800	0.01119000	2.70907000
H	0.99675100	−0.58957600	−2.64639100
O	−0.59416600	1.79298400	0.96545900
O	−0.37238000	1.20724300	−1.50062200
H	−0.73853700	2.61656100	0.42317300
O	−1.02170700	3.89724700	−0.66666700
H	−0.95085300	3.33231900	−1.45245400
H	−1.97459600	4.04426000	−0.57659000
O	6.91430050	0.47579515	0.04724544
O	5.81343642	−0.88170996	−1.40492680
C	8.18814580	−0.03633370	−0.42091208
C	9.27818928	0.67181206	0.35990964
C	5.82511592	−0.04207721	−0.53744781
H	8.20603336	−1.11992562	−0.26706631
H	8.26362767	0.14787369	−1.49726205
H	10.26017215	0.31160553	0.03466621
H	9.23646474	1.75350818	0.19729464
H	9.17861218	0.48002018	1.43301323
H	4.00370440	−1.34523650	−1.65510032

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (3):

N	1.62976907	0.11163309	−0.10326638
C	1.16680507	−0.78071391	1.00903562
C	1.98077407	−0.51200991	2.25199362
N	3.44565107	−0.44682291	1.96068662

C	4.09213307	-1.77767091	1.80134262
C	3.78481907	-2.37450791	0.44793262
N	3.84077307	-1.32230891	-0.62829338
C	1.55497707	-0.60354391	-1.41388638
C	2.75369807	-1.54838691	-1.64193538
C	5.19601507	-1.28791591	-1.24863438
C	6.12407507	-0.46502691	-0.40526938
N	5.55069807	0.54220109	0.28060262
C	6.28863107	1.41497709	0.97487862
C	7.66771907	1.30568709	1.03408962
C	8.24256307	0.24804809	0.35299362
C	7.49584707	-0.65583891	-0.38030938
Fe	3.58198007	0.53653709	0.12794462
C	0.77321407	1.32126609	-0.16611038
C	4.08440107	0.22487209	3.12136862
H	1.23105807	-1.81644291	0.68638662
H	0.11091507	-0.58040391	1.20683962
H	1.78812207	-1.27135491	3.01571862
H	1.70458607	0.46356209	2.65795762
H	3.76165707	-2.45359991	2.59618162
H	5.16739007	-1.63021891	1.91629662
H	2.80087907	-2.83229291	0.43614762
H	4.50318907	-3.16260991	0.21407362
H	1.54186507	0.15989109	-2.19002838
H	0.60773207	-1.14742491	-1.45622338
H	3.16289607	-1.35866791	-2.63312738
H	2.45590307	-2.59619591	-1.60344038
H	5.58011507	-2.29770291	-1.40606738
H	5.75103707	2.20211409	1.48854362
H	8.25574307	2.01448909	1.60116062
H	7.95169207	-1.47900991	-0.91501738
H	0.65578507	1.74380309	0.83327862
H	1.22480607	2.05535909	-0.83432038
H	-0.21490193	1.03855409	-0.54117338
H	3.68939707	1.23358609	3.22399562
H	3.86771607	-0.35327291	4.02580162
H	5.16456907	0.26839509	2.98541062
H	5.11879407	-0.79567791	-2.22181338
O	3.48137707	2.11630509	0.99835762
O	3.65377307	1.11457209	-1.43726838
H	2.59290607	2.31937909	1.32639962
O	3.87823707	3.36027509	-1.33999938
H	2.99648107	3.42278509	-1.73587238
H	3.70216107	3.13348109	-0.39573838

O	10.64612109	1.02826538	1.06778446
O	9.98260719	−0.73773617	−0.15745386
C	12.03088349	0.62782768	0.91701105
C	12.87382646	1.64887786	1.64146451
C	9.73742345	0.26267487	0.48804748
H	12.14310967	−0.37331260	1.34058801
H	12.26025916	0.58889568	−0.15071943
H	13.92790374	1.37145006	1.54725018
H	12.73968997	2.64519303	1.21007524
H	12.62010783	1.68371693	2.70500857

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (3):

N	−2.93011900	−0.09846900	−0.36321900
C	−3.36850500	−1.01526600	0.74452900
C	−2.58165400	−0.72786600	2.01139000
N	−1.11363700	−0.59280200	1.76062800
C	−0.41093900	−1.89332500	1.58971200
C	−0.67625100	−2.51400200	0.22864300
N	−0.70369900	−1.47892400	−0.87236300
C	−2.97237100	−0.78238500	−1.69298100
C	−1.80971000	−1.76940100	−1.85711800
C	0.62250500	−1.40192500	−1.56103700
C	1.58262200	−0.59727600	−0.73302700
N	1.01341100	0.37021300	0.01331700
C	1.76633400	1.23483000	0.71255000
C	3.15180900	1.15474700	0.70863500
C	3.72369600	0.14249700	−0.04419100
C	2.96080300	−0.75160100	−0.77757900
Fe	−0.98097700	0.40856600	−0.09331700
C	−3.84158000	1.08366800	−0.42578500
C	−0.51820900	0.09167600	2.94151900
H	−3.25857800	−2.04477300	0.41129100
H	−4.43558800	−0.85869000	0.92837500
H	−2.76760300	−1.51012200	2.75618600
H	−2.91198500	0.22085300	2.43981800
H	−0.70849100	−2.59468300	2.37838700
H	0.65457800	−1.69555900	1.71595400
H	−1.62523100	−3.04317900	0.22253100
H	0.09567300	−3.25514700	0.00439600
H	−2.91088100	0.00020700	−2.44888600
H	−3.93819100	−1.28762200	−1.79977100
H	−1.41728000	−1.68356000	−2.87002500

H	−2.13304700	−2.80268400	−1.72457000
H	1.00639200	−2.40369100	−1.77452500
H	1.23810600	1.99440300	1.27869500
H	3.75766000	1.85265500	1.27365500
H	3.42565000	−1.53373100	−1.36668300
H	−3.93871700	1.53088500	0.56397600
H	−3.45359100	1.81519400	−1.13591100
H	−4.83328900	0.75463300	−0.75034700
H	−0.95141300	1.08398300	3.05076500
H	−0.70929200	−0.49524200	3.84727400
H	0.55970900	0.18450800	2.80815300
H	0.48139200	−0.88021300	−2.51236400
O	−1.23237200	2.10181500	0.89076300
O	−0.90258600	1.20388700	−1.64385100
H	−2.17789500	2.30591700	1.04282000
O	−1.12793730	2.99587045	−1.49986691
H	−2.09820130	3.02786145	−1.56504991
H	−1.16454200	2.84341500	−0.19951100
O	5.93334500	1.15610900	0.77405000
O	5.66794900	−0.65323100	−0.53593900
C	7.37240900	0.98810800	0.73508100
C	7.97620100	2.10740300	1.54782000
C	5.21155900	0.27363500	0.10455800
H	7.61100200	0.00487700	1.14814700
H	7.69135500	1.02077500	−0.30961200
H	9.06548400	2.00587700	1.53913800
H	7.71748500	3.08261000	1.12500700
H	7.63432500	2.06692700	2.58618200

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (3):

N	2.36496700	−0.03683300	−0.43104000
C	2.86247400	0.63304000	0.80309900
C	2.11072300	0.10892400	2.00913400
N	0.63300300	0.07450700	1.78801800
C	−0.02504500	1.40647100	1.92662400
C	0.21102400	2.34626500	0.74714000
N	0.22644500	1.63830300	−0.56196200
C	2.37489000	0.87551700	−1.59565700
C	1.37627000	2.02983200	−1.41884200
C	−1.06591100	1.74998500	−1.25549400
C	−2.10166900	0.89323400	−0.57738400
N	−1.65454000	−0.25280100	−0.03497400

C	-2.52231800	-1.10982500	0.52365800
C	-3.87978200	-0.84644700	0.57933400
C	-4.34905900	0.34666800	0.03845400
C	-3.44825500	1.22721700	-0.54781800
Fe	0.38156300	-0.57634800	-0.13699100
C	3.17363700	-1.24040500	-0.72177000
C	0.05104200	-0.81603600	2.82039200
H	2.75340200	1.70948800	0.69635200
H	3.93254200	0.43859700	0.92422900
H	2.34000000	0.70326100	2.90007400
H	2.41683500	-0.92253100	2.20147900
H	0.32688000	1.88153900	2.84892300
H	-1.09263900	1.21381900	2.04229300
H	1.15054700	2.87983500	0.87449000
H	-0.57807300	3.10540300	0.75336000
H	2.11236100	0.27517400	-2.46786300
H	3.38552400	1.27133200	-1.74778600
H	1.01986500	2.33130800	-2.40565800
H	1.86708100	2.90336900	-0.98665800
H	-1.40425600	2.79039800	-1.31538900
H	-2.10438400	-2.02226900	0.93353500
H	-4.54853500	-1.56127100	1.04348700
H	-3.77599100	2.16564100	-0.98074700
H	3.19347900	-1.88741600	0.15797700
H	2.73028200	-1.78143700	-1.55854400
H	4.19968900	-0.95165300	-0.97561600
H	0.49176700	-1.80889200	2.74028800
H	0.25442800	-0.40406700	3.81527400
H	-1.02803100	-0.88869800	2.68232200
H	-0.94063100	1.37599200	-2.27583600
O	0.27285200	-2.67067900	0.38322700
O	0.26971300	-1.00416200	-1.88937400
H	1.16449800	-3.05190500	0.37998000
O	-0.73981600	-1.98779000	-2.12361300
H	-0.24315600	-2.64512600	-2.63855700
H	-0.15760600	-3.01195000	-0.42254200
O	-6.65216404	-0.08836062	0.54892287
O	-6.09738398	1.80722790	-0.57468291
C	-8.05982037	0.24420168	0.43921325
C	-8.84315565	-0.86117599	1.12029539
C	-5.79974092	0.78612196	-0.00337712
H	-8.22541179	1.21889450	0.90901410
H	-8.31407097	0.33884909	-0.62123867
H	-9.91558198	-0.64674408	1.05911008

H	−8.65656138	−1.82666943	0.63940595
H	−8.56750399	−0.94267584	2.17652677

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (3):

N	−2.27829600	0.07117700	−0.18466100
C	−2.69691200	−0.85212800	0.93167300
C	−1.79970500	−0.66360700	2.13724700
N	−0.34439900	−0.64103000	1.76565300
C	0.24097300	−1.99360100	1.49283700
C	−0.18589000	−2.55770500	0.14851000
N	−0.24200500	−1.48981000	−0.93204400
C	−2.50800800	−0.56110400	−1.52420200
C	−1.47261300	−1.65930800	−1.80552000
C	1.01221100	−1.51014800	−1.76060400
C	2.11826900	−0.84121400	−1.00315300
N	1.71357900	0.15984700	−0.18635300
C	2.61210400	0.91232100	0.47552000
C	3.97400300	0.67044300	0.35592600
C	4.40664300	−0.37281600	−0.46193200
C	3.46710200	−1.13904300	−1.15062200
Fe	−0.26993600	0.40110200	−0.10607700
C	−3.04626600	1.34872100	−0.10258200
C	0.39596300	−0.08303000	2.93490900
H	−2.68870600	−1.87566600	0.56693000
H	−3.73076000	−0.61819800	1.20000300
H	−1.98444600	−1.45035700	2.87653400
H	−2.01513500	0.30005600	2.60279600
H	−0.05052100	−2.68745300	2.28934100
H	1.32501100	−1.88189300	1.53255200
H	−1.16129800	−3.03020300	0.21413500
H	0.51983400	−3.33303600	−0.15918000
H	−2.43475900	0.23452400	−2.26411100
H	−3.52704100	−0.96015100	−1.54772600
H	−1.17157800	−1.60581400	−2.85110200
H	−1.87894000	−2.65568400	−1.63221500
H	1.25936900	−2.53560300	−2.04573400
H	2.21782600	1.70993400	1.09252800
H	4.67345800	1.29354000	0.90121200
H	−2.97631200	1.74674600	0.90934400
H	−2.63914500	2.06988500	−0.80974600
H	−4.09336800	1.13577900	−0.34205400
H	−0.02239200	0.88048800	3.23275100

H	0.29227400	−0.76780500	3.78406400
H	1.45307900	0.02993900	2.69625200
H	0.82151100	−0.93681900	−2.67151200
O	−0.25916200	1.98322500	0.71119000
O	−0.27927000	1.07574900	−1.60032500
H	−0.24959900	1.93292200	1.68449100
O	−0.87879100	3.98423100	−1.22453600
H	−0.69723100	3.33850300	−1.92728200
H	−0.71768100	3.44722100	−0.42322700
O	6.85701677	−0.28900876	−0.41666293
O	5.74231074	−1.83803437	−1.65014451
C	8.12674477	−0.85134139	−0.83583237
C	9.22432740	−0.03669663	−0.17931648
C	5.76213053	−0.88856250	−0.90465849
H	8.15744541	−1.90395773	−0.53714228
H	8.18079464	−0.81415129	−1.92846923
H	10.20347013	−0.43109453	−0.47181047
H	9.16965130	1.01269432	−0.48597396
H	9.14619733	−0.08200172	0.91159778
H	3.78450063	−1.95508557	−1.79164061

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (3):

N	−2.93011900	−0.09846900	−0.36321900
C	−3.36850500	−1.01526600	0.74452900
C	−2.58165400	−0.72786600	2.01139000
N	−1.11363700	−0.59280200	1.76062800
C	−0.41093900	−1.89332500	1.58971200
C	−0.67625100	−2.51400200	0.22864300
N	−0.70369900	−1.47892400	−0.87236300
C	−2.97237100	−0.78238500	−1.69298100
C	−1.80971000	−1.76940100	−1.85711800
C	0.62250500	−1.40192500	−1.56103700
C	1.58262200	−0.59727600	−0.73302700
N	1.01341100	0.37021300	0.01331700
C	1.76633400	1.23483000	0.71255000
C	3.15180900	1.15474700	0.70863500
C	3.72369600	0.14249700	−0.04419100
C	2.96080300	−0.75160100	−0.77757900
Fe	−0.98097700	0.40856600	−0.09331700
C	−3.84158000	1.08366800	−0.42578500
C	−0.51820900	0.09167600	2.94151900
H	−3.25857800	−2.04477300	0.41129100

H	−4.43558800	−0.85869000	0.92837500
H	−2.76760300	−1.51012200	2.75618600
H	−2.91198500	0.22085300	2.43981800
H	−0.70849100	−2.59468300	2.37838700
H	0.65457800	−1.69555900	1.71595400
H	−1.62523100	−3.04317900	0.22253100
H	0.09567300	−3.25514700	0.00439600
H	−2.91088100	0.00020700	−2.44888600
H	−3.93819100	−1.28762200	−1.79977100
H	−1.41728000	−1.68356000	−2.87002500
H	−2.13304700	−2.80268400	−1.72457000
H	1.00639200	−2.40369100	−1.77452500
H	1.23810600	1.99440300	1.27869500
H	3.75766000	1.85265500	1.27365500
H	3.42565000	−1.53373100	−1.36668300
H	−3.93871700	1.53088500	0.56397600
H	−3.45359100	1.81519400	−1.13591100
H	−4.83328900	0.75463300	−0.75034700
H	−0.95141300	1.08398300	3.05076500
H	−0.70929200	−0.49524200	3.84727400
H	0.55970900	0.18450800	2.80815300
H	0.48139200	−0.88021300	−2.51236400
O	−1.23738200	2.06857300	0.87127200
O	−0.90258600	1.20388700	−1.64385100
H	−2.18290500	2.27267500	1.02332900
O	−1.01013195	2.99493073	−1.48078006
H	−1.98039595	3.02692273	−1.54596306
H	−1.15858143	2.71693348	−0.16263790
O	6.02942144	0.98918672	0.63737286
O	5.62544898	−0.75893710	−0.71949503
C	7.45650301	0.76291773	0.52383690
C	8.14524365	1.82594850	1.34452627
C	5.23982373	0.16234595	−0.02657368
H	7.67118841	−0.24370182	0.89115321
H	7.72777237	0.82005817	−0.53319914
H	9.22753241	1.67952444	1.28024184
H	7.90967593	2.82574607	0.96816757
H	7.85045864	1.76219458	2.39607281

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (3):

N	2.36496700	−0.03683300	−0.43104000
C	2.86247400	0.63304000	0.80309900

C	2.11072300	0.10892400	2.00913400
N	0.63300300	0.07450700	1.78801800
C	-0.02504500	1.40647100	1.92662400
C	0.21102400	2.34626500	0.74714000
N	0.22644500	1.63830300	-0.56196200
C	2.37489000	0.87551700	-1.59565700
C	1.37627000	2.02983200	-1.41884200
C	-1.06591100	1.74998500	-1.25549400
C	-2.10166900	0.89323400	-0.57738400
N	-1.65454000	-0.25280100	-0.03497400
C	-2.52231800	-1.10982500	0.52365800
C	-3.87978200	-0.84644700	0.57933400
C	-4.34905900	0.34666800	0.03845400
C	-3.44825500	1.22721700	-0.54781800
Fe	0.38156300	-0.57634800	-0.13699100
C	3.17363700	-1.24040500	-0.72177000
C	0.05104200	-0.81603600	2.82039200
H	2.75340200	1.70948800	0.69635200
H	3.93254200	0.43859700	0.92422900
H	2.34000000	0.70326100	2.90007400
H	2.41683500	-0.92253100	2.20147900
H	0.32688000	1.88153900	2.84892300
H	-1.09263900	1.21381900	2.04229300
H	1.15054700	2.87983500	0.87449000
H	-0.57807300	3.10540300	0.75336000
H	2.11236100	0.27517400	-2.46786300
H	3.38552400	1.27133200	-1.74778600
H	1.01986500	2.33130800	-2.40565800
H	1.86708100	2.90336900	-0.98665800
H	-1.40425600	2.79039800	-1.31538900
H	-2.10438400	-2.02226900	0.93353500
H	-4.54853500	-1.56127100	1.04348700
H	3.19347900	-1.88741600	0.15797700
H	2.73028200	-1.78143700	-1.55854400
H	4.19968900	-0.95165300	-0.97561600
H	0.49176700	-1.80889200	2.74028800
H	0.25442800	-0.40406700	3.81527400
H	-1.02803100	-0.88869800	2.68232200
H	-0.94063100	1.37599200	-2.27583600
O	0.27285200	-2.67067900	0.38322700
O	0.26971300	-1.00416200	-1.88937400
H	1.16449800	-3.05190500	0.37998000
O	-0.73981600	-1.98779000	-2.12361300
H	-0.24315600	-2.64512600	-2.63855700

H	−0.15760600	−3.01195000	−0.42254200
O	−6.86348473	0.50718122	0.26867647
O	−5.53911198	2.08157475	−0.69612843
C	−8.03565718	1.32582496	0.02380023
C	−9.23697166	0.57348288	0.56247613
C	−5.69593011	1.01849596	−0.14575527
H	−7.89593380	2.29182242	0.51926540
H	−8.11223547	1.51209105	−1.05211822
H	−10.14655844	1.16072722	0.39628673
H	−9.35264025	−0.39144645	0.05870851
H	−9.13536807	0.39178287	1.63714474
H	−3.79268775	2.16241502	−0.97630974

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (4):

N	−2.93062100	−0.09075300	−0.37243000
C	−3.37693300	−1.00860000	0.74062300
C	−2.59847800	−0.72736200	2.01060900
N	−1.12412400	−0.59999900	1.76580100
C	−0.41515900	−1.90524200	1.59794900
C	−0.67439200	−2.52832700	0.23708500
N	−0.69442400	−1.49145200	−0.87162300
C	−2.96918000	−0.78649700	−1.70234700
C	−1.80618800	−1.78116200	−1.85912800
C	0.63539900	−1.41741600	−1.55968500
C	1.58864000	−0.59843200	−0.74244600
N	1.02064000	0.37628400	0.00198400
C	1.77379200	1.24454400	0.69809200
C	3.16062400	1.16697100	0.68966600
C	3.73393400	0.15055600	−0.06172200
C	2.96992100	−0.75027100	−0.78914200
Fe	−0.98818300	0.42456000	−0.10394600
C	−3.81504100	1.11229500	−0.42341100
C	−0.53810200	0.08433000	2.95243900
H	−3.27639100	−2.03856100	0.40849600
H	−4.44234500	−0.83733000	0.91774000
H	−2.78799600	−1.51227700	2.75103900
H	−2.92631500	0.22423600	2.43246800
H	−0.72336300	−2.60328300	2.38482300
H	0.64963600	−1.70952400	1.73156200
H	−1.62395800	−3.05484700	0.22690600
H	0.09928100	−3.26873300	0.01881600
H	−2.90789200	−0.00947500	−2.46272200

H	-3.93716300	-1.28797600	-1.80016600
H	-1.41041800	-1.70307300	-2.87123100
H	-2.13325800	-2.81106900	-1.71616800
H	1.02269500	-2.41983000	-1.75895400
H	1.24926400	2.00765200	1.25850800
H	3.75693200	1.87342500	1.25130200
H	3.42121700	-1.53989400	-1.37581100
H	-3.86535300	1.56410100	0.56681500
H	-3.41501200	1.82847400	-1.14032600
H	-4.81485800	0.79292300	-0.73475300
H	-0.98146500	1.07261000	3.06294200
H	-0.74324200	-0.51185500	3.84915700
H	0.54146800	0.17998000	2.83550900
H	0.49505500	-0.90821000	-2.51736000
O	-1.23677400	1.89565800	0.81231800
O	-0.91027600	1.09842800	-1.59883100
H	-1.31846200	2.67995900	0.18835700
O	-1.49490200	3.88676800	-0.98479600
H	-1.37734000	3.26745800	-1.72861700
H	-2.45609000	4.03911000	-0.96687200
N	5.20562500	0.02185400	-0.09285500
O	5.68527000	-0.87509400	-0.78234000
O	5.86236400	0.81969000	0.57158500

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (4):

N	-2.85025800	-0.12017500	-0.41560900
C	-3.31949200	-1.01826600	0.68896300
C	-2.55620200	-0.72743400	1.96659000
N	-1.08647500	-0.63591500	1.73582200
C	-0.40509300	-1.94878100	1.60437300
C	-0.63951600	-2.58980200	0.24418700
N	-0.65075800	-1.57400800	-0.86737500
C	-2.89269100	-0.82339100	-1.73141600
C	-1.75487100	-1.85352600	-1.85414900
C	0.68017100	-1.50731700	-1.53976400
C	1.63245200	-0.70923800	-0.69454100
N	1.05645500	0.28995000	0.00620800
C	1.80301000	1.15903500	0.70384500
C	3.18401900	1.04465300	0.75571800
C	3.76102400	-0.00382400	0.06135200
C	3.00354200	-0.89872800	-0.67828200
Fe	-0.92004400	0.34919700	-0.13580300

C	−3.71177300	1.09635600	−0.48070000
C	−0.50036800	0.07274800	2.90425300
H	−3.20743100	−2.05321000	0.37133300
H	−4.38945800	−0.85686400	0.84971600
H	−2.78282300	−1.48355100	2.72740100
H	−2.86872200	0.24134100	2.36242100
H	−0.72545600	−2.63544800	2.39720300
H	0.66130200	−1.76858600	1.75263600
H	−1.58530200	−3.12646200	0.23126000
H	0.13589500	−3.33732400	0.05260600
H	−2.79280100	−0.05840900	−2.50102800
H	−3.87179600	−1.29931600	−1.85203000
H	−1.35162100	−1.80895600	−2.86607900
H	−2.11262100	−2.87356400	−1.70507000
H	1.06026800	−2.50926700	−1.76050400
H	1.26718700	1.94641800	1.22113600
H	3.79191200	1.74268500	1.31937900
H	3.48212500	−1.70462600	−1.22371900
H	−3.75953600	1.55392200	0.50724800
H	−3.28679200	1.81435800	−1.18228900
H	−4.71632000	0.80574000	−0.80309900
H	−0.90267000	1.08358300	2.95372400
H	−0.73710400	−0.46758800	3.82719300
H	0.58374800	0.12310300	2.80072700
H	0.55443900	−0.97267100	−2.48593300
O	−1.15246800	1.81667200	0.73219100
O	−0.82658400	0.98234700	−1.62205100
H	−1.35282658	1.66660092	1.70165743
O	−1.13665390	3.66098633	−1.44648524
H	−1.04173340	3.08302209	−2.21563068
H	−1.17542768	3.07817767	−0.67740627
N	5.23643600	−0.18026500	0.10485000
O	5.67845600	−1.13384100	−0.50331900
O	5.85557300	0.64238200	0.74561000

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (4):

N	−2.93011900	−0.09846900	−0.36321900
C	−3.36850500	−1.01526600	0.74452900
C	−2.58165400	−0.72786600	2.01139000
N	−1.11363700	−0.59280200	1.76062800
C	−0.41093900	−1.89332500	1.58971200
C	−0.67625100	−2.51400200	0.22864300

N	-0.70369900	-1.47892400	-0.87236300
C	-2.97237100	-0.78238500	-1.69298100
C	-1.80971000	-1.76940100	-1.85711800
C	0.62250500	-1.40192500	-1.56103700
C	1.58262200	-0.59727600	-0.73302700
N	1.01341100	0.37021300	0.01331700
C	1.76633400	1.23483000	0.71255000
C	3.15180900	1.15474700	0.70863500
C	3.72369600	0.14249700	-0.04419100
C	2.96080300	-0.75160100	-0.77757900
Fe	-0.98097700	0.40856600	-0.09331700
C	-3.84158000	1.08366800	-0.42578500
C	-0.51820900	0.09167600	2.94151900
H	-3.25857800	-2.04477300	0.41129100
H	-4.43558800	-0.85869000	0.92837500
H	-2.76760300	-1.51012200	2.75618600
H	-2.91198500	0.22085300	2.43981800
H	-0.70849100	-2.59468300	2.37838700
H	0.65457800	-1.69555900	1.71595400
H	-1.62523100	-3.04317900	0.22253100
H	0.09567300	-3.25514700	0.00439600
H	-2.91088100	0.00020700	-2.44888600
H	-3.93819100	-1.28762200	-1.79977100
H	-1.41728000	-1.68356000	-2.87002500
H	-2.13304700	-2.80268400	-1.72457000
H	1.00639200	-2.40369100	-1.77452500
H	1.23810600	1.99440300	1.27869500
H	3.75766000	1.85265500	1.27365500
H	3.42565000	-1.53373100	-1.36668300
H	-3.93871700	1.53088500	0.56397600
H	-3.45359100	1.81519400	-1.13591100
H	-4.83328900	0.75463300	-0.75034700
H	-0.95141300	1.08398300	3.05076500
H	-0.70929200	-0.49524200	3.84727400
H	0.55970900	0.18450800	2.80815300
H	0.48139200	-0.88021300	-2.51236400
O	-1.23237181	2.10181517	0.89076327
O	-0.90258600	1.20388700	-1.64385100
H	-2.17789481	2.30591717	1.04282027
O	-1.12404060	2.95605588	-1.46644534
H	-2.09430460	2.98804688	-1.53162834
H	-1.16454200	2.84341500	-0.19951100
N	5.19228800	0.00878200	-0.07249900
O	5.64006900	-0.89229500	-0.76373900

O	5.82282000	0.80570000	0.60241400

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (4):

N	3.00556400	0.12972400	−0.33652300
C	3.49559400	0.27631100	1.07593000
C	2.70984300	−0.64790200	1.98610400
N	1.23031300	−0.56632700	1.73666200
C	0.57866400	0.64339300	2.33561900
C	0.82139400	1.90192100	1.51303600
N	0.80617000	1.62271600	0.01882300
C	3.06817100	1.42980300	−1.07324500
C	1.92052400	2.37772900	−0.67331500
C	−0.53148800	1.96281100	−0.56317300
C	−1.51359900	0.85878200	−0.28549300
N	−0.98675300	−0.38404500	−0.19206700
C	−1.79425600	−1.44825000	−0.03756100
C	−3.17488200	−1.32101400	0.04362600
C	−3.69681600	−0.03677300	−0.03585900
C	−2.88587600	1.07629400	−0.20156100
Fe	1.01246600	−0.34577400	−0.30066600
C	3.84299800	−0.86980300	−1.05450700
C	0.61294800	−1.76821500	2.36549400
H	3.41022700	1.31694700	1.38012600
H	4.55990500	0.02488000	1.12136000
H	2.92254300	−0.43164500	3.03927600
H	2.99772700	−1.68293200	1.78661700
H	0.94189500	0.79542700	3.35838000
H	−0.48925600	0.42740600	2.39298400
H	1.77810800	2.34945300	1.76723700
H	0.05440400	2.64469300	1.74638600
H	2.99202800	1.19002400	−2.13287200
H	4.04214700	1.90088700	−0.90217200
H	1.52189900	2.84983400	−1.57113700
H	2.26497100	3.17674500	−0.01575300
H	−0.88954900	2.92529300	−0.18814600
H	−1.31703200	−2.41777000	0.02099600
H	−3.80639700	−2.19001300	0.17010900
H	−3.29422000	2.07657600	−0.26335300
H	3.90181000	−1.78980600	−0.46910000
H	3.40103000	−1.08212100	−2.02856800
H	4.85630000	−0.47485500	−1.18998900
H	1.02995700	−2.67281800	1.92365300

H	0.81933400	−1.76353900	3.44224800
H	−0.46645600	−1.75493100	2.21586300
H	−0.41830500	2.04121000	−1.64743500
O	1.01378900	−2.33326500	−0.57814600
O	0.95979800	−0.09214700	−2.09892100
H	1.87797400	−2.76734300	−0.46118500
O	0.26304800	−1.18202300	−2.78485100
H	0.87534000	−1.34209400	−3.52894900
H	0.79922500	−2.38428800	−1.54304100
N	−5.15762100	0.15202300	0.06510400
O	−5.59651300	1.29602600	−0.03551100
O	−5.85171400	−0.84662400	0.24482900

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (4):

N	−2.93062100	−0.09075300	−0.37243000
C	−3.37693300	−1.00860000	0.74062300
C	−2.59847800	−0.72736200	2.01060900
N	−1.12412400	−0.59999900	1.76580100
C	−0.41515900	−1.90524200	1.59794900
C	−0.67439200	−2.52832700	0.23708500
N	−0.69442400	−1.49145200	−0.87162300
C	−2.96918000	−0.78649700	−1.70234700
C	−1.80618800	−1.78116200	−1.85912800
C	0.63539900	−1.41741600	−1.55968500
C	1.58864000	−0.59843200	−0.74244600
N	1.02064000	0.37628400	0.00198400
C	1.77379200	1.24454400	0.69809200
C	3.16062400	1.16697100	0.68966600
C	3.73393400	0.15055600	−0.06172200
C	2.96992100	−0.75027100	−0.78914200
Fe	−0.98818300	0.42456000	−0.10394600
C	−3.81504100	1.11229500	−0.42341100
C	−0.53810200	0.08433000	2.95243900
H	−3.27639100	−2.03856100	0.40849600
H	−4.44234500	−0.83733000	0.91774000
H	−2.78799600	−1.51227700	2.75103900
H	−2.92631500	0.22423600	2.43246800
H	−0.72336300	−2.60328300	2.38482300
H	0.64963600	−1.70952400	1.73156200
H	−1.62395800	−3.05484700	0.22690600
H	0.09928100	−3.26873300	0.01881600
H	−2.90789200	−0.00947500	−2.46272200

H	−3.93716300	−1.28797600	−1.80016600
H	−1.41041800	−1.70307300	−2.87123100
H	−2.13325800	−2.81106900	−1.71616800
H	1.02269500	−2.41983000	−1.75895400
H	1.24926400	2.00765200	1.25850800
H	3.75693200	1.87342500	1.25130200
H	3.42121700	−1.53989400	−1.37581100
H	−3.86535300	1.56410100	0.56681500
H	−3.41501200	1.82847400	−1.14032600
H	−4.81485800	0.79292300	−0.73475300
H	−0.98146500	1.07261000	3.06294200
H	−0.74324200	−0.51185500	3.84915700
H	0.54146800	0.17998000	2.83550900
H	0.49505500	−0.90821000	−2.51736000
O	−1.23677400	1.89565800	0.81231800
O	−0.91027600	1.09842800	−1.59883100
H	−2.22086800	2.06612100	0.92906800
O	−0.78782100	3.37897300	−1.58631900
H	0.15413800	3.60556300	−1.47674800
H	−0.99758800	2.88454900	−0.77455900
N	5.20562500	0.02185400	−0.09285500
O	5.68527000	−0.87509400	−0.78234000
O	5.86236400	0.81969000	0.57158500

Cartesian coordinates of transient state (TS2b) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (4):

N	−2.93011900	−0.09846900	−0.36321900
C	−3.36850500	−1.01526600	0.74452900
C	−2.58165400	−0.72786600	2.01139000
N	−1.11363700	−0.59280200	1.76062800
C	−0.41093900	−1.89332500	1.58971200
C	−0.67625100	−2.51400200	0.22864300
N	−0.70369900	−1.47892400	−0.87236300
C	−2.97237100	−0.78238500	−1.69298100
C	−1.80971000	−1.76940100	−1.85711800
C	0.62250500	−1.40192500	−1.56103700
C	1.58262200	−0.59727600	−0.73302700
N	1.01341100	0.37021300	0.01331700
C	1.76633400	1.23483000	0.71255000
C	3.15180900	1.15474700	0.70863500
C	3.72369600	0.14249700	−0.04419100
C	2.96080300	−0.75160100	−0.77757900
Fe	−0.98097700	0.40856600	−0.09331700

C	-3.84158000	1.08366800	-0.42578500
C	-0.51820900	0.09167600	2.94151900
H	-3.25857800	-2.04477300	0.41129100
H	-4.43558800	-0.85869000	0.92837500
H	-2.76760300	-1.51012200	2.75618600
H	-2.91198500	0.22085300	2.43981800
H	-0.70849100	-2.59468300	2.37838700
H	0.65457800	-1.69555900	1.71595400
H	-1.62523100	-3.04317900	0.22253100
H	0.09567300	-3.25514700	0.00439600
H	-2.91088100	0.00020700	-2.44888600
H	-3.93819100	-1.28762200	-1.79977100
H	-1.41728000	-1.68356000	-2.87002500
H	-2.13304700	-2.80268400	-1.72457000
H	1.00639200	-2.40369100	-1.77452500
H	1.23810600	1.99440300	1.27869500
H	3.75766000	1.85265500	1.27365500
H	3.42565000	-1.53373100	-1.36668300
H	-3.93871700	1.53088500	0.56397600
H	-3.45359100	1.81519400	-1.13591100
H	-4.83328900	0.75463300	-0.75034700
H	-0.95141300	1.08398300	3.05076500
H	-0.70929200	-0.49524200	3.84727400
H	0.55970900	0.18450800	2.80815300
H	0.48139200	-0.88021300	-2.51236400
O	-1.23738200	2.06857300	0.87127200
O	-0.90258600	1.20388700	-1.64385100
H	-2.18290500	2.27267500	1.02332900
O	-1.01856006	2.95736184	-1.42273610
H	-1.98882406	2.98935384	-1.48791910
H	-1.16012888	2.66887156	-0.15196177
N	5.19228800	0.00878200	-0.07249900
O	5.64006900	-0.89229500	-0.76373900
O	5.82282000	0.80570000	0.60241400

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (4):

N	3.00556400	0.12972400	-0.33652300
C	3.49559400	0.27631100	1.07593000
C	2.70984300	-0.64790200	1.98610400
N	1.23031300	-0.56632700	1.73666200
C	0.57866400	0.64339300	2.33561900
C	0.82139400	1.90192100	1.51303600

N	0.80617000	1.62271600	0.01882300
C	3.06817100	1.42980300	-1.07324500
C	1.92052400	2.37772900	-0.67331500
C	-0.53148800	1.96281100	-0.56317300
C	-1.51359900	0.85878200	-0.28549300
N	-0.98675300	-0.38404500	-0.19206700
C	-1.79425600	-1.44825000	-0.03756100
C	-3.17488200	-1.32101400	0.04362600
C	-3.69681600	-0.03677300	-0.03585900
C	-2.88587600	1.07629400	-0.20156100
Fe	1.01246600	-0.34577400	-0.30066600
C	3.84299800	-0.86980300	-1.05450700
C	0.61294800	-1.76821500	2.36549400
H	3.41022700	1.31694700	1.38012600
H	4.55990500	0.02488000	1.12136000
H	2.92254300	-0.43164500	3.03927600
H	2.99772700	-1.68293200	1.78661700
H	0.94189500	0.79542700	3.35838000
H	-0.48925600	0.42740600	2.39298400
H	1.77810800	2.34945300	1.76723700
H	0.05440400	2.64469300	1.74638600
H	2.99202800	1.19002400	-2.13287200
H	4.04214700	1.90088700	-0.90217200
H	1.52189900	2.84983400	-1.57113700
H	2.26497100	3.17674500	-0.01575300
H	-0.88954900	2.92529300	-0.18814600
H	-1.31703200	-2.41777000	0.02099600
H	-3.80639700	-2.19001300	0.17010900
H	-3.29422000	2.07657600	-0.26335300
H	3.90181000	-1.78980600	-0.46910000
H	3.40103000	-1.08212100	-2.02856800
H	4.85630000	-0.47485500	-1.18998900
H	1.02995700	-2.67281800	1.92365300
H	0.81933400	-1.76353900	3.44224800
H	-0.46645600	-1.75493100	2.21586300
H	-0.41830500	2.04121000	-1.64743500
O	1.01378900	-2.33326500	-0.57814600
O	0.95979800	-0.09214700	-2.09892100
H	1.87797400	-2.76734300	-0.46118500
O	0.26304800	-1.18202300	-2.78485100
H	0.87534000	-1.34209400	-3.52894900
H	0.79922500	-2.38428800	-1.54304100
N	-5.15762100	0.15202300	0.06510400
O	-5.59651300	1.29602600	-0.03551100

O	-5.85171400	-0.84662400	0.24482900

Cartesian coordinates of reactant state associated with the process of the water rotation for Fe^{IV}-oxyl radical (S=4) in complex (5):

N	-2.26653800	-0.11722300	-0.26197200
C	-2.61330700	-1.14288400	0.77295100
C	-1.76887500	-0.94114900	2.01067500
N	-0.32856000	-0.73637500	1.68538300
C	0.40835900	-1.98806700	1.37428200
C	0.08653500	-2.51002100	-0.01235000
N	-0.06052800	-1.39028700	-1.01029500
C	-2.38250300	-0.68566600	-1.63435800
C	-1.21869000	-1.63638900	-1.93774800
C	1.20907700	-1.20516500	-1.76861600
C	2.18858400	-0.46681300	-0.91162500
N	1.63108500	0.42749500	-0.07071700
C	2.39736900	1.22449900	0.68780900
C	3.77791700	1.13693400	0.64543100
C	4.36730300	0.20144800	-0.19859000
C	3.56254400	-0.61142500	-0.98948900
Fe	-0.34571600	0.42456700	-0.07476000
C	-3.17787400	1.04891900	-0.14047600
C	0.30520300	-0.13138700	2.88067600
H	-2.49227700	-2.13477300	0.34435000
H	-3.67123500	-1.03778000	1.02591100
H	-1.88341800	-1.78929900	2.69373800
H	-2.10196100	-0.03959100	2.52861700
H	0.17686600	-2.75520000	2.12051300
H	1.47256900	-1.76083200	1.45395700
H	-0.83007100	-3.09269800	-0.00216700
H	0.88057700	-3.18295800	-0.34347600
H	-2.37688700	0.15545700	-2.32664700
H	-3.34579700	-1.19648800	-1.72100800
H	-0.89281600	-1.47794100	-2.96481500
H	-1.51800700	-2.68039700	-1.85014000
H	1.59834500	-2.16674000	-2.11009300
H	4.37322400	1.79109600	1.27043900
H	5.44653100	0.10434200	-0.24301100
H	3.98448500	-1.34857900	-1.66255700
H	-3.17108700	1.40695500	0.88834000
H	-2.84226300	1.84131300	-0.80898900
H	-4.18822800	0.73288800	-0.41657700
H	-0.15887300	0.82968200	3.09541500

H	0.17335000	−0.80337000	3.73578400
H	1.37218800	0.01119000	2.70907000
H	0.99675100	−0.58957600	−2.64639100
O	−0.59416600	1.79298400	0.96545900
O	−0.37238000	1.20724300	−1.50062200
H	−0.73853700	2.61656100	0.42317300
O	−1.02170700	3.89724700	−0.66666700
H	−0.95085300	3.33231900	−1.45245400
H	−1.97459600	4.04426000	−0.57659000
F	1.75069536	2.10309640	1.48303212

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (5):

N	−2.25561400	0.08106000	−0.18740000
C	−2.66620400	−0.85618200	0.90856200
C	−1.77919000	−0.67264000	2.11701300
N	−0.33407200	−0.61304200	1.74960000
C	0.28101000	−1.94384000	1.48127300
C	−0.14256500	−2.51823100	0.14607700
N	−0.23993500	−1.45224900	−0.91774600
C	−2.48103100	−0.53734500	−1.52437800
C	−1.46331600	−1.64728000	−1.77695100
C	0.98892700	−1.45289800	−1.76160500
C	2.10991500	−0.82564600	−0.99939200
N	1.72487600	0.18374100	−0.17740500
C	2.66703000	0.86300700	0.47024500
C	4.01881000	0.58632700	0.37691600
C	4.40206600	−0.46077400	−0.44357400
C	3.43396500	−1.17960900	−1.14413100
Fe	−0.28756300	0.42115200	−0.08985700
C	−3.04230400	1.33835700	−0.09800900
C	0.38680900	−0.05689100	2.92317500
H	−2.64515500	−1.87515900	0.53231700
H	−3.70345300	−0.63866900	1.17319300
H	−1.95225700	−1.47393500	2.84190600
H	−2.01723700	0.27876600	2.59698400
H	0.01346700	−2.64184100	2.28122300
H	1.36286000	−1.80472300	1.51066100
H	−1.10154100	−3.02092900	0.22791000
H	0.58204200	−3.27149400	−0.17035200
H	−2.38441300	0.25657600	−2.26390000
H	−3.50469400	−0.92088200	−1.56032700
H	−1.17068400	−1.63211900	−2.82582900

H	−1.87920000	−2.63215800	−1.56876000
H	1.22549600	−2.46822500	−2.08631900
H	4.72349900	1.18258300	0.94247900
H	5.45095000	−0.71741600	−0.53994600
H	3.69952500	−2.00217400	−1.79666900
H	−2.96700900	1.74152500	0.91110400
H	−2.65658800	2.06395700	−0.81269800
H	−4.08611500	1.10426900	−0.32728100
H	−0.02213300	0.91100800	3.21250300
H	0.26185400	−0.73973400	3.77003500
H	1.44874300	0.04336300	2.70900800
H	0.79584700	−0.84414300	−2.64801800
O	−0.40205700	1.98165600	0.71118600
O	−0.27670800	1.08913800	−1.57140300
H	−0.55206735	1.95594420	1.66905038
O	0.85474940	3.29069139	−1.07993703
H	1.71594813	3.52248623	−0.70613225
H	0.41542711	2.87339446	−0.31731909
F	2.26212000	1.85145500	1.24587400

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (5):

N	−2.39407900	−0.01904000	−0.39251500
C	−2.81791100	−0.97045100	0.68433500
C	−2.05327000	−0.68905000	1.96563900
N	−0.57055800	−0.54756100	1.74889700
C	0.15060200	−1.84759400	1.56358900
C	−0.06402600	−2.48041100	0.19237300
N	−0.12949900	−1.47236000	−0.92289700
C	−2.38041200	−0.65568100	−1.73490700
C	−1.28139800	−1.73176600	−1.84868600
C	1.16193300	−1.38673200	−1.64885300
C	2.19665000	−0.67296500	−0.81723000
N	1.73302700	0.29848400	−0.00406500
C	2.59360100	1.04101800	0.71772100
C	3.96527500	0.82882300	0.66400900
C	4.45407300	−0.18608700	−0.15879900
C	3.55852000	−0.94723700	−0.90772600
Fe	−0.36199600	0.58507600	−0.02731800
C	−3.25831300	1.18907500	−0.39693300
C	−0.00376500	0.10603500	2.96465300
H	−2.67444100	−1.99115100	0.33760000
H	−3.89054400	−0.85288600	0.87138600

H	−2.24043900	−1.47417400	2.70701800
H	−2.39206800	0.26089500	2.38532200
H	−0.16967400	−2.54826600	2.34375800
H	1.20849800	−1.64040200	1.72558300
H	−0.97917400	−3.06768400	0.18795500
H	0.75469700	−3.18274100	0.00354900
H	−2.20763000	0.14200800	−2.45766800
H	−3.36130100	−1.09965800	−1.94328500
H	−0.92256900	−1.74995900	−2.87925600
H	−1.68694000	−2.72275600	−1.63905700
H	1.51625800	−2.38154900	−1.94049600
H	4.62757500	1.44430700	1.26228700
H	5.51965300	−0.38524500	−0.21422000
H	3.90080800	−1.74595600	−1.55700000
H	−3.27406200	1.63042200	0.60171700
H	−2.86370200	1.91624800	−1.10867900
H	−4.28008200	0.91440700	−0.68506200
H	−0.49849400	1.06062800	3.14117700
H	−0.16047500	−0.54630300	3.83181100
H	1.06588700	0.26929900	2.83267100
H	0.99749500	−0.80745200	−2.56266800
O	−0.53114000	2.26345100	0.97070500
O	−0.28213600	1.32645800	−1.57727800
H	−1.41518000	2.39225900	1.24297300
O	−0.33415610	3.22685606	−1.59496030
H	−1.28382410	3.43142706	−1.70513830
H	−0.38735800	2.99950600	−0.27796500
F	2.05442500	2.00252700	1.49700900

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=2) in complex (5):

N	−2.25976000	−0.48118500	0.02574300
C	−2.81861400	0.90495400	0.07832800
C	−2.07382000	1.78718300	−0.89863700
N	−0.59703800	1.62238200	−0.78595200
C	−0.00062500	2.36314600	0.35702100
C	−0.24958900	1.67505300	1.68838000
N	−0.20767200	0.17162300	1.55844800
C	−2.33240200	−1.13324900	1.35698800
C	−1.33489600	−0.48326100	2.31644500
C	1.10062400	−0.34799300	2.04481800
C	2.16314500	−0.05037300	1.03501400
N	1.73233800	−0.07138400	−0.25087200

C	2.63727900	0.10387200	-1.20458600
C	3.98428900	0.32575300	-0.97793300
C	4.40894400	0.36598800	0.33941500
C	3.48389200	0.17529600	1.36462600
Fe	-0.27793159	-0.36881497	-0.38926438
C	-3.05410500	-1.27363500	-0.94410100
C	-0.00398200	2.17896700	-2.02543800
H	-2.75992100	1.28113300	1.09675900
H	-3.88058700	0.87787100	-0.17922400
H	-2.34902400	2.83761600	-0.75707700
H	-2.34168500	1.50074200	-1.91855900
H	-0.39385800	3.38500000	0.39124000
H	1.07136300	2.42832500	0.16562900
H	-1.21263700	1.96685000	2.09759100
H	0.50667600	1.99451500	2.40873800
H	-2.09022000	-2.18353000	1.20701800
H	-3.35257900	-1.05597900	1.74709900
H	-0.92723700	-1.24238800	2.98334200
H	-1.81274600	0.26938200	2.94287400
H	1.33466000	0.07248000	3.02553500
H	4.65338900	0.46297100	-1.81787400
H	5.45378200	0.54492100	0.56713600
H	3.77911700	0.19997400	2.40660500
H	-3.12048800	-0.73824500	-1.89185700
H	-2.59053600	-2.24422600	-1.10929300
H	-4.06247800	-1.41823700	-0.54359500
H	-0.34625900	1.61694800	-2.89455700
H	-0.30924900	3.22554200	-2.13777600
H	1.08238800	2.13976100	-1.97501700
H	1.01856800	-1.43274400	2.14261100
O	-0.46083707	-0.97057072	-2.33929336
O	0.03574655	-2.08851884	0.11731696
H	-1.20386129	-0.55870435	-2.80690697
O	0.54095958	-2.97633724	-0.89230335
H	-0.19321538	-3.59668173	-1.02569311
H	-0.64746691	-1.93350233	-2.21107734
F	2.19748200	0.06137400	-2.45282600

Cartesian coordinates of reactant state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (5):

N	-2.25330000	0.07762100	-0.18095800
C	-2.66397400	-0.84023600	0.92974500
C	-1.75309400	-0.65969900	2.12209300

N	-0.31331300	-0.62898600	1.72907500
C	0.26615800	-1.97452100	1.45703200
C	-0.18736900	-2.53720200	0.12754100
N	-0.24948400	-1.47142100	-0.93774300
C	-2.50531000	-0.54968500	-1.50924800
C	-1.47068600	-1.63990100	-1.80342500
C	0.99679700	-1.49409700	-1.76077400
C	2.09689600	-0.83770500	-0.98922900
N	1.68550400	0.16871900	-0.19215100
C	2.57071000	0.91071800	0.48886700
C	3.92709000	0.64801200	0.41243800
C	4.36529000	-0.40427600	-0.38439600
C	3.43843500	-1.15732800	-1.09778900
Fe	-0.27536400	0.39858200	-0.11792900
C	-3.01542500	1.34920500	-0.08997000
C	0.44481100	-0.07921400	2.88100300
H	-2.66710700	-1.86284500	0.56288100
H	-3.69300600	-0.60355500	1.21031100
H	-1.92644600	-1.45044400	2.85855500
H	-1.96780000	0.30036300	2.59587400
H	-0.00877400	-2.66512700	2.26085700
H	1.35138000	-1.86296700	1.47246700
H	-1.16406200	-3.00311700	0.21439100
H	0.50524800	-3.31869700	-0.19155800
H	-2.44708400	0.24476800	-2.25214700
H	-3.52172900	-0.95336700	-1.51600900
H	-1.17508400	-1.57568600	-2.84948100
H	-1.87539000	-2.63802400	-1.63896700
H	1.24092700	-2.51722600	-2.05353000
H	4.61908700	1.26107600	0.97656200
H	5.42239100	-0.63648600	-0.45294700
H	3.74152400	-1.98129100	-1.73296400
H	-2.91732000	1.75766100	0.91546500
H	-2.62531700	2.06423200	-0.81310000
H	-4.06768900	1.13783900	-0.30227900
H	0.05066000	0.89072600	3.18465700
H	0.34375500	-0.76220900	3.73106100
H	1.50061100	0.01703300	2.62959000
H	0.81972700	-0.90921600	-2.66653400
O	-0.28252500	1.96499700	0.69305900
O	-0.27932000	1.06384200	-1.60078600
H	-0.38899500	1.93315200	1.65627600
O	-0.89857700	3.92710100	-1.23713200
H	-0.79092400	3.26647100	-1.93506300

H	−0. 73655900	3. 39526100	−0. 43677500
F	2. 06732301	1. 91446423	1. 23826344

Cartesian coordinates of transient state ($TS2_b$) associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (5):

N	−2. 39407900	−0. 01904000	−0. 39251500
C	−2. 81791100	−0. 97045100	0. 68433500
C	−2. 05327000	−0. 68905000	1. 96563900
N	−0. 57055800	−0. 54756100	1. 74889700
C	0. 15060200	−1. 84759400	1. 56358900
C	−0. 06402600	−2. 48041100	0. 19237300
N	−0. 12949900	−1. 47236000	−0. 92289700
C	−2. 38041200	−0. 65568100	−1. 73490700
C	−1. 28139800	−1. 73176600	−1. 84868600
C	1. 16193300	−1. 38673200	−1. 64885300
C	2. 19665000	−0. 67296500	−0. 81723000
N	1. 73302700	0. 29848400	−0. 00406500
C	2. 59360100	1. 04101800	0. 71772100
C	3. 96527500	0. 82882300	0. 66400900
C	4. 45407300	−0. 18608700	−0. 15879900
C	3. 55852000	−0. 94723700	−0. 90772600
Fe	−0. 36199600	0. 58507600	−0. 02731800
C	−3. 25831300	1. 18907500	−0. 39693300
C	−0. 00376500	0. 10603500	2. 96465300
H	−2. 67444100	−1. 99115100	0. 33760000
H	−3. 89054400	−0. 85288600	0. 87138600
H	−2. 24043900	−1. 47417400	2. 70701800
H	−2. 39206800	0. 26089500	2. 38532200
H	−0. 16967400	−2. 54826600	2. 34375800
H	1. 20849800	−1. 64040200	1. 72558300
H	−0. 97917400	−3. 06768400	0. 18795500
H	0. 75469700	−3. 18274100	0. 00354900
H	−2. 20763000	0. 14200800	−2. 45766800
H	−3. 36130100	−1. 09965800	−1. 94328500
H	−0. 92256900	−1. 74995900	−2. 87925600
H	−1. 68694000	−2. 72275600	−1. 63905700
H	1. 51625800	−2. 38154900	−1. 94049600
H	4. 62757500	1. 44430700	1. 26228700
H	5. 51965300	−0. 38524500	−0. 21422000
H	3. 90080800	−1. 74595600	−1. 55700000
H	−3. 27406200	1. 63042200	0. 60171700
H	−2. 86370200	1. 91624800	−1. 10867900
H	−4. 28008200	0. 91440700	−0. 68506200

H	−0.49849400	1.06062800	3.14117700
H	−0.16047500	−0.54630300	3.83181100
H	1.06588700	0.26929900	2.83267100
H	0.99749500	−0.80745200	−2.56266800
O	−0.53114000	2.26345100	0.97070500
O	−0.28213600	1.32645800	−1.57727800
H	−1.41518000	2.39225900	1.24297300
O	−0.33415600	3.22685600	−1.59496000
H	−1.28382400	3.43142700	−1.70513800
H	−0.38735800	2.99950600	−0.27796500
F	2.05442500	2.00252700	1.49700900

Cartesian coordinates of product state associated with the process of O-O bond formation for Fe^{IV}-oxyl radical (S=4) in complex (5):

N	2.36496700	−0.03683300	−0.43104000
C	2.86247400	0.63304000	0.80309900
C	2.11072300	0.10892400	2.00913400
N	0.63300300	0.07450700	1.78801800
C	−0.02504500	1.40647100	1.92662400
C	0.21102400	2.34626500	0.74714000
N	0.22644500	1.63830300	−0.56196200
C	2.37489000	0.87551700	−1.59565700
C	1.37627000	2.02983200	−1.41884200
C	−1.06591100	1.74998500	−1.25549400
C	−2.10166900	0.89323400	−0.57738400
N	−1.65454000	−0.25280100	−0.03497400
C	−2.52231800	−1.10982500	0.52365800
C	−3.87978200	−0.84644700	0.57933400
C	−4.34905900	0.34666800	0.03845400
C	−3.44825500	1.22721700	−0.54781800
Fe	0.38156300	−0.57634800	−0.13699100
C	3.17363700	−1.24040500	−0.72177000
C	0.05104200	−0.81603600	2.82039200
H	2.75340200	1.70948800	0.69635200
H	3.93254200	0.43859700	0.92422900
H	2.34000000	0.70326100	2.90007400
H	2.41683500	−0.92253100	2.20147900
H	0.32688000	1.88153900	2.84892300
H	−1.09263900	1.21381900	2.04229300
H	1.15054700	2.87983500	0.87449000
H	−0.57807300	3.10540300	0.75336000
H	2.11236100	0.27517400	−2.46786300
H	3.38552400	1.27133200	−1.74778600

H	1.01986500	2.33130800	-2.40565800
H	1.86708100	2.90336900	-0.98665800
H	-1.40425600	2.79039800	-1.31538900
H	-4.54853500	-1.56127100	1.04348700
H	-5.40575200	0.58927400	0.07548600
H	-3.77599100	2.16564100	-0.98074700
H	3.19347900	-1.88741600	0.15797700
H	2.73028200	-1.78143700	-1.55854400
H	4.19968900	-0.95165300	-0.97561600
H	0.49176700	-1.80889200	2.74028800
H	0.25442800	-0.40406700	3.81527400
H	-1.02803100	-0.88869800	2.68232200
H	-0.94063100	1.37599200	-2.27583600
O	0.36606019	-2.67682564	0.27220864
O	0.26971300	-1.00416200	-1.88937400
H	1.20878218	-3.02508349	0.60222763
O	0.24319085	-2.38986162	-2.36892419
H	1.12286345	-2.62096872	-2.71053027
H	0.28942387	-3.00757681	-0.64198729
F	-2.00186500	-2.24609100	1.03407800

Cartesian coordinates of complex (6):

N	-2.29314700	-0.06539500	-0.30081800
C	-2.68860500	-1.09439800	0.72884500
C	-1.86237000	-0.93058100	1.98870000
N	-0.39967000	-0.77260200	1.69789200
C	0.30443700	-2.05094700	1.37242100
C	0.00892700	-2.53709300	-0.03862300
N	-0.07437800	-1.39161300	-1.03091500
C	-2.38603100	-0.62294700	-1.69020200
C	-1.22708000	-1.58785700	-1.99407100
C	1.22568700	-1.22876700	-1.76196300
C	2.21046000	-0.50918400	-0.88965400
N	1.66316000	0.38643100	-0.03442800
C	2.44436200	1.17198500	0.73006100
C	3.82848000	1.07727700	0.67422300
C	4.40797700	0.14443900	-0.18553800
C	3.58910800	-0.66012500	-0.97660800
Fe	-0.33450300	0.43502500	-0.06548000
C	-3.18309000	1.12805400	-0.19131000
C	0.23338100	-0.20723700	2.92236200
H	-2.58836100	-2.08595400	0.29438600
H	-3.74810900	-0.95829400	0.96309100

H	-2.02097900	-1.78307400	2.65881200
H	-2.17406500	-0.02505900	2.51262000
H	0.02274000	-2.82598200	2.09435800
H	1.37203600	-1.86245700	1.49118200
H	-0.92569200	-3.08954100	-0.07291100
H	0.79444400	-3.22670600	-0.35852800
H	-2.35963300	0.22742800	-2.37007500
H	-3.35514700	-1.12026600	-1.79921000
H	-0.87436100	-1.40550400	-3.00869700
H	-1.54507200	-2.62916500	-1.94207400
H	1.59989700	-2.19974100	-2.09555300
H	4.43184300	1.72421200	1.30053900
H	5.48698500	0.04326500	-0.24097900
H	4.00323500	-1.39439400	-1.65860900
H	-3.20628400	1.46583200	0.84415500
H	-2.80636300	1.92407800	-0.83290600
H	-4.19069500	0.83915300	-0.50765100
H	-0.21230900	0.75925300	3.15236100
H	0.07180300	-0.89331500	3.76203800
H	1.30565300	-0.08853700	2.76763400
H	1.03945300	-0.61283500	-2.64588700
O	-0.56396700	1.81426000	0.99323100
O	-0.32203000	1.23912000	-1.49597500
H	-0.66187800	2.65185000	0.44838800
O	-0.84386700	3.96790600	-0.61294500
H	-0.76756100	3.40861700	-1.40806100
H	-1.79826500	4.14909100	-0.55478200
C	1.89965782	2.29428437	1.63022375
H	2.80927795	2.62993293	2.08280664
H	1.48880206	3.07939892	1.03047991
H	1.19975402	2.02494592	2.39343503

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