

Supporting information

## **Computational comparison of Ru(bda)(py)<sub>2</sub> and Fe(bda)(py)<sub>2</sub> as water oxidation catalysts**

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Table S1. The energy differences in kcal/mol of all species among different multiplicities

	Multiplicity	B3LYP-D3 LACV3P**** Energy difference	B3LYP*-D3 LACV3P**** Energy difference	M06-L LACV3P**** Energy difference
Ru <sup>II</sup> (bda)(py) <sub>2</sub>	1	0.00	0.00	0.00
Ru <sup>II</sup> (bda)(py) <sub>2</sub>	3	17.31	19.93	14.60
Ru <sup>II</sup> (bda)(py) <sub>2</sub>	5	38.72	44.26	30.35
Ru <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	2	0.00	0.00	0.00
Ru <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	4	21.06	23.51	17.47
Ru <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	6	45.96	50.71	39.10
Ru <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	1	0.00	0.00	0.00
Ru <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	3	8.09	9.87	10.35
Ru <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	5	38.31	41.37	35.48
Ru <sup>V</sup> (bda)(py) <sub>2</sub> -O <sup>+</sup>	2	0.00	0.00	0.00
Ru <sup>V</sup> (bda)(py) <sub>2</sub> -O <sup>+</sup>	4	10.50	12.27	12.14

	Multiplicity	B3LYP-D3 LACV3P**** Energy difference	B3LYP*-D3 LACV3P**** Energy difference	M06-L LACV3P**** Energy difference
Fe <sup>II</sup> (bda)(py) <sub>2</sub>	1	14.97	8.73	8.14
Fe <sup>II</sup> (bda)(py) <sub>2</sub>	3	17.38	17.44	14.28
Fe <sup>II</sup> (bda)(py) <sub>2</sub>	5	0.00	0.00	0.00
Fe <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	2	26.35	25.54	21.37
Fe <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	4	14.38	13.89	11.60
Fe <sup>III</sup> (bda)(py) <sub>2</sub> -H <sub>2</sub> O <sup>+</sup>	6	0.00	0.00	0.00
Fe <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	1	21.22	20.01	16.04
Fe <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	3	3.88	5.44	1.20
Fe <sup>IV</sup> (bda)(py) <sub>2</sub> -OH <sup>+</sup>	5	0.00	0.00	0.00
Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O <sup>+</sup>	2	14.21	11.35	12.07
Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O <sup>+</sup>	4	0.00	0.00	0.00

Table S2. Spin density contributions of different atoms from different orbitals

	O1	M2	O3	O4	N7
[Ru <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	0.18582 2px, 0.09188 2py, 0.50144 2pz	0.06872 4dxz, 0.15194 4dyz, 0.05924 4dx <sup>2</sup> y <sup>2</sup>	/	/	-0.01592 2px
[Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	0.34437 2px, 0.07189 2py, 0.63047 2pz	0.33035 3dxy, 0.27140 3dxz, 0.30380 3dyz, 0.40192 3dx <sup>2</sup> y <sup>2</sup> , 0.60219 3dz <sup>2</sup>	-0.01522 2py, 0.02607 2pz	-0.02301 2px, 0.03056 2pz	/
6- coordinate [Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	0.21543 2px, 0.38521 2py, 0.41354 2pz	0.15825 3dxy, 0.08868 3dxz, 0.09652 3dyz, 0.35535 3dx <sup>2</sup> y <sup>2</sup> , 0.29346 3dz <sup>2</sup>	/	-0.48617 2px, -0.01747 2py, -0.02822 2pz	/
	N8	O5	O6	N9 in pyridine	N10 in pyridine
[Ru <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	-0.01944 2py	/	/	/	/
[Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	0.01088 2py	-0.02980 2px, 0.02596 2pz	-0.03175 2py, 0.02839 2pz	-0.01532 2pz	-0.01456 2pz
6- coordinate [Fe <sup>V</sup> (bda)(py) <sub>2</sub> -O] <sup>+</sup>	/	/	-0.06195 2px, -0.13984 2py, -0.29028 2pz	/	/

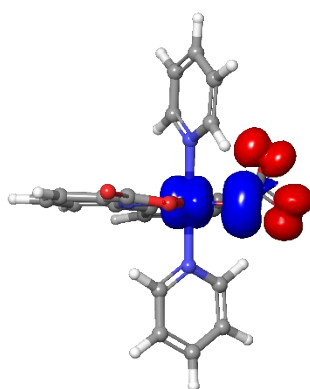
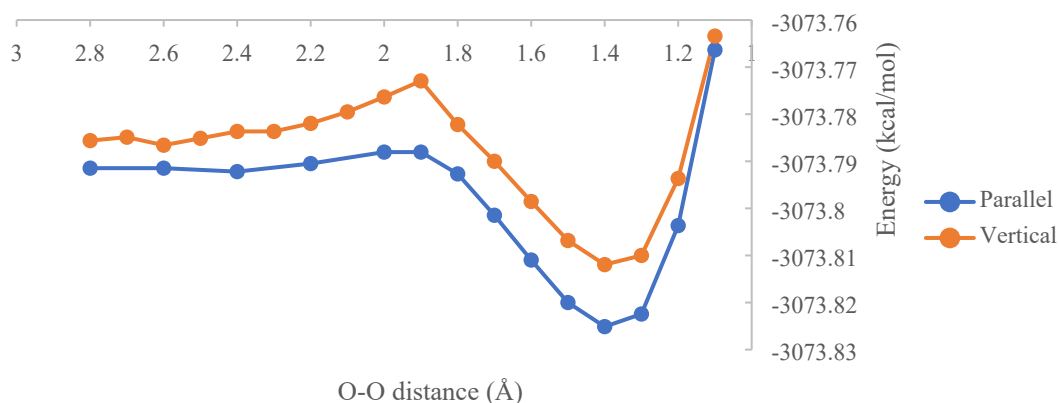
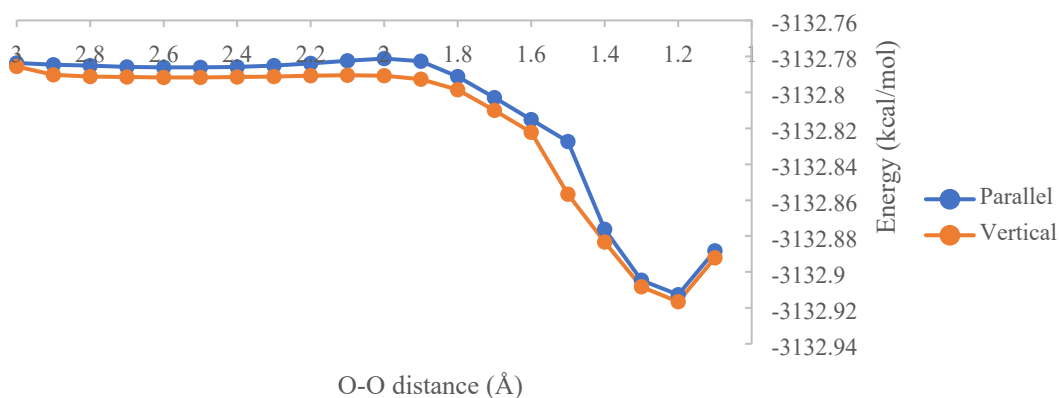


Figure S1 Spin density distribution of degenerated 6-coordinate [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> at doublet state at an isovalue of 0.005 electrons/bohr<sup>3</sup>

Energy profile of radical coupling of [RuV(bda)(py)<sub>2</sub>]<sup>+</sup> from different orientations



Energy profile of radical coupling of [FeV(bda)(py)<sub>2</sub>]<sup>+</sup> from different orientations



Energy profile of radical coupling of 6-coordinate [FeV(bda)(py)<sub>2</sub>]<sup>+</sup> from different orientations

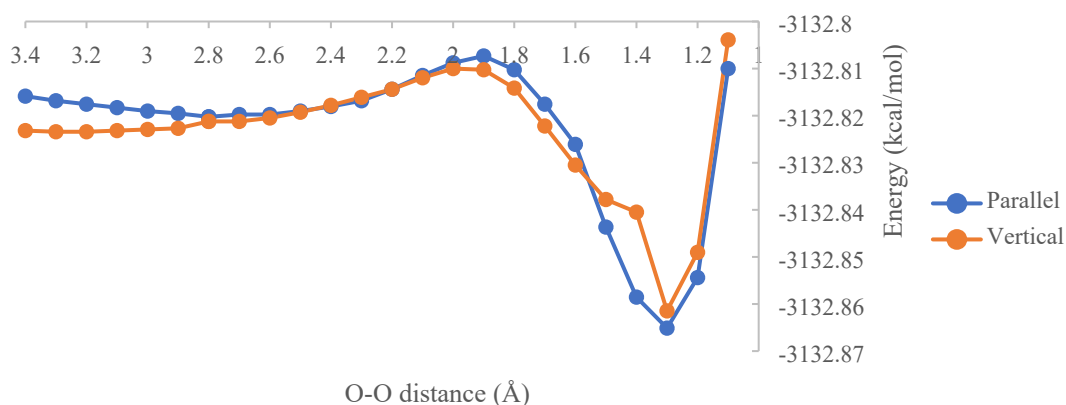


Figure S2 Energy profiles of vertical and parallel radical coupling

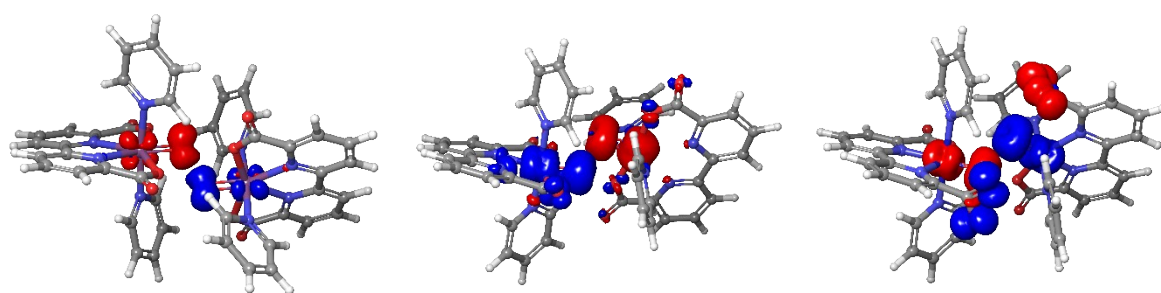


Figure S3 Spin density distributions of transition state structures of  $[\text{Ru}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (left),  $[\text{Fe}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (middle) and 6-coordinate  $[\text{Fe}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (right) at an isovalue of 0.005 electrons/bohr<sup>3</sup>

XYZ coordinates

Ru<sup>II</sup>(bda)(py)<sub>2</sub>—Singlet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1462.326276

G<sub>solv</sub> (kcal/mol) = -31.361

ZPE (kcal/mol) = 218.704

ΔH<sub>298</sub> (kcal/mol) = 16.363

ΔS<sub>298</sub> (cal/(K•mol)) = 173.692

XYZ coordinate

Ru2	-4.4001485345	9.6992911356	1.5754219261
C3	-8.3671666567	11.7399107655	0.0860503847
C4	-8.0901905657	10.4200859908	-0.2903218095
C5	-6.9121142395	9.8313068764	0.1566487413
N6	-6.0715798139	10.5296603604	0.9342457320
C7	-6.3002946412	11.8211743809	1.3219608684
C8	-7.4715945355	12.4496292762	0.8942171144
H9	-9.2801960695	12.2215569679	-0.2503530765
H10	-8.7514644491	9.8334567041	-0.9183258401
H11	-7.6801168438	13.4740727253	1.1843057216
C12	-2.9666995951	13.0419293113	3.6643269905
C13	-5.2126984333	12.3782005838	2.1539260791
N14	-4.2046874913	11.4847978898	2.3887617925
C15	-3.1107092856	11.7754455373	3.1088459927
H16	-2.0738202335	13.2500801644	4.2432812602
C17	-6.4348832426	8.4041878864	-0.1672126507
O18	-7.1686317668	7.7139982512	-0.8702430244
C19	-2.1139480396	10.6092664315	3.2435176701
O20	-1.0891474581	10.8201328389	3.8866704468
O21	-5.2919480755	8.0773022114	0.3553943639
O22	-2.4718233625	9.5122620158	2.6483170930
N23	-5.3497442185	8.8530664523	3.2778528207
C24	-5.8139681663	7.5863522705	3.1958719824
C25	-6.3653861797	6.9276714071	4.2894212959
H26	-5.7275500775	7.1218899682	2.2196925789
H27	-6.7219380635	5.9102396029	4.1688698991
N28	-3.2941079358	10.2501235393	-0.1465362496
C29	-3.8268861287	10.9004064788	-1.2009083323
C30	-3.1152154084	11.1417854090	-2.3696579240
H31	-4.8556921541	11.2226814205	-1.1001263955
H32	-3.5952698582	11.6668918296	-3.1887823542
C33	-3.9777183574	13.9878004486	3.4535348623
H34	-3.8885194517	14.9831306225	3.8779033613
C35	-5.1077594368	13.6610186390	2.6956758319
H36	-5.8926084921	14.3912611457	2.5287287660
C37	-6.4451296133	7.5853377557	5.5153655667
H38	-6.8696448317	7.0923931572	6.3848299454
C39	-5.9624640570	8.8902760199	5.6006789515
H40	-5.9937539491	9.4463134136	6.5317719794
C41	-5.4236023728	9.4857945201	4.4666180694
H42	-5.0295772794	10.4934641127	4.5028595102
C43	-1.7986235897	10.6937045886	-2.4640429076
H44	-1.2188604429	10.8616530995	-3.3666962026
C45	-1.2450410151	10.0243719602	-1.3741651277
H46	-0.2250181836	9.6558871193	-1.3955916174
C47	-2.0156178149	9.8215671477	-0.2344296516
H48	-1.6306367218	9.3217787951	0.6476844713

[Ru<sup>III</sup>(bda)(py)<sub>2</sub>-H<sub>2</sub>O]<sup>+</sup>—Doublet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1538.585679

G<sub>solv</sub> (kcal/mol) = -58.152

ZPE (kcal/mol) = 235.541

ΔH<sub>298</sub> (kcal/mol) = 18.129

ΔS<sub>298</sub> (cal/(K•mol)) = 185.379

XYZ coordinate

O1	-2.9983157188	7.5768373103	1.1119947608
Ru2	-4.3848560152	9.6281051969	1.5327514221
C3	-8.4183275947	11.7823302687	0.0695128436
C4	-8.1463153123	10.4699672518	-0.3195299577
C5	-6.9662562243	9.8781200161	0.1181384872
N6	-6.1101910298	10.5466171305	0.9031694089
C7	-6.3424932623	11.8280141724	1.2896901627
C8	-7.5094278659	12.4721488442	0.8772652409
H9	-9.3298522369	12.2727658308	-0.2564093688
H10	-8.8070143880	9.8875784822	-0.9523616918
H11	-7.7053247580	13.4943466444	1.1791723203
C12	-3.0425492114	13.0870314627	3.6253071700
C13	-5.2616374779	12.3835183145	2.1158406272
N14	-4.2687485534	11.4916589585	2.3623128888
C15	-3.1904145107	11.8119359756	3.0909179795
H16	-2.1539100334	13.2978548520	4.2101364885
C17	-6.5158178972	8.4751007169	-0.2458766472
O18	-7.2253831647	7.7625256864	-0.9318577489
C19	-2.2187546822	10.6629243920	3.2961349165
O20	-1.2014943491	10.8297051983	3.9424512585
O21	-5.3476521524	8.1728088916	0.2646323514
O22	-2.6256117203	9.5516277480	2.7340805033
N23	-5.4049074496	8.7706602395	3.2195699037
C24	-6.1363438998	7.6432556422	3.0805221450
C25	-6.7609222518	7.0257380353	4.1581849488
H26	-6.2006943757	7.2371205926	2.0794020417
H27	-7.3359757313	6.1216054735	3.9905608756
N28	-3.2525054045	10.3334476224	-0.1254919428
C29	-3.8051536077	10.9521197355	-1.1893846491
C30	-3.0553267295	11.3666807509	-2.2818330897
H31	-4.8754667072	11.1095409028	-1.1618397618
H32	-3.5488808561	11.8566549001	-3.1140217220
C33	-4.0456478162	14.0282469002	3.3888436995
H34	-3.9622601472	15.0322332665	3.7922037608
C35	-5.1663427336	13.6760511398	2.6319125993
H36	-5.9535394340	14.3972036855	2.4448585593
C37	-6.6298515810	7.5796752718	5.4301966244
H38	-7.1060416158	7.1176652544	6.2892493977
C39	-5.8675740328	8.7378866494	5.5759999727
H40	-5.7258825775	9.2044928072	6.5447364854
C41	-5.2713351552	9.2990282574	4.4540178825
H42	-4.6652717880	10.1900659417	4.5421503756
C43	-1.6797492204	11.1360490476	-2.2839294277
H44	-1.0675908166	11.4483337899	-3.1241366956
C45	-1.1099522661	10.4920229384	-1.1880182739
H46	-0.0465397094	10.2844121572	-1.1432660336
C47	-1.9220391496	10.1011831057	-0.1293862867
H48	-1.5266356938	9.5845835143	0.7344335865
H49	-2.6950744007	7.2478975363	1.9690466960
H50	-3.6556026933	6.9607763525	0.7558394524

[Ru<sup>IV</sup>(bda)(py)<sub>2</sub>-OH]<sup>+</sup>—Singlet  
E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1537.937692

G<sub>solv</sub> (kcal/mol) = -61.072

ZPE (kcal/mol) = 229.141

ΔH<sub>298</sub> (kcal/mol) = 17.272

ΔS<sub>298</sub> (cal/(K•mol)) = 177.732

XYZ coordinate

Ru2	-4.2907436818	9.4713041721	1.5417341117
C3	-8.5611235750	11.7735706892	0.4998457624
C4	-8.3407664190	10.4476222938	0.1332248310
C5	-7.1064943921	9.8764581502	0.4239630476
N6	-6.1433224817	10.5438220073	1.0672874718
C7	-6.3292869671	11.8422168018	1.4001573921
C8	-7.5373020626	12.4864600518	1.1264499408
H9	-9.5092569080	12.2565566302	0.2865515071
H10	-9.0734690177	9.8388605613	-0.3852489201
H11	-7.6735799128	13.5267016965	1.3981582431
C12	-2.8104443511	13.2269126090	3.2454462327
C13	-5.1531151088	12.4313071740	2.0276555184
N14	-4.1629786168	11.5314811077	2.2360808238
C15	-3.0386998900	11.9120917512	2.8559527824
H16	-1.8721381559	13.4554417644	3.7389408734
C17	-6.6831440369	8.5080968488	-0.0265904471
O18	-7.4580075142	7.7437428531	-0.5693924951
C19	-2.1209389964	10.7722029194	3.1851706102
O20	-1.0458526814	10.9439409439	3.7246757960
O21	-5.4104168885	8.3038266614	0.2008075885
O22	-2.6653962478	9.6210072697	2.8772050287
N23	-5.3389959459	8.6324574235	3.1855680043
C24	-5.9101968488	7.4163233158	3.0549136142
C25	-6.5803721175	6.8087862318	4.1111478796
H26	-5.8110419930	6.9445899846	2.0836693913
H27	-7.0269504540	5.8315132049	3.9652699517
N28	-3.1513656343	10.1482790169	-0.1060402054
C29	-3.7161473747	10.7559173114	-1.1667807077
C30	-2.9654615595	11.1825306834	-2.2538131790
H31	-4.7906422326	10.8881110968	-1.1346838727
H32	-3.4584144542	11.6651237199	-3.0905859936
C33	-3.8049015733	14.1725015112	3.0059091835
H34	-3.6676543316	15.2091205517	3.2962968727
C35	-4.9970053959	13.7655489170	2.4065681149
H36	-5.7973340347	14.4753062423	2.2330826447
C37	-6.6593335484	7.4701372743	5.3356559520
H38	-7.1768842264	7.0175482078	6.1756167814
C39	-6.0548489839	8.7213976037	5.4670930697
H40	-6.0811909562	9.2667109086	6.4041585977
C41	-5.3990963029	9.2683573764	4.3726145425
H42	-4.8985910865	10.2266970206	4.4324901005
C43	-1.5858822207	10.9708410433	-2.2449121693
H44	-0.9734457682	11.2958092745	-3.0801208191
C45	-1.0100758334	10.3273088576	-1.1511749732
H46	0.0555397728	10.1323088496	-1.1053615953
C47	-1.8230412258	9.9205574855	-0.0990209888
H48	-1.4359271763	9.3921213359	0.7632286773
O48	-3.2968842538	7.8514477973	1.3405185406
H50	-3.1856212064	7.4481742839	2.2179296402



[Ru<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup>—Doublet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1537.276968

G<sub>solv</sub> (kcal/mol) = -60.585

ZPE (kcal/mol) = 221.825

ΔH<sub>298</sub> (kcal/mol) = 17.149

ΔS<sub>298</sub> (cal/(K•mol)) = 179.079

XYZ coordinate

O1	-3.4110759284	7.8807772045	1.4298052428
Ru2	-4.2425537348	9.3925492948	1.5396964692
C3	-8.5437434640	11.8202176664	0.4546130605
C4	-8.3222529755	10.5037866950	0.0607520247
C5	-7.0921760379	9.9228997196	0.3580458794
N6	-6.1286245623	10.5724850679	1.0168221071
C7	-6.3247170881	11.8571412387	1.3892637925
C8	-7.5285979359	12.5105911035	1.1196534100
H9	-9.4880791801	12.3112701976	0.2420723044
H10	-9.0514305535	9.9068770383	-0.4760275319
H11	-7.6726296136	13.5394743736	1.4276619354
C12	-2.8795300186	13.2450679622	3.3702357451
C13	-5.1709096999	12.4380647967	2.0714968040
N14	-4.1817918172	11.5447350029	2.2987450010
C15	-3.0786800510	11.9346478563	2.9439401428
H16	-1.9543446488	13.4778251407	3.8856617868
C17	-6.7040085937	8.5415307924	-0.0868948758
O18	-7.4957085028	7.8201749128	-0.6658203152
C19	-2.1078101065	10.8231893332	3.2228614350
O20	-1.0466539637	11.0385424545	3.7797303853
O21	-5.4602452109	8.2649651714	0.1941090615
O22	-2.5601129730	9.6643913233	2.8299046550
N23	-5.3401749752	8.6536527001	3.2062041126
C24	-6.0047084913	7.4864896040	3.0776404390
C25	-6.7078564712	6.9319999078	4.1403332469
H26	-5.9497471162	7.0067721453	2.1075763094
H27	-7.2291107454	5.9918599439	3.9985893419
N28	-3.1335240625	10.1114792851	-0.1294235050
C29	-3.7486623814	10.5406126773	-1.2484368269
C30	-3.0320198041	10.9844498147	-2.3517677854
H31	-4.8299461876	10.5094371880	-1.2504370872
H32	-3.5636828471	11.3223620669	-3.2344577669
C33	-3.8815246167	14.1789249437	3.1248742514
H34	-3.7685638570	15.2114780228	3.4396817113
C35	-5.0468969824	13.7678898716	2.4756726133
H36	-5.8468860076	14.4729704255	2.2820734428
C37	-6.7184290988	7.5938335276	5.3674008259
H38	-7.2584829885	7.1799072992	6.2131731258
C39	-6.0131555113	8.7910584153	5.4950796185
H40	-5.9805674995	9.3317245802	6.4345527506
C41	-5.3290638844	9.2888447034	4.3941379809
H42	-4.7498004858	10.2007417579	4.4522222226
C43	-1.6376897893	10.9719702296	-2.3012094212
H44	-1.0526730950	11.3107749390	-3.1504874176
C45	-1.0084893563	10.5048001838	-1.1478871864
H46	0.0721179193	10.4618837914	-1.0691930785
C47	-1.7856957900	10.0760083610	-0.0786725115
H48	-1.3489285921	9.6868458255	0.8333190695

Fe<sup>II</sup>(bda)(py)<sub>2</sub>—Quintet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1491.931214

G<sub>solv</sub> (kcal/mol) = -28.348

ZPE (kcal/mol) = 218.371

ΔH<sub>298</sub> (kcal/mol) = 17.019

ΔS<sub>298</sub> (cal/(K•mol)) = 184.358

XYZ coordinate

Fe1	-4.3327285039	9.5663688431	1.5353825852
C3	-8.4846362685	11.9612799332	0.2132137481
C4	-8.2396403399	10.6421455696	-0.1722072219
C5	-7.0376231942	10.0551908993	0.2266696082
N6	-6.1470363846	10.7259488222	0.9535712774
C7	-6.3667647472	11.9916760772	1.3454505243
C8	-7.5439070794	12.6533739718	0.9834917202
H9	-9.4076317616	12.4539513443	-0.0792816864
H10	-8.9361116997	10.0570042363	-0.7617783528
H11	-7.7278597909	13.6761122205	1.2950022247
C12	-3.0172155997	13.1865682266	3.6496788454
C13	-5.2548441535	12.5315168600	2.1674097132
N14	-4.2897557043	11.6235422133	2.3870607630
C15	-3.2018763292	11.9190650196	3.0950935276
H16	-2.1152928308	13.3810394317	4.2185171002
C17	-6.6207873236	8.6187011546	-0.1113870415
O18	-7.4138989368	7.9192147138	-0.7359523706
C19	-2.2050435472	10.7618766958	3.2311735933
O20	-1.1616292547	10.9688719909	3.8451767498
O21	-5.4430167899	8.3024785454	0.3237520699
O22	-2.5925351840	9.6707616130	2.6525620485
N23	-5.3159624774	8.6219064461	3.2930721925
C24	-6.0809168978	7.5231038757	3.1605940421
C25	-6.6835174356	6.8963115932	4.2490132123
H26	-6.1906629480	7.1550488168	2.1463853339
H27	-7.2909450061	6.0112610507	4.0907882992
N28	-3.1435111150	10.1397136222	-0.2578155906
C29	-3.7580769633	10.3260696353	-1.4382541302
C30	-3.0782090291	10.7113832203	-2.5894524485
H31	-4.8266647850	10.1498633965	-1.4454507356
H32	-3.6227520558	10.8504161320	-3.5177291211
C33	-4.0101468262	14.1447017922	3.4399705661
H34	-3.9047838739	15.1431013658	3.8549937410
C35	-5.1458851257	13.8231898469	2.6897770606
H36	-5.9216017206	14.5615291254	2.5156718964
C37	-6.4860951950	7.4234867172	5.5241254836
H38	-6.9427928885	6.9580477499	6.3929434005
C39	-5.6857377921	8.5574634756	5.6647301923
H40	-5.4967382371	8.9996578349	6.6375051189
C41	-5.1187840985	9.1195785735	4.5254199362
H42	-4.4797928086	9.9923688545	4.5854252071
C43	-1.6985326217	10.9050857388	-2.5193490213
H44	-1.1368117150	11.2062756123	-3.3990190945
C45	-1.0542925404	10.6978461257	-1.3007146571
H46	0.0183217429	10.8263275125	-1.1989415901
C47	-1.8108362309	10.3137049101	-0.1959503410
H48	-1.3631252067	10.1252177911	0.7732201457

[Fe<sup>III</sup>(bda)(py)<sub>2</sub>-H<sub>2</sub>O]<sup>+</sup>—Sextet  
E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1568.190941

G<sub>solv</sub> (kcal/mol) = -56.580

ZPE (kcal/mol) = 235.490

ΔH<sub>298</sub> (kcal/mol) = 18.334

ΔS<sub>298</sub> (cal/(K•mol)) = 190.441

XYZ coordinate

Fe56	-4.3166605562	9.4693902187	1.6135022361
C57	-8.5176041600	11.8774488775	0.4136445101
C58	-8.3115374694	10.5391088181	0.0775516863
C59	-7.0901821997	9.9612094587	0.4215009996
N60	-6.1446452722	10.6497138844	1.0564295384
C61	-6.3256957263	11.9372088557	1.3976797661
C62	-7.5171279517	12.5932088869	1.0810899443
H63	-9.4530495368	12.3671145749	0.1611023087
H64	-9.0516790394	9.9361599539	-0.4364184788
H65	-7.6684852741	13.6323335983	1.3510571946
C66	-2.8677471999	13.1834676936	3.5005209173
C67	-5.1666777924	12.4991467134	2.1231404614
N68	-4.2020899379	11.5878166627	2.3414375566
C69	-3.0914410383	11.8990837163	3.0067568691
H70	-1.9485439042	13.3870980489	4.0380789042
C71	-6.6976334366	8.5294544428	0.1049426957
O72	-7.4881248005	7.7783006215	-0.4366378108
C73	-2.1312436344	10.7371055314	3.1758652183
O74	-1.0700768942	10.8925511866	3.7518509237
O75	-5.4691504334	8.2466175013	0.4677129791
O76	-2.5716372006	9.6284730895	2.6288994048
N77	-5.3935964497	8.8419487370	3.3870817755
C78	-5.9899564355	7.6335197847	3.3626699935
C79	-6.6435881046	7.1105903285	4.4729220816
H80	-5.9258306026	7.0966447535	2.4247036748
H81	-7.1117711049	6.1344893415	4.4082471240
N82	-3.2817904781	10.1062401833	-0.2201088166
C83	-3.9648652909	10.2507740180	-1.3718434584
C84	-3.3597050430	10.6664499051	-2.5516202070
H85	-5.0190169903	10.0141562310	-1.3340956730
H86	-3.9531516125	10.7677649215	-3.4538195666
C87	-3.8513082990	14.1477209685	3.2777865659
H88	-3.7183586708	15.1608680939	3.6444388352
C89	-5.0178205670	13.8085868162	2.5836368889
H90	-5.7907949308	14.5487291048	2.4088776220
C91	-6.6788437807	7.8577191623	5.6495412653
H92	-7.1815916053	7.4745052483	6.5322742980
C93	-6.0524746789	9.1048407662	5.6760524044
H94	-6.0475976427	9.7160376038	6.5720690790
C95	-5.4186738559	9.5585608388	4.5262921991
H96	-4.9120872086	10.5150947842	4.5032811358
C97	-1.9903526640	10.9344018393	-2.5470556708
H98	-1.4878591302	11.2584272038	-3.4532802333
C99	-1.2773561790	10.7699044541	-1.3596626585
H100	-0.2098747971	10.9554055467	-1.3099415708
C101	-1.9561767966	10.3542560778	-0.2196504524
H102	-1.4464794517	10.1977439618	0.7222446873
O54	-3.3824229179	7.4747639993	1.6233688436
H55	-2.4380243516	7.5377786689	1.8278025836
H56	-3.5237550969	6.9930237025	0.7964073555

[Fe<sup>IV</sup>(bda)(py)<sub>2</sub>-OH]<sup>+</sup>—Quintet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1567.483173

G<sub>solv</sub> (kcal/mol) = -54.098

ZPE (kcal/mol) = 227.931

ΔH<sub>298</sub> (kcal/mol) = 17.831

ΔS<sub>298</sub> (cal/(K•mol)) = 186.961

XYZ coordinate

Fe1	-4.2331967035	9.3065213665	1.5114342111
C3	-8.4421591917	11.9554498555	0.3547006972
C4	-8.2715491422	10.6158861131	0.0029206364
C5	-7.0657296264	10.0085270313	0.3457229765
N6	-6.0990286986	10.6494678191	0.9919628690
C7	-6.2494607610	11.9339442929	1.3469772731
C8	-7.4223491300	12.6287597862	1.0335860846
H9	-9.3617485335	12.4755914983	0.1055549376
H10	-9.0254447488	10.0399206448	-0.5224547565
H11	-7.5434914661	13.6680488540	1.3174844375
C12	-2.8231094493	13.1005498837	3.5334141415
C13	-5.0887862399	12.4596874829	2.0906547866
N14	-4.1579132489	11.5230862635	2.3319007034
C15	-3.0694256404	11.8239267633	3.0322085985
H16	-1.9168831938	13.2819178904	4.1004978842
C17	-6.6922797457	8.5913255451	0.0127430531
O18	-7.4575284765	7.8213540385	-0.5355721873
C19	-2.1564871871	10.6501888107	3.2332936906
O20	-1.1169067304	10.7308541260	3.8573790622
O21	-5.4572731219	8.2812481946	0.3535461717
O22	-2.5868426386	9.5416642040	2.6603756167
N23	-5.4515352263	8.7441793792	3.2594773620
C24	-5.9320537299	7.4856957430	3.2343654168
C25	-6.6753275797	6.9629834997	4.2876769926
H26	-5.7025478931	6.9116255566	2.3441080375
H27	-7.0459915567	5.9455585883	4.2285053120
N28	-3.2121328597	10.2118978107	-0.2304361483
C29	-3.8790182664	10.4749766676	-1.3677191479
C30	-3.2488233056	10.9817538023	-2.4984552640
H31	-4.9390981112	10.2598058661	-1.3618567185
H32	-3.8271538661	11.1785058814	-3.3946523617
C33	-3.7730884862	14.0892622468	3.2774838555
H34	-3.6272903075	15.1009131871	3.6429234053
C35	-4.9229597220	13.7691417828	2.5512575084
H36	-5.6736617020	14.5250267200	2.3508439148
C37	-6.9226964392	7.7637149356	5.4022557704
H38	-7.4979972666	7.3812332785	6.2397773842
C39	-6.4152731500	9.0639151485	5.4272319197
H40	-6.5787340936	9.7183900890	6.2766398831
C41	-5.6827961831	9.5153812535	4.3361185539
H42	-5.2649037259	10.5141465558	4.3098339214
C43	-1.8742628389	11.2159090258	-2.4533876386
H44	-1.3527622954	11.6100679595	-3.3201499503
C45	-1.1794774311	10.9233066010	-1.2798367909
H46	-0.1081907197	11.0743238923	-1.2032661317
C47	-1.8824986517	10.4187606067	-0.1915991659
H48	-1.3856350069	10.1553192504	0.7336790564
O48	-3.4165452121	7.6990266997	1.4134451100
H49	-2.6131660089	7.7656753533	1.9676765151

[Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup>—Quartet  
E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1566.800687

G<sub>solv</sub> (kcal/mol) = -53.084

ZPE (kcal/mol) = 221.663

ΔH<sub>298</sub> (kcal/mol) = 17.114

ΔS<sub>298</sub> (cal/(K•mol)) = 179.440

XYZ coordinate

O1	-3.3687727398	7.7911936121	1.4314906080
Fe2	-4.1546540481	9.2115119715	1.5407540356
C3	-8.6729786749	11.8865636338	0.5262452172
C4	-8.4291477928	10.5628339039	0.1555014112
C5	-7.1665810767	10.0422838570	0.4440125360
N6	-6.2247896311	10.7447310065	1.0549427410
C7	-6.4423518772	12.0137620866	1.4158551998
C8	-7.6716660831	12.6309377196	1.1598977327
H9	-9.6368798992	12.3421026163	0.3221666474
H10	-9.1670598961	9.9447448951	-0.3432319835
H11	-7.8514161110	13.6602751220	1.4493899025
C12	-2.8982711391	13.3667110014	3.3041338385
C13	-5.2592720191	12.6116479834	2.0815280817
N14	-4.2989979328	11.7077667603	2.3069166408
C15	-3.1668486192	12.0583239235	2.8987024828
H16	-1.9535404413	13.6001227652	3.7820020594
C17	-6.7071364290	8.6636777231	0.0768990528
O18	-7.4373172934	7.8458970155	-0.4462235396
C19	-2.2415087550	10.8978885946	3.1045818222
O20	-1.1377487673	11.0179164590	3.5977476561
O21	-5.4286756490	8.4012585322	0.3440659190
O22	-2.7209897191	9.7150150908	2.7242818089
N23	-5.2415052544	8.5466659375	3.0918929606
C24	-5.7824346929	7.3145470625	3.0132792430
C25	-6.4969497721	6.7768767907	4.0759888419
H26	-5.6295021776	6.7852619209	2.0805392200
H27	-6.9195445275	5.7828558253	3.9820363689
N28	-3.1093442500	9.9560505915	-0.0042371952
C29	-3.7302820366	10.5528303216	-1.0376683145
C30	-3.0152893808	11.0267703580	-2.1296184655
H31	-4.8051045863	10.6342624358	-0.9677810169
H32	-3.5445621738	11.5032496356	-2.9472457383
C33	-3.8890582986	14.3223237607	3.0726939598
H34	-3.7333801308	15.3548157764	3.3693496816
C35	-5.0889978142	13.9476373703	2.4586920958
H36	-5.8664199898	14.6815953097	2.2756854768
C37	-6.6468287136	7.5284830882	5.2414209514
H38	-7.1965452690	7.1277872961	6.0873710846
C39	-6.0744002342	8.7993968716	5.3087550130
H40	-6.1601657721	9.4135558079	6.1982381095
C41	-5.3695666196	9.2794896360	4.2128686060
H42	-4.8921919340	10.2486787815	4.2083391641
C43	-1.6292128825	10.8670059674	-2.1523211204
H44	-1.0483567862	11.2236317899	-2.9971934826
C45	-1.0009047557	10.2354143709	-1.0788854774
H46	0.0724482499	10.0834229909	-1.0572760526
C47	-1.7722450837	9.7847305582	-0.0153305268
H48	-1.3479479095	9.2861679933	0.8478432382

6-coordinate [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup>—Quartet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1566.806852

G<sub>solv</sub> (kcal/mol) = -57.438

ZPE (kcal/mol) = 220.748

ΔH<sub>298</sub> (kcal/mol) = 17.284

ΔS<sub>298</sub> (cal/(K•mol)) = 180.929

XYZ coordinate

O1	-1.9466060806	7.3587446367	1.8242756839
Fe2	-3.1887897630	7.9386142871	0.9438025935
C3	-6.6732358818	9.7962351938	-1.6022456090
C4	-6.5098259681	8.4110477785	-1.5046199355
C5	-5.4476381138	7.9376053393	-0.7377388674
N6	-4.6370244533	8.7853442918	-0.1102551801
C7	-4.7644598151	10.1167990533	-0.1797317999
C8	-5.7964865418	10.6688201419	-0.9425657567
H9	-7.4854518201	10.2056068433	-2.1948548583
H10	-7.1634834395	7.7031431690	-2.0020305711
H11	-5.9293804134	11.7418965298	-1.0195160014
C12	-1.8321590967	11.9022555189	2.2879395605
C13	-3.7499015381	10.8134503531	0.6411387503
N14	-3.0015020616	9.9889184795	1.4231447166
C15	-2.0941095650	10.5307040425	2.2503005669
H16	-1.0717841800	12.2828893981	2.9609239234
C17	-5.0249191718	6.4875549527	-0.5449627671
O18	-5.6866606436	5.5829230060	-1.0127562806
C19	-1.3704221372	9.6529075681	3.2302640055
O20	-0.1178912556	9.6239371424	3.2986778036
O21	-3.8883650793	6.3708539632	0.1139393931
O22	-1.9674941918	9.0091033453	4.1299727991
N23	-4.4592802884	7.5802626055	2.4512802871
C24	-4.4162064535	6.3394864887	2.9743891428
C25	-5.2394335119	5.9641644724	4.0295673607
H26	-3.7082136058	5.6591263283	2.5189518409
H27	-5.1748061536	4.9556214352	4.4221211413
N28	-1.8924278664	8.2301644640	-0.6076273072
C29	-2.2048047093	7.9285859129	-1.8804611242
C30	-1.2976791967	8.0767975827	-2.9235364834
H31	-3.1985678364	7.5439959308	-2.0588725051
H32	-1.5964191499	7.8146620707	-3.9325158969
C33	-2.5784179287	12.7467930742	1.4682032819
H34	-2.4051942147	13.8180214621	1.4762135945
C35	-3.5623216408	12.1974885843	0.6500003445
H36	-4.1697523174	12.8320949532	0.0147811191
C37	-6.1315802514	6.8949725196	4.5592024437
H38	-6.7861083970	6.6264767612	5.3824875644
C39	-6.1702872399	8.1784782768	4.0131625858
H40	-6.8481291490	8.9353201336	4.3924444965
C41	-5.3172538412	8.4822060285	2.9605054888
H42	-5.3127408203	9.4647990835	2.5062325681
C43	-0.0160309060	8.5469845075	-2.6422859256
H44	0.7151308328	8.6693071535	-3.4352275949
C45	0.3131702218	8.8420925180	-1.3194518669
H46	1.3027692763	9.1911160942	-1.0456068354
C47	-0.6460960376	8.6645717470	-0.3308311217
H48	-0.4200427682	8.8391758043	0.7132757017

Ru<sup>III</sup>(bda)(py)<sub>2</sub>-OH—Doublet  
E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1538.163901

G<sub>solv</sub> (kcal/mol) = -32.677

ZPE (kcal/mol) = 227.472

ΔH<sub>298</sub> (kcal/mol) = 17.825

ΔS<sub>298</sub> (cal/(K•mol)) = 184.716

XYZ coordinate

O1	-3.1767342610	7.7340165477	1.3030330392
Ru2	-4.2237633957	9.3429023696	1.4881899540
C3	-8.6101412445	11.9925436602	0.3431247228
C4	-8.3760827909	10.6752824559	-0.0438388699
C5	-7.1528145234	10.0954501572	0.3000914499
N6	-6.2223679379	10.7507778293	0.9925862417
C7	-6.4327219130	12.0257240549	1.3626789846
C8	-7.6255267300	12.6860341251	1.0513515201
H9	-9.5466326558	12.4831526548	0.0936352015
H10	-9.0889501246	10.0806323245	-0.6034529807
H11	-7.7854503118	13.7147276612	1.3553419065
C12	-3.0333802803	13.3898498273	3.4724351645
C13	-5.2919446583	12.6116894957	2.1010237981
N14	-4.3118774921	11.7264049360	2.3312253524
C15	-3.2226187279	12.0877299807	3.0035299625
H16	-2.1214967140	13.6199025746	4.0112696562
C17	-6.7634122238	8.6937923242	-0.1256676855
O18	-7.5887988633	7.9945040571	-0.7076626227
C19	-2.2415123204	10.9629126024	3.2641042786
O20	-1.1966461215	11.2055589222	3.8618765734
O21	-5.5382235000	8.3765865298	0.1555272472
O22	-2.6429178758	9.8048092820	2.8421908959
N23	-5.2832037017	8.5070922036	3.1009577495
C24	-5.9257153916	7.3329853023	2.9294811865
C25	-6.6372782292	6.7297799930	3.9620231028
H26	-5.8596605266	6.9055685345	1.9350321597
H27	-7.1445994795	5.7885023598	3.7795791839
N28	-3.1024576058	10.0824997017	-0.1243365312
C29	-3.6776973107	10.6013012122	-1.2244794382
C30	-2.9289163006	11.0977835532	-2.2845025659
H31	-4.7602530357	10.6034857724	-1.2369312684
H32	-3.4341550960	11.5095403164	-3.1518676850
C33	-4.0376724023	14.3243369788	3.2296659983
H34	-3.9347073649	15.3486164957	3.5765326096
C35	-5.1895316020	13.9351849013	2.5411153779
H36	-5.9844033056	14.6481325451	2.3514650924
C37	-6.6841419574	7.3509310415	5.2088193285
H38	-7.2351031887	6.9029070537	6.0304867823
C39	-6.0065303118	8.5583505514	5.3833051294
H40	-6.0071755985	9.0746514689	6.3375211299
C41	-5.3136499041	9.1026623395	4.3093438424
H42	-4.7592461306	10.0285404424	4.3923013470
C43	-1.5365489035	11.0499229986	-2.2077388658
H44	-0.9249804216	11.4351121138	-3.0184284176
C45	-0.9462487357	10.4923341201	-1.0750728784
H46	0.1317272191	10.4259739958	-0.9736862190
C47	-1.7589489136	10.0114902617	-0.0534002247
H48	-1.3635443386	9.5585791147	0.8474624210
H49	-3.0638062669	7.3660756271	2.1930870948

Fe<sup>III</sup>(bda)(py)<sub>2</sub>-OH—Sextet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1567.761426

G<sub>solv</sub> (kcal/mol) = -32.400

ZPE (kcal/mol) = 226.693

ΔH<sub>298</sub> (kcal/mol) = 18.303

ΔS<sub>298</sub> (cal/(K•mol)) = 194.500

XYZ coordinate

Fe56	-4.1933507516	9.2898737241	1.5788505144
C57	-8.3629010026	12.1767002813	0.4378165172
C58	-8.2454412220	10.8372122920	0.0773688289
C59	-7.0780433582	10.1577415939	0.4366188308
N60	-6.0930369018	10.7464799397	1.1081109000
C61	-6.1987199132	12.0344574446	1.4725688501
C62	-7.3282272426	12.7923240643	1.1483247855
H63	-9.2517067408	12.7432556330	0.1748419119
H64	-9.0109727030	10.2954995235	-0.4660687178
H65	-7.4051638806	13.8333389318	1.4422192194
C66	-2.7714093346	13.1166065026	3.7087436755
C67	-5.0320561084	12.5204085291	2.2460134121
N68	-4.0856374943	11.5841758951	2.4287692116
C69	-2.9906723946	11.8621999561	3.1357246708
H70	-1.8604122860	13.2742717530	4.2742739302
C71	-6.8358325128	8.6940853444	0.0947450088
O72	-7.7212134142	8.0778343084	-0.4951745935
C73	-1.9994242785	10.7095441702	3.2525494660
O74	-0.9757193938	10.8851856207	3.9084490711
O75	-5.6816362297	8.2563633247	0.4707720199
O76	-2.3695143156	9.6543531577	2.6106069102
N77	-5.3534591323	8.7794482773	3.3687575478
C78	-5.8466159820	7.5274560889	3.3526106994
C79	-6.5934120050	7.0163904254	4.4102682640
H80	-5.6260230097	6.9560684685	2.4583055240
H81	-6.9764368539	6.0030595213	4.3544649141
N82	-3.3721346702	10.0587566897	-0.2909868391
C83	-3.6738322285	9.3843588386	-1.4147342055
C84	-3.1409816498	9.7355022743	-2.6517039011
H85	-4.3557342516	8.5514210665	-1.2826465740
H86	-3.4138717699	9.1656909738	-3.5335621529
C87	-3.7392811140	14.1003132800	3.5193571345
H88	-3.6096013035	15.0919873099	3.9434594652
C89	-4.8869406038	13.8052405026	2.7792136833
H90	-5.6509413409	14.5592186420	2.6267289467
C91	-6.8304665920	7.8224126245	5.5226008366
H92	-7.4087547716	7.4492943934	6.3630461800
C93	-6.3095393418	9.1161991313	5.5395211815
H94	-6.4633372033	9.7779630580	6.3854724664
C95	-5.5760246217	9.5529869669	4.4413293863
H96	-5.1491279969	10.5480717118	4.4060203910
C97	-2.2603939016	10.8137161297	-2.7263602012
H98	-1.8290658024	11.1111456619	-3.6779054913
C99	-1.9352548170	11.4987205654	-1.5556918869
H100	-1.2442772914	12.3351572675	-1.5616249008
C101	-2.5100063315	11.0843423179	-0.3587995304
H102	-2.2778717342	11.5718127361	0.5791938682
O54	-3.4011413833	7.6107817144	1.4687505816
H55	-2.5501335501	7.6836066468	1.9307183573



[Ru<sup>IV</sup>(bda)(py)<sub>2</sub>-H<sub>2</sub>O]<sup>2+</sup>—Singlet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1538.226926

G<sub>solv</sub> (kcal/mol) = -152.984

ZPE (kcal/mol) = 236.794

ΔH<sub>298</sub> (kcal/mol) = 17.550

ΔS<sub>298</sub> (cal/(K•mol)) = 178.219

XYZ coordinate

O1	-3.1664635667	7.7317093245	1.2714878299
Ru2	-4.3381403193	9.5579062038	1.5207662218
C3	-8.5377528274	11.7252533805	0.3443387144
C4	-8.2622008564	10.4145815520	-0.0520369016
C5	-7.0307708420	9.8689021486	0.2864765830
N6	-6.1230706028	10.5545173477	0.9958089818
C7	-6.3582807698	11.8347261476	1.3668490566
C8	-7.5713070473	12.4481947498	1.0475439061
H9	-9.4882043383	12.1868742260	0.0959485680
H10	-8.9567118891	9.8090359542	-0.6260386549
H11	-7.7560793391	13.4740665476	1.3455963825
C12	-2.9215944130	13.1619602725	3.4161243877
C13	-5.2277147976	12.4182544454	2.0781148097
N14	-4.2384439140	11.5209738233	2.2912745621
C15	-3.1285313428	11.8677543768	2.9569924552
H16	-2.0017107040	13.3824792757	3.9485168516
C17	-6.5428137208	8.5230366674	-0.1493425444
O18	-7.2063341581	7.7066849949	-0.7331365667
C19	-2.2172340685	10.7086614024	3.2144020232
O20	-1.1448484539	10.7810625595	3.7537771074
O21	-5.2513990076	8.3685752867	0.1637973831
O22	-2.7960246604	9.5680013656	2.8211219783
N23	-5.4410692765	8.6886396781	3.1427665462
C24	-6.1200707387	7.5301053675	2.9809259161
C25	-6.8066308480	6.9257300377	4.0267771641
H26	-6.1051423273	7.0846950415	1.9940134818
H27	-7.3358803917	5.9958805779	3.8485296647
N28	-3.1734519278	10.3067318227	-0.0907117861
C29	-3.7451846015	10.8900544217	-1.1660470080
C30	-2.9958570581	11.3448300055	-2.2420017903
H31	-4.8236632092	10.9820366129	-1.1601730871
H32	-3.4969450365	11.8047111807	-3.0868451066
C33	-3.9191137021	14.1120970895	3.1871126400
H34	-3.7967471147	15.1342397146	3.5311259292
C35	-5.0890808366	13.7331701466	2.5253752546
H36	-5.8836836839	14.4507618710	2.3554783361
C37	-6.7950875770	7.5282232531	5.2849927019
H38	-7.3222078349	7.0766788417	6.1195145043
C39	-6.0874541951	8.7193224589	5.4517473631
H40	-6.0423361812	9.2200382048	6.4127663933
C41	-5.4211443043	9.2663570965	4.3634170735
H42	-4.8483310032	10.1787240939	4.4636605825
C43	-1.6085857623	11.1913570645	-2.2142575146
H44	-0.9983942828	11.5370600652	-3.0426998928
C45	-1.0223107755	10.5785379088	-1.1072466879
H46	0.0499964874	10.4290171923	-1.0443261167
C47	-1.8321655346	10.1428849691	-0.0654556060
H48	-1.4177394698	9.6428232720	0.8003164615
H49	-2.8207840038	7.3844274193	2.1107862115
H50	-3.6749013595	7.0523616305	0.7951340835

[Fe<sup>IV</sup>(bda)(py)<sub>2</sub>-H<sub>2</sub>O]<sup>2+</sup>—Quintet

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -1567.777399

G<sub>solv</sub> (kcal/mol) = -147.059

ZPE (kcal/mol) = 233.942

ΔH<sub>298</sub> (kcal/mol) = 18.654

ΔS<sub>298</sub> (cal/(K•mol)) = 191.437

XYZ coordinate

Fe56	-4.2170454906	9.5345851513	1.6769913281
C57	-8.5564414791	11.9354763191	0.5174673701
C58	-8.3889316133	10.5839057073	0.1890550343
C59	-7.1652301887	10.0038023003	0.5006271460
N60	-6.1654959433	10.6655832149	1.0931228524
C61	-6.3167717229	11.9579586322	1.4194474735
C62	-7.5173818852	12.6304151314	1.1346066903
H63	-9.4912330630	12.4395895193	0.2935175069
H64	-9.1714543627	10.0069314790	-0.2938248480
H65	-7.6406175283	13.6751135654	1.3971339609
C66	-2.8414214351	13.2502806716	3.4747347240
C67	-5.1415685591	12.5310272798	2.1100986941
N68	-4.1764601776	11.6223160150	2.3518257989
C69	-3.0682008407	11.9545155265	3.0137880723
H70	-1.9239742738	13.4702259126	4.0101970117
C71	-6.7681022188	8.6048724907	0.1980896489
O72	-7.5377891621	7.7397115164	-0.3147309231
C73	-2.1121576712	10.8028030408	3.2069831208
O74	-1.0492957892	10.9238624480	3.7659799362
O75	-5.5943068819	8.2092637735	0.4363319254
O76	-2.5760594231	9.6713333870	2.6725865028
N77	-5.3760634125	8.7792795056	3.3013966013
C78	-5.6468155131	7.4594489326	3.3927616122
C79	-6.3132330604	6.9189063851	4.4859552936
H80	-5.3058045302	6.8459068252	2.5699311562
H81	-6.5082655484	5.8525979422	4.5201079547
N82	-3.3126925851	10.0736155339	-0.1915487351
C83	-4.0055455045	10.4084730253	-1.3006123998
C84	-3.3823442368	10.7733467357	-2.4862613751
H85	-5.0837814998	10.3809832190	-1.2232173286
H86	-3.9816882416	11.0337677023	-3.3519324925
C87	-3.8218025664	14.2104042244	3.2219169346
H88	-3.6876315615	15.2334716285	3.5592421176
C89	-4.9887873313	13.8513489904	2.5354698281
H90	-5.7574041996	14.5913876108	2.3422442675
C91	-6.7122478057	7.7644077367	5.5214489803
H92	-7.2308717238	7.3681202419	6.3889875019
C93	-6.4293564534	9.1291373997	5.4267042923
H94	-6.7147596382	9.8208631690	6.2119318852
C95	-5.7605590142	9.5977344223	4.3046466808
H96	-5.5120676133	10.6456977145	4.1949913705
C97	-1.9868446352	10.7903128816	-2.5369599884
H98	-1.4711252978	11.0708272435	-3.4501619781
C99	-1.2670204950	10.4377312488	-1.3942755035
H100	-0.1823281844	10.4357993243	-1.3866090560
C101	-1.9603264218	10.0849618435	-0.2434792854
H102	-1.4443283392	9.8069524926	0.6669799767
O54	-3.3053195635	7.5618101813	1.4620970468
H55	-2.4166074127	7.5173417594	1.8479758937
H56	-3.3236546473	7.0694549727	0.6296727079

Pre-reactive structure of  $[\text{Ru}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (O-O distance 2.4 Å)

E (B3LYP-D3/LACV3P\*\*\*) (a.u.) = -3074.547919

$G_{\text{solv}}$  (kcal/mol) = -131.525

ZPE (kcal/mol) = 444.914

$\Delta H_{298}$  (kcal/mol) = 34.666

$\Delta S_{298}$  (cal/(K•mol)) = 305.398

XYZ coordinate

O1	-3.8983998204	11.8564765890	1.7619875401
Ru2	-4.9100786421	13.1287578386	2.3427310514
C3	-8.6332494290	16.2290176672	1.0023714108
C4	-8.0110112141	15.3940976279	0.0785815499
C5	-6.9539817134	14.6002177663	0.5122593402
N6	-6.5193875729	14.6008301054	1.7798452152
C7	-7.1028702498	15.4242848058	2.6820670894
C8	-8.1678234552	16.2491916142	2.3176488001
H9	-9.4647317672	16.8619153161	0.7086104732
H10	-8.3028452825	15.3305427284	-0.9641350025
H11	-8.6311631131	16.8969163788	3.0521795876
C12	-5.1700679985	14.9979467508	6.4023774283
C13	-6.4973471544	15.3530215918	4.0117595242
N14	-5.5394887831	14.4066766505	4.1101310108
C15	-4.9052080915	14.2283455747	5.2746101576
H16	-4.6127755765	14.7894639712	7.3092166424
C17	-6.1865452718	13.6860639510	-0.3956232619
O18	-6.4950856482	13.5308188604	-1.5654534737
C19	-3.9528130687	13.0703510079	5.2699835289
O20	-3.3153765331	12.7503896752	6.2646448856
O21	-5.1984714351	13.1015842057	0.2193049629
O22	-3.9530159031	12.4429220175	4.1344510227
N23	-6.4929371131	11.7066614579	2.6637998739
C24	-7.0847887179	11.1028573732	1.6129156644
C25	-7.9809816844	10.0544364491	1.7788324867
H26	-6.7961983076	11.4527444323	0.6312190875
H27	-8.4337872806	9.5943309546	0.9069738008
N28	-3.2953724601	14.4777989695	2.1121661397
C29	-3.4425364294	15.7210996213	1.6116543775
C30	-2.3664748285	16.5903658746	1.4983747420
H31	-4.4393456613	16.0079794572	1.3000136229
H32	-2.5223982175	17.5858193700	1.0964283996
C33	-6.1489614283	15.9845226907	6.3117612888
H34	-6.3917184936	16.6062721564	7.1679009528
C35	-6.8265530448	16.1583711465	5.1045907015
H36	-7.5983478749	16.9135001302	5.0149806834
C37	-8.2663916780	9.6017671555	3.0669218207
H38	-8.9451258661	8.7688953025	3.2222762756
C39	-7.6542475253	10.2326690341	4.1490633058
H40	-7.8390068693	9.9113883909	5.1680824532
C41	-6.7718052458	11.2775144909	3.9105086081
H42	-6.2470834997	11.7655140489	4.7187825999
C43	-1.1006140448	16.1571457652	1.9010851686
H44	-0.2440622706	16.8196207731	1.8212470318
C45	-0.9553851599	14.8632338803	2.3988873693
H46	0.0010087847	14.4613178726	2.7144683835
C47	-2.0743071915	14.0453723676	2.4957729779
H48	-2.0048050200	13.0358526422	2.8802921751
O49	-4.1721177174	9.9663322322	3.2154083824

Ru50	-2.9524900075	8.8156872750	2.7984768660
C51	2.0054357411	7.9662834758	2.3932730728
C52	1.5069036285	9.2275903274	2.7126735825
C53	0.1274650855	9.3990153240	2.7612164852
N54	-0.7324925272	8.4021452877	2.5240710889
C55	-0.2623406421	7.1817635725	2.1887576304
C56	1.1105230464	6.9315305860	2.1168798958
H57	3.0754187586	7.7891148370	2.3467916334
H58	2.1383136900	10.0859567280	2.9145370931
H59	1.4743414716	5.9457764539	1.8517811955
C60	-3.5139112403	4.5930363883	1.5086500701
C61	-1.3245099542	6.2146153563	1.9183884302
N62	-2.5649838136	6.6885145233	2.1831170187
C63	-3.6244970625	5.8906155683	1.9983929680
H64	-4.4241584393	4.0167654891	1.3832584643
C65	-0.5368368501	10.7237119755	2.9949195836
O66	0.1101961933	11.7494372341	3.1683838650
C67	-4.9314449655	6.5051945717	2.4018165669
O68	-5.9916208086	5.9229041447	2.2483641618
O69	-1.8299594708	10.6420333586	2.9289497601
O70	-4.7729836819	7.6904370716	2.9228367289
N71	-2.5924905559	8.5342548265	4.8682262392
C72	-2.5629306304	9.6448300497	5.6371069762
C73	-2.3331875476	9.5702943309	7.0050026718
H74	-2.7299413230	10.5940254264	5.1439989203
H75	-2.3288708370	10.4924029905	7.5756156820
N76	-3.3156855130	9.2652322938	0.7342193609
C77	-2.3768302756	9.8881862831	-0.0046470411
C78	-2.6758579364	10.4831388164	-1.2228162373
H79	-1.3794931487	9.9298620827	0.4114936063
H80	-1.8931176351	10.9887789195	-1.7774444356
C81	-2.2454138772	4.1020532316	1.2135210115
H82	-2.1134387786	3.0969400644	0.8256157027
C83	-1.1365180188	4.9208731627	1.4309508989
H84	-0.1369918374	4.5614650752	1.2149848634
C85	-2.1233265204	8.3230713277	7.5914889041
H86	-1.9361639661	8.2365787788	8.6576248148
C87	-2.1648371436	7.1806954658	6.7880344512
H88	-2.0171349006	6.1904037869	7.2052976849
C89	-2.4088568532	7.3224732860	5.4285696062
H90	-2.4658115066	6.4656987991	4.7678287880
C91	-3.9889615603	10.4444472843	-1.6908507911
H92	-4.2634150431	10.9375695890	-2.6176809435
C93	-4.9493749991	9.7743430354	-0.9350174926
H94	-5.9807154072	9.7155312275	-1.2655442958
C95	-4.5834335961	9.2038388648	0.2765745283
H96	-5.3048990041	8.7262539459	0.9277714348

Transition state structure of [Ru<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 1.9 Å)

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3074.544809

G<sub>solv</sub> (kcal/mol) = -129.533

ZPE (kcal/mol) = 444.486

ΔH<sub>298</sub> (kcal/mol) = 34.112

ΔS<sub>298</sub> (cal/(K•mol)) = 298.64

XYZ coordinate

O1	-3.9506661041	11.5614072088	2.1269220978
Ru2	-5.0690009441	12.8125698864	2.7205418159
C3	-9.0329519985	15.5801216990	1.4554725977
C4	-8.5050128246	14.6243711714	0.5902059257
C5	-7.3702752149	13.9264053679	0.9898068958
N6	-6.7905567178	14.1199708460	2.1814837920
C7	-7.2765935573	15.0622922637	3.0216728841
C8	-8.4024968399	15.8124868049	2.6790411368
H9	-9.9162246878	16.1483700097	1.1817883871
H10	-8.9246042429	14.4046364619	-0.3855743789
H11	-8.7847697790	16.5629194658	3.3614788302
C12	-4.9482708117	15.0822888736	6.5344098173
C13	-6.5092351975	15.1802250908	4.2610160254
N14	-5.5378233196	14.2483561135	4.3718765842
C15	-4.8013813214	14.1795780778	5.4873369741
H16	-4.3172296834	14.9627756572	7.4083778445
C17	-6.6381949416	12.9499537492	0.1160044599
O18	-7.0743328588	12.5809410720	-0.9618724932
C19	-3.9075488078	12.9751643550	5.5392743487
O20	-3.2213892781	12.7111727439	6.5144342508
O21	-5.5010561024	12.5926835768	0.6475859071
O22	-4.0241680794	12.2382707585	4.4740021383
N23	-6.5208346104	11.3398683319	3.2427378459
C24	-6.8705231411	10.4112532982	2.3294963521
C25	-7.5827111362	9.2701654556	2.6738247546
H26	-6.5307848127	10.5912373657	1.3190436554
H27	-7.7889622947	8.5163244563	1.9223981927
N28	-3.4926179155	14.1666528342	2.2681676762
C29	-3.6987971560	15.3601713101	1.6785563590
C30	-2.6520381933	16.2349717775	1.4191768751
H31	-4.7215884128	15.6005266213	1.4121850512
H32	-2.8551033077	17.1890162849	0.9448059445
C33	-5.9141085850	16.0801413253	6.4155168189
H34	-6.0590704972	16.8080324063	7.2075560349
C35	-6.7167768767	16.1182860583	5.2746201311
H36	-7.4951022013	16.8659798154	5.1747533967
C37	-7.9662556197	9.0931264690	4.0012811645
H38	-8.5137202646	8.2053865227	4.3019105404
C39	-7.6259090290	10.0688664764	4.9392391802
H40	-7.9059833513	9.9723035904	5.9825486988
C41	-6.8904809440	11.1717792501	4.5276600134
H42	-6.5698264831	11.9300577246	5.2296636270
C43	-1.3537230639	15.8600953566	1.7736720834
H44	-0.5191576235	16.5278790961	1.5828569133
C45	-1.1476171602	14.6165427021	2.3690737747
H46	-0.1628740057	14.2647839267	2.6576860132
C47	-2.2393056064	13.7891964748	2.6040903748
H48	-2.1229664362	12.8100100427	3.0529450215
O49	-4.0532357954	9.9705588680	3.1606921437

Ru50	-2.8393245957	8.7639492533	2.6755158311
C51	2.0255088255	7.6112744100	2.8214716633
C52	1.5706414067	8.8886982482	3.1461972355
C53	0.2103720084	9.1535985357	3.0322255245
N54	-0.6688544495	8.2236432864	2.6408238026
C55	-0.2379605276	6.9961931611	2.2758340089
C56	1.1147750754	6.6579665010	2.3620938775
H57	3.0790315763	7.3628350737	2.9025145707
H58	2.2253915524	9.6914588444	3.4678238570
H59	1.4502942165	5.6687376467	2.0735909275
C60	-3.5508553508	4.7419042083	0.9695970919
C61	-1.3152846121	6.1358179562	1.7885666748
N62	-2.5407920850	6.6932639076	1.9163979173
C63	-3.6279297554	6.0052942223	1.5454037648
H64	-4.4751400396	4.2515916152	0.6837800049
C65	-0.3992470114	10.5146773023	3.2099954712
O66	0.2667974668	11.4989726490	3.4894955058
C67	-4.9169919701	6.6946630323	1.8823599112
O68	-6.0017968794	6.2654851159	1.5271954656
O69	-1.6751179147	10.5127397351	2.9542861952
O70	-4.7139828643	7.7601622734	2.6065495595
N71	-2.6953652380	8.3652303411	4.7603701353
C72	-2.6674299996	9.4320917528	5.5891013384
C73	-2.5739841423	9.2765099158	6.9665501813
H74	-2.7375706618	10.4120658613	5.1337543828
H75	-2.5594603710	10.1675310101	7.5850527816
N76	-3.0023574861	9.3559912765	0.6327615760
C77	-1.9423995194	9.8883305460	-0.0073083215
C78	-2.0736272619	10.5343013398	-1.2287343619
H79	-0.9835965306	9.8057992943	0.4871337308
H80	-1.1951578247	10.9480951715	-1.7121101908
C81	-2.2933485268	4.1649532602	0.8067730468
H82	-2.1884191273	3.1797482833	0.3637707093
C83	-1.1636395866	4.8634563312	1.2356521137
H84	-0.1761378757	4.4281875276	1.1349925379
C85	-2.5081048419	7.9906048992	7.5008960496
H86	-2.4314542684	7.8398650953	8.5734116291
C87	-2.5489432337	6.8941155193	6.6358313952
H88	-2.5108324430	5.8771026374	7.0108812624
C89	-2.6469838566	7.1189040528	5.2689313646
H90	-2.6955869697	6.3017297359	4.5585602511
C91	-3.3430347606	10.6605617210	-1.7948479520
H92	-3.4790469515	11.1894993952	-2.7329329694
C93	-4.4364055770	10.1068746284	-1.1320804620
H94	-5.4440576473	10.2190417845	-1.5163992313
C95	-4.2263323632	9.4527501749	0.0745291121
H96	-5.0404203577	9.0236432331	0.6420317778

Product structure of [Ru<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 1.4 Å)  
E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3073.825172

XYZ coordinate

O1	-3.8800610000000	11.5530420000000	2.2832010000000
Ru2	-5.1408800000000	12.8564740000000	2.8899790000000
C3	-9.1764050000000	15.3724480000000	1.4997300000000
C4	-8.5827640000000	14.4337050000000	0.6577880000000
C5	-7.4243810000000	13.7987030000000	1.0892700000000
N6	-6.8828250000000	14.0363050000000	2.2914530000000
C7	-7.4266020000000	14.9685670000000	3.1061940000000
C8	-8.5816070000000	15.6561980000000	2.7296070000000
H9	-10.0812940000000	15.8914340000000	1.2004540000000
H10	-8.9692440000000	14.1835190000000	-0.3242880000000
H11	-9.0118900000000	16.3999410000000	3.3898610000000
C12	-5.1188300000000	15.1521290000000	6.6276080000000
C13	-6.6781310000000	15.1430980000000	4.3488770000000
N14	-5.6528610000000	14.2712510000000	4.4707020000000
C15	-4.9174490000000	14.2506250000000	5.5900830000000
H16	-4.4844120000000	15.0767440000000	7.5042870000000
C17	-6.6116630000000	12.8605340000000	0.2473220000000
O18	-6.9792630000000	12.4675570000000	-0.8477050000000
C19	-3.9674810000000	13.0919020000000	5.6527680000000
O20	-3.2401080000000	12.8796410000000	6.6072490000000
O21	-5.4784450000000	12.5685330000000	0.8271330000000
O22	-4.0923440000000	12.3185060000000	4.6084030000000
N23	-6.5463600000000	11.3421860000000	3.4243770000000
C24	-6.8682800000000	10.3875090000000	2.5310080000000
C25	-7.6134150000000	9.2673490000000	2.8752290000000
H26	-6.4885090000000	10.5268720000000	1.5293870000000
H27	-7.7836280000000	8.4956040000000	2.1334230000000
N28	-3.5973250000000	14.2276230000000	2.3941490000000
C29	-3.8394530000000	15.4111850000000	1.7962760000000
C30	-2.8163120000000	16.2961630000000	1.4841740000000
H31	-4.8746000000000	15.6355760000000	1.5652190000000
H32	-3.0511710000000	17.2397770000000	1.0035230000000
C33	-6.1426470000000	16.0901310000000	6.4993740000000
H34	-6.3331780000000	16.8124090000000	7.2867550000000
C35	-6.9436730000000	16.0724260000000	5.3571380000000
H36	-7.7669010000000	16.7694970000000	5.2506590000000
C37	-8.0576740000000	9.1379800000000	4.1884520000000
H38	-8.6367780000000	8.2714120000000	4.4919610000000
C39	-7.7354700000000	10.1343060000000	5.1124230000000
H40	-8.0583310000000	10.0722560000000	6.1460800000000
C41	-6.9686870000000	11.2145000000000	4.6986410000000
H42	-6.6682460000000	11.9899040000000	5.3912750000000
C43	-1.4996720000000	15.9449390000000	1.7936980000000
H44	-0.6823150000000	16.6202500000000	1.5599040000000
C45	-1.2549340000000	14.7149050000000	2.4010290000000
H46	-0.2552880000000	14.3791220000000	2.6562550000000
C47	-2.3264890000000	13.8780120000000	2.6891830000000
H48	-2.1767760000000	12.9055520000000	3.1381450000000
O49	-3.9331770000000	10.3621160000000	3.0172820000000
Ru50	-2.6900210000000	9.0316070000000	2.4411200000000
C51	2.0663910000000	7.6788060000000	2.5583940000000
C52	1.6645860000000	8.9622560000000	2.9291060000000
C53	0.3176690000000	9.2885310000000	2.8258370000000
N54	-0.5988020000000	8.4058860000000	2.4090140000000

C55	-0.2200030000000	7.1758820000000	1.9952340000000
C56	1.1181920000000	6.7813600000000	2.0647100000000
H57	3.1088770000000	7.3850940000000	2.6281880000000
H58	2.3530700000000	9.7251410000000	3.2764320000000
H59	1.4121720000000	5.7913600000000	1.7357280000000
C60	-3.6481460000000	5.1504270000000	0.6206390000000
C61	-1.3349340000000	6.3878800000000	1.4761170000000
N62	-2.5272110000000	7.0074600000000	1.6238610000000
C63	-3.6543870000000	6.3945400000000	1.2401610000000
H64	-4.5987660000000	4.7187900000000	0.3264560000000
C65	-0.2393950000000	10.6673400000000	3.0345850000000
O66	0.4448380000000	11.6149960000000	3.3767360000000
C67	-4.8951160000000	7.1389590000000	1.6364270000000
O68	-6.0134590000000	6.7818140000000	1.3064110000000
O69	-1.5073020000000	10.7218500000000	2.7214870000000
O70	-4.6083930000000	8.1592520000000	2.3993290000000
N71	-2.5975050000000	8.6050360000000	4.5224090000000
C72	-2.5393020000000	9.6469190000000	5.3790110000000
C73	-2.5075980000000	9.4589910000000	6.7555830000000
H74	-2.5499410000000	10.6374480000000	4.9469760000000
H75	-2.4748690000000	10.3357100000000	7.3936400000000
N76	-2.8454210000000	9.6532940000000	0.4129850000000
C77	-1.7477050000000	9.9698990000000	-0.3037850000000
C78	-1.8374450000000	10.5450460000000	-1.5633230000000
H79	-0.7895630000000	9.7675500000000	0.1585390000000
H80	-0.9308830000000	10.7827420000000	-2.1095570000000
C81	-2.4237520000000	4.5117780000000	0.4291200000000
H82	-2.3756370000000	3.5385540000000	-0.0488250000000
C83	-1.2554810000000	5.1287630000000	0.8787550000000
H84	-0.2940910000000	4.6415750000000	0.7624400000000
C85	-2.5317440000000	8.1611750000000	7.2628780000000
H86	-2.5051400000000	7.9836080000000	8.3337540000000
C87	-2.5978140000000	7.0879380000000	6.3706830000000
H88	-2.6280900000000	6.0618740000000	6.7213600000000
C89	-2.6336920000000	7.3493220000000	5.0075990000000
H90	-2.7014650000000	6.5497830000000	4.2782670000000
C91	-3.1002850000000	10.8258050000000	-2.0914100000000
H92	-3.1968640000000	11.2967980000000	-3.0647790000000
C93	-4.2321370000000	10.5049740000000	-1.3457180000000
H94	-5.2331870000000	10.7530360000000	-1.6812040000000
C95	-4.0627630000000	9.9108450000000	-0.1017460000000
H96	-4.9038280000000	9.6541960000000	0.5247350000000



Pre-reactive structure of  $[\text{Fe}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (O-O distance 2.5 Å)

E (B3LYP-D3/LACV3P\*\*\*) (a.u.) = -3133.587120

$G_{\text{solv}}$  (kcal/mol) = -125.180

ZPE (kcal/mol) = 444.402

$\Delta H_{298}$  (kcal/mol) = 34.665

$\Delta S_{298}$  (cal/(K•mol)) = 303.674

XYZ coordinate

O1	-2.0739242089	7.4791546230	2.4611895195
Fe2	-3.2858957305	8.4886651067	1.8062577924
C3	-7.5163038427	9.0782431642	-0.7991334601
C4	-6.8483962112	7.8572541033	-0.6913868815
C5	-5.6397843868	7.8408685095	0.0011131946
N6	-5.1255629362	8.9297089573	0.5620084425
C7	-5.7441326855	10.1176088853	0.4521943761
C8	-6.9564152460	10.2272796209	-0.2325454405
H9	-8.4616903357	9.1419447205	-1.3289146006
H10	-7.2227652134	6.9380269383	-1.1277677517
H11	-7.4550025104	11.1864465917	-0.3199504068
C12	-3.2974795178	12.9070645233	2.4766771792
C13	-4.9903304611	11.2015892017	1.1116796956
N14	-3.9508299881	10.7218553368	1.8059799722
C15	-3.1368216935	11.5218184654	2.4742651467
H16	-2.5997929493	13.5281316133	3.0275000488
C17	-4.7420715853	6.6398078660	0.1305217671
O18	-5.0336083299	5.5570904967	-0.3517071811
C19	-2.0712069064	10.7590475128	3.2287868635
O20	-1.1327315457	11.3088272019	3.7687509643
O21	-3.6106740466	6.9018197092	0.7426245394
O22	-2.3294335880	9.4635009659	3.2607801334
N23	-4.6033303957	7.8969732363	3.1616067252
C24	-4.7186669064	6.5756583645	3.3979173394
C25	-5.5921699497	6.0878685514	4.3622041065
H26	-4.0890581812	5.9134989823	2.8205462999
H27	-5.6368376947	5.0162045026	4.5174662005
N28	-2.0108653483	9.1181469832	0.3724639942
C29	-2.3723146696	9.1623575878	-0.9228492633
C30	-1.4734320060	9.4981424670	-1.9278043493
H31	-3.4004799371	8.9174582371	-1.1457189602
H32	-1.8083610599	9.5217121899	-2.9591430248
C33	-4.3781878115	13.4307672826	1.7617811731
H34	-4.5486224886	14.5026805102	1.7397563822
C35	-5.2459197873	12.5749897832	1.0731230490
H36	-6.0890792245	12.9706483274	0.5174293897
C37	-6.3601827544	6.9878697910	5.0988897071
H38	-7.0524296697	6.6343663903	5.8570467910
C39	-6.2161604887	8.3565576609	4.8584557805
H40	-6.7812771291	9.0929883625	5.4196887891
C41	-5.3200300622	8.7777655469	3.8860762066
H42	-5.1551241397	9.8245695808	3.6736728028
C43	-0.1533924339	9.7892723256	-1.5848480683
H44	0.5721215440	10.0500149415	-2.3490529931
C45	0.2184305617	9.7306437392	-0.2417819829
H46	1.2351548084	9.9424683046	0.0712192155
C47	-0.7331375481	9.3848236747	0.7091359025
H48	-0.4880576572	9.2951798804	1.7589748724
O49	-0.9353073768	6.0664827974	0.7413321903

Fe50	-0.2588754456	4.7524475829	1.4285329418
C51	4.2002677363	1.9313786058	2.0763035562
C52	4.0923727637	3.0728646860	1.2789857408
C53	2.8293130521	3.6545371550	1.1679386868
N54	1.7598552603	3.1769823093	1.7883923309
C55	1.8455741554	2.0813791437	2.5503140131
C56	3.0675658850	1.4207635193	2.7183664433
H57	5.1591620688	1.4370716789	2.1975031467
H58	4.9361752929	3.5053453616	0.7528966363
H59	3.1400330365	0.5335273136	3.3381961414
C60	-2.0305406501	1.3269714358	4.0809681222
C61	0.5380543697	1.7050176606	3.1403869142
N62	-0.4016665634	2.6304914819	2.9165217874
C63	-1.6355625462	2.4616269830	3.3713480454
H64	-3.0534606999	1.2368360250	4.4285200611
C65	2.5118188070	4.8521341462	0.3317411237
O66	3.3467602104	5.4822074548	-0.2845414476
C67	-2.5241812615	3.6345090546	3.0842324080
O68	-3.6936534508	3.6653821896	3.4429668746
O69	1.2197683141	5.1924439954	0.2914691015
O70	-1.9499904376	4.6426214091	2.4575069705
N71	0.5382354973	5.8874022389	2.9041401463
C72	1.1797853552	7.0223361498	2.5611121261
C73	1.6039598631	7.9291894921	3.5227325433
H74	1.3307299082	7.1765106688	1.4995533751
H75	2.1173889611	8.8343271348	3.2166709222
N76	-1.1047875336	3.5782472464	0.0508969110
C77	-0.4232595013	2.5805495602	-0.5437406956
C78	-1.0228754850	1.7884611558	-1.5133101977
H79	0.6002622061	2.4407340423	-0.2249519530
H80	-0.4531426780	0.9907178961	-1.9771347429
C81	-1.0618899774	0.3493220299	4.3171151428
H82	-1.3173701710	-0.5527280282	4.8643544850
C83	0.2433064317	0.5354935707	3.8504032555
H84	1.0040036195	-0.2154929207	4.0307859938
C85	1.3504621020	7.6583100539	4.8680894334
H86	1.6596323432	8.3584451941	5.6378228990
C87	0.6907265129	6.4772251549	5.2080105265
H88	0.4747203745	6.2266978495	6.2408073185
C89	0.2905355905	5.6123319093	4.1970395006
H90	-0.2410290968	4.6937095207	4.3980379769
C91	-2.3483095828	2.0437236440	-1.8747467807
H92	-2.8345136784	1.4375208551	-2.6330727567
C93	-3.0343499213	3.0878997299	-1.2552596414
H94	-4.0603176329	3.3415769173	-1.4964759082
C95	-2.3821523844	3.8443975164	-0.2913914266
H96	-2.8678532948	4.6646809635	0.2192191704

Transition state structure of [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 2.1 Å)

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3133.585527

G<sub>solv</sub> (kcal/mol) = -124.862

ZPE (kcal/mol) = 444.444

ΔH<sub>298</sub> (kcal/mol) = 34.151

ΔS<sub>298</sub> (cal/(K•mol)) = 298.35

XYZ coordinate

O1	-1.9128060380	7.2762751628	2.1222671600
Fe2	-3.1783928608	8.2504342934	1.4922122737
C3	-7.3095569862	9.1784614583	-1.0852637465
C4	-6.7483825841	7.9054467592	-0.9678258957
C5	-5.5528407733	7.7879845959	-0.2644680639
N6	-4.9534306399	8.8318896498	0.3053317551
C7	-5.4699396024	10.0686866834	0.1868481162
C8	-6.6601025807	10.2763121170	-0.5144953793
H9	-8.2400547508	9.3209601774	-1.6259742457
H10	-7.1938928796	7.0198504861	-1.4071486168
H11	-7.0740849209	11.2743998358	-0.6094901419
C12	-2.8787096173	12.6579833304	2.2941114815
C13	-4.6500422112	11.0919142684	0.8640173846
N14	-3.6626736569	10.5335627555	1.5739829824
C15	-2.8126318933	11.2650507466	2.2763547103
H16	-2.1563268700	13.2233164462	2.8724268565
C17	-4.7566631379	6.5178146143	-0.1366606757
O18	-5.1259664285	5.4552317965	-0.6057084296
C19	-1.8267893458	10.4120821735	3.0455014544
O20	-0.8476616660	10.8808200119	3.5969705749
O21	-3.5993812109	6.6964891913	0.4621666283
O22	-2.1983708795	9.1498974068	3.0693779316
N23	-4.4769551705	7.6769650627	2.8660208912
C24	-4.5692840595	6.3644147758	3.1549318327
C25	-5.4329010816	5.9027733875	4.1412717101
H26	-3.9279461689	5.6937102942	2.6006804881
H27	-5.4597820477	4.8377978264	4.3391532401
N28	-1.9245901229	8.8601535299	0.0224601524
C29	-2.2738625394	8.8184867099	-1.2759635102
C30	-1.3840438995	9.1528112586	-2.2899460687
H31	-3.2828476197	8.5038244477	-1.4976676313
H32	-1.7097403868	9.1057428009	-3.3233493420
C33	-3.9019357777	13.2644351806	1.5601332373
H34	-3.9980635030	14.3457714775	1.5505557228
C35	-4.8099474389	12.4803407767	0.8384763275
H36	-5.6108626009	12.9414725231	0.2710258242
C37	-6.2135519495	6.8201476681	4.8421592162
H38	-6.8987990310	6.4861485940	5.6153311122
C39	-6.0938552548	8.1804472319	4.5455500262
H40	-6.6714390151	8.9293782034	5.0765375639
C41	-5.2073788716	8.5756662446	3.5545345503
H42	-5.0607431944	9.6150494652	3.2962781862
C43	-0.0855123440	9.5327371118	-1.9533100034
H44	0.6324137526	9.7935912510	-2.7245284533
C45	0.2760313257	9.5608593296	-0.6061803749
H46	1.2774796113	9.8386100207	-0.2956822666
C47	-0.6658757210	9.2123803896	0.3523954027
H48	-0.4211166898	9.1848613601	1.4049115108
O49	-1.0623158466	5.9363023864	0.7470803506

Fe50	-0.2864892237	4.6542295417	1.4611192264
C51	4.3205475834	2.1082699850	2.0643337037
C52	4.1357044240	3.2376083233	1.2645332204
C53	2.8401410027	3.7447258328	1.1673193931
N54	1.8063644684	3.2098201320	1.8030190555
C55	1.9660370658	2.1216467530	2.5658816184
C56	3.2269034499	1.5348148869	2.7202101927
H57	5.3081484365	1.6719503614	2.1762831544
H58	4.9453744533	3.7173925263	0.7261245726
H59	3.3576678085	0.6549268894	3.3408070849
C60	-1.8423113545	1.1377897331	4.1394722698
C61	0.6920232375	1.6648542887	3.1728276018
N62	-0.3081821370	2.5215861902	2.9464374000
C63	-1.5257007736	2.2853627939	3.4119935917
H64	-2.8545418209	0.9860364607	4.4964901551
C65	2.4512568466	4.9192696494	0.3278040775
O66	3.2464260601	5.5876820968	-0.3008111990
C67	-2.4851556563	3.3991531475	3.1132681788
O68	-3.6553921870	3.3628038220	3.4649879071
O69	1.1434854762	5.1890519528	0.3023318360
O70	-1.9692799639	4.4386689546	2.4828187897
N71	0.4554726335	5.8440642377	2.9276840152
C72	1.0372560217	7.0089322077	2.5763804452
C73	1.3569326281	7.9711422205	3.5235422777
H74	1.2126625422	7.1458546067	1.5166979303
H75	1.8058503517	8.9070139437	3.2101319313
N76	-1.0846848087	3.4563459231	0.0576580209
C77	-0.3587772450	2.4903047190	-0.5363951702
C78	-0.9093678461	1.6944212678	-1.5318374772
H79	0.6622614370	2.3797966767	-0.1976017384
H80	-0.3030445666	0.9235438497	-1.9948143071
C81	-0.8102856041	0.2279191563	4.3804599639
H82	-1.0035030199	-0.6808380738	4.9418324694
C83	0.4777049139	0.4891982854	3.9015057834
H84	1.2856309596	-0.2090910534	4.0879951969
C85	1.0648675172	7.7231188363	4.8649712344
H86	1.2837693168	8.4703201793	5.6211090975
C87	0.4816796716	6.5060511429	5.2172952037
H88	0.2439405457	6.2698718724	6.2486651708
C89	0.1803178195	5.5875703302	4.2192124707
H90	-0.2974698484	4.6412990189	4.4284763051
C91	-2.2336182968	1.9126552100	-1.9208039433
H92	-2.6814541078	1.3048604394	-2.7011415696
C93	-2.9682439863	2.9227683764	-1.3003991928
H94	-3.9954030428	3.1480776124	-1.5651096261
C95	-2.3637781486	3.6831990050	-0.3086765162
H96	-2.8838294245	4.4841095140	0.1989041204

Product structure of  $[\text{Fe}^{\text{V}}(\text{bda})(\text{py})_2\text{-O}]^+$  dimer (O-O distance 1.2 Å)  
E (B3LYP-D3/LACV3P\*\*+) (a.u.) = -3132.916398

XYZ coordinate

O1	-3.3510089085447	10.8720144048234	2.1213594573362
Fe2	-5.1356608138623	12.8416563101569	2.8963154645607
C3	-9.0756105407525	15.4632907322357	1.3811963380470
C4	-8.4344867462458	14.5314632047830	0.5600615594432
C5	-7.3047302401573	13.8955629149471	1.0717862747888
N6	-6.8510759366544	14.1513964144821	2.2925096648067
C7	-7.4455368439594	15.0440959496687	3.0981374697140
C8	-8.5806909547210	15.7328868896449	2.6623019817168
H9	-9.9600896743473	15.9835984051110	1.0269091918260
H10	-8.7790025651961	14.2954354426619	-0.4401854794437
H11	-9.0729744002291	16.4572259143020	3.3016724714858
C12	-5.2389111479089	14.9568989299520	6.7194905640941
C13	-6.7571954623682	15.1454416096456	4.4090003751736
N14	-5.7635764692088	14.2504338860850	4.5131234838759
C15	-5.0302396983914	14.1336939630963	5.6131542486929
H16	-4.6220653995172	14.8387996141686	7.6035206737050
C17	-6.4475619245178	12.8971643047383	0.3269417832875
O18	-6.7191570610213	12.5680299758783	-0.8172926023720
C19	-4.0127486213070	13.0154695760402	5.5226674782087
O20	-3.2252510345466	12.7857658432658	6.4162147289039
O21	-5.4089307437652	12.4643596269848	1.0089519896306
O22	-4.0828918503717	12.3284050724481	4.3831058616867
N23	-6.4617239190453	11.4078549270381	3.3489871374201
C24	-6.5957863145878	10.3379177698375	2.5374692787867
C25	-7.4931445466560	9.3157581687012	2.8293145934146
H26	-5.9898031613292	10.3115279754408	1.6408062383125
H27	-7.5782674549159	8.4962963330116	2.1270718896905
N28	-3.6733645080849	14.1296420479470	2.3487357736936
C29	-3.9548219678070	15.1984139466475	1.5772666417559
C30	-2.9637008782047	16.0553398939890	1.1190841679974
H31	-4.9960866489751	15.3539862236258	1.3325761560955
H32	-3.2348244802349	16.9068053950347	0.5043910898673
C33	-6.2623584631695	15.9059936967487	6.6325395263673
H34	-6.4619029837058	16.5663957510928	7.4707231942445
C35	-7.0407835977617	16.0064624636336	5.4721514962283
H36	-7.8415266114497	16.7348765145155	5.4041553711726
C37	-8.2590952424447	9.3929463897885	3.9898537161843
H38	-8.9688895394683	8.6093867288929	4.2370064969314
C39	-8.1029707628100	10.4964256909448	4.8310007530271
H40	-8.6744976878210	10.5977414839438	5.7473798321857
C41	-7.1956815146007	11.4840698535599	4.4787304770994
H42	-7.0405266651228	12.3553277251382	5.0981997589934
C43	-1.6353424319413	15.7977229535299	1.4608814862934
H44	-0.8397414667368	16.4503772403225	1.1151758497196
C45	-1.3484717635130	14.6884711886254	2.2549662545170
H46	-0.3321372830521	14.4484773814390	2.5473075496146
C47	-2.3915084442558	13.8757142651664	2.6833178965270
H48	-2.2281826697813	13.0103794083230	3.3135399286150
O49	-2.8104190403001	11.0419024213220	1.0635778286725
Fe50	-2.7637078825387	8.9144346528459	-0.6774334340310
C51	0.3554767432609	6.0518871929544	-3.3501866561079
C52	0.7787260505360	7.1863802083082	-2.6511091339499
C53	-0.1927375892274	7.9134565443446	-1.9630378891877
N54	-1.4656696447945	7.5417451187756	-1.9599805955864

C55 -1.8996704390945 6.4654863563351 -2.6304586903657  
C56 -0.9954088461921 5.6816971489252 -3.3514397977419  
H57 1.0749583340970 5.4552438981406 -3.9023812984402  
H58 1.8122684073695 7.5139383542465 -2.6348345454888  
H59 -1.3274945600308 4.8071777958096 -3.9007844680597  
C60 -6.0993316978209 6.3472006080016 -2.0082645665915  
C61 -3.3705011790155 6.2952824646887 -2.5016952642274  
N62 -3.9055287101363 7.1931174199096 -1.6622328268644  
C63 -5.2070351367097 7.2339952942547 -1.4072538347277  
H64 -7.1576300967882 6.4083587482163 -1.7813644297411  
C65 0.0469835598104 9.1918313292802 -1.1877520179003  
O66 1.1547708164822 9.6616853571175 -1.0426898692031  
C67 -5.5754249692449 8.2949473418000 -0.3923652391109  
O68 -6.7290915051685 8.4362777643982 -0.0190533744826  
O69 -1.0661803287876 9.7366858490021 -0.6942521019105  
O70 -4.5548962575711 9.0010276039520 0.0524785548022  
N71 -2.2058348385746 7.8712887465553 0.9819234461492  
C72 -1.2617259117828 8.3639367192898 1.8093992728400  
C73 -0.9012181253200 7.7086790463186 2.9808687219321  
H74 -0.7975683100686 9.2918940340071 1.4994743396503  
H75 -0.1362855245435 8.1389250053734 3.6179512875515  
N76 -3.3456449246722 10.0924788255542 -2.2019311456443  
C77 -2.7740472939206 9.9779622137981 -3.4191835425809  
C78 -3.1432159623940 10.7909328518198 -4.4797954012395  
H79 -2.0130228517079 9.2186804371762 -3.5247247103721  
H80 -2.6611167582087 10.6649741241807 -5.4431029990006  
C81 -5.5684829440824 5.4024766483347 -2.8915495040503  
H82 -6.2240409513583 4.6921128088629 -3.3858485727652  
C83 -4.1919332296461 5.3644118785355 -3.1434823439334  
H84 -3.7775982394823 4.6315143537809 -3.8269929243516  
C85 -1.5313600560988 6.5087144654877 3.3075223398082  
H86 -1.2664946955282 5.9747014748006 4.2147170269114  
C87 -2.5085234906951 6.0050474923503 2.4475501878186  
H88 -3.0250036485714 5.0752946260083 2.6604225644834  
C89 -2.8223203509043 6.7149398418305 1.2967580492209  
H90 -3.5751001369262 6.3679203620403 0.6031160040356  
C91 -4.1333375930020 11.7547320719580 -4.2779541808578  
H92 -4.4465990238403 12.3997894715721 -5.0933177375111  
C93 -4.7130663477461 11.8734977637118 -3.0174954146362  
H94 -5.4942551086930 12.5905679811419 -2.7999462925534  
C95 -4.2938579697465 11.0290088404456 -1.9944370334567  
H96 -4.7276547291989 11.0866629873843 -1.0047976301146

Pre-reactive structure of 6-coordinate [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 3.3 Å)

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3133.613788

G<sub>solv</sub> (kcal/mol) = -125.157

ZPE (kcal/mol) = 443.160

ΔH<sub>298</sub> (kcal/mol) = 34.866

ΔS<sub>298</sub> (cal/(K•mol)) = 303.698

XYZ coordinate

O1	0.3205799565	5.5596123951	1.1519143496
Fe2	0.6513988852	4.5810419239	2.4123512228
C3	1.8873085511	1.7389497707	5.9514363834
C4	0.5681443355	2.1822151550	5.8159680764
C5	0.2795229460	3.0338236184	4.7532448693
N6	1.2295794279	3.3972691153	3.8954331397
C7	2.5017541048	2.9942723524	3.9953317558
C8	2.8730195380	2.1464586757	5.0429078635
H9	2.1554165516	1.0747233990	6.7673990777
H10	-0.2219944049	1.8953130684	6.5010386881
H11	3.8943075048	1.7990238960	5.1520098219
C12	4.6840405305	4.5020923094	0.7035431693
C13	3.3361618930	3.5156085199	2.8903044240
N14	2.6380926810	4.1681476969	1.9199748001
C15	3.2984210483	4.6163442908	0.8403666971
H16	5.1692716724	4.9008880502	-0.1805369368
C17	-1.0447053683	3.7060989113	4.4469247299
O18	-2.0237632482	3.5199583526	5.1511773413
C19	2.5473756973	5.2411200880	-0.3000022245
O20	2.7875189162	6.4087684990	-0.6861828596
O21	-0.9797004083	4.5263323497	3.4236708843
O22	1.7538406101	4.5976635169	-1.0386566426
N23	-0.0337731904	2.9955815268	1.4081235997
C24	-1.2903449381	3.1208530831	0.9368319453
C25	-1.9001734736	2.1064272627	0.2078280194
H26	-1.7973725521	4.0481301287	1.1651463697
H27	-2.9138698721	2.2663445932	-0.1408945435
N28	1.2628817557	6.2154177968	3.4761746092
C29	0.8988477490	6.4262235351	4.7528061739
C30	1.2332635152	7.5856706451	5.4413503111
H31	0.3100047742	5.6554481261	5.2260947831
H32	0.9055375671	7.7117054021	6.4671551459
C33	5.4056752933	3.8602298492	1.7084545674
H34	6.4828921401	3.7524115437	1.6317505524
C35	4.7205890590	3.3463085194	2.8060307882
H36	5.2531933689	2.8274446962	3.5953215958
C37	-1.1928071611	0.9323353272	-0.0414909891
H38	-1.6441460732	0.1225521242	-0.6069565576
C39	0.1091755951	0.8096323511	0.4501824672
H40	0.6955836365	-0.0872542746	0.2817879242
C41	0.6547866426	1.8628870388	1.1711580775
H42	1.6581909542	1.8082937171	1.5733674113
C43	1.9646162971	8.5725419670	4.7855430772
H44	2.2286165995	9.4947448221	5.2922505600
C45	2.3309328185	8.3596570416	3.4565719650
H46	2.8886583716	9.1043972482	2.8990489275
C47	1.9542639286	7.1777257501	2.8341282284
H48	2.1738561481	6.9953682052	1.7903046419
O49	-1.4316715178	7.6703169213	2.9861826479

Fe50	-2.6760188669	7.6905138140	1.9341699555
C51	-6.2974969341	8.0329798929	-1.0509144015
C52	-5.7515698243	6.7874511511	-0.7256918774
C53	-4.6714361490	6.7658610191	0.1519833527
N54	-4.1898301337	7.8941293785	0.6671807160
C55	-4.6871449380	9.1022287235	0.3779423754
C56	-5.7655443845	9.2080746060	-0.5047633697
H57	-7.1393813529	8.0952016137	-1.7335926612
H58	-6.1295609871	5.8553594974	-1.1309194780
H59	-6.1928903848	10.1715462736	-0.7591015067
C60	-2.6334435728	12.0162253144	2.6454461735
C61	-3.9922436019	10.1792715717	1.1151876353
N62	-3.0944614483	9.7374894461	2.0393992459
C63	-2.4593199779	10.6393874468	2.8049870886
H64	-2.0794064255	12.7023508771	3.2765447014
C65	-3.8665173084	5.5576616823	0.5873943006
O66	-4.1423755726	4.4389848945	0.1845552324
C67	-1.5442937648	10.1835446813	3.9065398745
O68	-0.3288384660	10.4877701982	3.9289380110
O69	-2.8466764952	5.8685849317	1.3537416153
O70	-1.9592202972	9.6064745421	4.9481893797
N71	-3.9568926408	7.2392604312	3.3994754146
C72	-3.6557416989	6.1229907728	4.0924429332
C73	-4.4445497519	5.6871706469	5.1503319555
H74	-2.7734175301	5.5847143769	3.7742451002
H75	-4.1513481497	4.7800050202	5.6660672297
N76	-1.3482471543	8.0520780298	0.4234051136
C77	-1.4026664581	7.4133700517	-0.7586049230
C78	-0.4347868822	7.5815411781	-1.7419421124
H79	-2.2314060995	6.7380800056	-0.9110616442
H80	-0.5180869676	7.0333364662	-2.6740325272
C81	-3.5332817210	12.4717648930	1.6827717641
H82	-3.6928101527	13.5353133728	1.5373880830
C83	-4.2337284109	11.5415830135	0.9200695705
H84	-4.9508174080	11.8660658259	0.1747475946
C85	-5.5729443313	6.4248661332	5.5026479906
H86	-6.2082540358	6.1079540895	6.3241065376
C87	-5.8780248078	7.5811671967	4.7805200218
H88	-6.7469137276	8.1850271978	5.0192134674
C89	-5.0461303343	7.9562960097	3.7345422313
H90	-5.2466810620	8.8429335354	3.1465939256
C91	0.6370279244	8.4360386997	-1.4948293528
H92	1.4163497899	8.5756796320	-2.2368128273
C93	0.6998957878	9.0891614975	-0.2636186868
H94	1.5222623780	9.7530118382	-0.0181041057
C95	-0.3013944439	8.8647157684	0.6712035987
H96	-0.2625723826	9.3113121681	1.6561328837



Transition state structure of 6-coordinate [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 2.0 Å)

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3133.598323

G<sub>solv</sub> (kcal/mol) = -125.725

ZPE (kcal/mol) = 442.416

ΔH<sub>298</sub> (kcal/mol) = 34.533

ΔS<sub>298</sub> (cal/(K•mol)) = 301.500

XYZ coordinate

O1	-0.2991292837	6.3579815444	1.9867701876
Fe2	0.1154061366	5.2114995492	3.1324144024
C3	1.3104280579	1.9609543512	6.2980253273
C4	-0.0276101498	2.3152773972	6.1020079363
C5	-0.3052005395	3.2911285233	5.1497581095
N6	0.6761289010	3.8550249589	4.4465955891
C7	1.9681253734	3.5519480018	4.6200029184
C8	2.3264568976	2.5848165815	5.5632176171
H9	1.5700085290	1.2031427387	7.0305586899
H10	-0.8423856447	1.8708959932	6.6628300416
H11	3.3635781813	2.3134332139	5.7251351188
C12	4.3099496905	5.8136026486	1.9231251801
C13	2.8488778932	4.3261861207	3.7187309287
N14	2.1904284876	5.0766195680	2.7921042257
C15	2.9144403235	5.7700239889	1.8986603263
H16	4.8407250031	6.4117859104	1.1904807243
C17	-1.6552779088	3.9116881487	4.8413570363
O18	-2.6612213212	3.5847515928	5.4469985972
C19	2.2148481682	6.5033598463	0.7950948848
O20	2.3690616163	7.7363408888	0.6136800638
O21	-1.5763916773	4.8585695814	3.9348936244
O22	1.5356856189	5.9254527594	-0.0930948997
N23	-0.2644169936	3.7404826710	1.8133763433
C24	-1.5069958226	3.7442506891	1.2930919919
C25	-1.9348596884	2.7684648872	0.3995316582
H26	-2.1594937275	4.5486183264	1.6012298859
H27	-2.9541948609	2.8224044356	0.0307489788
N28	0.4871744246	6.6735750610	4.5035562119
C29	0.0842718943	6.6041903073	5.7852518053
C30	0.3814636875	7.5950447612	6.7131795525
H31	-0.4948636126	5.7378947354	6.0693709691
H32	0.0327044980	7.4927060008	7.7349895997
C33	4.9844941116	5.0661808762	2.8876033022
H34	6.0687444226	5.0746357118	2.9323417756
C35	4.2455760905	4.2983678053	3.7833299813
H36	4.7430600085	3.6954032503	4.5340298389
C37	-1.0505465003	1.7595756512	0.0252722397
H38	-1.3550706027	0.9806950541	-0.6671782300
C39	0.2400024720	1.7634307148	0.5613791431
H40	0.9631587142	0.9986026943	0.2994489809
C41	0.5945139710	2.7665825221	1.4528586938
H42	1.5818028630	2.7978696781	1.8951969849
C43	1.1213114036	8.7034014183	6.3042180722
H44	1.3724199656	9.4914848894	7.0072152735
C45	1.5115816596	8.7896748347	4.9694193117
H46	2.0485377541	9.6507112656	4.5901480538
C47	1.1650540578	7.7650680047	4.0987436426
H48	1.3986908841	7.8194650338	3.0443114429
O49	-1.6035928651	7.7132225146	2.6662524075

Fe50	-2.9974233555	7.8572336853	1.7527280903
C51	-6.9708398958	8.3441215517	-0.6937006787
C52	-6.5058577354	7.0784662258	-0.3236559055
C53	-5.3125234834	7.0110121114	0.3891715916
N54	-4.6487990395	8.1205048035	0.7110414038
C55	-5.0542556418	9.3454309288	0.3565898907
C56	-6.2417833466	9.4940621074	-0.3650432331
H57	-7.8993161185	8.4406774089	-1.2478529785
H58	-7.0290110301	6.1624760225	-0.5756674324
H59	-6.6015340453	10.4727053458	-0.6623212476
C60	-2.3204193079	12.2051382946	1.8478578652
C61	-4.1286805724	10.3967794590	0.8312399073
N62	-3.1512993483	9.9532242809	1.6693338900
C63	-2.2972088440	10.8506534901	2.1872637435
H64	-1.5887613533	12.8790310244	2.2801125583
C65	-4.5605540204	5.7586483977	0.8020439568
O66	-4.9610736897	4.6466804007	0.5059848962
C67	-1.2948155998	10.4117189514	3.2101459266
O68	-0.0619622113	10.5912622939	3.0487873170
O69	-3.4332976006	6.0322939750	1.4185568262
O70	-1.6158068976	9.9655942540	4.3418371714
N71	-4.1177039502	7.7631249612	3.4244489718
C72	-3.9638635397	6.6437299225	4.1582365328
C73	-4.6924868797	6.4178278367	5.3208009830
H74	-3.2345933801	5.9302177278	3.8033727236
H75	-4.5225695576	5.4908071763	5.8587128134
N76	-1.9097726925	7.9230627157	0.0297517858
C77	-2.2698865083	7.2753302763	-1.0934110184
C78	-1.5340311033	7.3575549403	-2.2691233896
H79	-3.1650778437	6.6729521746	-1.0455692647
H80	-1.8674743332	6.8155379039	-3.1474151742
C81	-3.3038636883	12.6558901053	0.9689118635
H82	-3.3541740134	13.7022867293	0.6857288216
C83	-4.2292254515	11.7435680973	0.4710877063
H84	-5.0144074152	12.0674213518	-0.2025021871
C85	-5.6087854359	7.3787152105	5.7417398105
H86	-6.1967685474	7.2305588876	6.6423940496
C87	-5.7620105114	8.5411182540	4.9811386755
H88	-6.4628310601	9.3172621886	5.2695896487
C89	-5.0015264913	8.6964554057	3.8305036239
H90	-5.0969554505	9.5801045088	3.2131593177
C91	-0.3781154416	8.1362433016	-2.2888117268
H92	0.2153176194	8.2235767332	-3.1934687647
C93	0.0109112840	8.7830106120	-1.1174371092
H94	0.9234927763	9.3645300194	-1.0671443990
C95	-0.7706739720	8.6425128606	0.0218178152
H96	-0.4764489745	9.0822251827	0.9649870557

Product structure of 6-coordinate [Fe<sup>V</sup>(bda)(py)<sub>2</sub>-O]<sup>+</sup> dimer (O-O distance 1.3 Å)

E (B3LYP-D3/LACV3P<sup>\*\*\*</sup>) (a.u.) = -3132.861525

XYZ coordinate

O1	-3.8006154841449	10.9199682547253	2.5756870544181
Fe2	-1.9688740520031	10.3266696646148	2.3691212534541
C3	2.5284191806907	9.3559369890970	1.9563158275759
C4	2.1041746821503	10.5748775052052	2.5009450867687
C5	0.7372527995102	10.8047110308542	2.5749622032319
N6	-0.1314494377350	9.8769428159935	2.1585870266502
C7	0.2343464934013	8.7116200270699	1.6103541068247
C8	1.5984998516882	8.4199186518347	1.4947550253469
H9	3.5888293164715	9.1380470284475	1.8772516784840
H10	2.7944486866107	11.3369589824172	2.8454616015508
H11	1.9323313418905	7.4858661546833	1.0576938063152
C12	-3.2127816424085	6.4967403390677	0.6096021503272
C13	-0.9224350922505	7.8896538782810	1.2113691222363
N14	-2.1369144021520	8.4091519956282	1.5772776219232
C15	-3.2497629663073	7.7069879275387	1.3130735724417
H16	-4.1483684995171	5.9974124890828	0.3856890612948
C17	0.0362565314516	12.0756463178487	3.0019619326499
O18	0.6262525214647	13.0526800859851	3.4120397708082
C19	-4.6121573345909	8.2197871977579	1.7827988862771
O20	-5.4731638435726	8.3877596142900	0.9126225906240
O21	-1.2759543165181	12.0066948380460	2.8024155609526
O22	-4.6765050252685	8.3860360424650	3.0426303087508
N23	-1.9244932785432	9.6861314426253	4.2570839975146
C24	-2.0272197901646	10.6070144404588	5.2346740795221
C25	-2.1312556374310	10.2536437280152	6.5761845104743
H26	-2.0354382824997	11.6432647897035	4.9362890642549
H27	-2.2252692259166	11.0503078653005	7.3037030568753
N28	-2.1902283037608	10.9809728001101	0.4476277063559
C29	-1.2269736850446	11.7131965318939	-0.1519615342943
C30	-1.3947345368944	12.2641918784558	-1.4134711813183
H31	-0.3101014303012	11.8640592043841	0.3997212303168
H32	-0.5890125417867	12.8403169621638	-1.8559969360945
C33	-1.9867863308926	5.9771655566074	0.2184610835439
H34	-1.9311106193423	5.0379489622800	-0.3229770098606
C35	-0.8206498538438	6.6769586334252	0.5394082201538
H36	0.1510779489777	6.2853726604100	0.2616829385292
C37	-2.1297019426896	8.9053310310656	6.9222700200572
H38	-2.2099529408012	8.5986860617823	7.9605246644352
C39	-2.0299814505260	7.9521021003605	5.9069772956001
H40	-2.0332175010070	6.8893522594975	6.1244805370376
C41	-1.9323939778180	8.3755925427276	4.5893311623962
H42	-1.8636992591586	7.6652870165919	3.7800867253789
C43	-2.6083286902849	12.0740700302756	-2.0801634425304
H44	-2.7723331617665	12.5072485119394	-3.0622871130218
C45	-3.6033654013797	11.3250809675489	-1.4597140583664
H46	-4.5814702332363	11.1812980321837	-1.9045987776990
C47	-3.3556320725635	10.7881034385274	-0.2008313404004
H48	-4.1150208097699	10.2085984779823	0.3005527919938
O49	-3.8882868398427	12.0244943124943	3.2556397063002
Fe50	-5.3970758865953	13.0712116303124	2.8416207735868
C51	-8.9907281082416	15.5535147008505	1.2965756603785
C52	-8.4114923166021	14.5573886135474	0.4995214910883
C53	-7.3216262384332	13.8706877319716	1.0176927419780
N54	-6.8681255133199	14.1447524602728	2.2458564272936

C55 -7.3793253497403 15.1055805830584 3.0269926503488  
C56 -8.4721572621074 15.8451413697690 2.5620038475567  
H57 -9.8422667149891 16.1161357437981 0.9266701664856  
H58 -8.7689729345627 14.3195370034298 -0.4962746101137  
H59 -8.9137316239320 16.6274612511843 3.1687948403067  
C60 -5.2375426776467 15.2084151964760 6.6585195462090  
C61 -6.6692089201661 15.2159441180582 4.3135166198457  
N62 -5.7393060553072 14.2363241661659 4.5247327162936  
C63 -5.0723060804784 14.2108242631504 5.6909347191433  
H64 -4.6410556190360 15.1584706128018 7.5624076375768  
C65 -6.4580309980842 12.8433603764572 0.3125270028390  
O66 -6.6958382145855 12.4558866706454 -0.8141677740333  
C67 -4.1514623391158 13.0416123014007 5.9961417186974  
O68 -2.9838512214357 13.2914708165634 6.3311997059243  
O69 -5.4161515810012 12.4851133011133 1.0439959947261  
O70 -4.6810975309570 11.8892730495451 5.8992992590774  
N71 -6.6144927040078 11.5926880784105 3.4253274651166  
C72 -6.7056145640869 10.4798440836080 2.6772969610529  
C73 -7.3780724543917 9.3370300902805 3.1196113125450  
H74 -6.2230472383861 10.4924495371496 1.7130575031064  
H75 -7.4167155552834 8.4835695215843 2.4550650022518  
N76 -4.000601837619 14.4715141582283 2.3433481053918  
C77 -4.1043396379405 15.1977288119189 1.2116253412299  
C78 -3.1042771953154 16.0649807732769 0.7955860857776  
H79 -5.0057053306864 15.0698306048415 0.6286807225900  
H80 -3.2367805942295 16.6338600082162 -0.1182556662173  
C81 -6.1646136446873 16.2197013746595 6.4386217537158  
H82 -6.3202230659213 16.9992894973247 7.1778160646196  
C83 -6.9076005199664 16.2117345415552 5.2559837810909  
H84 -7.6528028986549 16.9761835884951 5.0670691899379  
C85 -7.9697826846892 9.3440065673150 4.3826427179267  
H86 -8.4981529685604 8.4708230682627 4.7521210799205  
C87 -7.8701105874096 10.4957982933490 5.1578956261776  
H88 -8.3115225059386 10.5553965918947 6.1467844873430  
C89 -7.1897672523049 11.6006340233905 4.6511004124775  
H90 -7.1165234713545 12.5124083103674 5.2198453172237  
C91 -1.9409092515528 16.1740919807064 1.5608562285533  
H92 -1.1373122664551 16.8353103507325 1.2515380578894  
C93 -1.8291479038186 15.4166947589806 2.7236315800076  
H94 -0.9358658277498 15.4295628593031 3.3377058822206  
C95 -2.8812019320339 14.5842684967823 3.0877256087316  
H96 -2.8152494586172 13.9827812965973 3.9822043210383