Electronic Supplementary Information for Dalton Transactions

Supplementary information

FOR

A Computational Study of Aerobic Oxidation of Ruthenium Porphyrins

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METHODS

DFT computations are used to elucidate the reaction pathway and characterize dimeric and monomeric Ru- intermediates considering all possible spin states as follows. First, geometry optimizations of all intermediate complexes were carried out using BP86 functional[i] including Slater local exchange[ia], Becke's 1988 non-local gradient correction to exchange[ib], Perdew and Zunger's 1981 local correlation[ic] and Perdew's 1986 gradient correction[id] with the lacvp*/6-31G(d) basis set.[ii,iii] A broad comparison of density functional calculations for structures, spin states and reaction pathways concerning organometallic complexes and metalloenzymes could be found in Ref.[iv] In particular, BP86 density functional has successfully been applied in studies of reactions involving Ru carbenes[v].

All degrees of freedom were optimized and only positive vibrational frequencies were obtained at the optimized geometries. High-valent oxoruthenium complexes were optimized within unrestricted DFT.

In the second step, BP86 energies were evaluated for the optimized geometry using much larger triple-ζ basis, lacv3p*+/6-311+G(d), with additional diffuse and polarization functions. All computations were performed with the Jaguar v4.0 suite of *ab initio* quantum chemistry programs.[vi] Thermal corrections to Gibbs free energies were calculated at BP86/LANL2DZ level[vii] at 298.15 K temperature with Gaussian 98 package.[viii] The NBO analysis was performed using the BP86 electron densities.

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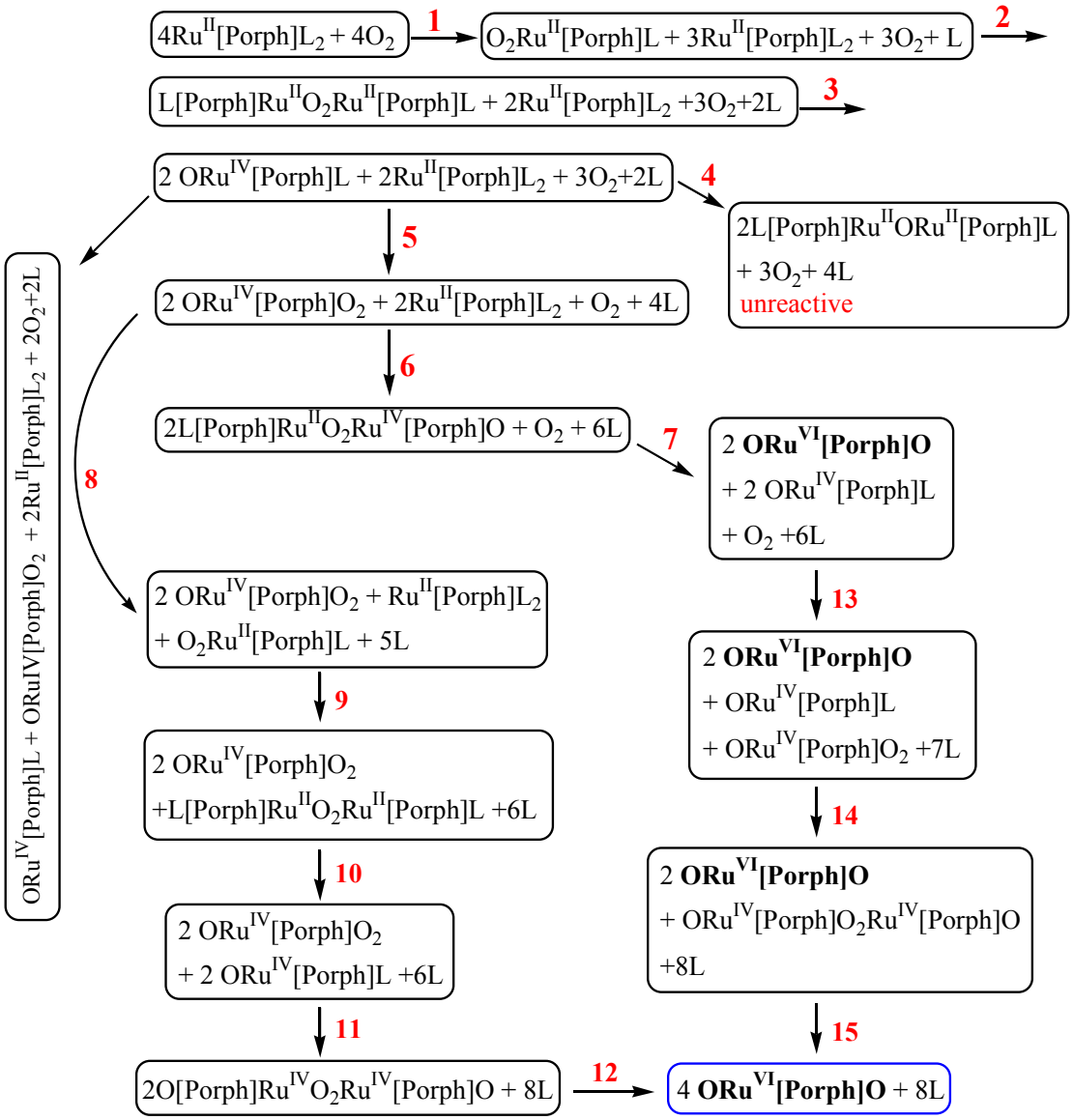

Scheme S1. Comepex branching reaction pathway of the Ru porphyrin autooxidation. A portion of this pathway was considered in the text. The manuscript provides all the information needed to assemble reaction energetics of such complex profiles.

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Table S1. Selected geometrical parameters: bond lengths (Å), bond angles (°) and vibrational frequencies (cm^{-1}), IR intensities ($km \cdot mol^{-1}$). Theoretical data calculated at DFT (BP86) level.

Complex And electronic state	bond length		bond angle		frequency		intensity
B singlet	Ru-N	1.995	N-Ru-N	179.9	δRing	992 *(1003)*[a]	33
E singlet	Ru-N	2.156	N-Ru-O	178.0	δRing	1002	43
	Ru-O	1.898	Ru-O-O	119.8	ν(RuO)	614	1
	O-O[b]	1.291					
H singlet	Ru-N	2.062	N-Ru-O	176.7	δRing	999	63
	Ru-O	1.941	Ru-O-O[b]	115.9	ν(RuO)	525	228
	O-O	1.367					
F triplet	Ru-N	2.297	N-Ru-O	179.8	δRing	998 *(1011)* [a]	43
	Ru-O	1.777			ν(RuO)	802 *(761)* [c]	32
I triplet	Ru-N	2.047	N-Ru-O	178.8	δRing	995	58
	Ru-O	1.899			ν(RuO)	734	69
J singlet	Ru-O1	1.744	O1-Ru-O2[b]	163.8	δRing	1006	51
	Ru-O2	1.929	Ru-O2-O3	140.7	ν(RuO1)	458	5
	O2-O3	1.271			ν(RuO3)	856	59
K triplet	Ru-N	2.096	O1-Ru-O2[b]	177.4	δRing	1006	37
	Ru-O1	1.774	Ru-O2-O3	140.7	ν(RuO1)	565	70
	O2-O3	1.357	N-Ru-O1	177.8	ν(RuO3)	811	332
	Ru-O2	2.094					
	Ru-O3	1.922					
L triplet	Ru-O1	1.762	O1-Ru-O2[b]	171.6	δRing	1002	67

	O2-O3	1.315	Ru-O2-O3	129.0	ν(RuO1)	795	160
	Ru-O2	2.068			ν(RuO3)	146	73
G singlet	Ru-O	1.760	O-Ru-O	167.7	δRing	1007*(1019)*[a]	53
					ν_{as}(RuO)	843 *(821)*[a,]	95

[a] Experimental data from ref. 1 (Groves, see paper). [b] Bond distance in molecular oxygen is 1.231 Å (BP86) and 1.21 Å (experimental New J. Chem. 1998, 327 F. Maseras (X-ray data for molecular oxygen [41]).[c] J. Am. Chem. Soc. 1989, 111, 8812, W. H. Leung, C. H. Ming.

$LRu^{II}L$ porphyrin
Total energy= -1347.967057 [au] (BP86/LACVP*)

Atom	x	y	z
Ru	0.0043	0.0034	-0.0020
N	0.0019	1.4718	1.4700
C	-0.0031	1.2608	2.8354
C	-0.0109	2.5465	3.5169
C	-0.0116	3.5183	2.5450
C	-0.0041	2.8369	1.2592
C	-0.0033	0.0021	3.4599
C	-0.0012	-1.2563	2.8347
C	-0.0057	-2.5424	3.5153
C	-0.0049	-3.5136	2.5426
C	0.0002	-2.8313	1.2572
N	0.0033	-1.4663	1.4692
C	-0.0056	3.4618	0.0005
C	-0.0035	2.8382	-1.2588
C	-0.0038	3.5207	-2.5440
C	0.0002	2.5497	-3.5168
C	0.0015	1.2634	-2.8366
N	-0.0004	1.4734	-1.4713
C	0.0039	0.0049	-3.4617
C	0.0033	-1.2541	-2.8375
C	0.0050	-2.5399	-3.5188
C	0.0032	-3.5117	-2.5468
C	0.0012	-2.8303	-1.2610
N	0.0011	-1.4652	-1.4723
C	0.0001	-3.4550	-0.0021
H	-0.0160	2.6762	4.6014
H	-0.0176	4.6027	2.6748
H	-0.0073	0.0020	4.5563
H	-0.0100	-2.6727	4.5997
H	-0.0083	-4.5981	2.6718

H	-0.0096	4.5582	0.0010
H	-0.0064	4.6052	-2.6727
H	0.0017	2.6803	-4.6011
H	0.0060	0.0051	-4.5581
H	0.0070	-2.6698	-4.6032
H	0.0035	-4.5962	-2.6763
H	-0.0014	-4.5514	-0.0025
N	1.9992	0.0009	-0.0118
C	3.1721	-0.0031	-0.0208
C	4.6304	-0.0050	-0.0246
H	5.0136	-0.0724	-1.0583
H	5.0175	0.9226	0.4334
H	5.0154	-0.8667	0.5492
N	-1.9905	0.0034	-0.0007
C	-3.1637	0.0043	-0.0028
C	-4.6221	0.0068	-0.0061
H	-5.0047	0.0090	-1.0423
H	-5.0100	-0.8898	0.5095
H	-5.0069	0.9033	0.5119

O_2-Ru^{II} porphyrin
Total energy= -1365.536893 [au] (BP86/LACVP*)

atom	x	y	z
N	0.0234	-1.4642	-1.4652
C	0.0372	-1.2552	-2.8355
C	0.0398	-2.5375	-3.5128
C	0.0275	-3.5080	-2.5379
C	0.0191	-2.8291	-1.2540
C	0.0348	-0.0012	-3.4627
C	0.0306	1.2533	-2.8351
C	0.0280	2.5356	-3.5111
C	0.0120	3.5059	-2.5349
C	0.0063	2.8267	-1.2518
N	0.0147	1.4617	-1.4647
C	-0.0034	3.4541	0.0056
C	-0.0059	2.8304	1.2638
N	0.0086	1.4660	1.4750
C	-0.0196	1.2552	2.8411
C	-0.0443	2.5391	3.5212
C	-0.0366	3.5105	2.5482
Ru	0.0580	-0.0009	-0.0066
N	-2.0978	0.0017	0.0489
C	-3.2678	0.0082	0.0588
C	-4.7265	0.0168	0.0711
C	-0.0322	-0.0019	3.4663
C	-0.0194	-1.2581	2.8394
C	-0.0419	-2.5420	3.5183
C	-0.0310	-3.5132	2.5446
C	-0.0003	-2.8331	1.2609

N	0.0101	-1.4685	1.4725
C	0.0080	-3.4570	0.0026
O	1.9556	0.0174	0.0065
O	2.6060	0.0025	-1.1083
H	-0.0630	2.6692	4.6050
H	-0.0456	4.5946	2.6783
H	-0.0529	-0.0028	4.5620
H	-0.0610	-2.6729	4.6020
H	-0.0373	-4.5974	2.6742
H	-0.0112	4.5500	0.0033
H	0.0136	4.5902	-2.6641
H	0.0426	2.6689	-4.5944
H	0.0455	-0.0009	-4.5583
H	0.0541	-2.6695	-4.5964
H	0.0321	-4.5923	-2.6675
H	0.0035	-4.5529	0.0003
H	-5.1200	0.0167	-0.9602
H	-5.1051	-0.8766	0.5972
H	-5.0948	0.9169	0.5931

LRu-O_2-RuL complex
Total energy= -2580.257682 [au] (BP86/LACVP*)

atom	x	y	z
N	4.2977	1.6768	-1.8796
C	4.4964	1.6526	-3.2612
C	4.6228	3.0231	-3.7441
C	4.4974	3.8569	-2.6508
C	4.2971	3.0113	-1.4795
C	4.5661	0.4950	-4.0506
C	4.4433	-0.8309	-3.6090
N	4.2389	-1.2240	-2.2857
C	4.1793	-2.6162	-2.2666
C	4.3464	-3.1155	-3.6267
C	4.5116	-2.0200	-4.4508
C	3.9976	-3.4035	-1.1197
C	3.8483	-2.9483	0.1986
C	3.6568	-3.7923	1.3718
C	3.5487	-2.9600	2.4685
C	3.6738	-1.5926	1.9864
N	3.8609	-1.6123	0.5989
C	3.6201	-0.4392	2.7792
C	3.7205	0.8840	2.3322
N	3.9153	1.2746	1.0030
C	3.9578	2.6686	0.9831
C	3.7890	3.1666	2.3434
C	3.6433	2.0714	3.1705

Ru	4.0568	0.0282	-0.6352
N	6.0984	-0.0293	-0.4720
C	7.2772	-0.0522	-0.3972
C	8.7317	-0.0808	-0.2828
C	4.1374	3.4603	-0.1604
O	2.1389	0.0926	-0.9363
O	1.3011	-0.0645	0.2614
Ru	-0.6106	-0.0718	-0.0494
N	-0.7627	-1.7159	1.2207
C	-0.9495	-1.6864	2.6028
C	-0.9789	-3.0552	3.1082
C	-0.8106	-3.8952	2.0267
C	-0.6746	-3.0541	0.8416
C	-1.0847	-0.5255	3.3767
C	-1.0451	0.7989	2.9161
N	-0.8693	1.1871	1.5868
C	-0.8882	2.5805	1.5529
C	-1.0816	3.0862	2.9068
C	-1.1780	1.9922	3.7437
C	-0.7464	3.3643	0.3985
C	-0.5660	2.9030	-0.9129
C	-0.4150	3.7459	-2.0932
C	-0.2583	2.9084	-3.1787
C	-0.3087	1.5391	-2.6823
N	-0.5006	1.5631	-1.2985
C	-0.1878	0.3808	-3.4601
C	-0.2172	-0.9426	-2.9972
N	-0.3976	-1.3286	-1.6649
C	-0.3573	-2.7225	-1.6244
C	-0.1518	-3.2278	-2.9748
C	-0.0665	-2.1356	-3.8167
C	-0.4868	-3.5108	-0.4702
N	-2.6648	-0.1170	-0.2491
C	-3.8405	-0.1456	-0.3501
C	-5.2905	-0.1848	-0.4969
H	-1.3208	1.9834	4.8237
H	-1.1293	4.1426	3.1725
H	-1.2276	-0.6673	4.4530
H	-1.1071	-3.3266	4.1557
H	-0.7745	-4.9852	2.0215
H	-0.7729	4.4512	0.5355
H	-0.4153	4.8367	-2.0804
H	-0.1060	3.1836	-4.2216
H	-0.0332	0.5238	-4.5342
H	0.1006	-2.1290	-4.8928
H	-0.0712	-4.2835	-3.2340
H	-0.4298	-4.5962	-0.6083
H	-5.5751	-0.1816	-1.5628
H	-5.7032	-1.0944	-0.0281
H	-5.7507	0.6920	-0.0123
H	4.6629	-2.0071	-5.5301
H	4.3344	-4.1694	-3.9040
H	4.7271	0.6417	-5.1242
H	4.7816	3.3003	-4.7860
H	4.5314	4.9459	-2.6292

H	3.9662	-4.4883	-1.2678
H	3.6009	-4.8806	1.3482
H	3.3839	-3.2370	3.5096
H	3.4611	-0.5864	3.8528
H	3.4831	2.0592	4.2484
H	3.7726	4.2207	2.6182
H	4.1505	4.5442	-0.0067
H	9.0392	-0.1504	0.7772
H	9.1476	-0.9508	-0.8224
H	9.1722	0.8355	-0.7129

ORu^{IV} porphyrin

Total energy= -1290.380987 [au] (BP86/LACVP*)

atom	x	y	z
Ru	0.3801	-0.0004	-0.0033
N	0.2530	1.4677	1.4665
C	0.2358	2.8324	1.2545
C	0.2116	3.5110	2.5384
C	0.2166	2.5382	3.5107
C	0.2440	1.2552	2.8310
C	0.2330	3.4591	-0.0024
C	0.2364	2.8331	-1.2595
C	0.2128	3.5122	-2.5431
C	0.2184	2.5393	-3.5155
C	0.2451	1.2558	-2.8359
N	0.2540	1.4685	-1.4715
C	0.2519	-0.0016	3.4569
C	0.2584	-1.2580	2.8308
C	0.2474	-2.5415	3.5105
C	0.2515	-3.5141	2.5382
C	0.2653	-2.8344	1.2549
N	0.2678	-1.4699	1.4666
C	0.2676	-3.4605	-0.0013
C	0.2631	-2.8349	-1.2584
C	0.2453	-3.5151	-2.5414
C	0.2408	-2.5432	-3.5148
C	0.2557	-1.2590	-2.8361
N	0.2667	-1.4706	-1.4714
C	0.2508	-0.0018	-3.4622
H	0.1956	4.5948	2.6688
H	0.2053	2.6677	4.5948
H	0.2207	4.5549	-0.0022
H	0.1968	4.5962	-2.6735
H	0.2079	2.6691	-4.5997
H	0.2471	-0.0017	4.5528
H	0.2407	-2.6718	4.5946
H	0.2486	-4.5982	2.6685
H	0.2682	-4.5564	-0.0010
H	0.2400	-4.5992	-2.6709
H	0.2306	-2.6740	-4.5988
H	0.2449	-0.0016	-4.5581

N	-1.9173	0.0014	-0.0097
C	-3.0874	0.0082	-0.0096
C	-4.5463	0.0136	-0.0077
H	-4.9294	-1.0213	-0.0204
H	-4.9223	0.5213	0.8974
H	-4.9256	0.5449	-0.8976
O	2.1575	0.0081	-0.0064

LRuORuL

Total energy= -2505.605573 [au] (BP86/LACVP*)

atom	x	y	z
N	4.4453	-0.8544	1.9096
C	4.4883	-0.1698	3.1079
C	4.5474	-1.1273	4.2003
C	4.5471	-2.3821	3.6376
C	4.4885	-2.2038	2.1961
C	4.5014	1.2275	3.2453
C	4.4923	2.1781	2.2115
N	4.4500	1.8908	0.8618
C	4.5001	3.0881	0.1761
C	4.5621	4.1812	1.1329
C	4.5571	3.6197	2.3885
C	4.5209	3.2246	-1.2217
C	4.5132	2.1915	-2.1733
C	4.5937	2.3689	-3.6140
C	4.6003	1.1137	-4.1758
C	4.5229	0.1570	-3.0841
N	4.4617	0.8420	-1.8868
C	4.5384	-1.2401	-3.2205
C	4.5161	-2.1899	-2.1867
N	4.4564	-1.9025	-0.8377
C	4.5011	-3.0995	-0.1520
C	4.5754	-4.1923	-1.1079
C	4.5848	-3.6310	-2.3632
Ru	4.3710	-0.0055	0.0115
N	6.4150	0.0007	0.0206
C	7.5882	0.0072	0.0273
C	9.0463	0.0140	0.0392
C	4.5059	-3.2364	1.2451
O	2.4709	-0.0066	0.0054
Ru	0.5700	-0.0080	0.0078
N	-1.4742	-0.0148	0.0144
C	-2.6466	-0.0184	0.0175
C	-4.1045	-0.0191	0.0169
N	0.4894	0.8407	1.9056
C	0.4378	2.1903	2.1936
C	0.3703	2.3662	3.6353
C	0.3723	1.1103	4.1962
C	0.4412	0.1544	3.1027
C	0.4221	3.2240	1.2427
C	0.4369	3.0873	-0.1551
C	0.3736	4.1803	-1.1118
C	0.3789	3.6183	-2.3673
C	0.4443	2.1766	-2.1903
N	0.4877	1.8895	-0.8407

C	0.4275	-1.2431	3.2383
C	0.4408	-2.1940	2.2050
C	0.3694	-3.6355	2.3817
C	0.3667	-4.1970	1.1264
C	0.4370	-3.1041	0.1703
N	0.4899	-1.9067	0.8557
C	0.4340	1.2253	-3.2232
C	0.4454	-0.1722	-3.0867
C	0.3820	-1.1287	-4.1797
C	0.3786	-2.3842	-3.6186
C	0.4400	-2.2073	-2.1771
N	0.4883	-0.8577	-1.8894
C	0.4235	-3.2405	-1.2267
H	0.3272	3.3329	4.1418
H	0.3303	0.8423	5.2541
H	0.3835	4.2473	1.6334
H	0.3319	5.2384	-0.8446
H	0.3424	4.1239	-3.3345
H	0.3898	-1.6341	4.2614
H	0.3258	-4.1415	3.3486
H	0.3212	-5.2548	0.8589
H	0.3850	-4.2635	-1.6177
H	0.3390	-3.3509	-4.1249
H	0.3455	-0.8612	-5.2378
H	0.4021	1.6159	-4.2466
H	-4.4871	-0.9852	-0.3574
H	-4.4883	0.1407	1.0401
H	-4.4867	0.7872	-0.6335
H	4.5937	4.1258	3.3555
H	4.6042	5.2392	0.8657
H	4.5329	1.6181	4.2687
H	4.5835	-0.8609	5.2587
H	4.5830	-3.3495	4.1426
H	4.5602	4.2480	-1.6120
H	4.6401	3.3360	-4.1192
H	4.6531	0.8466	-5.2333
H	4.5852	-1.6310	-4.2433
H	4.6333	-4.1369	-3.3297
H	4.6154	-5.2502	-0.8403
H	4.5387	-4.2597	1.6358
H	9.4405	-0.4041	-0.9040
H	9.4234	1.0461	0.1526
H	9.4243	-0.5945	0.8799

ORu-O_2 porphyrin
Total energy= -1307.959965 [au] (BP86/LACVP*)

atom	x	y	z
N	0.0250	-1.4665	1.4947
C	0.0005	-1.2566	2.8616
C	-0.0210	-2.5410	3.5320
C	-0.0186	-3.5115	2.5561
C	0.0054	-2.8356	1.2743
C	-0.0118	-0.0018	3.4896

C	-0.0043	1.2535	2.8622
N	0.0189	1.4642	1.4955
C	-0.0044	2.8333	1.2758
C	-0.0298	3.5085	2.5579
C	-0.0294	2.5374	3.5334
C	-0.0136	3.4634	0.0227
C	0.0019	2.8434	-1.2399
C	0.0196	3.5202	-2.5263
C	0.0566	2.5442	-3.4942
C	0.0561	1.2619	-2.8088
N	0.0188	1.4870	-1.4527
C	0.0812	0.0003	-3.4289
C	0.0595	-1.2618	-2.8095
N	0.0256	-1.4876	-1.4533
C	0.0114	-2.8442	-1.2413
C	0.0285	-3.5203	-2.5281
C	0.0618	-2.5437	-3.4956
Ru	-0.0307	-0.0008	0.0411
O	1.8712	0.0053	-0.2820
O	2.7055	0.0101	-1.2413
C	-0.0022	-3.4651	0.0209
O	-1.7635	-0.0044	-0.1580
H	-0.0477	2.6716	4.6165
H	-0.0486	4.5919	2.6885
H	-0.0335	-0.0021	4.5847
H	-0.0394	-2.6758	4.6150
H	-0.0344	-4.5951	2.6861
H	-0.0304	4.5586	0.0302
H	0.0093	4.6033	-2.6602
H	0.0811	2.6706	-4.5779
H	0.1158	0.0006	-4.5237
H	0.0847	-2.6696	-4.5793
H	0.0202	-4.6034	-2.6625
H	-0.0170	-4.5603	0.0278

ORu-O_2-RuL complex
Total energy= -2522.691047 [au] (BP86/LACVP*)

atom	x	y	z
N	4.5754	2.5742	-3.5513
C	4.1857	3.2244	-4.7240
C	4.3635	4.6610	-4.5498
C	4.8587	4.8615	-3.2767
C	4.9940	3.5514	-2.6503
C	3.7079	2.5923	-5.8813
C	3.5256	1.2148	-6.0696
N	3.7947	0.2257	-5.1196
C	3.4840	-1.0044	-5.6978
C	3.0025	-0.7805	-7.0559
C	3.0286	0.5811	-7.2843
C	3.6200	-2.2517	-5.0702
C	4.0937	-2.4915	-3.7719

C	4.2313	-3.8014	-3.1469
C	4.7386	-3.6041	-1.8779
C	4.9212	-2.1706	-1.7026
N	4.5206	-1.5149	-2.8722
C	5.4266	-1.5437	-0.5563
C	5.6020	-0.1661	-0.3676
N	5.3128	0.8231	-1.3140
C	5.6247	2.0549	-0.7381
C	6.1312	1.8301	0.6094
C	6.1181	0.4678	0.8362
Ru	4.5186	0.5229	-3.1917
N	6.4468	0.4033	-3.9802
C	7.5432	0.3283	-4.4130
C	8.8993	0.2320	-4.9418
C	5.4756	3.3054	-1.3561
O	2.7147	0.7317	-2.5334
O	2.3807	-0.0153	-1.3333
Ru	0.4947	0.2747	-0.5482
N	0.3827	-1.7978	-0.3910
C	0.7700	-2.5665	0.7051
C	0.4603	-3.9637	0.4310
C	-0.1074	-4.0202	-0.8265
C	-0.1574	-2.6587	-1.3433
C	1.3654	-2.0747	1.8747
C	1.6875	-0.7384	2.1493
N	1.4519	0.3408	1.3005
C	1.9192	1.4892	1.9342
C	2.4701	1.1180	3.2311
C	2.3267	-0.2488	3.3640
C	1.8685	2.7876	1.4084
C	1.3514	3.1699	0.1627
C	1.3272	4.5273	-0.3655
C	0.7456	4.4735	-1.6168
C	0.4058	3.0821	-1.8773
N	0.7806	2.3145	-0.7762
C	-0.1942	2.5913	-3.0441
C	-0.5050	1.2545	-3.3219
N	-0.2859	0.1775	-2.4645
C	-0.7204	-0.9755	-3.1136
C	-1.2373	-0.6084	-4.4253
C	-1.1056	0.7602	-4.5528
C	-0.6655	-2.2761	-2.5924
O	-1.1214	0.4958	0.2113
H	2.6230	-0.8769	4.2035
H	2.9067	1.8194	3.9412
H	1.6104	-2.8093	2.6483
H	0.6569	-4.7871	1.1165
H	-0.4629	-4.8988	-1.3636
H	2.2811	3.5861	2.0332
H	1.7098	5.4019	0.1593
H	0.5678	5.2937	-2.3108
H	-0.4275	3.3236	-3.8232
H	-1.3798	1.3849	-5.4018
H	-1.6414	-1.3142	-5.1501
H	-1.0528	-3.0765	-3.2308

H	2.7362	1.1163	-8.1872
H	2.6828	-1.5688	-7.7370
H	3.4459	3.2416	-6.7233
H	4.1344	5.4099	-5.3073
H	5.1087	5.8066	-2.7953
H	3.3249	-3.1299	-5.6539
H	3.9622	-4.7444	-3.6221
H	4.9625	-4.3538	-1.1200
H	5.6960	-2.1933	0.2827
H	6.4157	-0.0658	1.7379
H	6.4451	2.6198	1.2915
H	5.7641	4.1807	-0.7649
H	9.5500	-0.3281	-4.2473
H	8.8967	-0.2897	-5.9150
H	9.3292	1.2382	-5.0890

ORu-O_2-RuO
Total energy= -2465.123591 [au] (BP86/LACVP*)

atom	x	y	z
C	0.1553	-2.9891	-3.4287
C	0.0742	-1.5830	-3.0508
N	0.4090	-1.4616	-1.7075
C	0.7022	-2.7296	-1.2248
C	0.5396	-3.6940	-2.3056
C	-0.2832	-0.5268	-3.9010
C	-0.3759	0.8315	-3.5648
C	-0.7630	1.9054	-4.4704
C	-0.7339	3.0822	-3.7479
C	-0.3256	2.7460	-2.3903
N	-0.1188	1.3757	-2.3119
C	-0.1633	3.6534	-1.3316
C	0.2339	3.3511	-0.0238
N	0.5355	2.0753	0.4643
C	0.8758	2.2093	1.8102
C	0.7886	3.6144	2.1793
C	0.3945	4.3134	1.0557
C	1.2451	1.1600	2.6617
C	1.3420	-0.1946	2.3181
N	1.0712	-0.7297	1.0571
C	1.2777	-2.1122	1.1337
C	1.6959	-2.4477	2.4854
C	1.7365	-1.2731	3.2113
Ru	0.3921	0.3077	-0.5936
O	-1.3483	0.0610	-0.2755

C	1.1011	-3.0251	0.0876
O	2.3147	0.5272	-1.2883
O	2.7495	0.4593	-2.6041
Ru	4.7333	0.4723	-3.2055
O	6.4935	0.4758	-3.5423
N	4.9923	1.9592	-1.7694
C	4.9449	3.3306	-1.9950
C	5.2462	4.0222	-0.7489
C	5.4683	3.0571	0.2134
C	5.3092	1.7593	-0.4289
C	4.6498	3.9426	-3.2223
C	4.3457	3.2977	-4.4277
N	4.2907	1.9149	-4.6211
C	3.9626	1.6877	-5.9575
C	3.8025	2.9710	-6.6257
C	4.0380	3.9572	-5.6881
C	5.4551	0.5147	0.1988
C	5.3153	-0.7470	-0.3960
N	5.0021	-0.9813	-1.7312
C	4.9528	-2.3574	-1.9215
C	5.2545	-3.0174	-0.6575
C	5.4749	-2.0282	0.2799
C	3.8085	0.4282	-6.5522
C	3.9506	-0.8148	-5.9210
C	3.7772	-2.1154	-6.5513
C	4.0130	-3.0764	-5.5875
C	4.3348	-2.3840	-4.3491
N	4.2846	-1.0061	-4.5799
C	4.6477	-2.9988	-3.1306
H	1.0037	4.0072	3.1724
H	0.2257	5.3850	0.9581
H	1.4846	1.4251	3.6963
H	2.0055	-1.1411	4.2587
H	1.9253	-3.4557	2.8287
H	-0.3654	4.7062	-1.5517
H	-0.9624	4.0889	-4.0948
H	-1.0189	1.7679	-5.5200
H	-0.5124	-0.7909	-4.9379
H	-0.0514	-3.3748	-4.4260
H	0.7033	-4.7666	-2.2085
H	1.3002	-4.0767	0.3166
H	4.0074	5.0369	-5.8288
H	3.5426	3.0927	-7.6766
H	4.6536	5.0369	-3.2385
H	5.2777	5.1047	-0.6333
H	5.7152	3.2012	1.2644
H	3.5489	0.4136	-7.6153
H	3.5122	-2.2659	-7.5971
H	3.9764	-4.1595	-5.6977
H	4.6472	-4.0932	-3.1197
H	5.2879	-4.0968	-0.5151
H	5.7193	-2.1446	1.3349
H	5.7005	0.5294	1.2652

$ORu^{VI}O$
Total energy= -1232.800163 [au] (BP86/LACVP*)

atom	x	y	z
N	-1.4616	-1.4343	-0.0006
C	-1.2484	-2.7988	0.0007
C	-2.5347	-3.4665	0.0012
C	-3.5037	-2.4882	0.0002
C	-2.8264	-1.2058	-0.0007
C	0.0081	-3.4262	0.0006
C	1.2654	-2.7998	-0.0003
C	2.5518	-3.4680	-0.0006
C	3.5205	-2.4896	-0.0011
C	2.8430	-1.2071	-0.0011
N	1.4789	-1.4359	-0.0005
C	3.4711	0.0491	-0.0010
C	2.8547	1.3141	-0.0002
N	1.5006	1.5303	0.0002
C	1.2713	2.8853	0.0010
C	2.5558	3.5700	0.0011
C	3.5319	2.6021	0.0003
Ru	0.0078	0.0156	0.0000
O	0.0153	0.2049	-1.7497
C	0.0090	3.5047	0.0012
C	-1.2527	2.8845	0.0005
C	-2.5371	3.5695	-0.0009
C	-3.5137	2.6023	-0.0014
C	-2.8376	1.3143	-0.0005
N	-1.4828	1.5294	0.0005
C	-3.4546	0.0499	-0.0009
O	0.0189	0.2020	1.7501
H	2.6826	4.6541	0.0016
H	4.6149	2.7369	0.0002
H	0.0084	4.6002	0.0013
H	-2.6635	4.6537	-0.0014
H	-4.5967	2.7379	-0.0025
H	4.5664	0.0402	-0.0014
H	4.6045	-2.6175	-0.0014
H	2.6892	-4.5507	-0.0004
H	0.0075	-4.5213	0.0010
H	-2.6721	-4.5492	0.0022
H	-4.5876	-2.6164	0.0003
H	-4.5499	0.0412	-0.0015

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