Electronic Supplementary Material (ESI) for Dalton Transactions.

A Computational Study of the Mechanism for Water Oxidation by $(bpc)(bpy)Ru^{II}OH_2$

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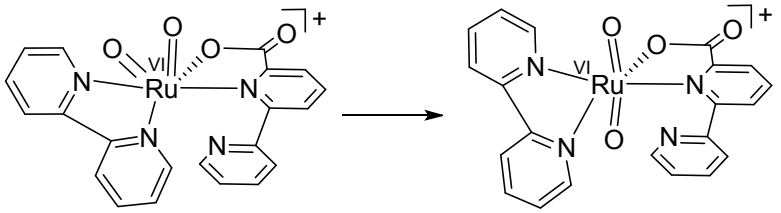
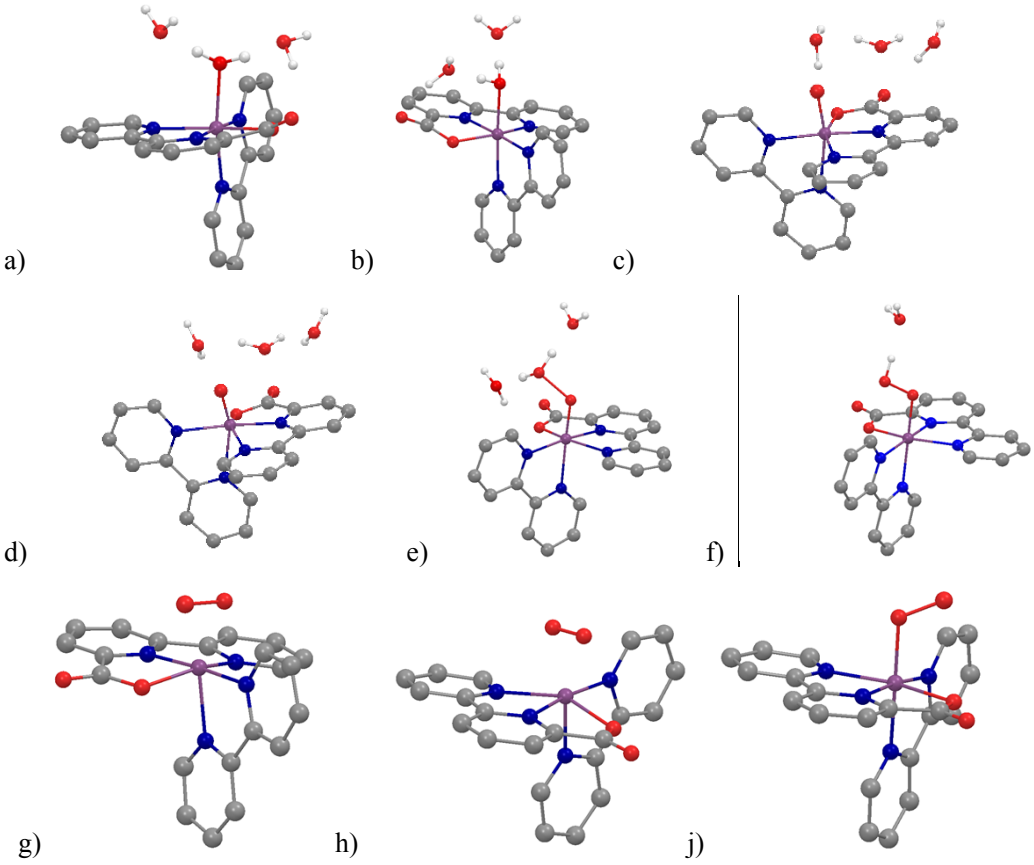


Scheme S1. Profile of the calculated relative G for the *cis*-bis-oxo and *trans*-bis-oxo of **23**.



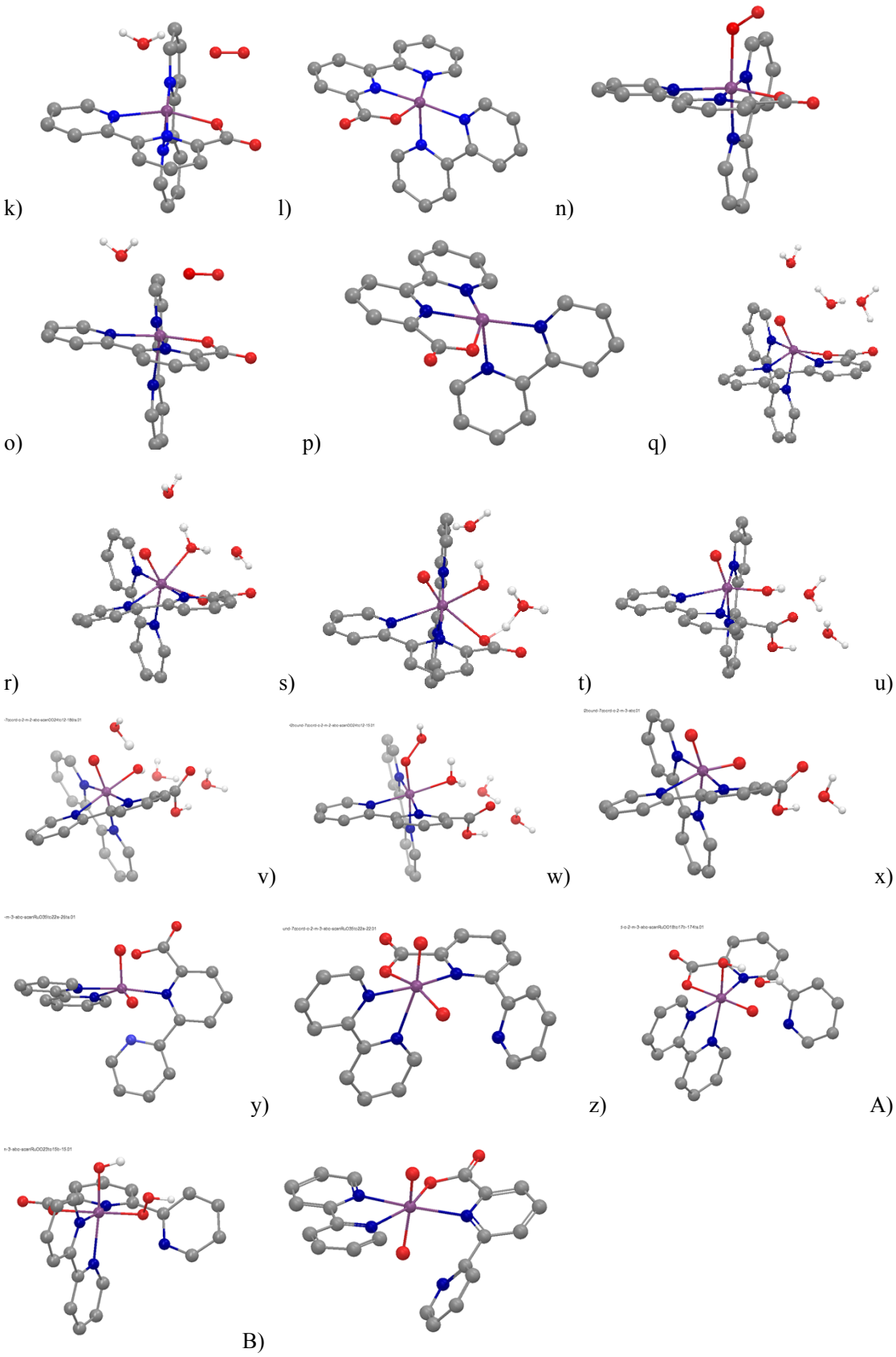


Figure S1. Optimized geometries of a) **1**; b) **2**; c) **3**; d) **4**; e) **ts5**; f) **6**; g) $\mathbf{7}_{\text{side-on}}$; h) $\mathbf{8}_{\text{side-on}}$; j) $\mathbf{9}_{\text{end-on}}$; k) **ts10**; l) **11**; n) $\mathbf{12}_{\text{end-on}}$; o) **ts13**; p) **14**; q) **ts15**; r) **16**; s) **ts17**; t) **18**; u) **ts19**; v) **20**; w) **21**; x) **ts22**; y) **23** z) **ts24**. A) **25**. B) *trans*-bis-oxo **23**. The hydrogen atoms except the HO type are omitted for

clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

Cartesian coordinates in Å and energies in atomic units unless stated otherwise of the calculated geometries.

Figure S1a

E (M06/LACV3P++ 2f(Ru)) =** -1501.30367241688

ZPE (kcal mol^{-1}) = 251.959

G_{solv} = -0.0864438

DH_{298} (kcal mol^{-1})= 19.151

DS_{298} (cal K^{-1} mol^{-1})= 193.271

Cartesian coordinates

atom	x	y	z
Ru1	3.4570286793	5.9941720223	1.7118276224
N2	2.4764436111	5.0323675762	3.2577943631
C3	3.0536477240	4.5892031544	4.3922077288
H4	4.1135289868	4.7875979396	4.4942303503
C5	2.3493173324	3.9101451247	5.3772576996
H6	2.8642911353	3.5735665309	6.2704848957
C7	0.9884750546	3.6717294041	5.1867872515
H8	0.4076273014	3.1413242215	5.9342429554
C9	0.3852326402	4.1234511583	4.0181495735
H10	-0.6699883641	3.9459116849	3.8504565938
C11	1.1439266131	4.8036740913	3.0601522341
C12	0.5914009402	5.3203418283	1.7941831212
C13	-0.7433813401	5.1800682448	1.4018843739
H14	-1.4507995510	4.6603165374	2.0369010539
C15	-1.1604077424	5.7084081491	0.1844753368
H16	-2.1933555258	5.6023903612	-0.1306331591
C17	-0.2316746472	6.3692278478	-0.6215602818
H18	-0.5145729106	6.7919977531	-1.5792278608
C19	1.0815603536	6.4765738005	-0.1791462544
H20	1.8568599768	6.9669464682	-0.7577235832
N21	1.4873498101	5.9674918570	1.0003519180
N22	5.3143079709	5.9085891702	2.4411430071
C23	6.0792875493	4.8763104791	2.0448168593
C24	7.3899621467	4.7610325837	2.4967912657
H25	7.9971611347	3.9328243964	2.1493441833
C26	7.8755866069	5.7370908740	3.3742905699
H27	8.8890818277	5.6694001630	3.7571810744
C28	7.0721766904	6.8201264942	3.7420228133
H29	7.4648586908	7.5903555581	4.3960620766
C30	5.7679400494	6.8982207074	3.2422548519
C31	4.7706839581	7.9682041821	3.4589118213
C32	4.9982252813	9.0851625118	4.2648788824

H33	5.9462933268	9.1959547602	4.7792302104
C34	4.0068738114	10.0520050541	4.4057804057
H35	4.1754034279	10.9223296830	5.0318811623
C36	2.7990057490	9.8816317924	3.7299875551
H37	1.9987019950	10.6093972505	3.8096786946
C38	2.6264445565	8.7495666725	2.9407519956
H39	1.7055095152	8.5731172656	2.3960631080
N40	3.5759870835	7.8062870875	2.7992083030
C41	5.4053826291	3.9900857713	0.9998323251
O42	4.1311032417	4.1713928715	0.8482771284
O43	6.1212725476	3.2568313161	0.3104931464
O44	4.1746123335	6.8475801820	-0.1610863076
H45	4.8750773181	7.5340202452	-0.0782328151
H46	4.5635830693	6.1334006325	-0.7428712588
O54	6.2500649361	8.6125958443	0.0365759557
H55	6.9967311647	8.2312876762	-0.4453840669
H56	6.1156536853	9.4838351208	-0.3594671894
O50	5.3514635932	5.0456808456	-1.7946127094
H51	5.6780689449	4.2827189371	-1.2730081669
H52	4.7038069391	4.6611383273	-2.3993059294

Figure S1b

E (M06/LACV3P++ 2f(Ru))** = -1500.97786853401

ZPE (kcal mol^{-1}) = 252.318

G_{solv} = -0.2281864

DH_{298} (kcal mol^{-1})= 19.088

DS_{298} (cal K^{-1} mol^{-1})= 191.916

Cartesian coordinates

atom	x	y	z
Ru1	3.4550806617	6.0162643348	1.7067174656
N2	2.4321953179	5.0953045818	3.2712167897
C3	2.9933697806	4.7040907638	4.4299994164
H4	4.0392786574	4.9507331048	4.5670607298
C5	2.2810495953	4.0123625143	5.4017048567
H6	2.7734819921	3.7138841979	6.3206814256
C7	0.9406292678	3.7114838253	5.1614608248
H8	0.3560582544	3.1676661747	5.8965230736
C9	0.3582940109	4.1145134886	3.9628069776
H10	-0.6809376884	3.8849698525	3.7628331849
C11	1.1228264740	4.8086817090	3.0212593472
C12	0.6028152522	5.2811143992	1.7247590009
C13	-0.7054335662	5.0845234156	1.2798905051
H14	-1.4211550382	4.5472643752	1.8901715839
C15	-1.0882297445	5.5808528765	0.0349633865
H16	-2.1025594679	5.4294324051	-0.3202518994

C17	-0.1575807564	6.2682315799	-0.7452638297
H18	-0.4200749317	6.6682761494	-1.7180825836
C19	1.1328482888	6.4306256736	-0.2540303118
H20	1.9068765527	6.9469622376	-0.8105242272
N21	1.5014583152	5.9502600975	0.9497189775
N22	5.3617056381	5.9426969350	2.4164052367
C23	6.0937091872	4.8914972817	2.0203141570
C24	7.4291190401	4.7797596759	2.3904177741
H25	8.0127263520	3.9300203289	2.0532951731
C26	7.9662694326	5.7899570836	3.1983409067
H27	9.0015236060	5.7326289742	3.5198623316
C28	7.1838620485	6.8804111622	3.5912235808
H29	7.6117038356	7.6614545153	4.2095108020
C30	5.8503818224	6.9454026374	3.1705132096
C31	4.8508078760	7.9988461842	3.4493178691
C32	5.1012057929	9.1312211519	4.2227333866
H33	6.0820199287	9.2883202549	4.6571355380
C34	4.0815852263	10.0583972022	4.4361976172
H35	4.2663768822	10.9428009417	5.0376664091
C36	2.8260840330	9.8322568330	3.8739387515
H37	2.0068327314	10.5275876457	4.0197091910
C38	2.6298514319	8.6823747282	3.1150083489
H39	1.6709799590	8.4597216987	2.6603678080
N40	3.6129271168	7.7902203310	2.8983078506
C41	5.3200701534	3.9561615597	1.1112292184
O42	4.0053080007	4.1714565108	1.1275333909
O43	5.8750221466	3.1369045004	0.4076668682
O44	4.2212151706	6.8722728014	-0.0968532428
H45	4.9862453301	7.5037218914	-0.0248277497
H46	4.4946594368	6.1614901058	-0.7566099940
O54	6.3040323125	8.5411825561	0.1189612529
H55	7.0880065499	8.2569082088	-0.3723920856
H56	6.1491775320	9.4529661323	-0.1659252274
O50	5.1329849963	5.0369559863	-1.7312923925
H51	5.3107664371	4.1471934517	-1.3821046299
H52	4.8974986024	4.9297515904	-2.6615698222

Figure S1c

E (M06/LACV3P++ 2f(Ru))** = -1576.45417544406

ZPE (kcal mol^{-1}) = 253.363

G_{solv} = -0.0964913

DH_{298} (kcal mol^{-1})= 20.335

DS_{298} (cal K^{-1} mol^{-1})= 202.234

Cartesian coordinates

atom	x	y	z

Ru1	3.1242869367	6.0779903354	1.6666441832
N2	2.3670137598	4.9967068853	3.4835532560
C3	3.1228630502	4.4097933051	4.4234577472
H4	4.1969956578	4.4918871638	4.2933357634
C5	2.5813466182	3.7263722743	5.5061447069
H6	3.2330087515	3.2650976827	6.2398284568
C7	1.1935282797	3.6521989849	5.6122279173
H8	0.7281944892	3.1285057581	6.4413060475
C9	0.4055484422	4.2577630078	4.6387341870
H10	-0.6734912534	4.2057596621	4.7123810136
C11	1.0162264924	4.9275298670	3.5725794554
C12	0.2550219557	5.5913049684	2.4881919624
C13	-1.1401775863	5.5607689061	2.3996881804
H14	-1.7281696964	5.0383346220	3.1437446632
C15	-1.7747221697	6.1959342538	1.3356350331
H16	-2.8568261523	6.1722035122	1.2548364476
C17	-1.0031934581	6.8495754180	0.3766096493
H18	-1.4562302129	7.3476409302	-0.4733508322
C19	0.3805105752	6.8476297829	0.5165389556
H20	1.0412310881	7.3215274627	-0.2020575343
N21	0.9917534066	6.2398446140	1.5495765323
N22	5.0768156785	5.6673276389	1.8964064406
C23	5.5154636421	4.5480182571	1.3108257893
C24	6.8674374548	4.2129301476	1.3873198546
H25	7.2292279152	3.3241490405	0.8841294286
C26	7.7218342626	5.0887025303	2.0545694827
H27	8.7820234346	4.8645087518	2.1165560063
C28	7.2346708004	6.2645747337	2.6394333245
H29	7.9104563719	6.9412846005	3.1492159583
C30	5.8729155577	6.5450412672	2.5419884811
C31	5.1513720014	7.7198541428	3.0828926521
C32	5.7809877796	8.7599746238	3.7680464282
H33	6.8526197435	8.7366224716	3.9267426971
C34	5.0237945981	9.8328660669	4.2334542234
H35	5.5046004983	10.6502964891	4.7613357726
C36	3.6487721602	9.8452113731	4.0083119268
H37	3.0253417963	10.6644142361	4.3488715682
C38	3.0772520599	8.7777652523	3.3217629663
H39	2.0140615623	8.7413986209	3.1109182785
N40	3.7997801433	7.7423059423	2.8730374411
C41	4.4241945349	3.7217746260	0.6423758487
O42	3.2070995754	4.2240040116	0.7212064086
O43	4.6814521683	2.6448842830	0.1211004278
O44	3.3199461233	7.0492651650	0.1914252700

O45	5.5705747565	5.3747452919	-1.2961042273
H46	6.1129943362	4.6307532184	-1.6141982104
H47	4.7116647400	5.2861590518	-1.7524393280
O49	2.9141535063	4.6730315541	-2.0991201707
H50	2.7880769073	4.4107967111	-1.1705483320
H51	2.9325060656	3.8386483946	-2.5850204841
O51	6.9540537628	2.8719403956	-1.4679991827
H52	6.1616673092	2.5109240199	-1.0296253665
H53	7.1455259868	2.2874883273	-2.2112435746

Figure S1d

E (M06/LACV3P++ 2f(Ru))** = -1576.102741342

ZPE (kcal mol^{-1}) = 253.165

G_{solv} = -0.2274867

DH_{298} (kcal mol^{-1})= 20.577

DS_{298} (cal K^{-1} mol^{-1})= 203.764

Cartesian coordinates

atom	x	y	z
Ru1	3.2003651395	6.0607005873	1.6121414792
N2	2.3950378053	5.1884780592	3.4782983160
C3	3.1437145287	4.7513727656	4.5058688747
H4	4.2152226100	4.8904660562	4.4200279270
C5	2.5877810533	4.1414633228	5.6227083918
H6	3.2282135193	3.7959660382	6.4266479358
C7	1.2026373524	3.9843112736	5.6723672111
H8	0.7299746726	3.5111635861	6.5273130773
C9	0.4277719690	4.4412276916	4.6103304083
H10	-0.6484828640	4.3261835422	4.6411907995
C11	1.0459741909	5.0443399952	3.5104435933
C12	0.3102880757	5.5565824034	2.3362078896
C13	-1.0738506640	5.4563279522	2.1851138778
H14	-1.6787352361	4.9828564400	2.9484135207
C15	-1.6785234694	5.9624294475	1.0360542398
H16	-2.7538862247	5.8868686050	0.9098253396
C17	-0.8866822148	6.5564398746	0.0559474594
H18	-1.3173361145	6.9584794288	-0.8543056436
C19	0.4883668321	6.6268062584	0.2558846853
H20	1.1556532264	7.0602412861	-0.4791078349
N21	1.0644406259	6.1487529831	1.3734629727
N22	5.1442054287	5.6184282129	1.9386907068
C23	5.5710576517	4.4899649318	1.3636785106
C24	6.9226894688	4.1645493103	1.3888440860
H25	7.2706745112	3.2708568731	0.8846940880
C26	7.7899384763	5.0577483189	2.0254674349
H27	8.8535364722	4.8428855204	2.0564459141

C28	7.3113919283	6.2285586574	2.6296240430
H29	7.9967772037	6.9075621862	3.1233659567
C30	5.9443909510	6.5025088144	2.5717457320
C31	5.2119582501	7.6486252974	3.1459022197
C32	5.8086671951	8.6764650274	3.8737073399
H33	6.8805785234	8.6794446566	4.0344659604
C34	5.0145017529	9.7021516133	4.3882335780
H35	5.4690994929	10.5114971858	4.9507279621
C36	3.6378620935	9.6772227981	4.1715778881
H37	2.9894307307	10.4589784891	4.5514882101
C38	3.0941126730	8.6262572420	3.4376125324
H39	2.0321500796	8.5676340103	3.2270290010
N40	3.8582632606	7.6425263351	2.9420942718
C41	4.4481997415	3.6741572082	0.7662117016
O42	3.2120818384	4.2147943993	0.9960753324
O43	4.5769967757	2.5970486981	0.2441593616
O44	3.3346798277	7.2104139368	0.3471969575
O45	5.0595599112	5.2794333031	-1.1363446223
H46	5.6723224769	4.6216651380	-1.5214042146
H47	4.2095653174	5.1832485578	-1.6073840983
O49	2.3921052590	4.8250201638	-1.9443648145
H50	2.2739710335	3.9067902890	-1.6644458727
H51	2.1539468323	4.8359701552	-2.8818418194
O51	6.7550180960	3.1032562667	-1.6053335173
H52	6.1770681903	2.3464266506	-1.4354026449
H53	7.2950175685	2.8642847547	-2.3702419041

Figure S1e

E (M06/LACV3P++ 2f(Ru))** = -1576.06966899183

ZPE (kcal mol^{-1}) = 252.82

G_{solv} = -0.2266143

DH_{298} (kcal mol^{-1})= 19.535

DS_{298} (cal K^{-1} mol^{-1})= 197.886

Cartesian coordinates

atom	x	y	z
Ru1	3.5702042631	6.1845748575	1.6660970984
N2	2.5739322566	5.0349647838	3.2267565071
C3	3.1443961181	4.5801219225	4.3573386770
H4	4.1684121378	4.8842991565	4.5389717762
C5	2.4746129428	3.7551265901	5.2515285644
H6	2.9750989095	3.4092672843	6.1491945599
C7	1.1624424816	3.3847039952	4.9584175020
H8	0.6083695886	2.7354919546	5.6289424170
C9	0.5664839649	3.8573385675	3.7922002430

H10	-0.4516815628	3.5747044297	3.5570687613
C11	1.2907717904	4.6897047758	2.9330313538
C12	0.7318142383	5.2540654444	1.6853004427
C13	-0.5772667811	5.0268511124	1.2555836070
H14	-1.2436151648	4.3960260568	1.8302976084
C15	-1.0296177756	5.6172180681	0.0777847274
H16	-2.0448789750	5.4422928097	-0.2633486153
C17	-0.1640334775	6.4314257512	-0.6486076996
H18	-0.4760795979	6.9132726800	-1.5683912504
C19	1.1314610627	6.6199536349	-0.1790552226
H20	1.8481113455	7.2320639314	-0.7129036736
N21	1.5675174797	6.0437367755	0.9573997729
N22	5.4049872724	6.0397076999	2.4955736630
C23	6.1608409348	5.0217469890	2.0629656039
C24	7.4582745168	4.8693436542	2.5392643473
H25	8.0693295696	4.0474158789	2.1826922749
C26	7.9215044021	5.8058112744	3.4719891869
H27	8.9286293200	5.7196450996	3.8680836209
C28	7.1049076451	6.8572266958	3.9040917612
H29	7.4810933751	7.5735062895	4.6255317515
C30	5.8085309311	6.9654412529	3.3882138824
C31	4.7776266904	7.9843917821	3.7062195315
C32	4.9771887949	9.0233993827	4.6135752688
H33	5.9268815904	9.1272921055	5.1259441006
C34	3.9468954974	9.9324066079	4.8574997527
H35	4.0941391178	10.7459172354	5.5607080982
C36	2.7345614377	9.7829337362	4.1888033241
H37	1.9108427990	10.4697904466	4.3488914967
C38	2.5909053753	8.7256878213	3.2923640518
H39	1.6704580423	8.5702951426	2.7406231247
N40	3.5782675311	7.8502988874	3.0564800903
C41	5.4760117293	4.1333291156	1.0373514465
O42	4.1882424687	4.4327120803	0.8084252126
O43	6.0688345832	3.2426016061	0.4747416826
O44	4.1997670510	7.3555220973	0.4368687587
O45	4.0353664636	7.0613571596	-1.3230418353
H46	3.9913560320	6.0418370052	-1.5102512744
O47	3.6725509690	4.6027721342	-1.8128740692
H48	4.0679059583	4.1116419508	-2.5451116161
H49	3.8371293132	4.1030236281	-0.9889914982
H50	4.9453189712	7.4296029064	-1.5769785246
O54	6.3834674465	8.0049797052	-1.9239220703
H55	6.8623745500	7.6709309397	-2.6950989646
H56	6.4447096211	8.9689147955	-1.9760297214

Figure S1f

E (M06/LACV3P++ 2f(Ru))** = -1499.34855671183

ZPE (kcal mol^{-1}) = 230.426

G_{solv} = -0.0928285

DH_{298} (kcal mol^{-1})= 18.231

DS_{298} (cal K^{-1} mol^{-1})= 189.768

Cartesian coordinates

atom	x	y	z
Ru1	3.5672650734	6.2708299432	1.7355880684
N2	2.5486899503	4.9511652985	3.0855261458
C3	3.1081196035	4.3566293067	4.1532451395
H4	4.1250695893	4.6512831498	4.3852196190
C5	2.4402228317	3.4091456330	4.9184215371
H6	2.9354348219	2.9520105523	5.7678145448
C7	1.1378692220	3.0636939314	4.5598567107
H8	0.5852343179	2.3224752537	5.1280889082
C9	0.5525002034	3.6793416796	3.4588094968
H10	-0.4563515449	3.4164948495	3.1670367828
C11	1.2789400755	4.6261891151	2.7282601192
C12	0.7417427473	5.3327522169	1.5473274677
C13	-0.5573135164	5.1438871595	1.0663756934
H14	-1.2289526755	4.4481030375	1.5532493471
C15	-0.9853301459	5.8557049026	-0.0498976192
H16	-1.9903460912	5.7160443956	-0.4346724591
C17	-0.1020847822	6.7407571846	-0.6640779753
H18	-0.3902238980	7.3106372777	-1.5404729347
C19	1.1794590867	6.8843368589	-0.1426959019
H20	1.9210279280	7.5269039940	-0.6014904907
N21	1.5938691080	6.2021952196	0.9403672793
N22	5.4038783441	6.1027372947	2.5238878020
C23	6.1599074915	5.1196502411	2.0171043105
C24	7.4710365249	4.9611299312	2.4560591134
H25	8.0716167373	4.1612602020	2.0378182303
C26	7.9559083157	5.8505779127	3.4210903864
H27	8.9741846923	5.7532059248	3.7846687807
C28	7.1439003852	6.8729504520	3.9233771730
H29	7.5309136981	7.5616958178	4.6655847697
C30	5.8346169211	6.9885866719	3.4434080976
C31	4.8074952936	7.9868929785	3.8190142907
C32	5.0206020758	8.9916934914	4.7640965540
H33	5.9798135633	9.0727670647	5.2626336284
C34	3.9975042787	9.8887072623	5.0591467956
H35	4.1547063977	10.6749062257	5.7905644825

C36	2.7753825647	9.7619936249	4.4013209485
H37	1.9533752035	10.4411396423	4.5985510306
C38	2.6210839472	8.7396559962	3.4697494206
H39	1.6925418368	8.6026582714	2.9264652155
N40	3.6015150369	7.8699859187	3.1794084185
C41	5.4551785765	4.2496664680	0.9687953330
O42	4.2089642398	4.5851302226	0.7185027479
O43	6.0716048378	3.3277043333	0.4649828354
O44	4.3739628613	7.5194694309	0.4879977746
O45	4.0379875160	7.3137564222	-0.8648344844
H50	4.6993826960	7.9035113485	-1.3175132979
O54	5.9326929616	8.7419149352	-2.1133468830
H55	5.7058873215	9.3771451663	-2.8045687753
H56	6.5807962414	8.1459700282	-2.5114831260

Figure S1g

E (M06/LACV3P++ 2f(Ru))** = -1422.2818695684

ZPE (kcal mol^{-1}) = 208.352

G_{solv} = -0.0895274

DH_{298} (kcal mol^{-1})= 15.438

DS_{298} (cal K^{-1} mol^{-1})= 162.82

Cartesian coordinates

atom	x	y	z
Ru1	3.6316785315	5.9908996473	1.7051438858
N2	2.3471871905	5.2503671656	3.2023588022
C3	2.7415004937	4.8491839449	4.4233532130
H4	3.7884958592	4.9964556650	4.6600520888
C5	1.8657922286	4.2713094201	5.3317734303
H6	2.2240857012	3.9604833187	6.3066665332
C7	0.5340243551	4.0984844332	4.9533079812
H8	-0.1794032619	3.6458750317	5.6345106288
C9	0.1266887426	4.5094170862	3.6888769022
H10	-0.9035306073	4.3781842436	3.3817995654
C11	1.0528163404	5.0865197490	2.8146636504
C12	0.7230086920	5.5538188758	1.4537757224
C13	-0.5374137931	5.4425450668	0.8639241437
H14	-1.3613596047	4.9866855161	1.3994262480
C15	-0.7234122814	5.9137153091	-0.4340903166
H16	-1.6954622046	5.8280039673	-0.9087693056
C17	0.3505711711	6.4852614995	-1.1136641786
H18	0.2449770978	6.8559961869	-2.1270444460
C19	1.5845998104	6.5684104984	-0.4750961870
H20	2.4665286665	6.9892314368	-0.9426065993
N21	1.7549653976	6.1183419261	0.7775624670

N22	5.4209668053	5.6407735515	2.5435075354
C23	5.9655755299	4.4523604870	2.2572027844
C24	7.2538679628	4.1581687218	2.6943545067
H25	7.6827931119	3.1904206049	2.4600319553
C26	7.9370179116	5.1325228509	3.4288069997
H27	8.9454780406	4.9384696222	3.7802662924
C28	7.3287413134	6.3548454659	3.7343712339
H29	7.8583508224	7.0956408573	4.3221008445
C30	6.0320120649	6.5940804953	3.2704106336
C31	5.1705769449	7.7716190071	3.5141342661
C32	5.5588767354	8.8838469435	4.2610915158
H33	6.5567279289	8.9327473220	4.6817449039
C34	4.6589510782	9.9290210076	4.4572560588
H35	4.9538731387	10.8007022035	5.0327193474
C36	3.3819883868	9.8424582445	3.9056806036
H37	2.6544120076	10.6363091492	4.0323221704
C38	3.0495050770	8.7095163571	3.1691663943
H39	2.0766293438	8.5970147170	2.7041949222
N40	3.9132047306	7.7014147006	2.9814823511
C41	5.0303357565	3.4963465000	1.5229302879
O42	3.8183998250	3.9836902848	1.2909794139
O43	5.3974942319	2.3710594221	1.2551908338
O44	4.2761729137	7.4068567313	0.4048280095
O45	4.5886258842	6.1636891193	-0.0740304483

Figure S1h

E (M06/LACV3P++ 2f(Ru))** = -1421.92082276717

ZPE (kcal mol^{-1}) = 208.51

G_{solv} = -0.2328763

DH_{298} (kcal mol^{-1})= 15.565

DS_{298} (cal K^{-1} mol^{-1})= 164.577

Cartesian coordinates

atom	x	y	z
Ru1	3.6360452233	5.9955602861	1.6808219320
N2	2.3862255274	5.3092241853	3.1680486104
C3	2.8091307625	4.9455755007	4.3959193606
H4	3.8538577548	5.1156180933	4.6203499476
C5	1.9532307436	4.3744440520	5.3248971731
H6	2.3300003079	4.0927946399	6.3018653145
C7	0.6192378198	4.1683023891	4.9679497491
H8	-0.0765741724	3.7172670914	5.6682861712
C9	0.1875890711	4.5449363214	3.7001940137
H10	-0.8447956605	4.3892073034	3.4128797878
C11	1.0876347511	5.1167581617	2.7969364882

C12	0.7307547875	5.5467040445	1.4352245021
C13	-0.5412958491	5.4043773663	0.8788668103
H14	-1.3443259062	4.9487895261	1.4450550946
C15	-0.7724564823	5.8435778415	-0.4231072787
H16	-1.7556337126	5.7329936400	-0.8688707003
C17	0.2737460980	6.4185533485	-1.1419725253
H18	0.1383077817	6.7706448916	-2.1585056789
C19	1.5207402456	6.5315452576	-0.5362225351
H20	2.3598779509	6.9622205342	-1.0680496584
N21	1.7434747442	6.1106616445	0.7216549580
N22	5.4270132163	5.6204473681	2.5564414560
C23	5.9543556023	4.4189998623	2.2888401046
C24	7.2262239318	4.0970886782	2.7506132626
H25	7.6483843867	3.1225842749	2.5284279162
C26	7.9087099940	5.0601732376	3.5041901416
H27	8.9055706507	4.8465150012	3.8769233292
C28	7.3119613165	6.2898691445	3.8064406008
H29	7.8378105644	7.0140035553	4.4183693720
C30	6.0302256828	6.5561453978	3.3140620451
C31	5.1687285389	7.7315151000	3.5587310838
C32	5.5355199670	8.8332515446	4.3283604698
H33	6.5262683438	8.8848785875	4.7657117014
C34	4.6206036663	9.8669995238	4.5315358889
H35	4.8994264484	10.7303470663	5.1274689516
C36	3.3496604212	9.7779053083	3.9650473055
H37	2.6120511563	10.5611461376	4.1011332479
C38	3.0326216623	8.6577149356	3.2021045367
H39	2.0627233836	8.5452294466	2.7308309161
N40	3.9164216329	7.6653525794	3.0020827234
C41	5.0101660362	3.5043768944	1.5344337254
O42	3.7836560485	4.0503510489	1.3217629116
O43	5.3013692676	2.3884511898	1.1994162174
O44	4.3266875146	7.4514396893	0.3587653521
O45	4.6704100439	6.3460768266	-0.1746424818

Figure S1j

E (M06/LACV3P++ 2f(Ru)) = -1422.27459235295**

ZPE (kcal mol^{-1}) = 207.402

G_{solv} = -0.0858208

DH_{298} (kcal mol^{-1})= 16.026

DS_{298} (cal K^{-1} mol^{-1})= 170.824

Cartesian coordinates

atom	x	y	z
Ru1	3.6319747418	5.9126841449	1.6836972087

N2	2.3773462961	5.1242105045	3.1491409517
C3	2.7980021448	4.6475924944	4.3346170453
H4	3.8603354078	4.7239589919	4.5307710613
C5	1.9312725334	4.0773474607	5.2572815912
H6	2.3166954282	3.7011056554	6.1982893053
C7	0.5764945956	3.9963524396	4.9379195152
H8	-0.1308736509	3.5541671628	5.6318972744
C9	0.1400305134	4.4867893407	3.7121470122
H10	-0.9087905917	4.4273826030	3.4492595163
C11	1.0588709234	5.0483091707	2.8203796015
C12	0.6952633278	5.5859617579	1.4954280114
C13	-0.6045264795	5.5735147659	0.9822225893
H14	-1.4193831892	5.1515894991	1.5575537850
C15	-0.8470713691	6.0987324337	-0.2830045910
H16	-1.8510843505	6.0902903421	-0.6944730421
C17	0.2183577314	6.6243881680	-1.0118462544
H18	0.0774837113	7.0354673346	-2.0052107257
C19	1.4893295082	6.6072293386	-0.4485131294
H20	2.3521933215	6.9815051753	-0.9848715962
N21	1.7261118327	6.1069958038	0.7774034521
N22	5.4021228096	5.5985622404	2.5807127871
C23	5.9829201262	4.4142534769	2.3454921465
C24	7.2440461948	4.1416127241	2.8683366395
H25	7.6989321539	3.1781819084	2.6673653586
C26	7.8675202913	5.1322296710	3.6325753576
H27	8.8519451482	4.9540719128	4.0537555601
C28	7.2345416406	6.3586062736	3.8635350984
H29	7.7253665124	7.1203088523	4.4585417941
C30	5.9689383403	6.5797605669	3.3126800961
C31	5.1208869291	7.7894365453	3.4358964798
C32	5.4950540432	8.9227423094	4.1593051919
H33	6.4546284300	8.9542841352	4.6619280508
C34	4.6318680962	10.0135966865	4.2284335800
H35	4.9168019443	10.8994239850	4.7869749188
C36	3.4043018934	9.9514880710	3.5718339896
H37	2.7050153614	10.7797590588	3.5980444992
C38	3.0843569619	8.7955162777	2.8664829861
H39	2.1454010941	8.6984924666	2.3326137179
N40	3.9109158609	7.7400368401	2.7954538998
C41	5.1366844529	3.4568512795	1.5057549906
O42	3.9744435265	3.9513921089	1.1257388028
O43	5.5569183022	2.3413270041	1.2652451380
O44	4.6950200291	7.0487541817	0.2514858868
O45	4.5656368246	6.2961331158	-0.7677360212

Figure S1k

E (M06/LACV3P++ 2f(Ru))** = -1498.653248

ZPE (kcal mol^{-1}) = 221.522

G_{solv} = -0.0828617

DH_{298} (kcal mol^{-1})= 18.521

DS_{298} (cal K^{-1} mol^{-1})= 193.868

Cartesian coordinates

atom	x	y	z
Ru1	3.4491510801	5.9419494311	2.2473784449
N2	1.9091788933	5.0912510400	3.8023090650
C3	2.2143488531	4.5588701390	4.9920746922
H4	3.2042983222	4.7862109577	5.3772833347
C5	1.3299001808	3.7540819742	5.7038119400
H6	1.6172241206	3.3427919843	6.6653646911
C7	0.0827702828	3.4870158522	5.1401443553
H8	-0.6315338818	2.8510883817	5.6533559374
C9	-0.2373296767	4.0390898617	3.9035705571
H10	-1.1970033968	3.8237076046	3.4498203467
C11	0.7001853645	4.8500049784	3.2516884342
C12	0.4445225197	5.4976675232	1.9420930135
C13	-0.8151160949	5.5083002096	1.3331820695
H14	-1.6570287722	5.0219294504	1.8098264557
C15	-0.9899053411	6.1573760282	0.1156491245
H16	-1.9635076516	6.1655091465	-0.3638682367
C17	0.0996255295	6.7997011141	-0.4702706705
H18	0.0084534390	7.3232089406	-1.4155503905
C19	1.3265419869	6.7561821500	0.1805327344
H20	2.2095803367	7.2420919195	-0.2205504263
N21	1.5017179155	6.1177718890	1.3546694459
N22	5.3090293880	5.7069855038	2.9600480910
C23	5.9133396181	4.5422736044	2.6670491219
C24	7.2187021749	4.3040467559	3.0797688918
H25	7.6843479735	3.3578338857	2.8280269433
C26	7.8719392256	5.2994116873	3.8150998070
H27	8.8916011891	5.1460574399	4.1537579857
C28	7.2133827609	6.4899259558	4.1326473205
H29	7.7165732134	7.2495978044	4.7197640113
C30	5.9000164784	6.6791672016	3.6900662697
C31	5.0136467664	7.8317053471	3.9489915071
C32	5.3849138813	8.9502150343	4.6988737480
H33	6.3830261684	9.0192556855	5.1155551528
C34	4.4648255670	9.9730680047	4.9107367829
H35	4.7439247166	10.8455963494	5.4929150216

C36	3.1828774013	9.8582685653	4.3725098299
H37	2.4360693162	10.6307939939	4.5192358968
C38	2.8692296093	8.7195163791	3.6385518920
H39	1.8863030354	8.5763689462	3.2031061367
N40	3.7540249630	7.7313226738	3.4218972970
C41	5.0276188363	3.5593394629	1.9079879031
O42	3.7895820671	3.9904766753	1.7169358087
O43	5.4712468777	2.4821763209	1.5622591405
O44	4.3157485392	5.5196903972	-0.7918033703
O45	3.9277253547	4.4812079685	-1.2941147783
O46	4.2714271685	8.1997017757	0.2931697924
H47	4.4422483381	9.1502104605	0.2803628351
H48	4.8327274681	7.8299119466	-0.4004524905

Figure S1l

E (M06/LACV3P++ 2f(Ru))** = -1271.957168

ZPE (kcal mol^{-1}) = 204.004

G_{solv} = -0.0939118

DH_{298} (kcal mol^{-1})= 14.082

DS_{298} (cal K^{-1} mol^{-1})= 154.535

Cartesian coordinates

atom	x	y	z
Ru1	3.5641284683	5.9206402252	1.7427361011
N2	2.3636641202	5.1982038079	3.1805847957
C3	2.8000174834	4.7707598036	4.3852616304
H4	3.8604538750	4.8742001231	4.5720075439
C5	1.9469982279	4.2196534740	5.3300407273
H6	2.3479165124	3.8873182724	6.2811250554
C7	0.5905139249	4.0994235722	5.0278305742
H8	-0.1023271645	3.6691087273	5.7432074026
C9	0.1385904899	4.5388820471	3.7891016784
H10	-0.9105696777	4.4543276391	3.5328912178
C11	1.0356562678	5.0871886981	2.8688370794
C12	0.6598568767	5.5807928221	1.5364537284
C13	-0.6326151862	5.5314384192	1.0073757151
H14	-1.4463973909	5.1055371180	1.5821030833
C15	-0.8659118730	6.0243829119	-0.2721795731
H16	-1.8630374786	5.9882421469	-0.6982408276
C17	0.2006000533	6.5568013726	-0.9982454506
H18	0.0637779611	6.9453899977	-2.0011410616
C19	1.4620560839	6.5776100545	-0.4163572573
H20	2.3248097128	6.9715066583	-0.9442605406
N21	1.6927285438	6.1056889630	0.8227250198
N22	5.3578830700	5.6078698158	2.5857054833

C23	5.9553531618	4.4454361792	2.2789515612
C24	7.2129046238	4.1558509468	2.7980706699
H25	7.6811286500	3.2114305349	2.5442000838
C26	7.8212640884	5.1059464723	3.6250768562
H27	8.8015771832	4.9087483565	4.0474105503
C28	7.1844855932	6.3193276811	3.9076829306
H29	7.6719326334	7.0565004718	4.5356047028
C30	5.9204539049	6.5601475825	3.3607527791
C31	5.0734608825	7.7678773744	3.5062537278
C32	5.4284192506	8.8662194206	4.2901686791
H33	6.3638247601	8.8614308863	4.8375934635
C34	4.5773427946	9.9658958930	4.3681541372
H35	4.8460249021	10.8229819363	4.9770623126
C36	3.3811335897	9.9452020307	3.6534927508
H37	2.6887010188	10.7792319238	3.6844704106
C38	3.0788108448	8.8234136266	2.8878057770
H39	2.1598902013	8.7609484111	2.3152192669
N40	3.8914322248	7.7545071015	2.8061558490
C41	5.1521135560	3.5537013088	1.3225557564
O42	4.0242402004	4.0844286471	0.8951845464
O43	5.6065048565	2.4676011360	1.0137596816

Figure S1n

E (M06/LACV3P++ 2f(Ru))** = -1421.915684

ZPE (kcal mol^{-1}) = 207.642

G_{solv} = -0.2313382

DH_{298} (kcal mol^{-1})= 16.313

DS_{298} (cal K^{-1} mol^{-1})= 175.676

Cartesian coordinates

atom	x	y	z
Ru1	3.5598761171	5.9363173759	1.7318357869
N2	2.3290529907	5.1978364804	3.1794873779
C3	2.7621762933	4.7612487259	4.3773295823
H4	3.8179663428	4.8772419019	4.5842165580
C5	1.9010184526	4.1828321299	5.3014041844
H6	2.2890070452	3.8424912302	6.2551308887
C7	0.5532686917	4.0476666403	4.9710292523
H8	-0.1446138281	3.5951203860	5.6681266028
C9	0.1100273289	4.4981958978	3.7303267958
H10	-0.9339984166	4.3988703289	3.4593756417
C11	1.0147265244	5.0725702845	2.8355884147
C12	0.6572208493	5.5794625216	1.5010848156
C13	-0.6202523069	5.5174227946	0.9454982645
H14	-1.4398752638	5.0691698298	1.4938769505
C15	-0.8360435141	6.0280253193	-0.3339282785

H16	-1.8249417649	5.9788928825	-0.7785405861
C17	0.2291151076	6.5945311819	-1.0353052309
H18	0.1001701268	6.9984336163	-2.0332182919
C19	1.4805671495	6.6256704457	-0.4337218877
H20	2.3415765252	7.0447136664	-0.9418433664
N21	1.6909164631	6.1333042617	0.8040709050
N22	5.3897938252	5.6117247526	2.5939258122
C23	5.9769769093	4.4390902388	2.3141916296
C24	7.2567497055	4.1603043951	2.7800400304
H25	7.7152304687	3.2055146066	2.5446175542
C26	7.9008336612	5.1407463219	3.5428800664
H27	8.9001461557	4.9593347413	3.9261733991
C28	7.2684767625	6.3584099797	3.8183124837
H29	7.7762752913	7.1122458798	4.4091825090
C30	5.9814991359	6.5834296584	3.3194023212
C31	5.1349601544	7.7845558854	3.4845185188
C32	5.5105708575	8.9165157253	4.2042778928
H33	6.4831880677	8.9620552643	4.6809733907
C34	4.6269389785	9.9916193350	4.3071108120
H35	4.9115136595	10.8787898774	4.8639290507
C36	3.3785432488	9.9096071563	3.6927500284
H37	2.6629672328	10.7222020892	3.7527545617
C38	3.0524890963	8.7527483851	2.9908780386
H39	2.0922278630	8.6414337241	2.4994025859
N40	3.9074220165	7.7197101529	2.8775810741
C41	5.1152631977	3.5185619717	1.4708954871
O42	3.8908595777	4.0354889474	1.2398342002
O43	5.4903057675	2.4451101913	1.0800112954
O44	4.7933508162	6.7182991921	-0.0667269913
O45	5.2958571665	6.0839047196	-0.9756399108

Figure S1o

E (M06/LACV3P++ 2f(Ru))** = -1498.307244

ZPE (kcal mol^{-1}) = 221.627

G_{solv} = -0.2258081

DH_{298} (kcal mol^{-1})= 18.579

DS_{298} (cal K^{-1} mol^{-1})= 194.644

Cartesian coordinates

atom	x	y	z
Ru1	3.4194266982	5.8400051812	2.0836904175
N2	1.9597267058	5.0328021640	3.6854398013
C3	2.2829974130	4.5284611477	4.8849673842
H4	3.2885080432	4.7308284903	5.2402278679
C5	1.3856321882	3.7817413869	5.6428632731
H6	1.6818144896	3.3897367604	6.6095358788

C7	0.1140935994	3.5501436304	5.1210321898
H8	-0.6115458045	2.9627091934	5.6745781200
C9	-0.2221590788	4.0777319482	3.8745686995
H10	-1.2068068498	3.8932549685	3.4630656472
C11	0.7242349237	4.8258667313	3.1690715271
C12	0.4551292201	5.4423041877	1.8453553030
C13	-0.7956339785	5.4153743943	1.2285771344
H14	-1.6319833543	4.9176204186	1.7027934089
C15	-0.9748466978	6.0392913131	-0.0060365281
H16	-1.9461874671	6.0130927465	-0.4899656600
C17	0.0966044354	6.7041091768	-0.6011498260
H18	-0.0091674256	7.2123911535	-1.5530323430
C19	1.3224690543	6.7065168089	0.0510437937
H20	2.1842554742	7.2403863059	-0.3397094675
N21	1.4988699653	6.0788291865	1.2359548843
N22	5.3081863851	5.5451327765	2.8641850831
C23	5.8905087104	4.3648279518	2.6078238509
C24	7.1633142124	4.0730295531	3.0806145123
H25	7.6098473926	3.1091684982	2.8596430696
C26	7.8192613290	5.0554484182	3.8310668046
H27	8.8165286858	4.8688644523	4.2169454183
C28	7.1964874311	6.2794185102	4.0883042247
H29	7.7087757206	7.0363871456	4.6705696160
C30	5.9112477801	6.5124057337	3.5861387799
C31	5.0825493965	7.7207484245	3.7498389592
C32	5.4603400723	8.8479067964	4.4751783892
H33	6.4262313978	8.8854096280	4.9650166733
C34	4.5820897896	9.9275108888	4.5717932136
H35	4.8639031221	10.8083676046	5.1401490924
C36	3.3430932928	9.8609177638	3.9353054313
H37	2.6339480818	10.6796013158	3.9908567903
C38	3.0192035191	8.7130046753	3.2197301149
H39	2.0701273450	8.6130860289	2.7060127787
N40	3.8624090612	7.6676116182	3.1323300857
C41	5.0190812505	3.4438055615	1.7916205212
O42	3.8419431817	4.0532423088	1.4528013837
O43	5.3050417348	2.3224533026	1.4846634155
O44	4.6263650197	6.0698878399	-0.4809170790
O45	5.1668601137	5.0661721221	-0.9051719866
O46	3.7951805708	8.7691825524	0.0435386053
H47	3.4781431752	9.6535080826	-0.1858765216
H48	4.5489039150	8.6288244213	-0.5451156027

Figure S1p

E (M06/LACV3P++ 2f(Ru)) =** -1271.604577

ZPE (kcal mol^{-1}) = 204.395

G_{solv} = -0.2566094

DH_{298} (kcal mol^{-1})= 14.087

DS_{298} (cal K^{-1} mol^{-1})= 155.541

Cartesian coordinates

atom	x	y	z
Ru1	3.5429340334	5.8939112611	1.8030222562
N2	2.2604311055	5.2069691796	3.2026578871
C3	2.6688322186	4.7779375552	4.4124633640
H4	3.7238819976	4.8765289126	4.6320241686
C5	1.7784571942	4.2311832155	5.3276013652
H6	2.1432917857	3.8949468371	6.2918121820
C7	0.4330728725	4.1215352841	4.9763534796
H8	-0.2854356750	3.6941608337	5.6684233607
C9	0.0189930843	4.5631052498	3.7222120466
H10	-1.0218702774	4.4817962378	3.4322509662
C11	0.9493814467	5.1045983852	2.8341369486
C12	0.6399285663	5.5930090580	1.4837246449
C13	-0.6164591272	5.5562471609	0.8815243563
H14	-1.4709972470	5.1476294364	1.4077232046
C15	-0.7621778327	6.0406244609	-0.4186312729
H16	-1.7335720586	6.0126751396	-0.9021330894
C17	0.3487656866	6.5507396806	-1.0930140570
H18	0.2722578375	6.9277811282	-2.1067760479
C19	1.5767055602	6.5595846055	-0.4421820726
H20	2.4750150774	6.9319202489	-0.9258018204
N21	1.7152626039	6.0990653877	0.8163825117
N22	5.4136037456	5.6185801607	2.5762600130
C23	6.0198857851	4.4655210819	2.2507696031
C24	7.3367725102	4.2299458321	2.6261719529
H25	7.8113273487	3.2924612988	2.3557114246
C26	7.9970737578	5.2311267889	3.3476142195
H27	9.0255294957	5.0825608650	3.6618192012
C28	7.3465438404	6.4287805558	3.6681676574
H29	7.8708366601	7.1993438827	4.2218078198
C30	6.0225839210	6.6117529709	3.2598321520
C31	5.1530451832	7.7889867293	3.4738232011
C32	5.5353770596	8.9280684164	4.1778578745
H33	6.5277809160	8.9958005188	4.6089666340
C34	4.6325390593	9.9825193672	4.3243329208
H35	4.9219708975	10.8749362096	4.8702258919
C36	3.3595367898	9.8728975145	3.7675976529
H37	2.6293965586	10.6691377392	3.8621042059
C38	3.0276703469	8.7091469859	3.0800304550

H39	2.0478801081	8.5768003149	2.6343725615
N40	3.8990006499	7.6945997026	2.9251961311
C41	5.1334631200	3.5203386761	1.4621038002
O42	3.8835435753	4.0079725954	1.2914081272
O43	5.5101670164	2.4538995073	1.0566529754

Figure S1q

E (M06/LACV3P++ 2f(Ru))** = -1576.09641357245

ZPE (kcal mol^{-1}) = 253.432

G_{solv} = -0.2297897

DH_{298} (kcal mol^{-1})= 19.836

DS_{298} (cal K^{-1} mol^{-1})= 196.632

Cartesian coordinates

atom	x	y	z
Ru1	3.5782105470	5.8977256399	1.5926420688
N2	2.4030957192	5.3235620521	3.3554154954
C3	2.9197319815	5.1054717033	4.5772368536
H4	3.9832835346	5.2765053626	4.6946176737
C5	2.1387700823	4.6740329351	5.6409786333
H6	2.5919384986	4.5031942510	6.6112240508
C7	0.7763154288	4.4640572625	5.4233895423
H8	0.1336355592	4.1261096509	6.2301669961
C9	0.2459834993	4.6909242309	4.1572469601
H10	-0.8101772239	4.5322075253	3.9782576244
C11	1.0824838160	5.1208851115	3.1216144616
C12	0.6191275992	5.3813233142	1.7440620485
C13	-0.6929178180	5.1812150039	1.3141021788
H14	-1.4478947521	4.8137443923	1.9980088752
C15	-1.0272389234	5.4477051706	-0.0125170465
H16	-2.0442853700	5.2921663307	-0.3579721404
C17	-0.0420601924	5.9058255118	-0.8837205966
H18	-0.2609579176	6.1175059723	-1.9242963171
C19	1.2525087629	6.0881895431	-0.4055282143
H20	2.0597172670	6.4227321355	-1.0517978787
N21	1.5625171448	5.8387536882	0.8803686034
N22	5.4318178800	5.6097176365	2.3746494992
C23	5.9667527964	4.4051764278	2.1521794474
C24	7.2859788925	4.1493931332	2.5055325261
H25	7.7163535114	3.1718941039	2.3179394929
C26	8.0046683331	5.1880920277	3.1106897998
H27	9.0392726478	5.0309086211	3.3994588228
C28	7.4001238765	6.4226511796	3.3779944414
H29	7.9586830082	7.2051840626	3.8790321051
C30	6.0698893316	6.6199089676	2.9974533329
C31	5.2001056505	7.7883175371	3.2445308199

C32	5.5983606619	8.9483009275	3.9057678339
H33	6.6210662963	9.0558066320	4.2485982163
C34	4.6716110670	9.9686309116	4.1222942388
H35	4.9740494833	10.8780524557	4.6318118427
C36	3.3603472232	9.8088420541	3.6778956979
H37	2.6134196122	10.5812001393	3.8247099221
C38	3.0151437139	8.6321949403	3.0175072825
H39	2.0164682449	8.4650233375	2.6306755787
N40	3.9085577074	7.6545629766	2.8150353233
C41	4.9659550948	3.4289030274	1.5784800620
O42	3.7158928722	3.9218208077	1.5396273655
O43	5.2502278733	2.3015136948	1.2506424208
O44	3.8887299190	7.0614218445	0.3488304567
O45	4.9407452506	4.8034454594	-0.7416872626
H46	4.6464368486	3.9265885334	-1.0830882093
H47	4.6657240179	5.4491841136	-1.4189286190
O49	3.6979121308	6.5197206272	-2.6511549353
H50	4.1342580255	7.3565841578	-2.8610537991
H51	3.5940579037	6.0731570058	-3.5029116846
O51	3.9905791677	2.3179893433	-1.3672160352
H52	4.2064901352	1.8666650586	-0.5357545009
H53	4.3704886662	1.7653453043	-2.0627847896

Figure S1r

E (M06/LACV3P++ 2f(Ru))** = -1576.10281022977

ZPE (kcal mol^{-1}) = 254.164

G_{solv} = -0.2282873

DH_{298} (kcal mol^{-1})= 19.624

DS_{298} (cal K^{-1} mol^{-1})= 193.156

Cartesian coordinates

atom	x	y	z
Ru1	3.6311047570	5.8221773562	1.5451977002
N2	2.3492437146	5.1387938266	3.2162487695
C3	2.8499210477	4.7362206412	4.3952844930
H4	3.9261775848	4.7817974704	4.5074631136
C5	2.0315526632	4.2693751623	5.4158594235
H6	2.4685428987	3.9536060474	6.3568351068
C7	0.6550101838	4.2067701864	5.1924430531
H8	-0.0128151463	3.8390838867	5.9650468852
C9	0.1437231917	4.6154802362	3.9642856826
H10	-0.9213833629	4.5654981147	3.7765887246
C11	1.0193801650	5.0840011792	2.9783466920
C12	0.5989818367	5.5496943657	1.6443070090
C13	-0.7283513667	5.5818654454	1.2127700235
H14	-1.5250555171	5.2392615882	1.8616835045

C15	-1.0232417876	6.0581881191	-0.0626285266
H16	-2.0511610179	6.0860291176	-0.4099693102
C17	0.0172767484	6.4973709589	-0.8784757838
H18	-0.1677175904	6.8799115577	-1.8760284900
C19	1.3214042677	6.4405176759	-0.3977641596
H20	2.1604509031	6.7617451122	-1.0035993382
N21	1.6016750483	5.9761300711	0.8337329660
N22	5.5652641081	5.7056018850	2.2887605138
C23	6.2209405490	4.5520360444	2.1253694247
C24	7.5758494351	4.4573890530	2.4234295609
H25	8.0960914947	3.5176505040	2.2733360943
C26	8.2037954995	5.5933496898	2.9475803224
H27	9.2603987855	5.5636282574	3.1949714960
C28	7.4677366395	6.7533219767	3.2127520614
H29	7.9431823072	7.6027036230	3.6899087538
C30	6.1100469152	6.7855459473	2.8792361815
C31	5.1175553587	7.8254842275	3.2123214029
C32	5.4180873690	9.0387083057	3.8283569247
H33	6.4482505903	9.3009180111	4.0415188272
C34	4.3837512869	9.9118060939	4.1648400314
H35	4.6061084481	10.8619276875	4.6401452668
C36	3.0673871427	9.5507587645	3.8833391453
H37	2.2361535984	10.2015052210	4.1311474032
C38	2.8269554788	8.3306582347	3.2571369933
H39	1.8236039359	8.0149598116	2.9967089171
N40	3.8215355749	7.4917450658	2.9374466025
C41	5.2837999729	3.4285659046	1.7551429802
O42	4.0152758780	3.7661806603	1.9213148468
O43	5.6669635177	2.3234775368	1.4185199418
O44	4.0512605697	7.1240334027	0.4492358915
O45	3.9842108917	4.7211907315	-0.3086989236
H46	3.7204679924	3.7518657735	-0.4298816340
H47	3.9441005550	5.2349015991	-1.1553291790
O49	3.8196998075	6.1970311993	-2.5528435185
H50	4.5360869578	6.8392569865	-2.6522964045
H51	3.7527994434	5.7478562927	-3.4073706508
O51	3.7072429797	2.1843968667	-0.6692309615
H52	4.3508156287	1.8322764859	-0.0262949132
H53	2.9218710472	1.6277662901	-0.5971474939

Figure S1s

E (M06/LACV3P++ 2f(Ru))** = -1576.07675468096

ZPE (kcal mol^{-1}) = 252.021

G_{solv} = -0.2274033

DH_{298} (kcal mol^{-1})= 18.932

DS_{298} (cal K^{-1} mol^{-1})= 187.966

Cartesian coordinates

atom	x	y	z
O42	0.0000000000000	0.0000000000000	0.0000000000000
H52	0.0000000000000	0.0000000000000	1.2192836561000
Ru1	2.2225475762649	0.0000000000000	-0.7179272024747
N2	1.5086992065542	-2.0543975751595	-0.6146302129536
C3	0.4768521507195	-2.4919783852345	-1.3587705319242
H4	-0.0010177694142	-1.7640858724367	-2.0007854408137
C5	0.0381747020334	-3.8072874062495	-1.2928551820512
H6	-0.7980190292918	-4.1270466747573	-1.9048312298328
C7	0.6867023355328	-4.6874416601932	-0.4243792902453
H8	0.3656498100998	-5.7213077943352	-0.3448083734910
C9	1.7511206939161	-4.2262296021278	0.3439617952684
H10	2.2610359353959	-4.8961380887162	1.0253359279744
C11	2.1535827999575	-2.8918136934298	0.2316516198024
C12	3.2682083614342	-2.2895613303870	0.9804116743176
C13	4.0626988300573	-2.9835809860827	1.8943086415255
H14	3.8750671407462	-4.0291467219981	2.1052614996774
C15	5.1045271614554	-2.3154966972609	2.5350045880452
H16	5.7330258633335	-2.8405943081362	3.2471765615753
C17	5.3259116072838	-0.9706139850293	2.2464951718751
H18	6.1277686848536	-0.4149306171851	2.7201404489128
C19	4.4989305107006	-0.3277572445275	1.3294353483262
H20	4.6337595922074	0.7202406836964	1.0851184071293
N21	3.4963780014551	-0.9786973265821	0.7118658822926
N22	0.9874676037100	0.8936915493484	-2.1801668613533
C23	-0.1284449455939	1.5244534951461	-1.7820149120880
C24	-0.8500300010666	2.3372210263148	-2.6467187204979
H25	-1.7412535400739	2.8404745386000	-2.2877126171299
C26	-0.4052956982652	2.4395348424114	-3.9681011647200
H27	-0.9395857688955	3.0639041216285	-4.6772498736541
C28	0.6937826713125	1.6918201593883	-4.3932861939569
H29	0.9915943055995	1.7111398813811	-5.4349544758487
C30	1.3862835676369	0.9001741986207	-3.4693794552867
C31	2.4764461918041	-0.0491672547657	-3.7847792093323
C32	3.0696167197539	-0.1643919140927	-5.0424042877245
H33	2.7826768374047	0.4977428099059	-5.8507479880619
C34	4.0457121641435	-1.1385524930215	-5.2496814069386
H35	4.5190659348660	-1.2370269278532	-6.2214526719680
C36	4.4044508792418	-1.9776418305135	-4.1967283993190
H37	5.1569517520255	-2.7489024819562	-4.3189829807184
C38	3.7800652394011	-1.8027747306319	-2.9633030894897
H39	4.0385823399164	-2.4209290937785	-2.1100442466260

N40	2.8397518517027	-0.8714971201383	-2.7655289295033
C41	-0.5807385980501	1.1544923562010	-0.4008239090484
O43	-1.4114423061719	1.7544360201209	0.2352143997897
O44	3.6025871124212	0.9522816494511	-1.1775365092274
O45	1.9145886935399	1.3720357866911	0.7631268697292
H46	1.1068813774304	0.8286389507591	2.0069637993888
H47	2.7251246000210	1.9203449477793	0.8674075326468
O49	4.2089088313622	2.9005007748031	1.0422199023629
H50	4.4806921075276	3.3744909466694	0.2447337882024
H51	4.2539182706255	3.5487116283728	1.7588621395824
O51	0.3532087631891	0.2269388450416	2.3449103207215
H53	-0.3103185861838	0.7666057399244	2.8045368172692

Figure S1t

E (M06/LACV3P++ 2f(Ru))** = -1576.1125944554

ZPE (kcal mol^{-1}) = 255.136

G_{solv} = -0.2244191

DH_{298} (kcal mol^{-1})= 19.342

DS_{298} (cal K^{-1} mol^{-1})= 192.199

Cartesian coordinates

atom	x	y	z
O42	0.0000000000000	0.0000000000000	0.0000000000000
H52	0.0000000000000	0.0000000000000	0.9931053769000
Ru1	3.1938766838406	0.0000000000000	-1.7220862815942
N2	2.6522392785238	-2.0267490112695	-1.0719720574922
C3	1.4400797747469	-2.5848697047981	-1.2289438799393
H4	0.6916519323033	-1.9817051930974	-1.7267049516059
C5	1.1535774737960	-3.8600672562496	-0.7541295625660
H6	0.1642847681653	-4.2802525634034	-0.8971516788530
C7	2.1574269684401	-4.5677657266422	-0.0942125973042
H8	1.9693451916232	-5.5652146762701	0.2903823068241
C9	3.4108208792714	-3.9825486405657	0.0717364312844
H10	4.1946688700401	-4.5233901244767	0.5868306671682
C11	3.6406781801713	-2.6993552784953	-0.4286777320630
C12	4.9313532463341	-1.9883171556231	-0.3134506069873
C13	6.0585362511688	-2.5130503172463	0.3229192121687
H14	6.0241759524094	-3.4940737277527	0.7798879513595
C15	7.2324564921366	-1.7632331637965	0.3728213984386
H16	8.1121022086054	-2.1619903815540	0.8680654591833
C17	7.2631735056075	-0.5011229027212	-0.2187232551883
H18	8.1568079931571	0.1130866467491	-0.2038770215669
C19	6.1138097070736	-0.0262551196688	-0.8398790039405
H20	6.0756847423556	0.9450506086402	-1.3207816260657
N21	4.9827965066868	-0.7538796986198	-0.8841402165007

N22	1.2939323241584	0.6205945421385	-2.5473322068463
C23	0.3471146115513	1.3373629138533	-1.9045808265817
C24	-0.5868360891777	2.0996701619978	-2.6035492711569
H25	-1.3069475830100	2.6900974250595	-2.0481452153656
C26	-0.5810988532001	2.0661048261665	-3.9958220811424
H27	-1.2954449717973	2.6537908085338	-4.5635360578895
C28	0.3326289343130	1.2458067725312	-4.6532748164982
H29	0.3233364193980	1.1843905851832	-5.7340235657032
C30	1.2690759813149	0.5272633330855	-3.9067219475700
C31	2.2467424361721	-0.4056955901721	-4.5180033332196
C32	2.2257602066267	-0.7637388422820	-5.8687127923669
H33	1.4890746036442	-0.3438792546994	-6.5415140431054
C34	3.1609748924222	-1.6777366822348	-6.3509591954522
H35	3.1550498717515	-1.9579120890548	-7.3995376330787
C36	4.0980182088735	-2.2256914455565	-5.4760614711770
H37	4.8428312552723	-2.9370651695386	-5.8149645145811
C38	4.0684925657860	-1.8323569460768	-4.1427270770183
H39	4.7827526432643	-2.2148724939202	-3.4224450677208
N40	3.1660922358149	-0.9532868838896	-3.6817267583167
C41	0.2016062553730	1.2560709460806	-0.3983505716596
O43	0.1527994571869	2.2418641147355	0.3071922232458
O44	4.0797745571683	1.2452803300087	-2.5373635867177
O45	2.6678336621761	0.6558526680921	-0.0618896745964
H46	0.4029914608219	1.5223906817490	2.2511474059782
H47	3.0868267409356	0.3214726202938	0.7929241901541
O49	3.1918498825589	-0.1777611997295	2.3338675218264
H50	3.7777223009761	0.3065560338174	2.9312255135004
H51	2.2803255728876	0.0318991675285	2.6293396831718
O51	0.4979987286707	0.6115258054034	2.5917194741290
H53	-0.0839870718206	0.5396470655840	3.3621025203473

Figure S1u

E (M06/LACV3P++ 2f(Ru)) =** -1652.50737360353

ZPE (kcal mol^{-1}) = 268.188

G_{solv} = -0.223912

DH_{298} (kcal mol^{-1})= 20.533

DS_{298} (cal K^{-1} mol^{-1})= 200.816

Cartesian coordinates

atom	x	y	z
O42	0.1548433282	0.0142807059	0.0306113501
H52	0.1410278071	0.0650399621	1.0253095501
Ru1	3.1689394068	-0.0441186526	-1.7330100887
N2	2.5838888313	-2.0372582364	-1.0177342901
C3	1.3604097817	-2.5848822794	-1.1295560216
H4	0.5996352806	-1.9701600655	-1.5926822272

C5	1.0741328587	-3.8604807920	-0.6562936766
H6	0.0748911419	-4.2666998976	-0.7670234996
C7	2.0920321090	-4.5879616227	-0.0415943520
H8	1.9050535751	-5.5859343676	0.3421472761
C9	3.3594361041	-4.0214879448	0.0753326248
H10	4.1569504061	-4.5790002989	0.5504489520
C11	3.5868041793	-2.7382173574	-0.4254480067
C12	4.8988005582	-2.0582316888	-0.3671237002
C13	6.0408068675	-2.6117195920	0.2153854334
H14	6.0031015369	-3.5944070237	0.6685831886
C15	7.2342815087	-1.8925494450	0.2174540901
H16	8.1249391027	-2.3180390125	0.6687321673
C17	7.2667701867	-0.6253568040	-0.3611920895
H18	8.1727218986	-0.0296283742	-0.3770010417
C19	6.1029373626	-0.1183349651	-0.9278662643
H20	6.0594826828	0.8662610985	-1.3791813110
N21	4.9556051591	-0.8232512795	-0.9355112288
N22	1.2910215574	0.5688039724	-2.5765936365
C23	0.3332505045	1.2815004472	-1.9456278355
C24	-0.6252293441	2.0056375575	-2.6511997591
H25	-1.3527986216	2.5926700274	-2.1022973775
C26	-0.6289458575	1.9403288028	-4.0422171517
H27	-1.3651363779	2.4918473182	-4.6182277531
C28	0.3135601740	1.1446377714	-4.6880564806
H29	0.3088885133	1.0730736221	-5.7683518077
C30	1.2755001837	0.4674561947	-3.9354077302
C31	2.3092112410	-0.4055884857	-4.5427715835
C32	2.3131830849	-0.7676957793	-5.8913920385
H33	1.5475726961	-0.4024380226	-6.5644123252
C34	3.3081286928	-1.6168383200	-6.3728527889
H35	3.3191759939	-1.9015281969	-7.4201194775
C36	4.2814058624	-2.0935631846	-5.4968672216
H37	5.0725685774	-2.7543061037	-5.8332437428
C38	4.2256387586	-1.6984265789	-4.1646291510
H39	4.9646336827	-2.0291200088	-3.4442375234
N40	3.2657570207	-0.8812724659	-3.7024434991
C41	0.2297023071	1.2572399265	-0.4358479241
O43	0.1157113922	2.2727884508	0.2204103156
O44	3.9884683475	1.4111326021	-2.3216055335
O45	2.8608382468	0.9562027744	-0.0017100071
H46	0.3722968282	1.6298072422	2.2486217069
H47	3.1330497277	0.5123458574	0.8494949192
O49	3.1368700347	-0.1951011073	2.3592528127
H50	3.7505401148	0.1409242350	3.0258714037

H51	2.2448001366	0.0660690591	2.6638943194
O51	0.4707658144	0.7229143327	2.5958070950
H53	-0.1547451772	0.6348577263	3.3294348945
O54	4.3243434333	2.6845681980	-0.7633985408
H55	3.8732537696	3.4050028992	-1.2362577222
H56	3.5616154044	1.9658340221	-0.2585398799

Figure S1v

E (M06/LACV3P++ 2f(Ru))** = -1652.54116364267

ZPE (kcal mol^{-1}) = 272.127

G_{solv} = -0.2214088

DH_{298} (kcal mol^{-1})= 20.643

DS_{298} (cal K^{-1} mol^{-1})= 200.678

Cartesian coordinates

atom	x	y	z
O42	0.2430545703	-0.0133757049	0.0842135917
H52	0.1560156114	0.0494775310	1.0727464016
Ru1	3.1696714370	-0.0768116725	-1.7346532998
N2	2.6160215516	-2.0168755976	-1.0328235468
C3	1.3933589930	-2.5648308890	-1.1536088689
H4	0.6432762796	-1.9577688274	-1.6419650922
C5	1.0955525460	-3.8306801939	-0.6616713827
H6	0.0961880126	-4.2341273332	-0.7812360950
C7	2.1006323843	-4.5534672803	-0.0216443982
H8	1.9040023383	-5.5437296667	0.3767531297
C9	3.3699174072	-3.9924636216	0.0950072437
H10	4.1622960359	-4.5475720761	0.5816880661
C11	3.6103526344	-2.7186031671	-0.4243118438
C12	4.9299952298	-2.0552650204	-0.3915316465
C13	6.0731882611	-2.6218309968	0.1771921175
H14	6.0250128848	-3.5941628595	0.6516731811
C15	7.2827324246	-1.9327021927	0.1300834780
H16	8.1758152032	-2.3679677530	0.5670166042
C17	7.3270897879	-0.6835804536	-0.4858531322
H18	8.2474765513	-0.1134562425	-0.5484471939
C19	6.1578211469	-0.1636293312	-1.0306963644
H20	6.1319788388	0.8104684582	-1.5031265408
N21	4.9893785855	-0.8311438061	-0.9860136373
N22	1.2775846501	0.5461636594	-2.5436397081
C23	0.3118955516	1.2468530348	-1.9108873741
C24	-0.6602817010	1.9625205184	-2.6064253480
H25	-1.3899908273	2.5390091353	-2.0494942867
C26	-0.6743686495	1.9030138831	-3.9979330699
H27	-1.4228034835	2.4455153854	-4.5665387813

C28	0.2782316484	1.1274639263	-4.6496946478
H29	0.2732329490	1.0616305424	-5.7304790008
C30	1.2548876138	0.4628092009	-3.9019761771
C31	2.3084473751	-0.3752966655	-4.5149859863
C32	2.3223612728	-0.7327880515	-5.8654099773
H33	1.5464306994	-0.3826502922	-6.5347632565
C34	3.3341855836	-1.5571109126	-6.3509765049
H35	3.3516248927	-1.8394369881	-7.3987185946
C36	4.3160779343	-2.0141537949	-5.4737400844
H37	5.1210958869	-2.6582943318	-5.8096869745
C38	4.2524848568	-1.6252836097	-4.1406975188
H39	4.9976090337	-1.9449583542	-3.4227666047
N40	3.2757997692	-0.8282555119	-3.6713479086
C41	0.2089204473	1.2242871670	-0.4053401278
O43	0.0115528696	2.2321105270	0.2468785448
O44	3.8339405124	1.5970919641	-2.4561232033
O45	2.9353480420	0.9962182149	0.1161288290
H46	0.1161676629	1.6690548666	2.2422332185
H47	3.0508179198	0.5927596979	1.0342783101
O49	2.9252491219	-0.0026350753	2.4927621671
H50	3.5403514510	0.2775683631	3.1831363325
H51	2.0303702952	0.2654592786	2.7899900862
O51	0.2785174680	0.7958606342	2.6499850446
H53	-0.3807530819	0.6775759479	3.3486994743
O54	4.5461243855	2.4027891143	-1.5023698871
H55	4.6131146295	3.2462831430	-1.9844432091
H56	3.5011480604	1.7834506510	0.0254611997

Figure S1w

E (M06/LACV3P++ 2f(Ru))** = -1499.00599845474

ZPE (kcal mol^{-1}) = 230.689

G_{solv} = -0.227187

DH_{298} (kcal mol^{-1})= 18.033

DS_{298} (cal K^{-1} mol^{-1})= 186.383

Cartesian coordinates

atom	x	y	z
O42	0.1064689775	0.1535473579	0.0790322114
H52	0.0020548306	0.2393645595	1.0954023613
Ru1	3.1689235588	-0.0009100473	-1.6382018802
N2	2.6651631858	-2.0556613167	-1.0618300434
C3	1.4361077623	-2.5897557255	-1.1468506124
H4	0.6644573423	-1.9643412086	-1.5777597924
C5	1.1651552151	-3.8704712342	-0.6753593540
H6	0.1620544529	-4.2740244495	-0.7571440248
C7	2.2004503658	-4.6031373890	-0.0970979949

H8	2.0233821864	-5.6046840330	0.2822064998
C9	3.4709260074	-4.0366031082	-0.0001525667
H10	4.2782076091	-4.5943267536	0.4587081030
C11	3.6849990842	-2.7474001281	-0.4900445701
C12	4.9837042852	-2.0440398838	-0.4269535895
C13	6.1462762979	-2.5870990894	0.1213703240
H14	6.1399518890	-3.5861101164	0.5397021122
C15	7.3210476598	-1.8351986866	0.1363218688
H16	8.2259616348	-2.2514756398	0.5677239607
C17	7.3194184321	-0.5502637516	-0.4034634102
H18	8.2110293874	0.0669486198	-0.4093056308
C19	6.1369749873	-0.0537212451	-0.9398859878
H20	6.0692364056	0.9396800919	-1.3695822748
N21	5.0088893760	-0.7871688042	-0.9497903799
N22	1.2869542237	0.6122351409	-2.5400060778
C23	0.3534203388	1.3709353821	-1.9232905209
C24	-0.5603012415	2.1352374747	-2.6485457969
H25	-1.2610720634	2.7600971141	-2.1066224652
C26	-0.5518956301	2.0656489491	-4.0367984246
H27	-1.2514452363	2.6511936893	-4.6248145048
C28	0.3577221558	1.2180264822	-4.6653564233
H29	0.3609516582	1.1367266372	-5.7447710443
C30	1.2794454647	0.5026985620	-3.9012611892
C31	2.2640745791	-0.4260306593	-4.5006006934
C32	2.2554457359	-0.7918149820	-5.8502224039
H33	1.5147706247	-0.3890918130	-6.5293116720
C34	3.2077967806	-1.6930550995	-6.3217570021
H35	3.2116312037	-1.9810402931	-7.3682867413
C36	4.1491014888	-2.2192757482	-5.4376659907
H37	4.9067758376	-2.9215445383	-5.7672241272
C38	4.1028973521	-1.8200286764	-4.1066569469
H39	4.8173043205	-2.1936342997	-3.3820358644
N40	3.1836180588	-0.9520434576	-3.6550697674
C41	0.2138658510	1.3775486020	-0.4138014908
O43	0.1280878582	2.4192897824	0.2010872729
O44	4.0032417602	1.3173320831	-2.4269875513
O45	2.7647281796	0.5222280397	-0.0259955567
H46	0.0044093820	1.6346686864	2.5268761219
O51	-0.0282909343	0.6666023758	2.5851602413
H53	-0.7717751058	0.4529208383	3.1655061408

Figure S1x

E (M06/LACV3P++ 2f(Ru))** = -1422.23793552482

ZPE (kcal mol^{-1}) = 206.666

G_{solv} = -0.0932754

DH_{298} (kcal mol^{-1})= 15.584

DS_{298} (cal K^{-1} mol^{-1})= 166.838

Cartesian coordinates

atom	x	y	z
O42	0.0000000000000	0.0000000000000	0.0000000000000
Ru1	0.0000000000000	0.0000000000000	2.5526449436000
N2	2.0665654439772	0.0000000000000	1.8054266258788
C3	2.5094822847868	0.8602027176879	0.8758775848849
H4	1.7910462627269	1.5816251917550	0.5134763802898
C5	3.8088874784897	0.7967287966875	0.3847507080485
H6	4.1341244657792	1.5060582118880	-0.3677714350371
C7	4.6588129380139	-0.1978323690148	0.8650957217063
H8	5.6757953134180	-0.2813908900425	0.4952981769419
C9	4.1896082648911	-1.0937320103996	1.8223679025304
H10	4.8358229817717	-1.8774117791424	2.1983129307130
C11	2.8769344166659	-0.9736653886341	2.2841966595140
C12	2.2720519382309	-1.8631390697593	3.2966326271656
C13	2.9324472203039	-2.9279860523952	3.9134494627959
H14	3.9590899538291	-3.1608810391044	3.6587788523785
C15	2.2547083984547	-3.6944558451204	4.8588461645714
H16	2.7548860303883	-4.5290006543284	5.3396936821263
C17	0.9352162901923	-3.3790706486594	5.1797799044713
H18	0.3765105660368	-3.9516619207882	5.9113643561721
C19	0.3312531075808	-2.3038172596424	4.5371072741423
H20	-0.6861029243530	-1.9901370442749	4.7431631803419
N21	0.9908364625654	-1.5780880919222	3.6225775424220
N22	-0.9573038879075	1.7318301030246	1.7080648509179
C23	-1.5853198219708	1.6506573048895	0.5276259510803
C24	-2.5136736779604	2.6149314413092	0.1404012219891
H25	-3.0025227705244	2.4945488490156	-0.8197332217070
C26	-2.7320135235115	3.7017172988534	0.9815915916705
H27	-3.4519838612425	4.4695063226850	0.7159082586383
C28	-1.9652850637067	3.8387610866686	2.1416479694177
H29	-2.0566385575565	4.7304819170560	2.7497804314619
C30	-1.0600272024978	2.8340989795069	2.4873457248941
C31	-0.0635071801324	2.9406758329215	3.5809252201927
C32	-0.0294555545010	3.9973088039034	4.4934413305563
H33	-0.7949518496916	4.7638344114813	4.4803561913595
C34	0.9994636785776	4.0533917089189	5.4310505063347
H35	1.0360184953247	4.8651364438974	6.1506514101466
C36	1.9759666484692	3.0596988853828	5.4320047193711
H37	2.7961330875315	3.0713611061401	6.1412067881872
C38	1.8707128662366	2.0317563110743	4.4976156209426
H39	2.5985312637893	1.2262292234325	4.4667212581137

N40	0.8827432848766	1.9720982177852	3.5993415193839
C41	-1.0618884056799	0.5898831068005	-0.4388128877283
O43	-1.5900866278006	0.4818064081075	-1.5378038289528
O44	-0.9829354303410	0.2423787425593	3.9778037645285
O45	-0.8568049009207	-1.3357389066380	1.7542144338199

Figure S1y

E (M06/LACV3P++ 2f(Ru))** = -1422.28019385315

ZPE (kcal mol^{-1}) = 207.325

G_{solv} = -0.0761177

DH_{298} (kcal mol^{-1})= 15.93

DS_{298} (cal K^{-1} mol^{-1})= 171.142

Cartesian coordinates

atom	x	y	z
O42	0.0000000000000	0.0000000000000	0.0000000000000
Ru1	0.0000000000000	0.0000000000000	2.0311991905000
N2	2.1902711158980	0.0000000000000	1.4979342175763
C3	2.9683520017762	1.0850327889635	1.4097558041396
H4	2.5230118572821	2.0198755012068	1.7377693011345
C5	4.2864521145192	0.9984664014690	0.9660222572137
H6	4.8946409786801	1.8936970933164	0.8993120302897
C7	4.7931524690621	-0.2519594894000	0.6193495888021
H8	5.8136341363372	-0.3553719183299	0.2644428114901
C9	3.9834019749241	-1.3790949893153	0.7454640690790
H10	4.3771455908843	-2.3572011427139	0.4982948597968
C11	2.6701886628491	-1.2251872472859	1.1964855217553
C12	1.7350493834259	-2.3539511664005	1.4136633110117
C13	2.0629346131978	-3.6878715666868	1.1621059831206
H14	3.0371264137697	-3.9433985819948	0.7648262835483
C15	1.1320719215017	-4.6912228794249	1.4172122740702
H16	1.3839555745804	-5.7280022882616	1.2183137385691
C17	-0.1199649194950	-4.3501770752431	1.9245232372552
H18	-0.8737769950959	-5.1001578853436	2.1351015537915
C19	-0.4011289613349	-3.0088158716121	2.1508201712231
H20	-1.3626726426467	-2.6715484081392	2.5211865705182
N21	0.5050020673828	-2.0475922750594	1.9041982608622
N22	-0.4638700453673	2.0748073963775	1.6074940519265
C23	-0.8741739510634	2.1937598330017	0.3243450352478
C24	-1.5144026873790	3.3310433930844	-0.1467351211949
H25	-1.8091014837637	3.3587502669640	-1.1896514680013
C26	-1.7553070401610	4.3732605363054	0.7452271487328
H27	-2.2735643413972	5.2704851501473	0.4214603145283
C28	-1.2889345463944	4.2632760557200	2.0527237374265
H29	-1.4050947254392	5.0781160126390	2.7585498819422
C30	-0.6151925246599	3.1088011207602	2.4669968215259

C31	0.0267115947258	3.0628183372002	3.8111852184176
C32	-0.7234946279732	3.2242262643048	4.9781269159017
H33	-1.8034037436463	3.3219327637901	4.9307693192662
C34	-0.0498294241150	3.2336265853787	6.1992723736159
H35	-0.5989395860176	3.3441258968199	7.1292150316901
C36	1.3363873532787	3.0992982005652	6.2004117962292
H37	1.9013643303445	3.1072270736066	7.1266654951233
C38	1.9950365166712	2.9548209410648	4.9774657210310
H39	3.0773497488706	2.8528284810234	4.9436736302374
N40	1.3645849545188	2.9349831527835	3.7988732702231
C41	-0.5765105509911	1.0329402264094	-0.5973660542936
O43	-0.8325581482569	1.0847525298832	-1.7805792359932
O44	0.6310596292925	0.2362482136036	3.6525358346264
O45	-1.7022033729456	-0.3622091145858	2.2213201337112

Figure S1z

E (M06/LACV3P++ 2f(Ru))** = -1498.65508574755

ZPE (kcal mol^{-1}) = 219.974

G_{solv} = -0.084671

DH_{298} (kcal mol^{-1})= 17.054

DS_{298} (cal K^{-1} mol^{-1})= 179.333

Cartesian coordinates

atom	x	y	z
O42	-0.3138364167	-0.0977225385	0.1087619444
Ru1	0.2481618955	0.0476270472	2.0647596556
N2	2.2780091406	0.1921795680	1.2523583755
C3	2.9230719990	1.3346835448	0.9777813734
H4	2.4331292312	2.2461888146	1.3021145584
C5	4.1729018002	1.3364600635	0.3633830281
H6	4.6670614348	2.2779496665	0.1514360861
C7	4.7604599240	0.1168571110	0.0364674228
H8	5.7313423789	0.0829646249	-0.4473437180
C9	4.0946859083	-1.0679002064	0.3450844437
H10	4.5475491358	-2.0221816772	0.1073888185
C11	2.8435322319	-1.0042248154	0.9610337739
C12	2.0622428982	-2.1964081464	1.3554441829
C13	2.4938770858	-3.5101224743	1.1643853105
H14	3.4483080245	-3.7099712569	0.6943497226
C15	1.6871855825	-4.5668986560	1.5808025228
H16	2.0160299759	-5.5907143580	1.4345799356
C17	0.4585649282	-4.2967285382	2.1793285175
H18	-0.1997735222	-5.0905333751	2.5132224950
C19	0.0739924691	-2.9715251781	2.3415079684
H20	-0.8767315431	-2.6904229352	2.7786921709

N21	0.8622524671	-1.9587962250	1.9455479791
N22	-0.4607665386	2.0635298354	1.6832643604
C23	-1.1625435031	2.0836461411	0.5261180767
C24	-1.9674354989	3.1567509526	0.1652827974
H25	-2.4929032813	3.0996515166	-0.7810571758
C26	-2.0692049551	4.2372017250	1.0351819670
H27	-2.7027198156	5.0858611203	0.7964088945
C28	-1.3214734225	4.2259803571	2.2103534358
H29	-1.3352718840	5.0720423288	2.8882732784
C30	-0.5018683489	3.1344951550	2.5149819961
C31	0.3769100625	3.1951348198	3.7170121376
C32	-0.1537506974	3.5122064179	4.9726594022
H33	-1.2213706646	3.6652802843	5.0974745323
C34	0.7194821989	3.6191932049	6.0556261998
H35	0.3421094996	3.8585577499	7.0453449409
C36	2.0808055330	3.4162718455	5.8408799388
H37	2.7965684171	3.4934432469	6.6525266217
C38	2.5125170535	3.1138701499	4.5478115475
H39	3.5693117721	2.9570542890	4.3438271439
N40	1.6882596628	3.0044977664	3.5010114819
C41	-1.0364561176	0.8792302646	-0.3927061016
O43	-1.5634371717	0.8920408570	-1.4864150283
O44	0.8162848252	0.2940436832	3.7476185483
O45	-1.4285474823	-0.4351762709	2.7210967234
O46	-0.6064127871	-0.4670115020	4.9729674589
H47	-1.2272517330	-0.4288942105	3.8563104734
H48	-0.6010344851	0.3930707337	5.4245059420

Figure S1A

E (M06/LACV3P++ 2f(Ru)) =** -1498.6893422336

ZPE (kcal mol^{-1}) = 223.565

G_{solv} = -0.0849466

DH_{298} (kcal mol^{-1})= 17.393

DS_{298} (cal K^{-1} mol^{-1})= 180.981

Cartesian coordinates

atom	x	y	z
O42	-0.4261083418	-0.2232294958	0.2063545518
Ru1	0.2075940864	0.0385193441	2.1094436346
N2	2.2193942360	0.1918336963	1.3117865930
C3	2.8655114227	1.3426806627	1.0654999040
H4	2.3836448702	2.2438156534	1.4278157029
C5	4.1065100101	1.3629429899	0.4347594561
H6	4.5966954318	2.3114381676	0.2454660662
C7	4.6907808899	0.1550652401	0.0624182551
H8	5.6553628299	0.1369830872	-0.4349793050

C9	4.0288648141	-1.0382057182	0.3446714637
H10	4.4789146617	-1.9853320717	0.0750676405
C11	2.7843134823	-0.9949201753	0.9754182795
C12	2.0036544881	-2.1954329647	1.3389392205
C13	2.4047841321	-3.5021297230	1.0584663397
H14	3.3386021961	-3.6894133358	0.5432091473
C15	1.5890702554	-4.5667962163	1.4332095191
H16	1.8904846298	-5.5858334810	1.2131271133
C17	0.3836871068	-4.3055270382	2.0799917281
H18	-0.2857128817	-5.1043209291	2.3782798648
C19	0.0317084812	-2.9842570999	2.3319500601
H20	-0.9033103732	-2.7051053048	2.8011691185
N21	0.8297538491	-1.9638424855	1.9788965685
N22	-0.4378361384	2.0537455492	1.6666227610
C23	-1.0919326561	2.0507011519	0.4785342296
C24	-1.8342795359	3.1370438960	0.0329701561
H25	-2.3152357667	3.0578335308	-0.9352150219
C26	-1.9341286790	4.2585418464	0.8491312974
H27	-2.5211237395	5.1190466505	0.5431473136
C28	-1.2439707205	4.2701365185	2.0588922716
H29	-1.2592517249	5.1432588438	2.7014947773
C30	-0.4778712415	3.1654497713	2.4432990899
C31	0.3542051210	3.2546953303	3.6759251549
C32	-0.2170552068	3.6178234855	4.8999407441
H33	-1.2878954700	3.7743698698	4.9825707210
C34	0.6187332525	3.7591160390	6.0066290968
H35	0.2088559929	4.0358388239	6.9733701518
C36	1.9862816241	3.5430006697	5.8464635803
H37	2.6750524939	3.6512626269	6.6779289856
C38	2.4598904344	3.1909750379	4.5814580908
H39	3.5221740977	3.0224623680	4.4180577774
N40	1.6699544604	3.0490289393	3.5123658058
C41	-0.9920943069	0.8042196696	-0.3837390623
O43	-1.4198087312	0.8185299534	-1.5216132597
O44	0.7899578997	0.3506868431	3.9525519251
O45	-1.5052348886	-0.4922018592	2.7838140865
O46	0.4290477598	-0.7402756559	4.8044357626
H47	-1.5131381864	-0.3685799472	3.7509858692
H48	0.7193627644	-0.3986134718	5.6678733760

Figure S1B

E (M06/LACV3P++ 2f(Ru))** = -1422.23880131319

ZPE (kcal mol^{-1}) = 206.878

G_{solv} = -0.0770534

DH_{298} (kcal mol^{-1})= 16.026

DS_{298} (cal K^{-1} mol^{-1})= 171.538

Cartesian coordinates

atom	x	y	z
O42	-1.7395298447	-0.1056099928	2.3052635310
Ru1	0.1322509879	0.0709106260	1.8145580965
N2	2.4166945712	-0.3220486146	1.4686172572
C3	3.3982224182	0.5785467287	1.3794477323
H4	3.1049041741	1.6187196345	1.4534519236
C5	4.7320894786	0.2143369669	1.2074115715
H6	5.4993338064	0.9775967216	1.1390904270
C7	5.0442919474	-1.1405081393	1.1318487228
H8	6.0703699710	-1.4677318471	0.9967239439
C9	4.0227720462	-2.0787109389	1.2517795536
H10	4.2584372585	-3.1353084364	1.2252994187
C11	2.7058432242	-1.6396074743	1.4292242554
C12	1.5721268835	-2.5686909877	1.6459287042
C13	1.7003700990	-3.9588850290	1.5928629625
H14	2.6505074737	-4.4094442489	1.3360031071
C15	0.6029674062	-4.7702795622	1.8680646104
H16	0.7015238490	-5.8503065581	1.8245516694
C17	-0.6137115678	-4.1798507804	2.1994999568
H18	-1.4926471654	-4.7718671948	2.4277332291
C19	-0.6949712763	-2.7928066136	2.2257780246
H20	-1.6144214613	-2.2686745057	2.4591491468
N21	0.3687088193	-2.0168238745	1.9511476257
N22	-0.5421896919	2.1556875473	1.6522539866
C23	-1.7187106378	2.2782897256	2.3005168110
C24	-2.2982105699	3.5055437758	2.5932511621
H25	-3.2478530895	3.5183727006	3.1160341816
C26	-1.6309450448	4.6593074940	2.1919616520
H27	-2.0378084860	5.6414550093	2.4105351097
C28	-0.4548757595	4.5306290107	1.4601357519
H29	0.0455174265	5.4058446433	1.0622320386
C30	0.0695794529	3.2610007596	1.1778715676
C31	1.2276510348	3.1323921664	0.2528512398
C32	2.2974812305	4.0389000928	0.2757625384
H33	2.3587979802	4.8063770600	1.0405487732
C34	3.2872707709	3.9207334143	-0.6998833733
H35	4.1277396936	4.6081071917	-0.7117982171
C36	3.1805859794	2.9102096442	-1.6548750847
H37	3.9238462735	2.7929805950	-2.4367274047
C38	2.0881373153	2.0412721050	-1.5859919256
H39	1.9655879621	1.2288420827	-2.2977893117
N40	1.1362202248	2.1574567706	-0.6602092475

C41	-2.4262326316	1.0003637433	2.6424872956
O43	-3.5225513698	0.9642770039	3.1446281070
O44	0.8962879889	0.5295421510	3.3612910335
O45	0.2626147332	-0.0810813128	-0.0107347636

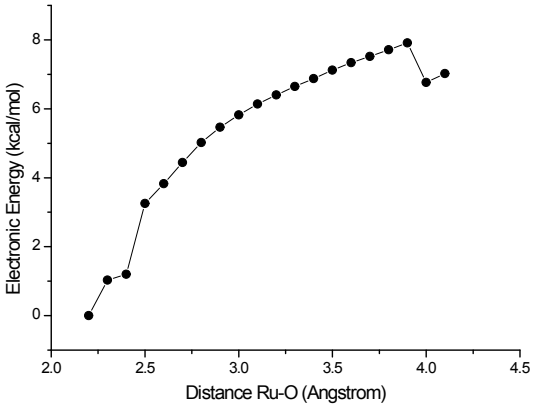


Figure S2. Scan result of dissociation of oxygen $\mathbf{9}_{\mathbf{end\text{-}on}}$ [(bpc)(bpy)$Ru^{IV}OO]^{+}$. The electronic energies were obtained using Becke's three-parameter hybrid functional and the LYP correlation functional (B3LYP) together with the LACVP** core potential and basis set.

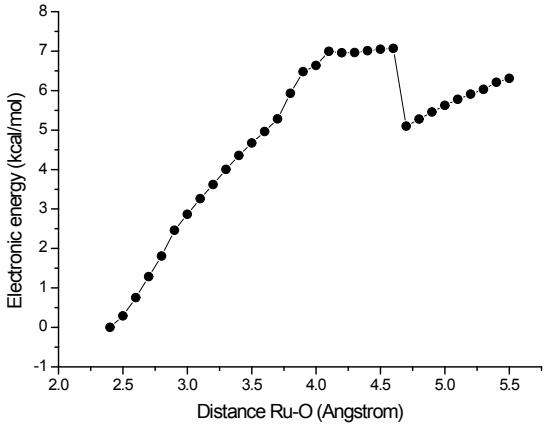


Figure S3. Scan result of dissociation of oxygen $\mathbf{12}_{\mathbf{end\text{-}on}}$ [(bpc)(bpy)$Ru^{V}OO]^{+}$. The electronic energies were obtained using Becke's three-parameter hybrid functional and the LYP correlation functional (B3LYP) together with the LACVP** core potential and basis set.