

Supporting Information for

Half-sandwich Ruthenium Phenolate-Oxazoline Complexes: Experimental and Theoretical Studies in Catalytic Transfer Hydrogenation of Nitroarene

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Table S1 Crystallographic Data and Structure Refinement Parameters for Ru complexes

	1	2	3	4	5
Empirical formula	C ₁₉ H ₂₂ ClNO ₂ Ru	C ₂₀ H ₂₄ ClNO ₂ Ru	C ₂₁ H ₂₆ ClNO ₂ Ru	C ₂₅ H ₂₆ ClNO ₂ Ru	C ₄₂ H ₅₂ Cl ₂ N ₂ O ₄ Ru
Formula weight	432.90	446.92	460.95	508.99	921.90
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic
Space group	P2 ₁ /c	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ /c	Pbca
a(Å)	9.7633(8)	10.1321(6)	10.3160(5)	13.2107(7)	13.7849(13)
b (Å)	14.3925(14)	12.5288(7)	13.1204(6)	11.5403(6)	19.1553(19)
c (Å)	12.9991(8)	15.0763(9)	14.5756(7)	15.3298(8)	30.872(3)
α (°)	90.00	90.00	90.00	90.00	90.00
β (°)	98.53	90.00	90.00	110.4930(10)	90.00
γ (°)	90.00	90.00	90.00	90.00	90.00
Volume (Å ³), Z	1806.4(3), 4	1913.83(19), 4	1972.81(16), 4	2189.2(2), 4	8151.7(14), 8
D _c (mg / m ³)	1.592	1.551	1.552	1.544	1.502
μ (Mo-Kα) (mm ⁻¹)	1.026	0.971	0.945	0.860	0.915
F(000)	880	912	944	1040	3776
θ range (°)	2.11 ~ 24.99	2.42 ~ 27.42	2.09 ~ 27.55	1.65 ~ 27.53	1.32 ~ 27.52
Reflections/unique[R	3177 / 2818 [0.0210]	4319/3725 [0.0309]	4510/4368 [0.0211]	4965/4498 [0.0184]	9295/7722 [0.0380]
Completeness to θ (°)	24.99 (99.8 %)	27.51 (98 %)	27.55 (99 %)	27.53 (98.8 %)	27.52 (99.2 %)
Data/restraints/param	3177 / 253 / 217	4319 / 0 / 230	4510 / 0 / 236	4965 / 0 / 274	9295 / 0 / 479
Goodness-of-fit on F ²	1.020	1.035	1.165	1.040	1.056
R ₁ , wR ₂ [I > 2σ(I)] ^a	R ₁ = 0.0300, wR ₂ = 0.1142	R ₁ = 0.0256, wR ₂ = 0.0554	R ₁ = 0.0176, wR ₂ = 0.0416	R ₁ = 0.0228, wR ₂ = 0.0258	R ₁ = 0.0305, wR ₂ = 0.0735
R ₁ , wR ₂ (all data)	R ₁ = 0.0366, wR ₂ = 0.1364	R ₁ = 0.0340, wR ₂ = 0.0589	R ₁ = 0.0189, wR ₂ = 0.0430	R ₁ = 0.0604, wR ₂ = 0.0624	R ₁ = 0.0415, wR ₂ = 0.0810

^a R₁ = Σ||F_o|-|F_c||/Σ|F_o|; wR₂ = [Σw(|F_o²|-|F_c²|)²/Σw|F_o²|²]^{1/2}.

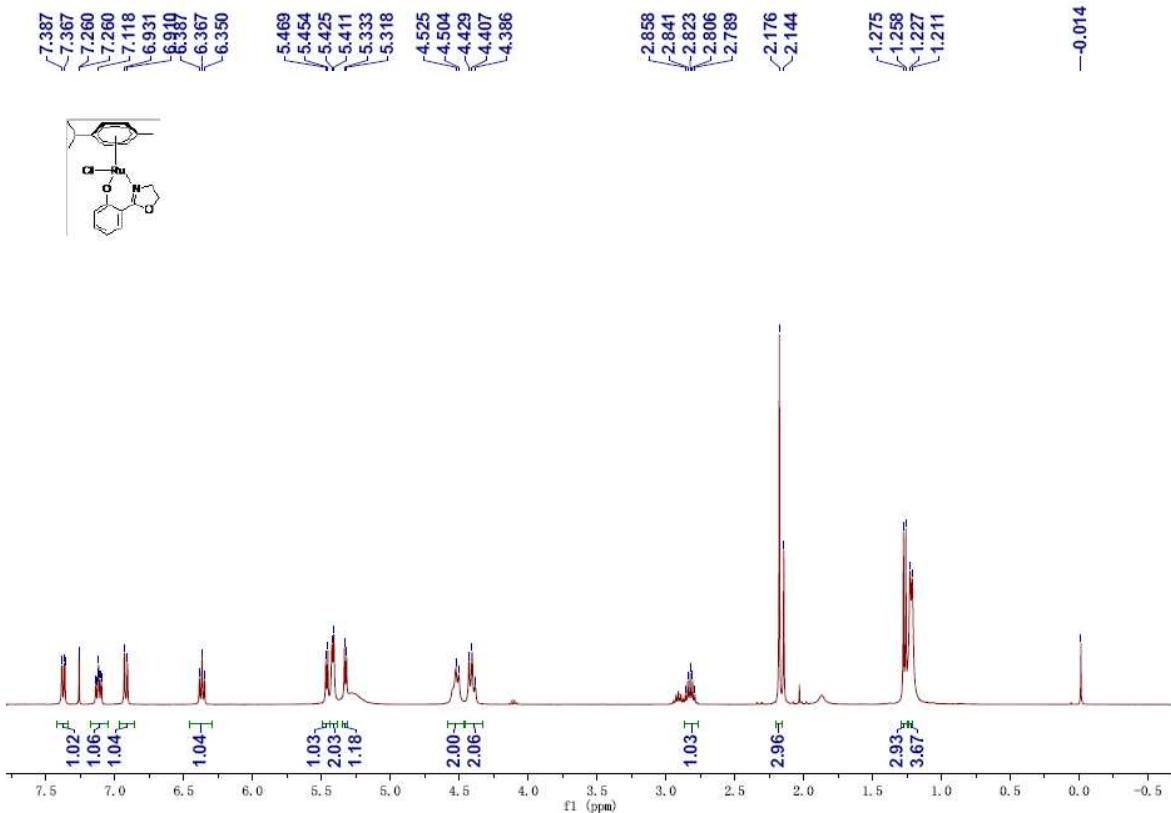


Figure S1. The ^1H NMR of half-sandwich ruthenium complex **1**

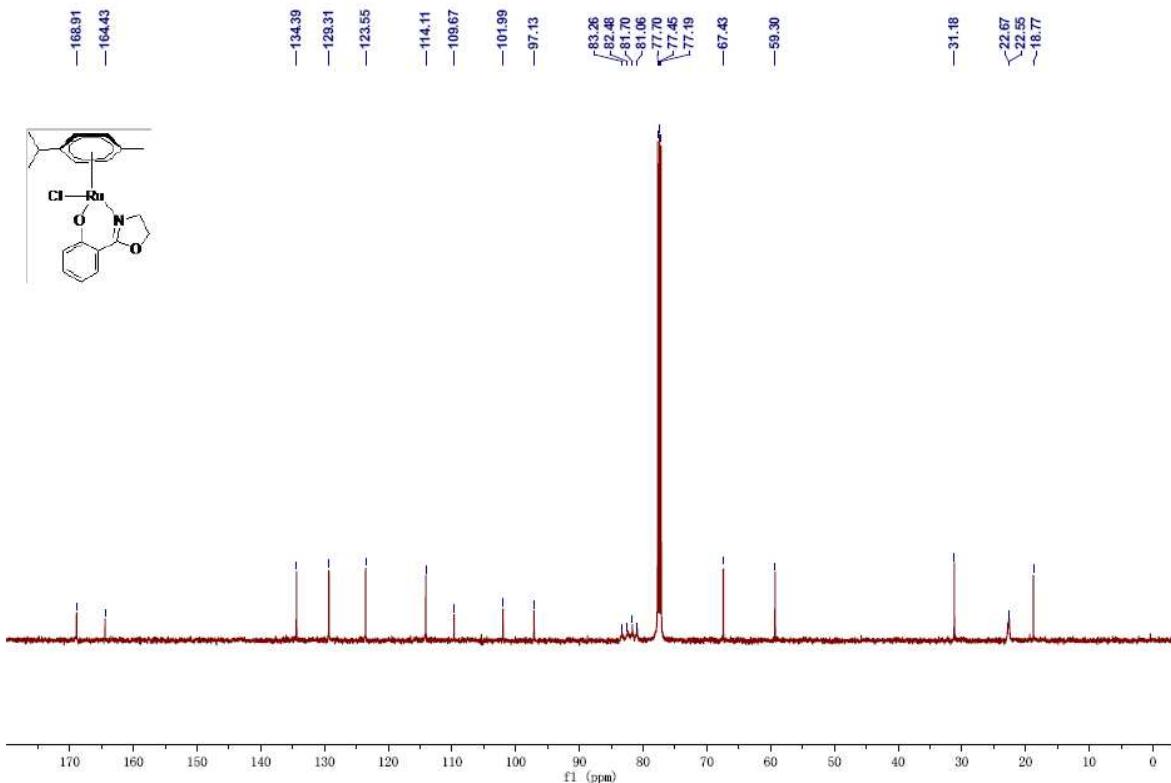


Figure S2. The ^{13}C NMR of half-sandwich ruthenium complex **1**

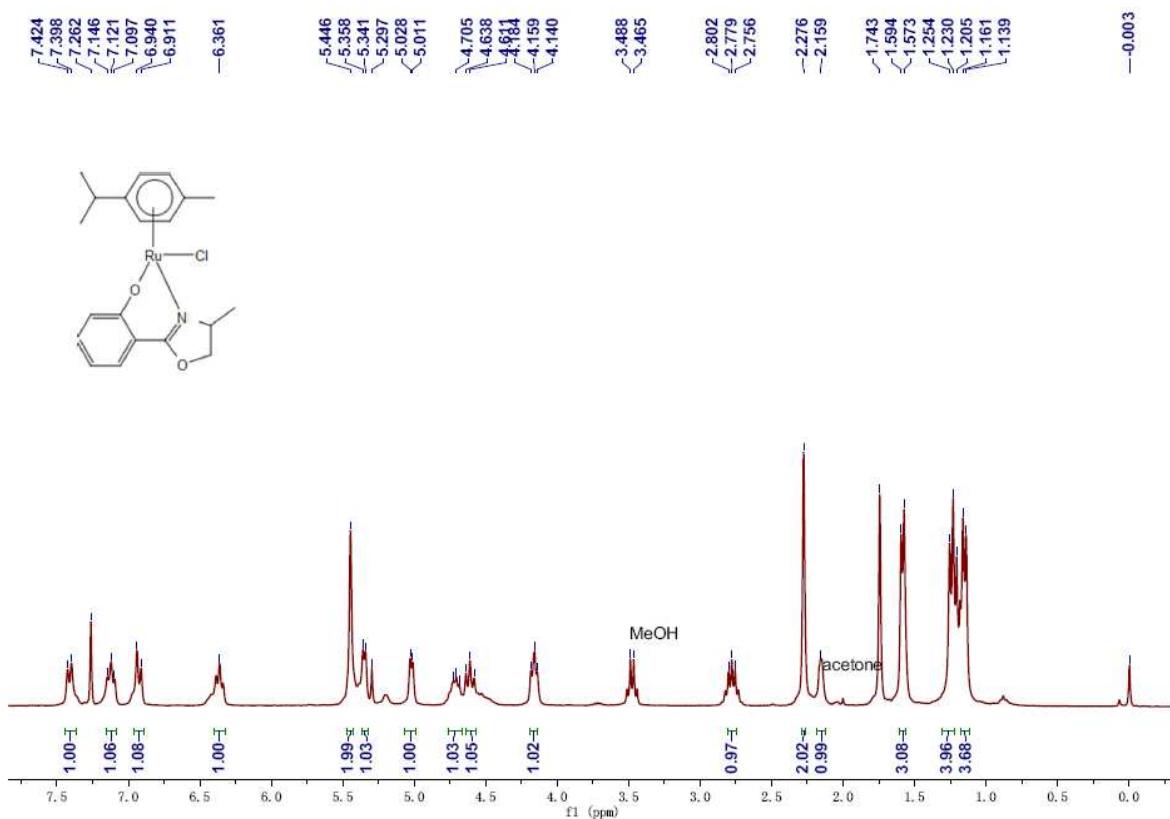


Figure S3. The ¹H NMR of half-sandwich ruthenium complex **2**

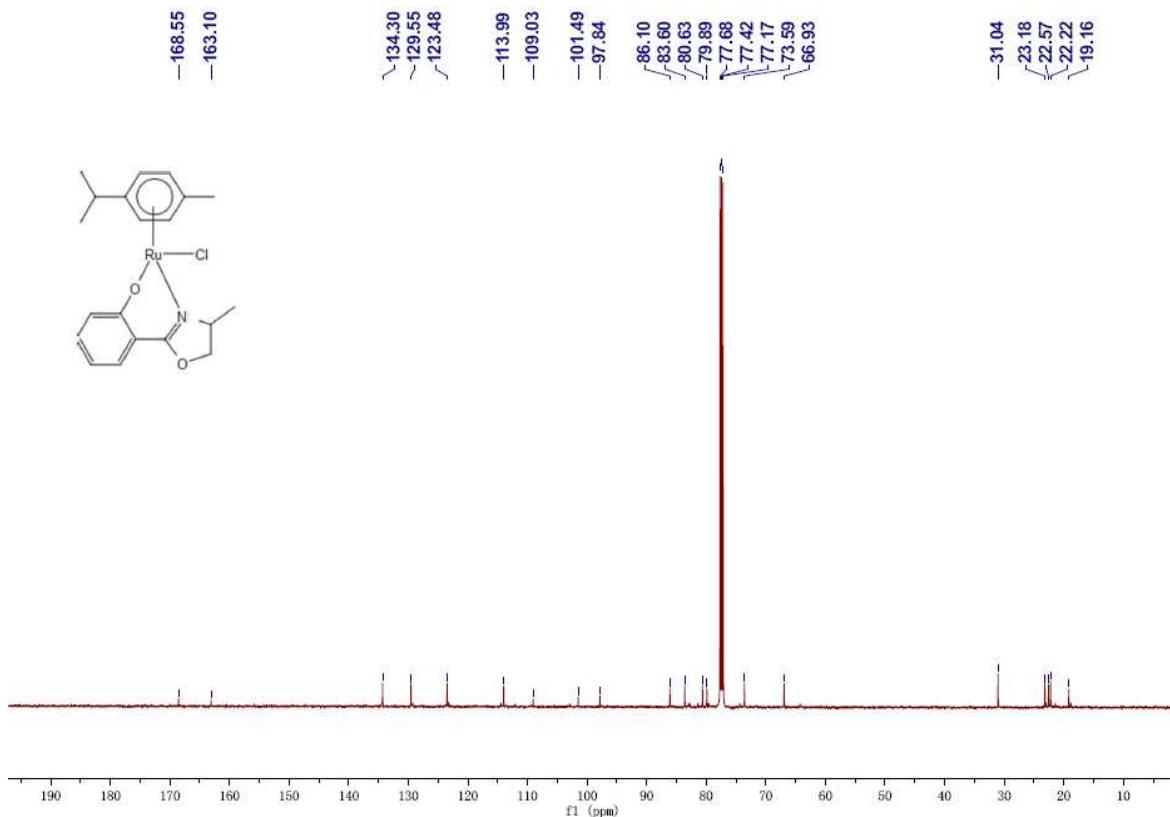


Figure S4. The ¹³C NMR of half-sandwich ruthenium complex **2**

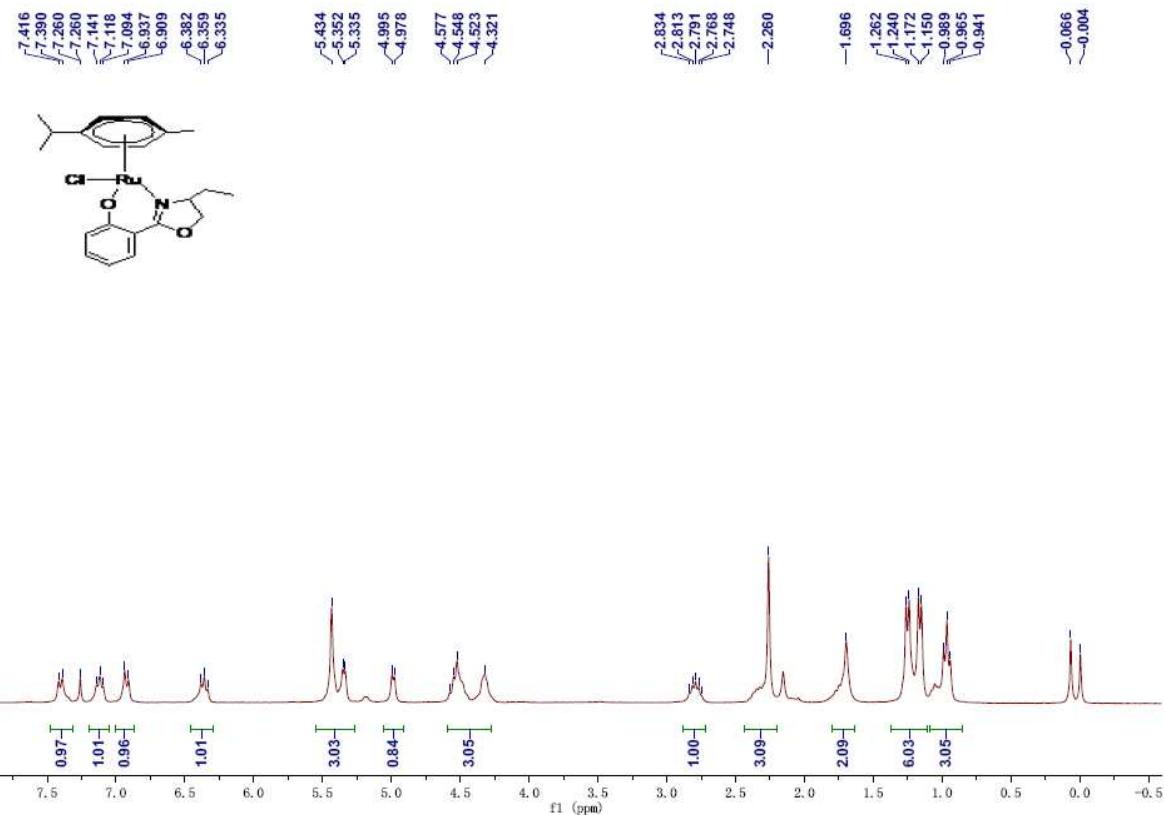


Figure S5. The ¹H NMR of half-sandwich ruthenium complex **3**

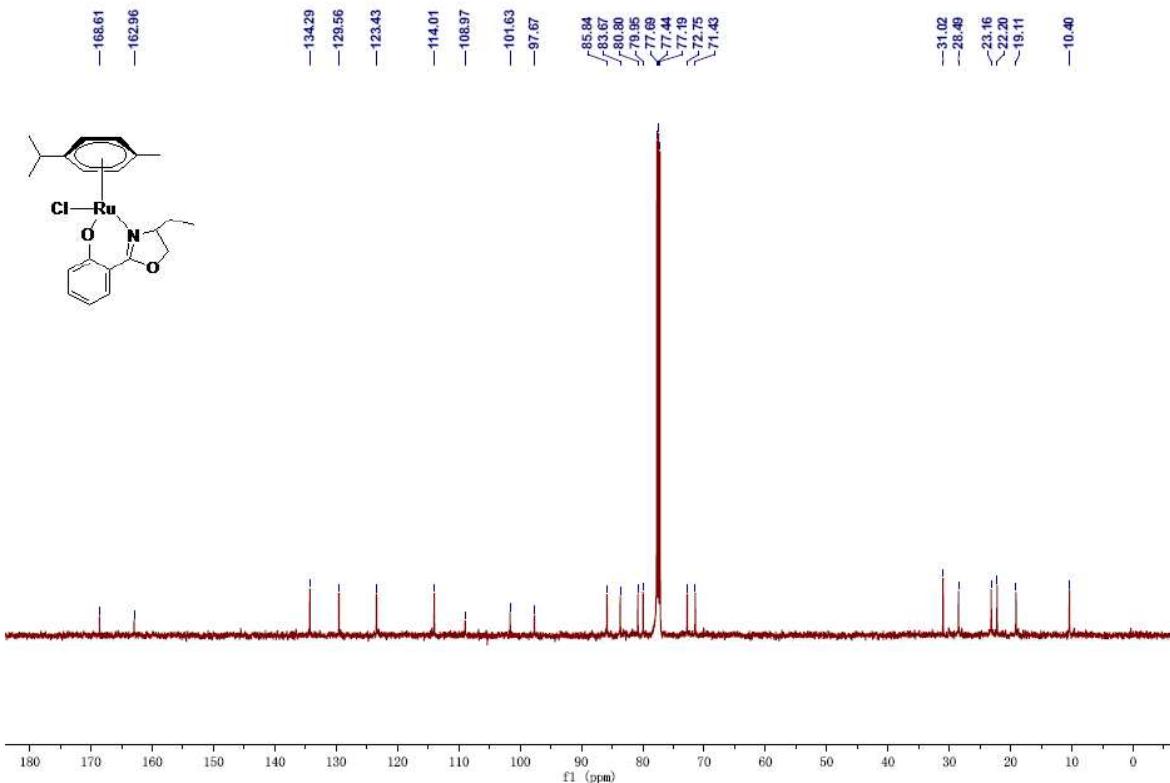


Figure S6. The ¹³C NMR of half-sandwich ruthenium complex **3**

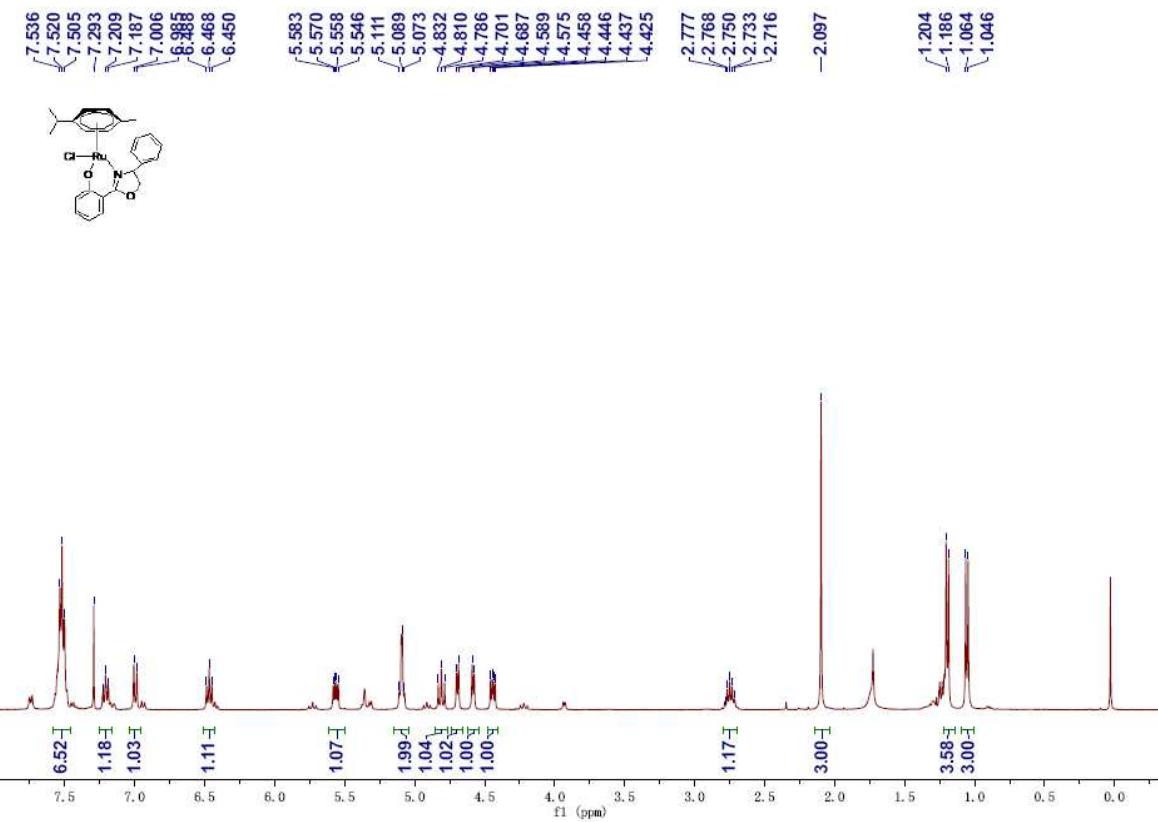


Figure S7. The ^1H NMR of half-sandwich ruthenium complex 4

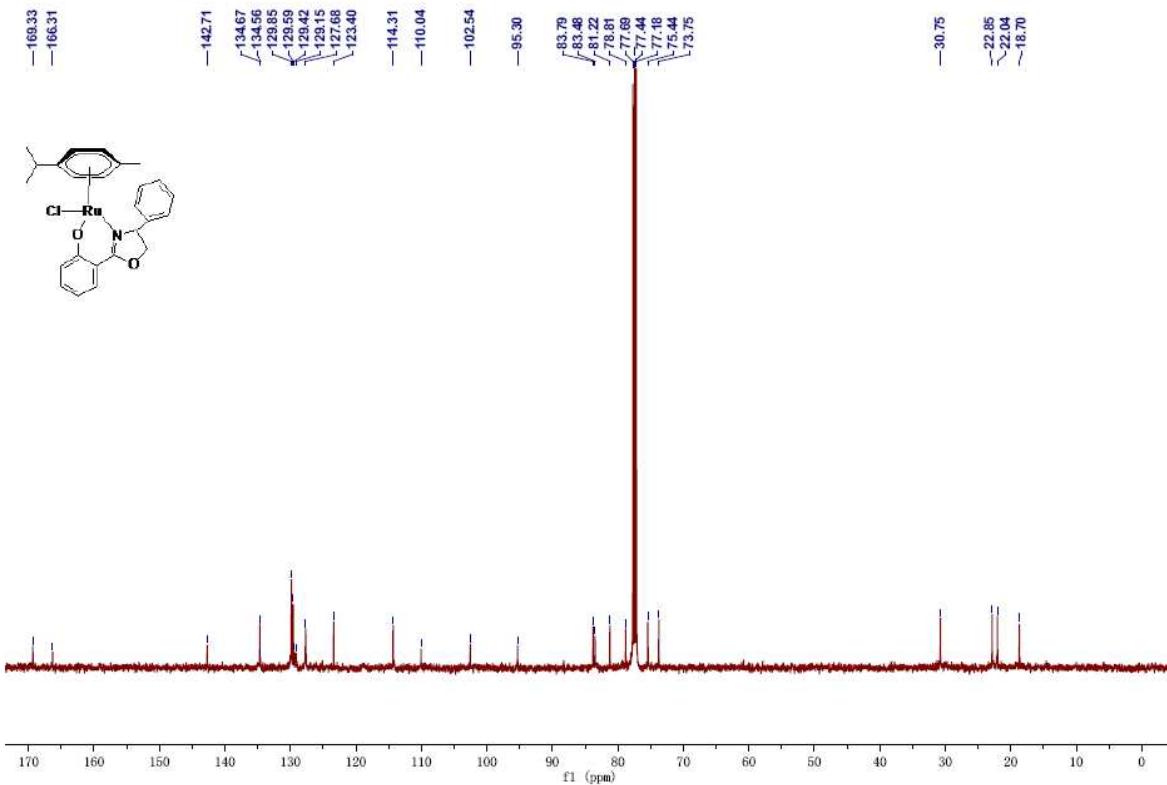


Figure S8. The ^{13}C NMR of half-sandwich ruthenium complex 4

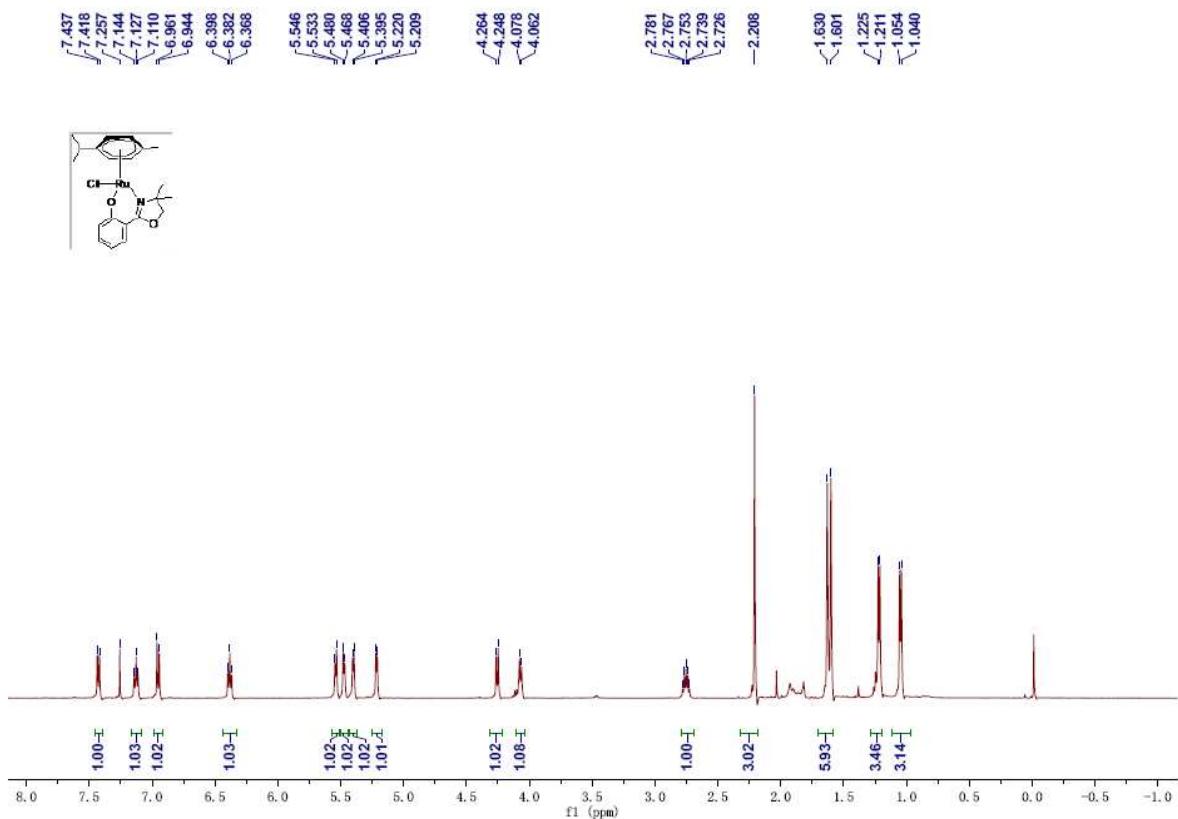


Figure S9. The ¹H NMR of half-sandwich ruthenium complex **5**

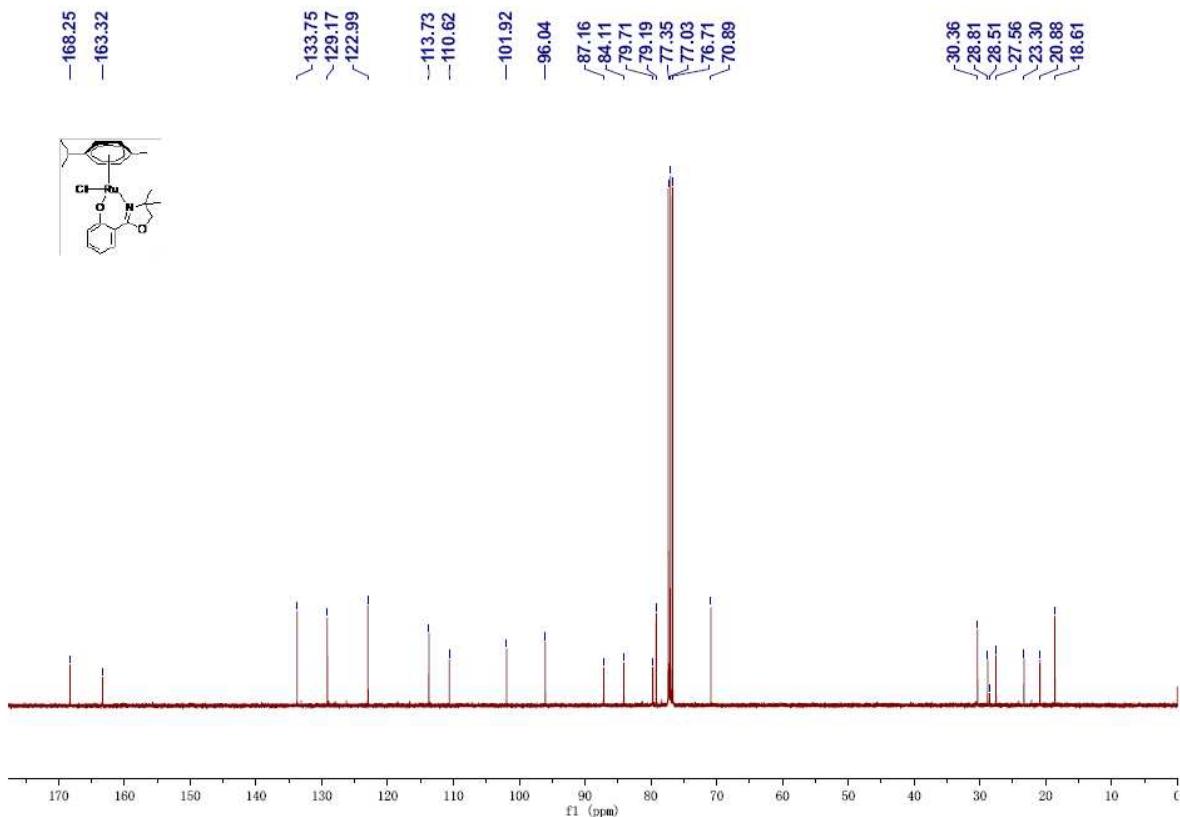


Figure S10. The ¹³C NMR of half-sandwich ruthenium complex **5**

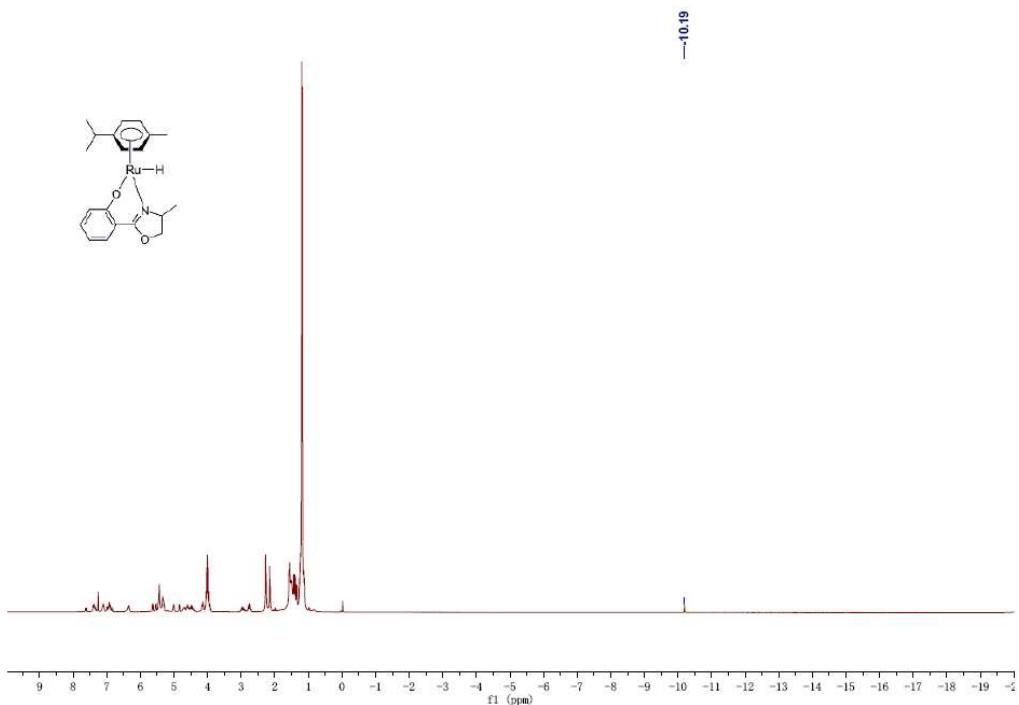


Figure S11. The *in situ* ^{1}H NMR of complex **2** reaction with isopropanol

Theoretical details

Density functional theory studies were carried out with Gaussian 09¹ computational chemistry suite. Geometries of gas phase minimum and transition state electronic structures were optimised using the Minnesota meta hybrid functional M11-L² with Stuttgart-Dresden effective core potential SDD^{3,4} for Cu and Pople's basis set 6-31+G(d,p)^{5,6} for rest of the atoms. Frequency calculations were carried out at that level to ensure convergence (all positive eigenvalues for minima and single negative for saddle points). Thermochemical corrections and zero point vibrational energies, as well as the infrared, were determined at the gas phase M11-L/6-31+G(d,p)+SDD level using the unscaled frequencies. Solvation energies were considered with single point calculations with the SMD model⁷ (2-propanol parameters) on gas phase optimized structures carried out with same functional M11-L and basis set. The electronic energies together with thermal and vibrational corrections based on gas-phase vibrations and solvation energies constitute the solution free energy, ΔG_{sol} , reported throughout the manuscript.

REFERENCES

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Table S2 Table of energies: minimum and transition state structures

	Energy	$G_{\text{correction}}$	$H_{\text{correction}}$	ZPE	G	$\Delta G_{\text{solvation}}$	ΔG_{sol}
cymene	-389.4302305	0.17202	0.219937	0.208382	-389.25821	-5.72	-389.267326
acetone	-193.1032413	0.055117	0.087647	0.082076	-193.04812	-6.19	-193.0579889
nitrobenzene	-436.6232413	0.07035	0.10993	0.102134	-436.55289	-5.73	-436.5620227
iPrOH	-194.3108964	0.07919	0.112989	0.106564	-194.23171	-6.47	-194.2420172
h2o	-76.40449206	0.004499	0.025896	0.022117	-76.399993	-8.33	-76.41326796
cpxA	-1152.478895	0.35503	0.433772	0.407958	-1152.1239	-20.36	-1152.156311
cpxB	-1346.814177	0.454613	0.549431	0.516873	-1346.3596	-19.25	-1346.390241
cpxC	-1270.390798	0.431386	0.51956	0.489428	-1269.9594	-17.45	-1269.987221
cpxD	-1077.267668	0.350632	0.426246	0.401902	-1076.917	-16.1	-1076.942693
cpxE	-1151.69191	0.358942	0.442234	0.415117	-1151.333	-19.24	-1151.363629
TS1	-1151.686276	0.35813	0.438779	0.412192	-1151.3281	-17.95	-1151.356751
cpxF	-1151.678084	0.352951	0.43909	0.410723	-1151.3251	-22.21	-1151.360528
TS2-os	-1513.876589	0.438962	0.533246	0.500618	-1513.4376	-19.16	-1513.468161
cpxG	-1513.923534	0.445776	0.540744	0.50821	-1513.4778	-22.46	-1513.51355
cpxJ	-1395.21313	0.369675	0.460645	0.430479	-1394.8435	-22.24	-1394.878897
TS2-is	-1395.160187	0.366633	0.457235	0.427414	-1394.7936	-21.63	-1394.828024

cpxK	-1395.211302	0.370415	0.463066	0.432529	-1394.8409	-29.23	-1394.887468
cpxH	-1318.796091	0.348493	0.434457	0.406574	-1318.4476	-23.89	-1318.48567
TS3	-1318.791166	0.346824	0.431496	0.403903	-1318.4443	-23.6	-1318.481952
cpxL	-1242.392941	0.319647	0.403333	0.376852	-1242.0733	-27.81	-1242.117613
cpxM	-1242.391319	0.315342	0.400427	0.373484	-1242.076	-27.84	-1242.120343
cpxN	-1243.632503	0.345409	0.428574	0.401468	-1243.2871	-20.78	-1243.32021
cpxO	-1243.644789	0.346817	0.429791	0.403135	-1243.298	-20.87	-1243.331231

All values in hartrees except for $\Delta G_{\text{solvation}}$ in kcal/mol.

1. Gaussian archive files

cymene

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nitrobenzene

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 987,0.101589\|O,3.190913,-1.725245,0.089971\|C,2.622422,-2.973342,-0.264
 855\|H,3.143128,-3.76201,0.299717\|H,2.791252,-3.128408,-1.34575\|C,1.154
 706,-2.818254,0.091864\|H,0.495287,-3.229653,-0.694655\|C,0.848505,-3.42
 3102,1.441631\|H,1.528784,-3.02539,2.212797\|H,0.970137,-4.517318,1.4119
 28\|H,-0.177798,-3.215637,1.767324\|C,-2.701686,-3.064748,0.15023\|H,-3.7
 63551,-3.325915,0.292636\|H,-2.128389,-3.635966,0.894066\|H,-2.406155,-3
 .417258,-0.850406\|C,-1.704179,2.690593,0.553476\|H,-0.667827,2.75545,0.
 945094\|C,-1.750433,3.415704,-0.769941\|H,-1.381038,4.445569,-0.645931\|H
 ,-2.782515,3.496786,-1.153212\|H,-1.12843,2.92082,-1.530073\|C,-2.633603
 ,3.348434,1.557179\|H,-2.383855,4.414253,1.678186\|H,-2.581604,2.878197,
 2.551351\|H,-3.682073,3.290732,1.21859\|O,-0.416379,-1.218631,-2.103393\|
 H,0.338897,-0.742386,-2.457372\\Version=ES64L-G09RevE.01\\State=1-A\\HF=
 -1152.4788947\\RMSD=2.901e-09\\RMSF=3.976e-06\\Dipole=-0.6163589,-0.73640
 14,1.199672\\Quadrupole=-0.3864965,7.97243,-7.5859335,-3.1462252,0.6808
 292,-2.5667691\\PG=C01 [X(C20H25N1O3Ru1)]\\@\\

cpxB

1\\1\\GINC-R2447\\FOpt\\RM11L\\GenECP/Auto\\C23H33N1O4Ru1\\ROOT\\28-Mar-2017\\0
 \\# m11l/genecp/auto opt=(cartesian,maxcyc=200) scf=(maxcyc=200,novara
 cc) # iop(5/13=1,2/11=1,1/8=1) int=ultrafine freq\\Complex A2 Ru(II)-O
 H---iPrOH substrate\\0,1\\H,-2.2424996401,-1.3360784661,2.1281104817\\C,
 -1.4155397184,-1.7566931424,1.548638849\\C,0.7447260855,-2.6730102823,0
 .0183421178\\C,-0.1054007284,-1.6716788543,2.0317734402\\C,-1.6555692518
 ,-2.2801442125,0.2547937771\\C,-0.5659632533,-2.7683794536,-0.495227600
 3\\C,1.0129584378,-2.1498474399,1.2954791078\\H,0.064708972,-1.192424029
 1,3.0020707174\\H,-0.7113425778,-3.1046940727,-1.5225648279\\H,1.5910237
 954,-2.924636765,-0.6311822064\\Ru,-0.1484859518,-0.7007498846,0.059219
 3633\\O,-1.5459101406,0.2981489738,-1.0251736335\\C,-2.1505762801,1.3795
 68765,-0.7012984279\\C,-3.5026608561,3.8245641999,-0.2379684096\\C,-1.53
 41990096,2.4509769313,-0.0063132915\\C,-3.481321618,1.5805382128,-1.124
 7945926\\C,-4.1325945828,2.7690961519,-0.897355091\\C,-2.2066360403,3.65
 96766608,0.1905505279\\H,-3.9634364159,0.7630868669,-1.6711296427\\H,-5.
 1634572481,2.889606094,-1.2477321479\\H,-1.6862590086,4.4732333331,0.70
 49025539\\H,-4.0275584839,4.7666227501,-0.0669811653\\C,-0.1893733379,2.
 2934688644,0.4577073632\\N,0.431646656,1.1916814972,0.6959808421\\O,0.50
 52894028,3.4031450847,0.6986459064\\C,1.854236064,2.9864248138,0.830447
 8184\\H,2.3442502899,3.6373572882,1.5697070157\\H,2.348402656,3.10892853
 91,-0.1515750479\\C,1.7286200375,1.5393645873,1.2556723137\\H,2.51163370
 24,0.9013442974,0.8057843889\\C,1.7211547518,1.420159599,2.7626020047\\H
 ,0.9984999062,2.1257475559,3.2052054378\\H,2.7166060288,1.6466305955,3.
 17537187\\H,1.4438416113,0.4140562465,3.0975733913\\C,2.3955233812,-2.13
 31349546,1.8389725685\\H,2.6526818517,-3.1214427953,2.2555980058\\H,2.50
 72236231,-1.4070633496,2.6565029398\\H,3.1311514366,-1.8893379485,1.058

6797045\|C,-3.0598561498,-2.2556680744,-0.2821474577\|H,-3.4824285863,-1
 .2734633453,0.0142076473\|C,-3.1481628688,-2.3667278873,-1.7846489676\|H
 ,-4.1884977448,-2.214501929,-2.1114179764\|H,-2.8526526764,-3.369562316
 2,-2.1384193929\|H,-2.5225643615,-1.6139196822,-2.2859931944\|C,-3.86884
 15535,-3.3473208054,0.3939147337\|H,-4.9193373111,-3.3123294501,0.06566
 22602\|H,-3.8590553541,-3.2598444473,1.4916649101\|H,-3.4748984021,-4.34
 54735692,0.1379811416\|O,0.9968839647,-0.2481815555,-1.502026388\|H,0.55
 31568044,0.4751259706,-1.948403118\|H,2.6185275213,-0.477768136,-1.1900
 865473\|O,3.5192700408,-0.7106015469,-0.8875441222\|C,4.4387712038,-0.12
 04468091,-1.7377305504\|H,4.2904161974,-0.4877065472,-2.7830149025\|C,4.
 2900454553,1.3842639413,-1.7493609767\|H,4.4824065542,1.7927413236,-0.7
 400452747\|H,3.2687385028,1.6769573685,-2.045367226\|H,4.9936049881,1.86
 41982251,-2.4488295659\|C,5.8093798096,-0.5369690248,-1.2798802242\|H,5.
 9049647551,-1.6326572204,-1.2739116052\|H,5.9902911448,-0.1788166588,-0
 .252027593\|H,6.5971755195,-0.1254150819,-1.9286910324\|Version=ES64L-G
 09RevE.01\State=1-A\HF=-1346.8141769\RMSD=4.626e-09\RMSF=6.141e-05\Dep
 ole=-0.1837162,-0.3195635,1.2199084\Quadrupole=-0.4016288,1.4526586,-1
 .0510298,6.1933055,3.3631406,1.5058535\PG=C01 [X(C23H33N1O4Ru1)]\@\@

cpxC

1\1\GINC-CN474\FOpt\RM11L\GenECP/Auto\C23H31N1O3Ru1\HNAN_JZY\22-Mar-20
 17\0\#\ m11l/genecp/auto opt=maxcyc=200 scf=(maxcyc=200,novaracc) # io
 p(5/13=1,2/11=1) int=ultrafine freq\Complex B Ru(II)-OiPr\0,1\H,2.70
 44827042,0.3660059633,1.6093938351\|C,2.2312271662,1.0292970488,0.87988
 63695\|C,0.8965256214,2.6649777206,-0.9601448974\|C,1.3484095136,2.03735
 06079,1.3116843195\|C,2.409780822,0.8033383993,-0.4997218909\|C,1.759031
 5711,1.660040852,-1.4230156136\|C,0.6748544166,2.8993540702,0.414240312
 8\|H,1.1561732949,2.1361609617,2.3860150988\|H,1.8257187666,1.4711618972
 ,-2.4959199906\|H,0.2787053129,3.2021627894,-1.6880972242\|Ru,0.24264215
 5,0.7959653303,-0.1005869765\|O,0.3046431766,-1.0958349531,-0.837251390
 4\|C,0.1371245102,-2.18933325,-0.1976712592\|C,-0.3049460114,-4.71411804
 73,1.0162427808\|C,-0.7402845572,-2.3437939228,0.9069167321\|C,0.7979786
 077,-3.3549246501,-0.6450016301\|C,0.581518199,-4.5746999616,-0.0521044
 223\|C,-0.9666104082,-3.6002264587,1.4746860273\|H,1.4681585836,-3.25315
 77833,-1.5047831459\|H,1.11065567,-5.4549330965,-0.4333349259\|H,-1.6769
 299307,-3.6807057839,2.303383962\|H,-0.4745278903,-5.6898031563,1.47619
 95155\|C,-1.4562585973,-1.2016841145,1.3863406793\|N,-1.1270008071,0.034
 9515012,1.2633734749\|O,-2.5936584855,-1.4263181597,2.0397849199\|C,-3.2
 634822683,-0.179510246,2.0838798498\|H,-3.7974466007,-0.1088368149,3.04
 3792554\|H,-3.9965442985,-0.1578950805,1.2559693859\|C,-2.1470067496,0.8
 338445564,1.9154944232\|H,-2.4385194893,1.6540099747,1.2328728706\|C,-1.
 6773173024,1.363154843,3.2504389072\|H,-1.4216293158,0.5350830539,3.932
 1111167\|H,-2.4664376712,1.9654683308,3.7275799296\|H,-0.7888973545,2.00
 00440226,3.1576443022\|C,-0.2631981021,3.9618406645,0.8563469313\|H,0.18
 57495955,4.9634878125,0.7537255344\|H,-0.5496485839,3.8428802895,1.9111
 584109\|H,-1.1822984319,3.9464046242,0.2493229964\|C,3.2616395439,-0.355

666668,-0.9426983972\H,2.9570900894,-1.2182830317,-0.3150119726\C,3.07
 60110627,-0.7412198917,-2.3903913305\H,3.6384274069,-1.662455922,-2.60
 77687924\H,3.4669361576,0.0340449198,-3.0720632023\H,2.0191715533,-0.9
 267825469,-2.6334933541\C,4.7191274656,-0.0449424666,-0.6536035152\H,5
 .3584855791,-0.9012977232,-0.9193171885\H,4.8983044564,0.188594297,0.4
 073661161\H,5.0626081164,0.8204590731,-1.245384185\O,-1.4800777022,1.1
 849622305,-1.0348213456\C,-2.1164060221,0.247587198,-1.7938254747\H,-2
 .1363731188,-0.7570374883,-1.2894474377\C,-3.5548762483,0.691596993,-1
 .9658963496\H,-3.5934658765,1.6705178862,-2.4740229274\H,-4.0479563271
 ,0.8115720176,-0.9863194619\H,-4.1423985995,-0.0283904171,-2.559283901
 5\C,-1.4477776769,0.0699670405,-3.1423317588\H,-0.3981939841,-0.238420
 8331,-3.0129423305\H,-1.460334197,1.0278111184,-3.6935086439\H,-1.9474
 447102,-0.6912069903,-3.7654880395\\Version=ES64L-G09RevE.01\\State=1-A
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 255,1.2023252\Quadrupole=0.7953114,0.007572,-0.8028833,-1.8307564,-7.6
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cpxD

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1\1\GINC-R95\FOpt\RM11L\GenECP/Auto\C20H25N1O2Ru1\ROOT\11-Jan-2017\0\\
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=1,2/11=1) int=ultrafine freq\Complex 1 Ru(II)-hydride\\0,1\H,0.92807
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8417\C,-1.1594575028,0.5646619215,2.6581568049\C,-1.0358133819,-1.7909
286556,2.0435154926\C,1.0135305945,-0.5178397092,2.3979166485\C,0.2519
978039,0.6029349959,2.7617909372\C,-1.8121740886,-0.6032096669,2.22715
26111\H,-1.5411380097,-2.7258248904,1.7761760034\H,0.7458992856,1.5428
22977,3.0172053701\H,-1.7481098183,1.4625819316,2.8683040389\Ru,-0.285
7121867,0.0548612379,0.7410314067\H,-0.2462865543,1.5726448595,0.34178
34786\O,1.3563239334,-0.0663197238,-0.4374840638\C,1.5148316906,0.4521
33399,-1.5898657615\C,2.0183841838,1.6077908247,-4.1323013668\C,0.4572
777834,0.7644936724,-2.4902141273\C,2.8280115103,0.7131164276,-2.04293
31684\C,3.0663953541,1.2814057965,-3.2683258625\C,0.7317775359,1.33450
04606,-3.7402791515\H,3.6468044395,0.4597626742,-1.3624595629\H,4.0993
385746,1.4884123043,-3.5695496312\H,-0.10609705,1.5596222403,-4.406491
599\H,2.2184205277,2.0641517779,-5.103946938\C,-0.8814487521,0.3855062
382,-2.1730110329\N,-1.3474229052,-0.0202416717,-1.0414183671\O,-1.764
2257382,0.4087765367,-3.1739576719\C,-3.0321697861,0.1983199695,-2.590
6638452\H,-3.6243643458,-0.4300195173,-3.2735002065\H,-3.5324049547,1.
1779712865,-2.4785723365\C,-2.709194973,-0.4572177016,-1.2613520476\H,
-3.3570767526,-0.0601996841,-0.4594660941\C,-2.7976122937,-1.963953738
8,-1.3071239781\H,-2.2315209782,-2.3584248752,-2.166627461\H,-3.842266
2159,-2.3018528819,-1.3990452275\H,-2.3678663065,-2.4141361779,-0.4005
880141\C,-3.297563227,-0.6677212079,2.1898017514\H,-3.665015119,1.395
8602257,1.4502021326\H,-3.7428742956,0.3115068993,1.9587455527\H,-3.69
5778389,-0.9846232884,3.1692979735\C,2.5156255966,-0.4971901367,2.3432
38906\H,2.790803253,-1.1090457435,1.4608461243\C,3.0967788893,0.880316

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312,2.1341825232\H,4.1802706961,0.8112184295,1.9521825613\H,2.96944710
 01,1.5225187766,3.0230069976\H,2.6398958354,1.3832030521,1.267616879\C
 ,3.0880114777,-1.1534615155,3.584744724\H,4.1860501571,-1.2216194978,3
 .5254664765\H,2.7000931498,-2.1737681057,3.7360261863\H,2.8395624939,-
 0.5706627571,4.4883651949\\Version=ES64L-G09RevE.01\State=1-A\HF=-1077
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 7240212\Quadrupole=7.717276,-3.7893565,-3.9279195,0.850596,3.5631031,0
 .3177423\PG=C01 [X(C20H25N1O2Ru1)]\\@

cpxE

1\1\GINC-R284\FOpt\RM11L\GenECP/Auto\C16H27N1O5Ru1\ROOT\28-Apr-2017\0\
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 3=1,2/11=1) int=ultrafine freq\Complex B1b Ru(II)-OiPr\0,1\Ru,0.5543
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 9655054\O,-1.3251950111,-0.9315885617,-0.9246619621\O,1.6086791894,-0.
 1757669486,-2.0132371969\O,-0.4659227,-1.1240957406,1.4708603333\N,0.0
 234686149,1.3209514153,0.2432291068\H,-0.1348840461,-2.5644565867,-1.4
 801586218\C,-2.1506184844,-0.0338567459,-1.3577484941\H,1.2108954617,-
 2.0672641219,-1.9936822029\C,2.6472504163,-0.0537117152,-1.1840321588\
 C,-0.1123765673,-2.3627443795,2.0671893011\H,-1.3139240565,-1.23793264
 87,1.017836869\C,-1.0799303175,1.8699801039,-0.1336942689\C,0.70605463
 78,2.2439496732,1.1308233252\C,-2.0915366018,1.3419159213,-1.007939006
 \C,-3.210628725,-0.443680916,-2.184797962\H,2.3103018816,-0.2288827365
 ,-0.0262750785\C,3.7198504419,-1.1147574832,-1.3531279683\C,3.23450682
 2,1.3437364672,-1.1895585764\H,0.0456053566,-3.1102739325,1.259108063\
 C,1.1798253699,-2.1454442106,2.7946347388\C,-1.2231859652,-2.815956688
 1,2.9740543579\O,-1.3069953863,3.0946416824,0.3538868823\C,-0.35350249
 18,3.3056693553,1.3675980505\H,1.5731568142,2.6770544566,0.589749121\C
 ,1.2011264566,1.5973544148,2.3940502455\C,-3.0799568426,2.2179616096,-
 1.4770613509\C,-4.156208518,0.4415107116,-2.6433381642\H,-3.2545355307
 ,-1.5040790311,-2.448815748\H,4.1411033408,-1.0411101694,-2.3685437204
 \H,3.3114221505,-2.12802414,-1.2220774666\H,4.5436562386,-0.9875524971
 ,-0.632175354\H,3.8734279661,1.5510106333,-0.3151557779\H,2.4264992448
 ,2.0857803243,-1.2422995612\H,3.8494261324,1.4668399001,-2.0957156441\
 H,1.5344417307,-3.0842912548,3.2430874266\H,1.0524094034,-1.4038408459
 ,3.6005053172\H,1.9554241271,-1.7786368796,2.1047603967\H,-0.977263921
 5,-3.7793115034,3.4446445257\H,-2.1684752977,-2.952526931,2.4248920859
 \H,-1.3975906296,-2.0788578328,3.7741529462\H,-0.8528753587,3.17215669
 75,2.3490075419\H,0.0093746886,4.3413269322,1.2968135716\H,1.644784174
 4,2.3513176029,3.0641195966\H,0.3744850033,1.0966881351,2.9235362151\H
 ,1.9714429452,0.8408472479,2.1821797086\C,-4.0985356027,1.7880022916,-
 2.2924638473\H,-3.0226404596,3.2696396943,-1.1844813569\H,-4.961089924
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O5Ru1)]\\@

TS1

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1\1\GINC-R337\FTS\RM11L\GenECP/Auto\C16H27N1O5Ru1\ROOT\02-May-2017\0\\
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novaracc) # iop(5/13=1,2/11=1) int=ultrafine freq\\TS for beta hydride
trsf - cpxB1a\\0,1\Ru,-0.8013380406,0.0641499216,-0.4996867711\O,-1.5
582884069,1.446423921,-1.9566672483\O,0.7532601775,1.389133908,-0.7009
654902\O,-0.7113392961,-0.9839395367,-2.2164063977\O,-0.9468973508,1.3
76519272,1.1919619012\N,0.3182987669,-1.0949995349,0.7004897843\H,-0.7
628176795,1.9951303771,-1.9602008436\C,1.9981839487,1.0497207102,-0.63
77317765\H,-1.3950509904,0.8189417259,-2.6798028682\C,-1.7499380335,-1
.5120333938,-1.6122902638\C,-2.0342416223,2.292133886,1.2439925984\H,-
0.1509556969,1.865344242,0.9344093808\C,1.6039030981,-0.9996433254,0.7
557579625\C,-0.098645087,-2.0254703719,1.7353263589\C,2.4771018663,-0.
0997068164,0.0508374833\C,2.9576846265,1.8752638191,-1.2501284062\H,-2
.1218775337,-0.8797560046,-0.2453193629\C,-3.0977600536,-1.2699908017,
-2.2550882042\C,-1.5552031369,-2.9518455183,-1.2047060641\H,-2.2902963
989,2.5892746068,0.2041083749\C,-3.1959555991,1.564562733,1.8492510979
\C,-1.6256621257,3.5022456539,2.0369285015\O,2.1967313337,-1.845459332
5,1.604003783\C,1.199385881,-2.7548713646,2.0195124561\H,-0.861792553,
-2.7114709993,1.3293834172\C,-0.6708299775,-1.3016079937,2.9281500456\
C,3.8543075826,-0.357026557,0.0957985544\C,4.3013408109,1.5924697377,-
1.1960832338\H,2.5885719569,2.7597277578,-1.7770646398\H,-3.12180324,-
1.7660469073,-3.2405606365\H,-3.3007748156,-0.2000620677,-2.4029547855
\H,-3.9180067854,-1.6827922315,-1.64715846\H,-2.2924433586,-3.29563653
37,-0.461864298\H,-0.5362738112,-3.1067808483,-0.8234209433\H,-1.66649
73079,-3.5832894793,-2.1027741175\H,-4.0933174032,2.1993937486,1.84278
9421\H,-2.9800370418,1.2872083044,2.8942183379\H,-3.4183102486,0.64841
91064,1.282222802\H,-2.4470200373,4.2319278584,2.087303827\H,-0.761860
886,4.0149324152,1.5837689831\H,-1.3549196518,3.2211304816,3.067284942
3\H,1.369460715,-2.9865753907,3.082033579\H,1.3060269911,-3.6834454217
,1.4270826621\H,-0.9661816303,-2.0191101255,3.7103389282\H,0.063803753
3,-0.6008657066,3.3570406522\H,-1.556301682,-0.7196922208,2.6371080419
\C,4.7648718487,0.4668907511,-0.5199374525\H,4.1979345963,-1.242882921
4,0.6360619933\H,5.0115984929,2.2613133853,-1.6938551812\H,5.832301036
,0.2400430822,-0.477956425\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-115
1.6862756\\RMSD=5.421e-09\\RMSF=1.480e-06\\Dipole=-0.8316157,0.1576109,0.
9749596\\Quadrupole=-3.6187316,6.136352,-2.5176205,-1.2440588,-0.849550
5,-4.2418502\\PG=C01 [X(C16H27N1O5Ru1)]\\@
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cpxF

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203\O,-0.6663247301,-1.3583147164,-0.6913207387\O,0.6389152376,1.14317
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 6986426,1.0273682521,0.9018188711\H,0.8240951091,-1.9689031712,-1.8184
 055712\C,-1.8845839315,-0.9568463585,-0.6074211806\H,2.3194704094,-2.2
 102050767,-1.5166726593\C,1.2895650895,1.5100671259,-2.7310467717\C,2.
 0052311413,-2.4809710681,1.5820864559\H,0.1997777865,-1.9998875475,0.9
 570654768\C,-1.3822713188,1.0410656378,0.8638283236\C,0.3563921294,2.0
 94633065,1.7687549755\C,-2.2939016979,0.1985168731,0.1274664762\C,-2.8
 988130801,-1.6960254354,-1.2485763851\H,2.3968482227,0.6275911644,0.08
 25826717\C,0.643086683,2.4068469743,-3.7234447206\C,2.6978648663,1.103
 1355702,-2.9463052677\H,2.387340088,-2.9092881881,0.6236509596\C,3.112
 5655298,-1.7300194819,2.2563717085\C,1.4444314852,-3.5944481177,2.4231
 953208\O,-1.9603138998,1.9932863642,1.6102641347\C,-0.9447387558,2.586
 137962,2.3831318371\H,0.825784614,2.8729280202,1.1297340509\C,1.358574
 9274,1.6328418898,2.7897134695\C,-3.6555697567,0.5321413333,0.17734974
 66\C,-4.222947466,-1.3349447005,-1.1881021768\H,-2.5817488308,-2.58163
 16728,-1.8079539224\H,-0.4103969175,2.5755259978,-3.4715419353\H,0.713
 9166252,1.9848014227,-4.7396078324\H,1.1669655914,3.3768947155,-3.7657
 734053\H,2.7338674506,0.1565543514,-3.5092317775\H,3.1727196845,0.9166
 945503,-1.970833065\H,3.2528052306,1.8545867218,-3.52762096\H,3.968117
 3255,-2.3922922619,2.4523690504\H,2.7622264276,-1.3215214928,3.2183570
 261\H,3.4438298563,-0.8914170137,1.6264864038\H,2.2189488401,-4.340486
 7046,2.6537072931\H,0.6225122001,-4.120758193,1.9116409306\H,1.0555806
 151,-3.1988334939,3.3746290541\H,-1.0588670549,2.2422343492,3.43112450
 29\H,-1.0825269911,3.6779334254,2.3599018162\H,1.6223157611,2.45557421
 04,3.4742430314\H,0.9413632305,0.8048016471,3.3877409128\H,2.274924986
 5,1.277253399,2.2996324654\C,-4.6156445014,-0.2090953421,-0.4696234917
 \H,-3.9517407046,1.4146190948,0.7497485815\H,-4.972050474,-1.940445659
 5,-1.710394213\H,-5.6669326649,0.0828388139,-0.4161189918\\Version=ES6
 4L-G09RevE.01\State=1-A\HF=-1151.6780844\RMSD=2.874e-09\RMSF=3.092e-06
 \Dipole=1.3738958,-0.4664809,-0.3171074\Quadrupole=-10.0941657,6.82967
 63,3.2644894,-5.2184006,-2.7672136,-0.88043\PG=C01 [X(C16H27N1O5Ru1)]\
 \@\n

TS2-os

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1\1\GINC-R231\FTS\RM11L\GenECP/Auto\C26H30N2O4Ru1\ROOT\06-Feb-2017\0\\
# m11l/genecp/auto opt=(ts,calcfc,noeigen,maxcyc=200) scf=(maxcyc=200,
novaracc) # iop(5/13=1,2/11=1) int=ultrafine freq\TS for hydride tran
sfer to O of ArNO2 (outer-sphere)\0,1\H,3.4538485752,-0.5515280797,1.
9627353674\C,3.2684649236,-0.2987738283,0.913742069\C,2.7158454832,0.3
835926215,-1.7532737916\C,3.52790586,0.9829122101,0.4481990758\C,2.658
4666575,-1.2536052653,0.0534314399\C,2.4667997133,-0.9317849925,-1.300
2094113\C,3.2319635333,1.3664019957,-0.8860015115\H,3.9459678146,1.729
9695304,1.1336408764\H,1.996012947,-1.6445956902,-1.9792393982\H,2.481
1989884,0.6484926424,-2.7895744639\Ru,1.3286088767,0.5032715702,-0.099
0187572\H,0.1224547499,0.5324558735,-1.3769715421\O,-0.097732132,-0.63

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3544833,0.7494192676\|C,-1.2007454395,-0.3354094461,1.3095071383\|C,-3.7
 116809313,0.1400545357,2.5322837071\|C,-1.7266379488,0.9821483197,1.433
 4509605\|C,-1.9842196351,-1.3886066452,1.8362890287\|C,-3.1988581792,-1.
 1561802233,2.4241890893\|C,-2.9768178003,1.1877273867,2.0379091759\|H,-1
 .5819209395,-2.4012771677,1.7317514746\|H,-3.7804491427,-2.0025839922,2
 .8061372303\|H,-3.3553262578,2.2104806626,2.1191505452\|H,-4.6801331224,
 0.317663534,3.0055111854\|C,-0.9720932496,2.1105284835,0.9970674752\|N,0
 .2136878594,2.1358797207,0.481624997\|O,-1.5376251329,3.3089240947,1.17
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 763050586,1.0305555609\|H,-1.1871371735,4.4044909683,-0.5252162307\|C,0.
 606432306,3.5306383968,0.3903118514\|H,1.1002595322,3.7123032325,-0.580
 6470407\|C,1.5212860956,3.9091784586,1.5304382888\|H,0.9909895246,3.8284
 043083,2.4933945086\|H,1.8836736161,4.9439432297,1.4238842375\|H,2.39143
 96669,3.2410805971,1.5804815918\|C,3.5790795034,2.7218839897,-1.3886252
 898\|H,3.5214974324,3.4859859603,-0.5975789878\|H,2.9178183861,3.0308269
 128,-2.2123880223\|H,4.6120903781,2.7438564062,-1.7761142936\|C,2.272230
 2892,-2.5915128843,0.625418473\|H,1.7880719645,-2.3737687867,1.59949406
 8\|C,1.2824963827,-3.3622077277,-0.2156090345\|H,0.963861723,-4.26962412
 7,0.3210220034\|H,1.7248911426,-3.6973419593,-1.1694605045\|H,0.38481363
 68,-2.7675700332,-0.4427208146\|C,3.5200270075,-3.4151537673,0.88323412
 9\|H,3.2665510716,-4.3694843927,1.3717912694\|H,4.2439210225,-2.89283179
 66,1.5290603279\|H,4.0352977608,-3.65330532,-0.0629087971\|N,-1.11475467
 6,-0.812072485,-2.327816181\|O,-0.801980452,0.4082507002,-2.2083750527\|
 O,-0.3248218508,-1.6220310037,-2.8052214711\|C,-2.3184181264,-1.2324805
 868,-1.7519849015\|C,-4.7229573658,-2.0900267163,-0.7117565811\|C,-2.588
 4068172,-2.5961988154,-1.6941808235\|C,-3.239740673,-0.2930675127,-1.29
 72931\|C,-4.4405271321,-0.734071328,-0.7804465775\|C,-3.7927170405,-3.01
 45587089,-1.1649611729\|H,-1.8399156452,-3.3001818989,-2.0625506283\|H,-
 3.0021796393,0.7698526658,-1.3596444995\|H,-5.1655056452,-0.0034010473,
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 =-1513.8765894\\RMSD=5.919e-09\\RMSF=4.613e-06\\Dipole=0.5222016,1.242781
 8,0.6153444\\Quadrupole=3.5946033,10.3612514,-13.9558546,5.8861469,-1.1
 987144,-3.347594\\PG=C01 [X(C26H30N2O4Ru1)]\\@\\

cpxG

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1\\1\\GINC-R229\\FOpt\\RM11L\\GenECP/Auto\\C26H30N2O4Ru1\\ROOT\\12-Jan-2017\\0\\
  # m11l/genecp/auto opt=maxcyc=200 scf=(maxcyc=200,novaracc) # iop(5/1
  3=1,2/11=1) int=ultrafine freq\\Complex 3 Ru(II)-hydride-ON(OH)Ar\\0,1
  \\H,1.466970011,-3.1186298895,1.5591395646\\C,0.9653692725,-2.2830477853
  ,2.0550770282\\C,-0.3704046565,-0.0963305172,3.1851508384\\C,-0.43399410
  91,-2.2694663058,2.1634204024\\C,1.7106711757,-1.1590834633,2.470656890
  7\\C,1.0305197335,-0.0744760907,3.0739743745\\C,-1.1449348116,-1.1900469
  618,2.7479415402\\H,-0.9965742862,-3.1144161909,1.7532385052\\H,1.569639
  25,0.8341809852,3.3452982828\\H,-0.8842682597,0.8139460026,3.5147640076
  \\Ru,0.1303855916,-0.4411515908,1.1100371735\\O,1.6853574348,0.211777326
  
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1,-0.0416227815\|C,2.0037816547,-0.2044157572,-1.2156867977\|C,2.8090804
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 3538\|C,3.3541852655,-0.1424027445,-1.6135761423\|C,3.7419835183,-0.4767
 528614,-2.889269866\|C,1.4843219184,-0.9645713395,-3.4773037355\|H,4.079
 6989546,0.2100625345,-0.8726508383\|H,4.8005086864,-0.4091639649,-3.162
 2535001\|H,0.7322032516,-1.2810857669,-4.205836446\|H,3.1219240821,-1.14
 79509659,-4.8519796463\|C,-0.3185922025,-0.7648837653,-1.8397520949\|N,-
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 ,-2.8506371334\|C,-2.4646479238,-0.6277890093,-2.2779111705\|H,-3.163858
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 34001,-0.1317377127\|C,-2.669662528,-2.5524418521,-0.697119918\|H,-2.142
 5780182,-3.1813001185,-1.4332972019\|H,-3.7523112604,-2.6700024082,-0.8
 631239905\|H,-2.4449632024,-2.9525842804,0.2993333041\|C,-2.6233761038,-
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 ,2.7169869866\|C,3.1961260886,-1.1462594574,2.2324323486\|H,3.3427551565
 ,-1.5112833717,1.1950417502\|C,3.8274616774,0.2203622046,2.3405425452\|H
 ,4.8844744809,0.1700904323,2.0372349851\|H,3.81590905,0.5947584317,3.37
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 37729225,3.1834422891\|H,4.9460319185,-2.1736673792,2.9916104611\|H,3.46
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 8458891\|O,-0.7051051073,1.3538680762,0.8090188973\|N,-0.4440730192,1.87
 51436679,-0.3979213123\|C,-1.5369079869,2.5972042924,-0.8940741761\|C,-3
 .732481478,3.8127786599,-2.1044275046\|C,-1.3611414603,3.3968916298,-2.
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 3.0322279608,-0.9731634578\|C,-2.4541614808,3.9957726841,-2.6156271025\|H,
 -0.3534423189,3.5402556007,-2.4179537943\|H,-2.9299523352,1.827789388
 3,0.5425674765\|H,-4.8964505496,2.8979952737,-0.5433660432\|H,-2.3059679
 819,4.621673634,-3.5012734085\|H,-4.5938804752,4.2865086378,-2.58305362
 76\|O,0.6427022416,2.7709831034,-0.2946568328\|H,1.374663578,2.144410108
 8,-0.2890448609\\Version=ES64L-G09RevE.01\State=1-A\HF=-1513.9235337\R
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 adrupole=8.4560841,-11.0410072,2.5849232,4.3496151,1.3279538,-1.352177
 1\PG=C01 [X(C26H30N2O4Ru1)]\\@

cpxJ

1\1\GINC-CN434\FOpt\RM11L\GenECP/Auto\C19H26N2O6Ru1\HNAN_JZY\05-Sep-20
 17\0\\# m11l/genecp/auto opt=maxcyc=200 scf=(xqc,maxcyc=200) # iop(1/8
 =1) int=ultrafine freq\\Complex 2 Ru(II)-H + PhNO2\\0,1\Ru,-0.58337307
 22,-0.9172227422,-0.2753937106\O,-0.3528215452,-1.8570627251,-2.195436
 6765\O,-0.9413144233,0.6698440749,-1.6024851787\O,1.3473725639,-0.9294
 053588,-0.3556764182\O,-2.6888589651,-0.8807867721,-0.4803870091\N,-0.
 8335805316,0.3039963667,1.2784005652\H,-0.3180151282,-1.0235235286,-2.
 6832315133\|C,-0.8472125169,1.9217341104,-1.3084318252\|H,0.5329794215,-
 2.2215006828,-2.2378814683\|C,-3.3892238429,-1.9727521083,-1.0741132223

\H,-2.6826286227,-0.1414512621,-1.1063533213\|C,-0.8524504254,1.5875581
 938,1.1949740581\|C,-1.0014677514,-0.0699733343,2.6676967265\|C,-0.79302
 8558,2.4289786032,0.0240654162\|C,-0.8153735643,2.8651465189,-2.3531219
 787\|H,-0.5918433449,-2.2003601572,0.68874668\|H,-2.7451954354,-2.412191
 9367,-1.8639181693\|C,-3.6235717629,-2.9849245035,0.0049483154\|C,-4.664
 7142439,-1.457982381,-1.6803137944\|O,-0.9365679668,2.2247636341,2.3671
 141208\|C,-0.7311032906,1.247398988,3.3696169656\|H,-0.2403515876,-0.827
 3941929,2.9156387754\|C,-2.3819815237,-0.6259980108,2.9095428436\|C,-0.7
 024608129,3.8130404798,0.229445079\|C,-0.723330963,4.2157146977,-2.1177
 573896\|H,-0.8627315958,2.4725462945,-3.3732177573\|H,-4.114033984,-3.87
 72732911,-0.4098703737\|H,-4.2748858368,-2.5687483738,0.7908252601\|H,-2
 .6735952094,-3.2937477748,0.4642408504\|H,-5.2283370478,-2.2759066407,-
 2.1522813145\|H,-4.473170851,-0.7028900864,-2.4599245214\|H,-5.307114472
 2,-1.0011859178,-0.9106816653\|H,-1.4174599042,1.4667307943,4.202756141
 9\|H,0.3111400361,1.3338772025,3.7266441798\|H,-2.5079449122,-0.91375588
 09,3.965520282\|H,-3.1589492754,0.1147616096,2.6570044953\|H,-2.54773525
 86,-1.5171038308,2.2872316378\|C,-0.6644313823,4.7047358867,-0.81591694
 51\|H,-0.6608288645,4.1804501651,1.2577662254\|H,-0.6942534188,4.9093245
 255,-2.9651059746\|H,-0.5894721466,5.777369296,-0.6238752658\|N,2.178856
 7603,-0.7232374843,0.5725202898\|O,1.8463295187,-0.4788592683,1.7206555
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 859,-0.4172549768\|C,4.478188469,-0.7243714406,1.2270613874\|C,3.9111646
 43,-0.9768743051,-1.1158749612\|C,5.2543901258,-1.0623237474,-1.4192960
 967\|C,5.8166318805,-0.8156136656,0.9007267367\|H,4.1402896415,-0.588793
 2112,2.2551645643\|H,3.1530385737,-1.0144808383,-1.8985034085\|H,5.56186
 72415,-1.184332031,-2.4613912994\|H,6.5675042743,-0.7513445625,1.692780
 6549\|H,7.2732804171,-1.0529457633,-0.6682776746\|Version=ES64L-G09RevE
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 5,1.2362086,-0.8020138,5.6795355\PG=C01 [X(C19H26N2O6Ru1)]\@\|

TS2-is

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1\1\GINC-R1152\FTS\RM11L\GenECP/Auto\C19H26N2O6Ru1\ROOT\04-May-2017\0\  

\# m11l/genecp/auto opt=(ts,calcfc,noeigen,maxcyc=200) scf=(maxcyc=200  

,novaracc) # iop(5/13=1,2/11=1) int=ultrafine freq\PES 1 for hydride  

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95\O,0.5416826914,-1.1469272464,-2.2953665818\O,-1.8335795916,-0.27234  

58012,-1.3875039834\O,1.5021222693,0.6597795629,-0.7310745102\O,-1.131  

0136942,-2.2190684662,-0.0386578715\N,-0.9925594872,0.3886710182,1.233  

0386241\H,-0.1816071092,-0.7652313839,-2.8059312898\|C,-2.6674483683,0.  

7061878453,-1.2547551805\|H,1.3239257501,-0.627392855,-2.5043428731\|C,-  

0.5942496885,-3.4805359571,-0.4294482579\|H,-1.8860768008,-2.0025066028  

,-0.6057808542\|C,-2.0518035947,1.113142903,1.1236904342\|C,-0.736663733  

8,0.2025630677,2.6542507001\|C,-2.8030249734,1.4512332969,-0.0577156738  

\|C,-3.5089529323,1.0447160469,-2.3267596933\|H,1.147006011,-0.496933742  

3,0.9596946743\|H,-0.0553402814,-3.3480076442,-1.3900434694\|C,0.3754696

```

994,-3.9003553574,0.6325516282\|C,-1.72539032,-4.4545170924,-0.60678874
 77\O,-2.5389304042,1.5954563301,2.2652616424\|C,-1.5802108298,1.3043994
 797,3.2640104548\H,0.3303872281,0.3724460643,2.855392927\|C,-1.13257511
 89,-1.1841502905,3.0942719553\|C,-3.7408720231,2.4862707407,0.016734472
 9\|C,-4.4157087614,2.0747603772,-2.2305400419\H,-3.4144591857,0.4600069
 591,-3.2462490389\H,0.8954064421,-4.8214344889,0.3325750036\H,-0.14661
 44007,-4.0969825677,1.5833675516\H,1.1289807619,-3.1168479903,0.802247
 1201\H,-1.344771736,-5.4412916947,-0.9082459391\H,-2.4320535319,-4.126
 4600389,-1.3863005302\H,-2.2852852155,-4.5782621021,0.3340360731\H,-2.
 1201993795,1.0093990233,4.176977072\H,-1.0036761735,2.2247522949,3.467
 2776514\H,-0.942171248,-1.3180118304,4.1710999166\H,-2.2021609446,-1.3
 74178534,2.9042344991\H,-0.5554440261,-1.9404295814,2.5441494967\|C,-4.
 5377747816,2.8113016627,-1.0560790342\H,-3.8285833888,3.0415360595,0.9
 544017117\H,-5.0454170435,2.3163141153,-3.0934036853\H,-5.2564840778,3
 .6302015523,-0.9831974067\N,2.267902734,1.0597774419,0.2571437782\O,1.
 8556683008,0.6254675883,1.3890306797\|C,3.6352386455,0.9762269535,-0.03
 83497835\|C,6.3496179646,0.940153324,-0.5844125227\|C,4.5364694663,0.699
 8399243,0.9814264993\|C,4.0832746026,1.257421904,-1.3248141733\|C,5.4389
 273663,1.2334811465,-1.5885517114\|C,5.8891005212,0.6748393258,0.695220
 6941\H,4.1552506211,0.4958498873,1.9830485052\H,3.3609124981,1.5075913
 239,-2.1046315014\H,5.7922990183,1.4526234345,-2.6005898803\H,6.599567
 3149,0.4422359931,1.4941409171\H,7.4212593352,0.9272565258,-0.79937954
 77\\Version=ES64L-G09RevE.01\\State=1-AHF=-1395.1601866\\RMSD=2.844e-09
 \\RMSF=1.125e-06\\Dipole=-0.2549977,-1.0960997,-0.4237338\\Quadrupole=-6.
 2676428,-2.0864911,8.3541338,0.2150906,-2.2601323,1.8024755\\PG=C01 [X(
 C19H26N2O6Ru1)]\\@

cpxK

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1\\1\\GINC-R181\\FOpt\\RM11L\\GenECP/Auto\\C19H26N2O6Ru1\\ROOT\\05-May-2017\\0\\
\\# m11l/genecp/auto opt=maxcyc=200 scf=(maxcyc=200,novaracc) # iop(5/
3=1,2/11=1,1/8=1) int=ultrafine freq\\Complex 2b Ru(II)-ON(OH)Ph\\0,1\\
Ru,-1.0211614621,-0.8549957611,0.2943275796\O,-0.735898181,-2.80214661
45,-0.5771489306\O,-0.5323800239,-0.3556479534,-1.5426350268\O,0.73010
28349,-1.3774634412,0.9968734347\O,-2.9381079736,-0.3797853462,-0.5961
746026\N,-0.9169854643,1.0240268618,0.9344225214\H,-0.4873759092,-2.48
00214301,-1.4518343996\|C,0.1481132346,0.7111122129,-1.8479761474\H,0.1
149777134,-2.9744458222,-0.1505135719\|C,-3.8836942655,-1.4211309821,-0
.7754046872\H,-2.567957154,-0.1452621243,-1.4575032884\|C,-0.2758021001
,1.9376836144,0.2974398192\|C,-1.336151755,1.5600019991,2.2095281838\|C,
0.2927500064,1.8545909189,-1.0190717901\|C,0.7632747475,0.7407388724,-3
.1092443399\H,1.6688980037,-0.8556622654,2.9973831714\H,-3.3443159274,
-2.3362063275,-1.1067396383\|C,-4.5004386592,-1.6719148811,0.5679554076
\|C,-4.8936461086,-1.0184440189,-1.8138718429\O,-0.1276520154,3.0891465
334,0.9532600214\|C,-0.505617113,2.8302301514,2.2929234482\H,-1.0441974
155,0.8506668797,3.0074008428\|C,-2.8285687068,1.7817076717,2.233579094
9\|C,1.0265382123,2.9519620712,-1.4891266789\|C,1.4748570598,1.83363237,

```

-3.5432808921\H,0.6541046191,-0.1483208389,-3.737180011\H,-5.208699523
 8,-2.5111488595,0.5227811971\H,-5.0439645171,-0.7787592429,0.917118433
 6\H,-3.7281751493,-1.9199042078,1.3130298291\H,-5.6337802874,-1.816908
 9539,-1.9704064511\H,-4.4199789218,-0.8184156459,-2.7882009346\H,-5.43
 10975735,-0.1086330133,-1.5029421793\H,-1.057919348,3.7068615355,2.666
 4863453\H,0.4140565314,2.6917481333,2.8879865924\H,-3.1631835411,2.145
 1328575,3.2180518759\H,-3.1269469017,2.5193148219,1.4707949248\H,-3.36
 21696098,0.844273778,2.0109881034\C,1.6112759405,2.9562409769,-2.73224
 83769\H,1.1311282177,3.8195213902,-0.8328770073\H,1.9442385987,1.81060
 89976,-4.5321499879\H,2.1827137029,3.8232683007,-3.0703720794\N,1.6344
 695961,-0.374767428,1.1724541014\O,1.6171480408,-0.0144242103,2.518720
 2466\C,2.9129515874,-0.8136752057,0.7792762009\C,5.4163124669,-1.55779
 73309,-0.1819191119\C,4.0546833668,-0.5241067436,1.5158231337\C,3.0299
 244329,-1.4537397235,-0.4527543673\C,4.2741386825,-1.821552683,-0.9238
 184129\C,5.2958753277,-0.9050136624,1.0321237884\H,3.9648772116,0.0115
 946636,2.4621485673\H,2.1282425456,-1.6323413663,-1.046549693\H,4.3551
 068915,-2.3216323778,-1.8938774393\H,6.1895704322,-0.681496448,1.62318
 45325\H,6.39999603,-1.8515867022,-0.5575665087\Version=ES64L-G09RevE
 .01\State=1-A\HF=-1395.2113017\RMSD=4.331e-09\RMSF=2.121e-06\Dipole=-1
 .5260884,-0.4316382,0.1600682\Quadrupole=1.2705408,-4.6665371,3.395996
 3,2.0522453,-0.7124958,6.2813556\PG=C01 [X(C19H26N2O6Ru1)]\@\n

cpxH

1\1\GINC-CN190\FOpt\RM11L\GenECP/Auto\C19H24N2O5Ru1\ROOT\06-Sep-2017\0
 \#\ m11l/genepc/auto opt=maxcyc=200 scf=(maxcyc=200) # int=ultrafine f
 req\Complex 5 Ru(II)-PhNO2H + iPrOH\0,1\Ru,0.1422510469,0.6631247497
 ,0.0117513284\O,2.0900295792,0.8687523217,0.0213577519\O,-1.112068098,
 0.4344599128,-1.5299487781\O,0.1450819124,2.6514183204,-0.712555648\N,
 0.3437441633,-1.2059993876,0.7283483068\C,3.0038018843,-0.0330908973,0
 .0914340012\C,0.6895936165,3.6661936609,0.1179749817\H,-0.785525176,2.
 8457975845,-0.8844491132\C,1.4705906003,-1.8402097546,0.8193101885\C,-
 0.6591542744,-2.0168853988,1.4047446171\C,2.771876728,-1.3882638861,0.
 4489807289\C,4.3329606752,0.3439266557,-0.1818837317\H,-3.025249493,1.
 9266443093,-1.3630316494\H,1.6493971425,3.2372303592,0.4574203734\C,0.
 9447416,4.892466764,-0.7142228284\C,-0.2048531312,3.9328809364,1.29783
 88473\O,1.4010335932,-3.0524712853,1.3784253452\C,0.0311669721,-3.3631
 343591,1.4934448081\H,-1.564914377,-2.0910059677,0.7817183624\C,-1.011
 9596384,-1.4166312115,2.7431540095\C,3.846239975,-2.2887885665,0.50784
 33122\C,5.3636465478,-0.5600135701,-0.1250737271\H,4.5059927709,1.3884
 566574,-0.4542323589\H,1.4521090436,5.6706626191,-0.1244486137\H,-0.00
 1271023,5.324553716,-1.0841225085\H,1.5723752748,4.6537752814,-1.58371
 52483\H,0.2518496694,4.6625503347,1.9833937496\H,-0.4018963507,3.00557
 35989,1.8582717426\H,-1.1771974773,4.3434276287,0.9728359525\H,-0.1232
 382665,-3.8892716427,2.4484907562\H,-0.2460452848,-4.0397907208,0.6636
 848164\H,-1.8122535589,-1.9916385507,3.2367049487\H,-0.132682171,-1.39
 89128259,3.4086727867\H,-1.3566673952,-0.3782483832,2.6187935987\C,5.1

278430419,-1.8919154059,0.2196871781\H,3.6421482385,-3.3250385907,0.79
 04683491\H,6.3818186193,-0.2305691476,-0.3575495508\H,5.9504625766,-2.
 6094730969,0.2621652615\N,-1.8700855167,0.6753712112,-0.4791612694\O,-
 2.4745287794,1.983920732,-0.5707788107\C,-2.9335540971,-0.2644237961,-
 0.293953792\C,-4.8964921216,-2.1349318288,0.1791109997\C,-3.7485391433
 ,-0.1243013196,0.8175548602\C,-3.0895981701,-1.314144275,-1.1806517374
 \C,-4.0811000094,-2.2507449475,-0.934063117\C,-4.7306870035,-1.0676129
 078,1.0510741451\H,-3.596154742,0.7225056269,1.4925875993\H,-2.4129063
 87,-1.3927414516,-2.0334198334\H,-4.2138317321,-3.0882726797,-1.625026
 6024\H,-5.3755823805,-0.9714176663,1.929054294\H,-5.6717194734,-2.8817
 494598,0.3709909175\\Version=ES64L-G09RevE.01\\State=1-A\\HF=-1318.79609
 13\\RMSD=6.046e-09\\RMSF=4.764e-06\\Dipole=-1.928563,-0.0759394,0.4765226
 \\Quadrupole=0.6201778,6.7333811,-7.3535589,5.3153748,-0.134936,-1.5291
 565\\PG=C01 [X(C19H24N2O5Ru1)]\\@\\

TS3

1\\1\\GINC-CN155\\FTS\\RM11L\\GenECP/Auto\\C19H24N2O5Ru1\\ROOT\\09-Sep-2017\\
 # m11l/genecp/auto opt=(ts,calcfc,noeigen,maxcyc=200) scf=(maxcyc=200
 ,novaracc) # iop(5/13=1,2/11=1,1/8=1) int=ultrafine freq\\TS 2 for -OH
 transfer to Ru: cpx5_nw\\0,1\\Ru,-0.0574512452,0.6172292612,-1.0970327
 107\\O,1.5946816997,1.0757043394,-0.1424292919\\O,-2.1899055406,0.238108
 3747,-1.5775448068\\O,-0.5234054851,2.6471274601,-1.1825432622\\N,0.5180
 873066,-1.3233106281,-1.1231775114\C,2.2689427699,0.3078378101,0.63923
 08025\\C,0.3005738998,3.6260059777,-0.5681756017\\H,-1.3970046644,2.6223
 848788,-0.6996142535\C,1.477617546,-1.7985175194,-0.3980445842\C,-0.00
 1084204,-2.4150892109,-1.9379306733\C,2.2559608247,-1.1103911754,0.585
 5356956\\C,3.1136755306,0.9100477763,1.5915327284\\H,-3.3333305763,1.928
 1466964,-0.3024392689\\H,1.3361494329,3.3516171327,-0.8397855023\\C,-0.0
 433793128,4.965833969,-1.1620252875\\C,0.1516248352,3.6028890974,0.9296
 239916\\O,1.7849513396,-3.0734370037,-0.6142356984\\C,1.0794835943,-3.47
 15503083,-1.7714517916\\H,-0.0717361571,-2.0772345728,-2.9876745654\\C,-
 1.355755582,-2.8843631972,-1.4703408891\\C,3.0765316184,-1.8521664914,1
 .4461035871\\C,3.8899600908,0.1588321714,2.4385659276\\H,3.1228797657,2.
 0034672141,1.6258091025\\H,0.6188270933,5.7525784795,-0.7687989363\\H,-1
 .0805274774,5.2494637,-0.9163375813\\H,0.0529346875,4.9500488353,-2.256
 9865883\\H,0.8523736201,4.3114861404,1.3980786399\\H,0.3608647398,2.5998
 921623,1.3305639247\\H,-0.8706472712,3.8836343858,1.2319364139\\H,0.6856
 452431,-4.4858460091,-1.602636276\\H,1.7959253559,-3.5032518171,-2.6120
 543513\\H,-1.6562985385,-3.7824681102,-2.0330484584\\H,-1.3380952665,-3.
 141670878,-0.3969242705\\H,-2.1217083833,-2.1150376161,-1.6283126737\\C,
 3.8777921738,-1.2350342633,2.3743641098\\H,3.0616899519,-2.9429821591,1
 .370785234\\H,4.5268025455,0.6632618514,3.1726881244\\H,4.4994120977,-1.
 8279847691,3.048669211\\N,-1.7843058107,0.4010374689,-0.393184556\\O,-2.
 5152229897,2.0035784428,0.1980236851\\C,-2.3110966142,-0.3968043645,0.6
 50321711\\C,-3.2073862161,-2.0343915252,2.6584947939\\C,-1.5349427955,-0
 .5532929803,1.7833487599\\C,-3.5298159142,-1.0334243131,0.4989002809\\C,

-3.9738201895,-1.8573432845,1.5160882314\|C,-1.9907773072,-1.3815971017
 ,2.7912669178\|H,-0.5757046505,-0.0277976202,1.8500438376\|H,-4.10445865
 61,-0.8879137395,-0.4194160207\|H,-4.9319946309,-2.3744644806,1.4139238
 702\|H,-1.3858148198,-1.5233362193,3.6905937144\|H,-3.5633914639,-2.6917
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 63\\RMSD=7.679e-09\\RMSF=2.734e-06\\Dipole=-0.1887205,-1.417501,0.0194066
 \\Quadrupole=-2.2476428,3.481586,-1.2339432,5.5065358,0.3804239,2.22371
 9\\PG=C01 [X(C19H24N2O5Ru1)]\\@\\

cpxL

1\\1\\GINC-CN155\\FOpt\\RM11L\\GenECP/Auto\\C19H22N2O4Ru1\\ROOT\\12-Sep-2017\\0
 \\# m11l/genecp/auto opt=maxcyc=200 scf=(novaracc,maxcyc=200) # iop(5/
 13=1,2/11=1) int=ultrafine freq\\Complex 6 Ru(II)-PhNO-OiPr product co
 mplex\\0,1\\Ru,0.7252614642,1.0227096206,-0.7052001734\\O,0.8696932957,-
 0.759941522,-1.439969705\\O,-0.775733188,1.803319036,-1.5469465783\\O,1.
 9800551406,2.0989930198,0.1936498018\\N,-0.0692700709,0.3097101814,0.97
 31281157\\C,0.6894530052,-1.8965483467,-0.8374194908\\C,2.7833190729,2.6
 951421973,-0.7610792232\\C,-0.2970108885,-0.9328831559,1.224334665\\C,-0
 .630115995,1.1112726746,2.0452783583\\C,0.1191335935,-2.0616907691,0.44
 76389069\\C,1.0622078596,-3.0536995964,-1.5387999741\\H,2.3786212712,2.4
 088726594,-1.7849358563\\C,2.6965292858,4.1954277779,-0.6415238313\\C,4.
 1931215762,2.1706657249,-0.6632544748\\O,-0.9978402985,-1.1640221949,2.
 3212557125\\C,-1.5252247317,0.0919676354,2.7312139941\\H,-1.2257459819,1
 .931182244,1.5972149992\\C,0.449218385,1.6748056702,2.9347390375\\C,-0.0
 83858058,-3.3478728004,0.9600567793\\C,0.8664907014,-4.3050201207,-1.00
 52417292\\H,1.5024200305,-2.9179315899,-2.5293701013\\H,3.2954005317,4.6
 945385703,-1.4179011964\\H,3.077049849,4.5144579063,0.3416396053\\H,1.65
 57993873,4.5377848744,-0.7320754861\\H,4.8345812598,2.5893169329,-1.453
 3106936\\H,4.2106616101,1.0742050148,-0.7481381938\\H,4.6279932097,2.441
 9889302,0.3115668466\\H,-1.4827597302,0.13371812,3.8298684133\\H,-2.5779
 599915,0.1378470364,2.3981066674\\H,0.0026015419,2.2850799645,3.7347474
 148\\H,1.0272188176,0.862888479,3.405437331\\H,1.1472519131,2.3004108958
 ,2.3642620834\\C,0.2879913581,-4.4650192061,0.2516876307\\H,-0.544318292
 2,-3.4468289034,1.9465732332\\H,1.1677879023,-5.1848358066,-1.582459075
 7\\H,0.129443003,-5.4615477741,0.6689121354\\N,-1.9207994159,2.144542833
 6,-1.0733244526\\C,-2.7137766711,1.1086830285,-0.65979114\\C,-4.49788733
 48,-0.8384294706,0.2660995351\\C,-3.8822783151,1.4730437653,0.027951182
 7\\C,-2.4768726151,-0.2523458446,-0.9070167895\\C,-3.3587066706,-1.20500
 4026,-0.4402838262\\C,-4.7575942479,0.5099907349,0.4832978584\\H,-4.0709
 913469,2.5383384328,0.1946854934\\H,-1.5982509954,-0.5516885739,-1.4853
 115894\\H,-3.1546521606,-2.2635635769,-0.6361353566\\H,-5.6610201055,0.8
 118414059,1.0224474236\\H,-5.1890184403,-1.6016066489,0.6335453133\\Ver
 sion=ES64L-G09RevE.01\\State=1-A\\HF=-1242.3929409\\RMSD=7.689e-09\\RMSF=4
 .968e-06\\Dipole=0.5765995,-0.3384212,1.0533183\\Quadrupole=-1.3714486,1
 .6968878,-0.3254392,4.6264933,-9.1055257,3.0665015\\PG=C01 [X(C19H22N2O
 4Ru1)]\\@\\

cpxM

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1\1\GINC-CN155\FOpt\RM11L\GenECP/Auto\C19H22N2O4Ru1\ROOT\14-Sep-2017\0
\# m11l/genecp/auto opt=maxcyc=200 scf=(novaracc,maxcyc=200) # iop(5/
13=1,2/11=1) int=ultrafine freq\\Complex 7a Ru(II)-H-PhNO + acetone co
mplex\\0,1\Ru,1.2302146571,-1.0258720729,-0.3865021908\O,0.0660806254,
-2.5282529965,-0.8623756559\O,0.3059342935,0.4511006425,-1.0560143254\
O,2.5651358591,0.2903626151,0.3603809386\N,0.1652997003,-0.9256822484,
1.4680560043\C,-1.0333186495,-2.9362678886,-0.3373930651\C,3.036977203
6,1.322065985,-0.1027532515\C,-0.9743832615,-1.4771635221,1.6836110527
\C,0.4894965571,-0.1092096028,2.6138409849\C,-1.62926505,-2.4490187106
,0.8619443756\C,-1.7159060686,-3.9699053192,-1.0140664017\H,1.93500811
2,-1.2012310202,-1.8143123831\C,3.7433265244,2.2442527238,0.8215964344
\C,2.94321727,1.6892110446,-1.533708711\O,-1.5858411911,-1.1269152547,
2.8177622929\C,-0.8357352916,-0.0584432253,3.3604017013\H,0.7856008135
,0.8968564602,2.2590849264\C,1.6192907228,-0.721148106,3.405583659\C,-
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