SUPPLEMENTARY INFORMATION

The Formation of $[Ru(NHC)_4(\eta^2\text{-}O_2)H]^+$: An Unusual, High Frequency Hydride Chemical Shifts and the Facile, Reversible Coordination of O_2

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I. Synthesis and characterisation of **1**, **2** and **3**

All manipulations were carried out under argon using standard Schlenk, high vacuum and glovebox techniques. Solvents were purified using an Innovative Technologies solvent system (THF, CH_2Cl_2, hexane) or dried over molecular sieves (CH_3CN). Deuterated solvents (Fluorochem) were vacuum transferred from CaH_2 (CD_2Cl_2) or dried over molecular sieves (C_5D_5N). Oxygen (BOC, 99 %) and CO (BOC, 99.9 %) were used as received. $Ru(PPh_3)_3HCl$ and $I^iPr_2Me_2$ were prepared according to the literature.[1,2] NMR spectra were recorded on Bruker Avance 400 and 500 (Bath) and 700 (ETHZ) MHz NMR spectrometers, and ^1H and $^{13}C\{^1H\}$ spectra referenced as follows: CD_2Cl_2 (δ 5.32, δ 53.7), C_5D_5N (δ 7.21, δ 123.5). 2D experiments (^1H COSY, ^1H-^{13}C HMQC/HMBC/*J*-resolved HMBC, NOESY) were performed using standard Bruker pulse sequences. IR spectra were recorded as KBr discs on a Nicolet Protégé 460 FTIR spectrometer. Mass spectra were recorded using a micrOTOF electrospray time-of-flight (ESI-TOF) mass spectrometer (Bruker Daltonik GmbH) coupled to an Agilent 1200 LC system (Agilent Technologies). Elemental analyses were performed by Elemental Microanalysis Ltd, Okehampton, Devon, UK.

$[Ru(I^iPr_2Me_2)_4H]^+$, 1. $Ru(PPh_3)_3HCl$ (300 mg, 0.32 mmol) and $I^iPr_2Me_2$ (234 mg, 1.30 mmol) was heated at 70 °C in THF (5 mL) for 12 h in an ampule fitted with a J. Youngs PTFE valve. The reaction mixture was cooled to room temperature and the purple solid formed isolated by cannula filtration, washed with hexane (2 x 5 mL) and dried under vacuum. The resulting solid (229 mg) and $NaBAr_4^F$ (234 mg)[3] were stirred at room temperature in acetonitrile (10 mL) for 5 h. The suspension was cannula filtered, the filtrate reduced to dryness and the resultant purple solid washed with hexane (2 x 5 mL) and dried under vacuum. This afforded **$1[BAr_4^F]$** as a deep purple solid in 78% yield (350 mg). Crystals suitable for X-ray diffraction were obtained

by slow diffusion of hexane into a concentrated solution of **1[BAr$_4^F$]** in CH_2Cl_2. ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K): δ 5.76 (sept, $^3J_{HH}$ = 7.2 Hz, 4H, NC*H*$(CH_3)_2$), 4.56 (sept, $^3J_{HH}$ = 6.9 Hz, 4H, NC*H*$(CH_3)_2$), 2.16 (s, 24H, NCC*H*$_3$), 1.32 (d, $^3J_{HH}$ = 7.2 Hz, 12H, NCH(C*H*$_3)_2$), 1.24 (d, $^3J_{HH}$ = 7.2 Hz, 12H, NCH(C*H*$_3)_2$), 0.72 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$), 0.62 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$), -41.2 (s, 1H, Ru-*H*). ^{13}C{^{1}H} NMR (100 MHz, C_5D_5N, 298 K): δ 199.1 (s, N*C*N), 124.9 (s, N*C*CH$_3$), 124.2 (s, N*C*CH$_3$), 53.1 (s, N*C*H), 51.1 (s, N*C*H), 21.2 (s, NCH(*C*H$_3)_2$), 20.8 (s, NCH(*C*H$_3)_2$), 20.3 (s, NCH(*C*H$_3)_2$), 20.2 (s, NCH(*C*H$_3)_2$), 10.5 (s, NC*C*H$_3$), 10.4 (s, NC*C*H$_3$). IR (cm^{-1}): 2054 (ν_{RuH}). Analysis for $C_{76}H_{93}N_8RuBF_{24}$ [found (calculated)]: C, 53.75 (54.13); H, 5.50 (5.56); N, 6.52 (6.64).

[Ru(I^{i}Pr$_2$Me$_2$)$_4$(η^2-O$_2$)H]$^+$, 2. [Ru(I^{i}Pr$_2$Me$_2$)$_4$H][BAr$_4^F$] (**1[BAr$_4^F$]**, 20 mg, 0.012 mmol) was dissolved in either CD_2Cl_2 or C_5D_5N in a J. Youngs resealable NMR tube, which was freeze-pump-thaw degassed (x 3) and then placed under 1 atm of O_2. This afforded instantaneously a pink solution of **2[BAr$_4^F$]**. Crystals suitable for X-ray diffraction were obtained by slow diffusion of hexane into a concentrated CH_2Cl_2 solution of **2[BAr$_4^F$]**. ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K): δ 5.62 (sept, $^3J_{HH}$ = 6.9 Hz, 4H, NC*H*$(CH_3)_2$), 5.36 (sept, $^3J_{HH}$ = 6.9 Hz, 4H, NC*H*$(CH_3)_2$), 4.85 (s, 1H, Ru-H), 2.18 (s, 12H, NCC*H*$_3$), 2.16 (s, 12H, NCC*H*$_3$), 1.59 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$), 1.43 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$), 0.72 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$), 0.61 (d, $^3J_{HH}$ = 6.9 Hz, 12H, NCH(C*H*$_3)_2$). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 298 K): δ 176.8 (s, N*C*N), 127.6 (s, N*C*CH$_3$), 126.0 (s, N*C*CH$_3$), 53.1 (s, N*C*H), 50.1 (s, N*C*H), 24.0 (s, NCH(*C*H$_3)_2$), 21.0 (s, NCH(*C*H$_3)_2$), 20.3 (s, NCH(*C*H$_3)_2$), 20.2 (s, NCH(*C*H$_3)_2$), 11.0 (s, NC*C*H$_3$), 10.7 (s, NC*C*H$_3$). IR (cm^{-1}): 1992 (ν_{RuH}), 1047 (ν_{OO}). [Ru(I^{i}Pr$_2$Me$_2$)$_4$(η^2-^{18}O$_2$)H]:IR (cm^{-1}): 1994 (ν_{RuH}), 992 (calc. 987) (ν_{OO}). ESI-TOF MS: 855.5497 (calc. 855.5532).

[Ru(I^{i}Pr$_2$Me$_2$)$_4$(CO)H]$^+$, 3. [Ru(I^{i}Pr$_2$Me$_2$)$_4$H][BAr$_4^F$] (**1[BAr$_4^F$]**, 20 mg, 0.012 mmol) was dissolved in CD_2Cl_2 in a J. Youngs resealable NMR tube. The tube was freeze-pump-thaw

degassed (x 3) and 1 atm of CO added, affording a colorless solution in the time of warming. Crystals suitable for X-ray diffraction were obtained by slow diffusion of hexane into a concentrated solution of **3[BAr$_4^F$]** in CH_2Cl_2. ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K): δ 6.09 (sept, $^3J_{HH}$ = 7.2 Hz, 4H, NC*H*$(CH_3)_2$), 5.61 (sept, $^3J_{HH}$ = 7.2 Hz, 4H, NC*H*$(CH_3)_2$), 2.19 (s, 12H, NCC*H*$_3$), 2.18 (s, 12H, NCC*H*$_3$), 1.46 (d, $^3J_{HH}$ = 7.2 Hz, 12H, NCH(C*H*$_3)_2$), 1.32 (d, $^3J_{HH}$ = 7.2 Hz, 12H, NCH(C*H*$_3)_2$), 0.78 (d, $^3J_{HH}$ = 7.1 Hz, 12H, NCH(C*H*$_3)_2$), 0.61 (d, $^3J_{HH}$ = 7.2 Hz, 12H, NCH(C*H*$_3)_2$), -3.08 (s, 1H, Ru-*H*). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, 298 K): δ 203.9 (s, Ru-*C*O), 187.7 (s, N*C*N), 126.3 (s, N*C*CH$_3$), 125.9 (s, N*C*CH$_3$), 52.9 (s, N*C*H), 52.8 (s, N*C*H), 22.9 (s, NCH(*C*H$_3)_2$), 20.4 (s, NCH(*C*H$_3)_2$), 19.8 (s, NCH(*C*H$_3)_2$), 11.1 (s, NC*C*H$_3$). IR (cm^{-1}): 1898 (ν_{CO}). Analysis for $C_{77}H_{93}N_8RuOBF_{24}$ [found (calculated)]: C, 54.38 (53.94); H, 5.35 (5.47); N, 6.70 (6.54).

II Molecular structures of complexes **1[BAr$_4^F$]** and **3[BAr$_4^F$]**

Figure S-1. Molecular structure of **1[BAr$_4^F$]**

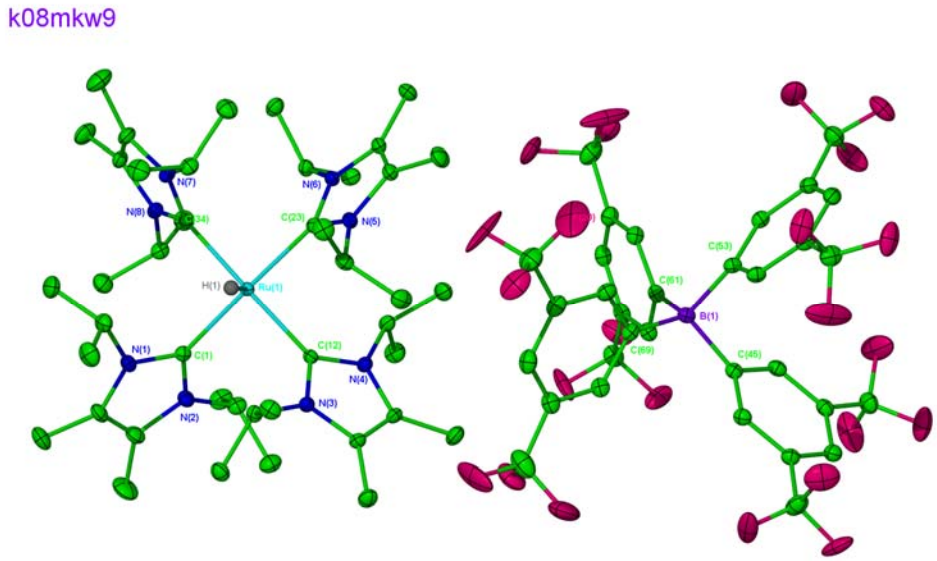
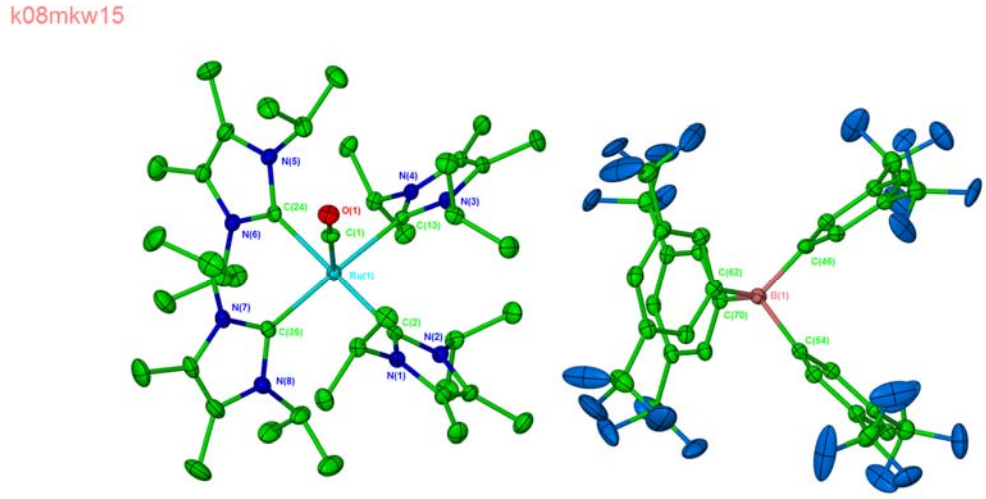


Figure S-2. Molecular structure of **3[BAr$_4^F$]**



III. **Table S-1** Crystal data and structure refinement for **1[BAr_4^F]**, **2[BAr_4^F]** and **3[BAr_4^F]**

Compound	**1[BAr_4^F]**	**2[BAr_4^F]**	**3[BAr_4^F]**
Empirical formula	$C_{76}H_{93}BF_{24}N_8Ru$	$C_{76}H_{93}BF_{24}N_8O_2Ru$	$C_{77}H_{93}BF_{24}N_8ORu$
Formula weight	1686.46	1718.46	1714.47
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/a$	$P2_1/a$	$P2_1/a$
a / Å	19.3420(2)	19.0490(2)	19.5720(3)
b / Å	21.1490(2)	21.2720(3)	21.1740(3)
c / Å	20.2090(2)	20.3250(3)	20.2440(3)
α / °	90	90	90
β / °	104.358(1)	103.628(1)	104.875(1)
γ / °	90	90	90
U / Å^3	8008.56(14)	8004.03(18)	8108.3(2)
Z	4	4	4
D_c / gcm^{-3}	1.399	1.426	1.404
μ / mm^{-1}	0.298	0.302	0.297
F(000)	3480	3544	3536
Crystal size / mm	0.45 x 0.30 x 0.06	0.40 x 0.14 x 0.13	0.33 x 0.15 x 0.12
Theta min., max for data collection	3.61, 27.49	3.54, 27.48	3.56, 27.49
Index ranges	-25<=h<=25; -27<=k<=27; -26<=l<=26	-24<=h<=24; -27<=k<=27; -26<=l<=26	-25<=h<=24; -27<=k<=27; -25<=l<=26
Reflections collected	141976	129475	77117
Independent reflections, R_{int}	18302, 0.0703	18297, 0.1018	18500, 0.1177
Reflections observed (>2σ)	13441	10977	12214
Data Completeness	0.996	0.997	0.994
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Max., min. transmission	0.99, 0.91	0.98, 0.90	0.96 and 0.77
Data / restraints / parameters	18302 / 122 / 1098	18297 / 48 / 1183	18500 / 81 / 1241
Goodness-f-fit n F^2	1.048	1.066	1.057
Final $R1$, $wR2$ [I>2σ(I)]	0.0533, 0.1183	0.0673, 0.1492	0.0664, 0.1453
Final $R1$, $wR2$ (all data)	0.0825, 0.1355	0.1340, 0.1796	0.1121, 0.1739
Largest diff. peak, hole / eÅ^{-3}	1.213, -0.684	0.990, -0.452	1.373, -1.113

Single crystals of compounds **1[BAr_4^F]** and **2[BAr_4^F]** were analysed at 150 K, using Mo(*K*α) radiation on a Nonius Kappa CCD diffractometer. Details of the data collections, solutions and refinements are given in Table S-1. The structures were solved using SHELXS-97[4] and refined using full-matrix least squares in SHELXL-97.[4] Refinements were generally straightforward with the following exceptions and points of note.

In **1[BAr_4^F]**, the hydride location was evenly spread between positions H1 and H1A. Both partial ligands were refined at a distance of 1.6 Å from the ruthenium center. Moreover, the fluorine atoms in many of the CF_3 groups of the BAr_4^F anion were disordered in a 65:35 ratio (the only exception is F1-3/F1A-3A where disorder was observed to be 50:50). All 50% and 65% occupancy partials refined anisotropically. C-F and F-F distances were restrained to be similar during the final least squares cycles in all disordered CF_3 moieties. The asymmetric unit in **2[BAr_4^F]** consists of one cation and one anion. The ruthenium center in the former is disordered over 2 sites in a 90:10 ratio. This feature necessarily means disorder of the peroxo moiety (and consequent inability to reliably locate the associated hydrogen). The major 90% component of this ligand is itself also disordered over 2 sites in a 70:20 ratio. Of these two regions, only the fractional rutheniums plus the 70% occupancy portion of the peroxyo moiety were treated anisotropically. Ru-O distances and O-O bond distances were refined subject to similarity restraints. There is one short O…H contact distance associated with one of the partial oxygens at 10% occupancy (H26…O2B). It is most likely that there is some additional disorder present in the associated carbene ligand which (if modelled) would eliminate this short contact. However, this was not readily evident (probably because of the small occupancy level) from the electron density map. Several of the fluorine atoms in the anion also exhibited disorder. In particular, F1-3, 13-15, 22-24 and 19-21 all exhibited 50:50 disorder while F4-6 had 60:40 disorder. Associated C-F distances were restrained to ideal values during the final least squares. The asymmetric unit

in **3[BAr$_4^F$]** comprises of one cation and one anion. The carbonyl ligand in the former is disordered in a 60:40 ratio. Several fluorines in the anion CF_3 groups also exhibit disorder. In particular, F1-3 and F7-9 are split evenly over two sites, F10-18 are located over two positions (ratio 45:55), F19-21 are disordered 60:40 and F22-24 are divided between two locations in a relative proportions of 65:35.

Crystallographic data for compounds **1[BAr$_4^F$]**, **2[BAr$_4^F$]** and **3[BAr$_4^F$]** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publications CCDC 713540-713542. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax(+44) 1223 336033, e-mail: deposit@ccdc.cam.ac.uk].

IV. Computational Details.

Full Reference 6. Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Calculations and employed the BP86 functional.[5] Ru and P were described using the Stuttgart RECPs and the associated basis sets[6] and a polarisation function was added for P ($\zeta = 0.387$).[7] 6-31G** basis sets were used for C, N, O and H atoms except backbone Me groups where the 6-31G basis set was applied.[8] All stationary points were characterized via analytical frequency calculations as minima (no imaginary eigenvalues). The energy curves in Figure 2 are based on computed SCF energies and so for consistency all energies are reported at this level. Inclusion of zero-point energy corrections or the inclusion of solvents effects (PCM method, CH_2Cl_2) did not significantly the energetics given in the main text.

The MECP was computed with the same basis sets as above but with 6-31G** also on the backbone Me groups. The MECP energy was then compared with single point calculation in ^{1}**2** and ^{3}**2b** with this basis set.

Full Reference 14. (a) te Velde, G.; Bickelhaupt, F. M.; van Gisbergen, S. J. A.; Fonseca Guerra, C.; Baerends, E. J.; Snijders, J. G.; Ziegler, T. *J. Comput. Chem.* **2001**, *22*, 931. (b) Fonseca Guerra, C.; Snijders, J. G.; te Velde, G.; Baerends, E. J. *Theor. Chem. Acc*. 1998, *99*, 391. (c) ADF2007.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com

All calculations are single points performed on the geometries optimized with Gaussian 03 as per reference 6. Calculations used the BP86 functional with TZ2P all electron basis sets on all atoms. The integration parameter was set to 5.0 and SCF convergence to10^{-7} a.u. Relativistic effects were included through the ZORA scalar correction and spin orbit coupling NMR chemical shifts were calculated[9] including relativistic effects via the mass-velocity, Darwin, and spin-Zeeman terms.

Tables of Cartesian Coordinates (Å) and Computed Energies (a.u.) for all Stationary Points (see main text for compound numbering)

$[Ru(IMe_4)_4H]^+$

```
Energy            = -1629.34618373
Enthalpy 0K       = -1628.617985
Enthalpy 298K     = -1628.569981
Free Energy 298K  = -1628.700044

N  -2.43823 -1.81154 -0.90484
C  -1.40506 -1.55000 -0.01576
N  -1.53887 -2.59314  0.89481
C  -2.60502 -3.45362  0.58630
C  -3.17429 -2.95767 -0.56087
Ru  0.00004 -0.00005 -0.00821
C   1.40498  1.55002 -0.01560
N   2.43797  1.81195 -0.90473
C   3.17409  2.95794 -0.56038
C   2.60483  3.45354  0.58695
N   1.53886  2.59281  0.89536
C   2.74184  1.00634 -2.08219
C   0.71152  2.74772  2.08428
C  -0.71147 -2.74846  2.08363
C  -2.74223 -1.00563 -2.08208
C  -1.54995  1.40496 -0.01564
N  -1.81167  2.43793 -0.90487
C  -2.95775  3.17404 -0.56086
C  -3.45360  2.60487  0.58642
N  -2.59296  1.53889  0.89507
C  -1.00581  2.74176 -2.08218
C  -2.74834  0.71153  2.08392
C   1.55009 -1.40504 -0.01598
N   2.59301 -1.53904  0.89480
C   3.45383 -2.60483  0.58600
C   2.95815 -3.17383 -0.56143
N   1.81195 -2.43786 -0.90536
C   2.74800 -0.71188  2.08383
C   1.00599 -2.74198 -2.08253
H  -0.00011  0.00004 -1.56410
C   2.95324  4.64836  1.42169
C   4.33424  3.45100 -1.37063
C  -4.33444 -3.45046 -1.37128
C  -2.95358 -4.64862  1.42073
C   3.45125 -4.33368 -1.37209
C   4.64881 -2.95334  1.42047
C  -3.45074  4.33399 -1.37144
C  -4.64863  2.95337  1.42081
H   2.58303 -1.29825  3.00547
H   3.75644 -0.26796  2.12609
H   2.00783  0.09880  2.02316
H   1.97513  0.22390 -2.15003
H   2.72279  1.62765 -2.99386
H   3.73759  0.53929 -1.99392
H   1.29785  2.58285  3.00597
H   0.26737  3.75607  2.12653
H  -0.09901  2.00738  2.02349
H  -0.53922  3.73773 -1.99405
H  -0.22299  1.97539 -2.14958
H  -1.62683  2.72216 -2.99405
H  -3.75679  0.26759  2.12578
H  -2.00816 -0.09916  2.02339
H  -2.58369  1.29780  3.00568
H  -2.72327 -1.62673 -2.99391
H  -3.73798 -0.53861 -1.99359
H  -1.97558 -0.22315 -2.14976
H  -1.29777 -2.58408  3.00542
H  -0.26727 -3.75680  2.12535
H   0.09901 -2.00804  2.02318
H   0.53968 -3.73809 -1.99432
H   0.22298 -1.97584 -2.14977
H   1.62688 -2.72223 -2.99448
H   4.77077  4.35077 -0.90730
H   5.13985  2.69673 -1.44947
H   4.03981  3.72282 -2.40229
H   2.13037  5.38751  1.46120
H   3.19688  4.37409  2.46583
H   3.83425  5.16287  1.00467
H   5.16332 -3.83421  1.00316
H   5.38791 -2.13043  1.46004
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H   2.69712 -5.13941 -1.45099
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H   4.35120 -4.77016 -0.90907
H  -4.35055  4.77064 -0.90830
H  -2.69647  5.13958 -1.45045
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H  -5.38797  2.13066  1.45995
H  -4.37468  3.19683  2.46508
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H  -4.77080 -4.35055 -0.90841
H  -3.83463 -5.16294  1.00353
H  -2.13080 -5.38787  1.46008
H  -3.19726 -4.37461  2.46493
```

$[Ru(IMe_4)_4H(\eta^2\text{-}O_2)]^+$

```
Energy            = -1779.71660566
Enthalpy 0K       = -1778.977541
Enthalpy 298K     = -1778.929119
Free Energy 298K  = -1779.057449

N  -0.12020 -3.15897 -0.41449
C   0.38468 -2.03195  0.20368
N   1.21409 -2.55360  1.17839
C   1.24164 -3.95652  1.15326
C   0.39631 -4.33913  0.14107
Ru -0.00000  0.00003 -0.27279
```

C	2.10792	0.33729	-0.22007
N	2.84658	1.09198	0.68233
C	4.21997	1.08503	0.38677
C	4.36579	0.30133	-0.73132
N	3.07896	-0.13734	-1.07748
C	2.32245	1.81941	1.83408
C	5.23526	1.83254	1.19786
C	5.58767	-0.07132	-1.51443
C	2.84709	-1.01872	-2.22450
C	2.00630	-1.78349	2.13362
C	2.07860	-4.77815	2.08660
C	0.03362	-5.70095	-0.36806
C	-1.11551	-3.20404	-1.48945
C	-0.38468	2.03198	0.20373
N	0.12018	3.15902	-0.41443
C	-0.39633	4.33916	0.14115
C	-1.24165	3.95653	1.15335
N	-1.21410	2.55361	1.17845
C	1.11546	3.20410	-1.48941
C	-2.00631	1.78347	2.13366
C	-2.07861	4.77814	2.08670
C	-0.03365	5.70099	-0.36795
O	-0.09336	-0.68936	-2.25560
O	0.09337	0.68948	-2.25558
C	-2.10791	-0.33729	-0.22008
N	-2.84655	-1.09200	0.68231
C	-4.21993	-1.08511	0.38672
C	-4.36577	-0.30142	-0.73137
N	-3.07895	0.13731	-1.07750
C	-2.32242	-1.81940	1.83407
C	-5.23522	-1.83266	1.19779
C	-5.58766	0.07118	-1.51450
C	-2.84711	1.01873	-2.22449
H	-0.00000	0.00000	1.33716
H	-3.25247	0.55521	-3.13844
H	-3.35518	1.98530	-2.06413
H	-1.76039	1.16097	-2.34227
H	-1.51274	0.81786	2.29619
H	-2.06379	2.33298	3.08503
H	-3.02733	1.60752	1.75564
H	0.71169	3.76260	-2.34884
H	2.02761	3.71138	-1.13244
H	1.34716	2.18092	-1.80831
H	2.34190	2.90946	1.66148
H	1.28619	1.50501	2.00320
H	2.92757	1.59680	2.72821
H	3.35511	-1.98532	-2.06414
H	1.76037	-1.16089	-2.34230
H	3.25251	-0.55520	-3.13842
H	2.06378	-2.33302	3.08498
H	3.02732	-1.60752	1.75561
H	1.51272	-0.81788	2.29618
H	-0.71176	-3.76251	-2.34890
H	-2.02765	-3.71133	-1.13247
H	-1.34723	-2.18085	-1.80831
H	-2.34170	-2.90945	1.66143
H	-1.28621	-1.50486	2.00329
H	-2.92763	-1.59691	2.72817
H	-1.98312	5.84727	1.83759
H	-3.15210	4.52029	2.02295
H	-1.77258	4.66195	3.14391
H	1.05114	5.90274	-0.29226
H	-0.31797	5.83716	-1.42817
H	-0.55394	6.47794	0.21489
H	-6.48656	-0.37538	-1.05936
H	-5.74321	1.16568	-1.55009
H	-5.53489	-0.28388	-2.56078
H	-5.02381	-2.91788	1.23785
H	-5.29281	-1.47211	2.24273
H	-6.23754	-1.71093	0.75612
H	6.23759	1.71073	0.75623
H	5.02392	2.91776	1.23789
H	5.29280	1.47200	2.24280
H	5.74317	-1.16582	-1.55004
H	5.53494	0.28377	-2.56071
H	6.48659	0.37518	-1.05926
H	3.15208	-4.52030	2.02285
H	1.77257	-4.66198	3.14381
H	1.98311	-5.84728	1.83747
H	0.55390	-6.47791	0.21477
H	-1.05117	-5.90269	-0.29238
H	0.31795	-5.83710	-1.42829

1

Energy = -2258.32755599
Enthalpy 0K = -2257.157299
Enthalpy 298K = -2257.088924
Free Energy 298K = -2257.255299

N	-2.64182	-1.49733	0.93456
C	-1.61716	-1.37407	-0.00628
N	-1.93244	-2.36690	-0.93406
C	-3.10362	-3.06480	-0.58215
C	-3.54934	-2.51992	0.60012
Ru	-0.00001	-0.00002	0.00683
C	1.37408	-1.61715	-0.00631
N	2.36692	-1.93237	-0.93410
C	3.06490	-3.10350	-0.58219
C	2.52008	-3.54923	0.60011
N	1.49742	-2.64179	0.93453
C	2.66479	-1.07182	-2.10784
C	2.51537	-1.80204	-3.45460
C	4.15584	-3.74809	-1.39051
C	2.94421	-4.73490	1.42048
C	0.58262	-2.75372	2.09630
C	1.30045	-2.70739	3.45728
C	-1.07191	-2.66483	-2.10780
C	-0.36380	-4.02573	-1.98261
C	-3.74833	-4.15568	-1.39046
C	-4.73515	-2.94389	1.42039
C	-2.75361	-0.58260	2.09639
C	-2.70723	-1.30055	3.45730
C	1.61715	1.37404	-0.00631
N	2.64182	1.49733	0.93450
C	3.54929	2.51997	0.60005

C	3.10355	3.06481	-0.58222
N	1.93238	2.36687	-0.93411
C	4.73504	2.94401	1.42036
C	2.75370	0.58256	2.09630
C	3.97183	-0.35208	1.98618
C	1.07181	2.66477	-2.10783
C	1.80198	2.51533	-3.45462
C	3.74818	4.15572	-1.39055
C	0.36369	4.02566	-1.98266
C	2.70731	1.30043	3.45724
C	-1.37407	1.61715	-0.00625
N	-2.36693	1.93240	-0.93401
C	-3.06482	3.10359	-0.58211
C	-2.51995	3.54930	0.60017
N	-1.49733	2.64180	0.93458
C	-2.66490	1.07182	-2.10771
C	-2.51572	1.80203	-3.45450
C	-4.15564	3.74830	-1.39049
C	-2.94392	4.73506	1.42049
C	-0.58251	2.75367	2.09634
C	-1.30030	2.70721	3.45733
C	-4.02573	0.36362	-1.98237
C	0.35210	3.97183	1.98618
C	4.02566	-0.36366	-1.98268
C	-0.35202	-3.97184	1.98606
C	-1.80213	-2.51541	-3.45456
C	-3.97168	0.35214	1.98632
H	4.61090	-4.57067	-0.81536
H	4.97060	-3.05180	-1.65202
H	3.77827	-4.18382	-2.33346
H	3.71171	-5.30857	0.87624
H	2.11710	-5.43367	1.63491
H	3.38879	-4.44113	2.38873
H	1.87247	-0.30814	-2.04254
H	3.33861	-2.50498	-3.65673
H	2.51977	-1.05669	-4.26805
H	1.56434	-2.35450	-3.51046
H	4.08241	0.22986	-1.05756
H	4.15983	0.32417	-2.83457
H	4.87418	-1.06639	-2.00261
H	-0.03796	-1.84337	1.99734
H	1.84934	-3.63625	3.67724
H	0.55072	-2.57885	4.25644
H	2.00670	-1.86518	3.51790
H	-0.92431	-3.95081	1.04682
H	-1.06968	-3.96610	2.82332
H	0.19831	-4.92436	2.04329
H	-3.05206	-4.97040	-1.65216
H	-4.18424	-3.77805	-2.33330
H	-4.57080	-4.61081	-0.81519
H	-5.30898	-3.71116	0.87601
H	-5.43371	-2.11664	1.63490
H	-4.44153	-3.38867	2.38860
H	-0.30819	-1.87255	-2.04253
H	0.22971	-4.08247	-1.05749
H	0.32402	-4.15996	-2.83450
H	-1.06656	-4.87423	-2.00251
H	-2.50524	-3.33853	-3.65659
H	-1.05680	-2.52003	-4.26803
H	-2.35441	-1.56427	-3.51050
H	-1.84323	0.03793	1.99740
H	-3.63604	-1.84955	3.67720
H	-2.57875	-0.55089	4.25654
H	-1.86496	-2.00674	3.51786
H	-3.95078	0.92434	1.04702
H	-3.96568	1.06988	2.82351
H	-4.92424	-0.19808	2.04380
H	-4.97048	3.05213	-1.65204
H	-3.77796	4.18398	-2.33343
H	-4.61060	4.57096	-0.81537
H	-2.11673	5.43374	1.63485
H	-3.38849	4.44139	2.38879
H	-3.71138	5.30879	0.87626
H	-1.87254	0.30818	-2.04251
H	-3.33906	2.50488	-3.65653
H	-2.52018	1.05666	-4.26793
H	-1.56475	2.35457	-3.51051
H	-4.08237	-0.22987	-1.05723
H	-4.16000	-0.32423	-2.83422
H	-4.87428	1.06632	-2.00220
H	0.03810	1.84335	1.99728
H	-1.84935	3.63597	3.67732
H	-0.55053	2.57877	4.25648
H	-2.00641	1.86488	3.51797
H	0.92426	3.95097	1.04685
H	1.06989	3.96592	2.82333
H	-0.19821	4.92434	2.04368
H	4.57074	4.61079	-0.81537
H	3.05191	4.97048	-1.65211
H	4.18395	3.77813	-2.33347
H	5.30867	3.71154	0.87613
H	5.43381	2.11687	1.63466
H	4.44137	3.38853	2.38867
H	0.30810	1.87248	-2.04252
H	2.50508	3.33845	-3.65669
H	1.05661	2.51995	-4.26806
H	2.35425	1.56420	-3.51058
H	-0.22975	4.08245	-1.05749
H	-0.32421	4.15982	-2.83449
H	1.06643	4.87417	-2.00266
H	1.84336	-0.03803	1.99731
H	3.95100	-0.92422	1.04683
H	3.96586	-1.06988	2.82332
H	4.92435	0.19821	2.04374
H	3.63609	1.84949	3.67715
H	2.57892	0.55071	4.25644
H	1.86499	2.00655	3.51789
H	-0.00003	-0.00001	-1.54705

^{1}2

Energy = -2408.67447201
Enthalpy 0K = -2407.494129
Enthalpy 298K = -2407.424042
Free Energy 298K = -2407.592978

N	2.53755	-1.99395	-0.65957
C	1.40684	-1.66993	0.09245
N	1.36922	-2.66631	1.05893
C	2.41907	-3.58642	0.90240
C	3.14290	-3.17123	-0.18899
Ru	0.00003	-0.00002	-0.21426
O	0.60906	-0.31731	-2.20458
O	-0.60914	0.31725	-2.20450
C	0.33199	-2.77278	2.11623
C	-0.56659	-4.00640	1.91272
C	2.74411	-4.74028	1.81037
C	4.37019	-3.82871	-0.75773
C	3.09224	-1.19830	-1.80077
C	4.55937	-0.77461	-1.60337
C	-1.68403	-1.36688	-0.09521
N	-2.04112	-2.34584	-1.00772
C	-3.23349	-2.99418	-0.64198
C	-3.64139	-2.43034	0.54455
N	-2.69339	-1.44199	0.87114
C	-1.20272	-2.69915	-2.18987
C	-0.56377	-4.09333	-2.05359
C	-2.75087	-0.59819	2.09995
C	-2.77258	-1.41019	3.41057
C	-4.84566	-2.80354	1.36388
C	-3.93113	-4.05910	-1.44110
C	-1.40680	1.66989	0.09246
N	-1.36918	2.66623	1.05897
C	-2.41899	3.58639	0.90242
C	-3.14278	3.17127	-0.18902
N	-2.53746	1.99397	-0.65960
C	-0.33192	2.77278	2.11622
C	0.56666	4.00637	1.91255
C	-2.74414	4.74016	1.81046
C	-4.36991	3.82896	-0.75788
C	-3.09236	1.19823	-1.80065
C	-4.55953	0.77479	-1.60305
C	1.68401	1.36685	-0.09527
N	2.04106	2.34584	-1.00776
C	3.23339	2.99425	-0.64199
C	3.64132	2.43040	0.54453
N	2.69339	1.44198	0.87109
C	1.20267	2.69908	-2.18994
C	1.94676	2.51614	-3.52330
C	3.93093	4.05928	-1.44105
C	4.84556	2.80366	1.36387
C	2.75092	0.59819	2.09990
C	3.90641	-0.41848	2.09590
C	-0.92812	2.69539	3.53414
C	-2.86842	1.89328	-3.15630
C	-3.90630	0.41854	2.09598
C	-1.94679	-2.51633	-3.52325
C	0.56374	4.09327	-2.05379
C	2.77266	1.41022	3.41051
C	0.92819	-2.69530	3.53414
C	2.86826	-1.89356	-3.15630
H	-3.45344	5.41588	1.30499
H	-1.86764	5.34539	2.08917
H	-3.23084	4.41005	2.74701
H	-4.40096	4.88634	-0.44648
H	-5.30715	3.36099	-0.40505
H	-4.38596	3.81841	-1.85830
H	0.27447	1.87079	1.95442
H	-1.46476	3.61003	3.82796
H	-0.11131	2.55171	4.26105
H	-1.61719	1.84095	3.63120
H	1.06838	3.97204	0.93432
H	1.34509	4.03275	2.69240
H	0.01350	4.95484	1.98611
H	-2.49161	0.28180	-1.79674
H	-3.51568	2.77311	-3.30518
H	-3.10028	1.17843	-3.96357
H	-1.81758	2.19436	-3.26899
H	-4.71514	0.27895	-0.63318
H	-4.80460	0.04182	-2.38998
H	-5.27928	1.60104	-1.70048
H	-5.46492	-1.93536	1.64554
H	-4.57831	-3.33623	2.29440
H	-5.49291	-3.47905	0.78175
H	-4.76186	-4.48367	-0.85467
H	-3.26864	-4.89773	-1.71228
H	-4.36201	-3.66356	-2.37834
H	-1.80255	-0.04100	2.05750
H	-3.86362	1.08634	1.22623
H	-3.83473	1.04069	3.00439
H	-4.89464	-0.06748	2.12055
H	-3.76459	-1.83428	3.62942
H	-2.52108	-0.73525	4.24629
H	-2.04024	-2.22906	3.40891
H	-0.38753	-1.96056	-2.16608
H	-2.68919	-3.30541	-3.72404
H	-1.20969	-2.54578	-4.34309
H	-2.44337	-1.53438	-3.56353
H	0.02362	-4.17255	-1.12491
H	0.12690	-4.24869	-2.89975
H	-1.29301	-4.91947	-2.07806
H	1.86768	-5.34607	2.08815
H	3.22986	-4.41023	2.74741
H	3.45417	-5.41546	1.30527
H	5.30730	-3.36022	-0.40526
H	4.38609	-3.81867	-1.85816
H	4.40169	-4.88593	-0.44586
H	-0.27440	-1.87081	1.95435
H	1.46454	-3.61006	3.82812
H	0.11141	-2.55125	4.26101
H	1.61751	-1.84105	3.63108
H	-1.06827	-3.97227	0.93446
H	-1.34505	-4.03264	2.69254
H	-0.01342	-4.95484	1.98651
H	2.49133	-0.28197	-1.79693
H	3.51558	-2.77334	-3.30512
H	3.09997	-1.17879	-3.96369
H	1.81743	-2.19475	-3.26885
H	4.71504	-0.27880	-0.63350
H	4.80420	-0.04156	-2.39029
H	5.27923	-1.60074	-1.70096
H	5.49286	3.47910	0.78171

H	5.46479	1.93549	1.64565
H	4.57818	3.33644	2.29434
H	4.76190	4.48358	-0.85477
H	3.26848	4.89808	-1.71180
H	4.36148	3.66394	-2.37853
H	1.80262	0.04097	2.05749
H	3.76468	1.83431	3.62932
H	2.52119	0.73529	4.24625
H	2.04033	2.22909	3.40886
H	3.86375	-1.08626	1.22613
H	3.83489	-1.04065	3.00430
H	4.89472	0.06759	2.12046
H	0.38747	1.96050	-2.16609
H	-0.02355	4.17263	-1.12506
H	-0.12703	4.24850	-2.89990
H	1.29297	4.91941	-2.07847
H	2.68915	3.30522	-3.72415
H	1.20966	2.54553	-4.34314
H	2.44334	1.53420	-3.56349
H	-0.00001	0.00002	1.39034

^{3}2

Energy = -2408.67364599
Enthalpy 0K = -2407.495593
Enthalpy 298K = -2407.424215
Free Energy 298K = -2407.598603

N	2.99511	-0.93739	-0.83459
C	1.90617	-1.03878	0.02675
N	2.34166	-1.95393	0.98256
C	3.64481	-2.40870	0.71193
C	4.05263	-1.77503	-0.43827
Ru	0.00859	-0.00103	-0.08150
C	-1.03909	-1.89431	0.04990
N	-1.93931	-2.32069	1.02558
C	-2.41162	-3.62028	0.76481
C	-1.80781	-4.03280	-0.39985
N	-0.96908	-2.98282	-0.81340
C	-2.36573	-1.48738	2.18213
C	-2.04384	-2.12938	3.54461
C	-3.35807	-4.40641	1.62898
C	-2.02630	-5.32530	-1.13589
C	-0.06366	-3.04322	-1.99621
C	-0.82363	-3.24466	-3.31837
C	1.51858	-2.39485	2.14045
C	1.09220	-3.86992	2.03719
C	4.45048	-3.34959	1.56376
C	5.38263	-1.90460	-1.12721
C	3.03072	-0.03698	-2.02199
C	2.98240	-0.81079	-3.35103
C	-1.89013	1.04398	0.05259
N	-2.99034	0.95336	-0.79315
C	-4.03533	1.80036	-0.38388
C	-3.60719	2.42973	0.76171
N	-2.30395	1.96394	1.01405
C	-5.33775	2.00183	-1.10701
C	-3.06035	0.02961	-1.96112
C	-4.08111	-1.10588	-1.76462
C	-1.45393	2.40799	2.15094
C	-2.06730	2.09325	3.52803
C	-4.38027	3.39692	1.61432
C	-1.03970	3.88562	2.03805
C	-3.26313	0.77241	-3.29278
C	1.04166	1.89964	0.01870
N	1.97386	2.33433	0.95715
C	2.41757	3.64019	0.68277
C	1.75856	4.05005	-0.45276
N	0.91785	2.99046	-0.83637
C	2.43239	1.50662	2.10476
C	2.13814	2.15264	3.47137
C	3.37428	4.44437	1.51801
C	1.86803	5.38242	-1.14037
C	0.00046	3.01755	-2.01158
C	0.75765	2.99407	-3.35100
C	3.90743	1.08690	1.98064
C	-1.03249	4.15572	-1.94067
C	-3.84028	-1.05605	2.09201
C	1.08049	-4.05811	-1.81898
C	2.17429	-2.08250	3.49852
C	4.18809	0.97665	-1.97506
H	-3.66994	-5.32057	1.09887
H	-4.27934	-3.85474	1.87951
H	-2.89467	-4.72715	2.57957
H	-2.60121	-6.02134	-0.50414
H	-1.08663	-5.83674	-1.40178
H	-2.60051	-5.18301	-2.06904
H	-1.73782	-0.59048	2.07517
H	-2.72464	-2.95526	3.80189
H	-2.15258	-1.36501	4.33274
H	-1.01004	-2.50570	3.58343
H	-4.04558	-0.51842	1.15514
H	-4.06998	-0.37602	2.92946
H	-4.53788	-1.90467	2.17055
H	0.38594	-2.04460	-2.01432
H	-1.18697	-4.27578	-3.45107
H	-0.14194	-3.02398	-4.15553
H	-1.67356	-2.55007	-3.39884
H	1.66780	-3.84666	-0.91252
H	1.75888	-3.97747	-2.68495
H	0.73365	-5.10284	-1.77800
H	3.88713	-4.24254	1.87940
H	4.83978	-2.86277	2.47709
H	5.32512	-3.70591	0.99509
H	5.88900	-2.82382	-0.78906
H	6.06198	-1.06174	-0.90245
H	5.29072	-1.97287	-2.22285
H	0.61897	-1.76800	2.04749
H	0.53995	-4.06381	1.10637
H	0.42760	-4.11539	2.88247
H	1.94494	-4.56504	2.08975
H	3.01613	-2.75166	3.73347
H	1.42358	-2.21533	4.29595
H	2.53294	-1.04257	3.54630
H	2.09557	0.52903	-1.93291
H	3.90148	-1.38631	-3.54657

H	2.86118	-0.09393	-4.17988
H	2.12205	-1.49499	-3.38225
H	4.20582	1.52260	-1.01876
H	4.03480	1.71698	-2.77810
H	5.17553	0.52035	-2.14242
H	4.27900	3.88393	1.80445
H	2.90901	4.82121	2.44761
H	3.70987	5.32711	0.94929
H	1.02134	6.05345	-0.90517
H	1.92511	5.29264	-2.23687
H	2.78597	5.89710	-0.81150
H	1.80733	0.60506	2.01417
H	2.80425	2.99926	3.69797
H	2.29250	1.39933	4.26244
H	1.09634	2.50154	3.54033
H	4.09327	0.55704	1.03533
H	4.16123	0.40278	2.80770
H	4.60041	1.94042	2.04820
H	-0.54660	2.07192	-1.92141
H	1.26387	3.94675	-3.57575
H	0.04063	2.79896	-4.16474
H	1.50333	2.18553	-3.37097
H	-1.58102	4.14070	-0.98565
H	-1.76758	4.01017	-2.75007
H	-0.59196	5.15440	-2.08247
H	-5.31640	3.67340	1.10331
H	-3.83606	4.33598	1.80989
H	-4.66259	2.96700	2.59220
H	-6.02020	2.60316	-0.48509
H	-5.85935	1.05701	-1.33199
H	-5.20703	2.54253	-2.06152
H	-0.55353	1.78688	2.03229
H	-2.90111	2.76282	3.78954
H	-1.29256	2.22632	4.30219
H	-2.42409	1.05356	3.58660
H	-0.54784	4.09007	1.07600
H	-0.32308	4.12418	2.84175
H	-1.88967	4.57615	2.15442
H	-2.06627	-0.42778	-1.98076
H	-3.87020	-1.68200	-0.85088
H	-4.00633	-1.79609	-2.62187
H	-5.12409	-0.75371	-1.72636
H	-4.29557	1.13003	-3.43097
H	-3.03515	0.08212	-4.12031
H	-2.57455	1.62691	-3.38158
H	-0.02268	-0.02203	1.50966
O	0.05053	0.03136	-2.15150
O	-0.28676	-0.14777	-3.39556

^{3}2b

Energy = -2408.66334827
Enthalpy 0K = -2407.485256
Enthalpy 298K = -2407.414411
Free Energy 298K = -2407.585894

N	3.11723	-0.52160	-0.83863
C	2.02900	-0.76626	-0.00350
N	2.56781	-1.60133	0.97779
C	3.92811	-1.87009	0.74441
C	4.27125	-1.19763	-0.40412
Ru	-0.00244	-0.00575	-0.11548
C	-0.75490	-2.04244	0.02685
N	-1.68219	-2.54142	0.94297
C	-1.97163	-3.89598	0.70899
C	-1.21050	-4.28026	-0.36983
N	-0.46312	-3.15655	-0.76002
C	-2.24076	-1.75051	2.07117
C	-1.74298	-2.23480	3.44641
C	-2.97311	-4.73259	1.45595
C	-1.22225	-5.61642	-1.05884
C	0.52654	-3.16460	-1.87346
C	-0.11916	-3.50960	-3.22689
C	1.80199	-2.10142	2.15176
C	1.55273	-3.61964	2.11434
C	4.83357	-2.68933	1.62139
C	5.62428	-1.14721	-1.05772
C	3.06403	0.35289	-2.04467
C	3.14704	-0.44784	-3.35605
C	-2.03020	0.74970	0.00758
N	-3.09349	0.48338	-0.84594
C	-4.26349	1.15454	-0.45331
C	-3.95052	1.85600	0.68749
N	-2.59376	1.60417	0.95839
C	-5.59930	1.07045	-1.13729
C	-2.97410	-0.39454	-2.04293
C	-3.93995	-1.59126	-2.00933
C	-1.85959	2.13631	2.13898
C	-2.50194	1.73704	3.48146
C	-4.88008	2.69123	1.52313
C	-1.61079	3.65329	2.07200
C	-3.06331	0.39436	-3.36090
C	0.75003	2.05929	0.00973
N	1.69324	2.56451	0.90183
C	1.97529	3.91843	0.65404
C	1.19269	4.29517	-0.41100
N	0.44214	3.16559	-0.78319
C	2.25683	1.79099	2.04041
C	1.74195	2.29071	3.40363
C	2.98021	4.76379	1.38717
C	1.13585	5.65088	-1.05991
C	-0.57226	3.17457	-1.88146
C	0.07375	3.28496	-3.27485
C	3.79143	1.69359	2.00593
C	-1.68777	4.21624	-1.68244
C	-3.77470	-1.64501	2.02067
C	1.76817	-4.02567	-1.58175
C	2.41596	-1.67220	3.49842
C	4.07454	1.51307	-1.99716
H	-2.81390	-5.79781	1.22121
H	-4.01582	-4.49508	1.17451
H	-2.89452	-4.63072	2.55016
H	-1.69008	-6.36945	-0.40347
H	-0.21431	-5.98522	-1.30600
H	-1.80669	-5.59717	-1.99691
H	-1.81532	-0.75161	1.89787

H -2.13897 -3.22310 3.72770
H -2.07545 -1.52210 4.22013
H -0.64470 -2.28083 3.48374
H -4.11723 -1.28787 1.03783
H -4.11284 -0.91790 2.77758
H -4.27600 -2.59805 2.24783
H   0.84987 -2.11807 -1.92829
H -0.34004 -4.58233 -3.33800
H   0.57971 -3.23326 -4.03357
H -1.04475 -2.93397 -3.38019
H   2.28711 -3.68975 -0.67229
H   2.46981 -3.91790 -2.42603
H   1.54624 -5.10019 -1.48216
H   4.37837 -3.63815 1.94826
H   5.15136 -2.14370 2.52912
H   5.75110 -2.94709 1.06706
H   6.24154 -1.98805 -0.70002
H   6.17680 -0.21927 -0.82045
H   5.57273 -1.22983 -2.15498
H   0.83446 -1.58706 2.03974
H   1.00694 -3.91964 1.20930
H   0.94246 -3.90536 2.98743
H   2.48469 -4.20429 2.17112
H   3.30979 -2.25634 3.76611
H   1.67285 -1.83684 4.29717
H   2.68366 -0.60486 3.50581
H   2.06080 0.79373 -1.99470
H   4.12441 -0.93461 -3.50586
H   2.98903 0.23873 -4.20456
H   2.35583 -1.21084 -3.40051
H   3.99881 2.07182 -1.05091
H   3.83641 2.21317 -2.81549
H   5.11842 1.19470 -2.13957
H   4.02276 4.49067 1.14162
H   2.87411 4.71086 2.48310
H   2.84820 5.82116 1.10713
H   0.23212 6.22147 -0.77892
H   1.16634 5.59829 -2.15996
H   2.00650 6.24889 -0.74572
H   1.84403 0.78644 1.87593
H   2.12495 3.28799 3.67121
H   2.07436 1.59494 4.19259
H   0.64260 2.32596 3.42890
H   4.14658 1.33599 1.02783
H   4.12096 0.96599 2.76633
H   4.28861 2.64694 2.24012
H -1.03568 2.18476 -1.80160
H   0.44160 4.29957 -3.49744
H -0.68175 3.04038 -4.04053
H   0.90066 2.56912 -3.38352
H -2.15636 4.12742 -0.69103
H -2.46949 4.02499 -2.43681
H -1.35107 5.25387 -1.82641
H -5.78662 2.92905 0.94246
H -4.43757 3.65103 1.83517
H -5.21425 2.16709 2.43758
H -6.24907 1.89048 -0.78939
H -6.12947 0.12522 -0.91756
H -5.52453 1.16045 -2.23282
H -0.88720 1.62577 2.06330
H -3.40579 2.32066 3.71427
H -1.77786 1.92757 4.29179
H -2.76187 0.66817 3.50993
H -1.02947 3.92779 1.18090
H -1.03251 3.96128 2.95940
H -2.54362 4.23941 2.07913
H -1.95289 -0.79289 -1.97182
H -3.84791 -2.15320 -1.06634
H -3.67582 -2.27575 -2.83294
H -4.99397 -1.30701 -2.15254
H -4.07803 0.76826 -3.57373
H -2.77093 -0.26754 -4.19194
H -2.36658 1.24601 -3.35885
H   0.02459 0.13882 1.47676
O   0.11232 0.51153 -2.17791
O -0.08495 -0.55871 -2.91959

Singlet-triplet MECP point

SCF energy (singlet): -2408.73907398
SCF energy (triplet): -2408.73892157

The energy in the text is an average value of the singlet and the triplet energies

N -2.59420 1.92502 -0.67201
C -1.45127 1.63438 0.07487
N -1.42938 2.64791 1.02893
C -2.49868 3.54393 0.86281
C -3.22092 3.09722 -0.21701
Ru -0.00481 -0.00635 -0.16519
O -0.58164 0.33802 -2.18160
O   0.52649 -0.26008 -2.62699
C -0.41686 2.76931 2.11064
C   0.48353 4.00680 1.93813
C -2.83649 4.71276 1.74111
C -4.45939 3.72087 -0.78811
C -3.14661 1.08526 -1.78142
C -4.59891 0.63226 -1.54362
C   1.64251 1.40842 -0.07723
N   1.96428 2.42411 -0.96776
C   3.13807 3.09900 -0.59398
C   3.57083 2.52002 0.57790
N   2.65507 1.49545 0.88406
C   1.11465 2.78586 -2.13731
C   0.41640 4.14466 -1.95908
C   2.74544 0.62118 2.08874
C   2.71137 1.40021 3.41882
C   4.75818 2.92359 1.40081
C   3.79440 4.20373 -1.36723
C   1.44014 -1.64420 0.04851
N   1.46059 -2.63972 1.02514
C   2.54490 -3.51700 0.85710
C   3.23937 -3.07393 -0.24526
N   2.57704 -1.92565 -0.70832

C	0.45621	-2.77512	2.11168
C	-0.42107	-4.02653	1.92147
C	2.92601	-4.66233	1.75039
C	4.48865	-3.67199	-0.82052
C	3.04824	-1.11356	-1.86652
C	4.47542	-0.56407	-1.69531
C	-1.63620	-1.41583	-0.05683
N	-1.95486	-2.40695	-0.97315
C	-3.12640	-3.09478	-0.61462
C	-3.55906	-2.54583	0.56952
N	-2.64632	-1.52777	0.90373
C	-1.10413	-2.73225	-2.15304
C	-1.85775	-2.59201	-3.48738
C	-3.78507	-4.17508	-1.42010
C	-4.75391	-2.95988	1.37573
C	-2.73359	-0.69305	2.13594
C	-3.91612	0.29158	2.12735
C	1.08008	-2.70121	3.51976
C	2.86327	-1.85483	-3.20218
C	3.95492	-0.33051	2.06234
C	1.85757	2.66954	-3.47885
C	-0.39628	-4.09051	-2.00837
C	-2.73257	-1.51823	3.43782
C	-1.04757	2.69008	3.51398
C	-2.96731	1.74898	-3.15912
H	3.61713	-5.33154	1.21550
H	2.07253	-5.27818	2.07174
H	3.45173	-4.32688	2.66232
H	4.57901	-4.72067	-0.49625
H	5.40278	-3.15094	-0.48528
H	4.49055	-3.67559	-1.91985
H	-0.17061	-1.88140	1.97865
H	1.65005	-3.60272	3.79196
H	0.27211	-2.59541	4.26356
H	1.74221	-1.82658	3.62202
H	-0.99112	-3.96895	0.98269
H	-1.14012	-4.11024	2.75271
H	0.16431	-4.95908	1.91386
H	2.36370	-0.25749	-1.86361
H	3.58809	-2.67218	-3.34735
H	3.00327	-1.13995	-4.02895
H	1.84608	-2.26418	-3.28342
H	4.57682	0.01698	-0.76609
H	4.67684	0.12090	-2.53613
H	5.25663	-1.33952	-1.71908
H	5.41721	2.07885	1.65611
H	4.47143	3.41920	2.34446
H	5.36990	3.64191	0.83408
H	4.60970	4.63968	-0.77210
H	3.10456	5.02642	-1.61473
H	4.23594	3.84667	-2.31349
H	1.82688	0.01785	2.01834
H	3.97827	-0.93746	1.14790
H	3.88843	-1.01783	2.92307
H	4.91338	0.20464	2.15661
H	3.66601	1.90216	3.64102
H	2.52347	0.68835	4.24065
H	1.91180	2.15369	3.43950
H	0.32880	2.02343	-2.12549
H	2.55738	3.50094	-3.66048
H	1.11487	2.68298	-4.29362
H	2.40355	1.71603	-3.54934
H	-0.18410	4.16240	-1.03599
H	-0.27015	4.29913	-2.80838
H	1.11422	4.99718	-1.94513
H	-1.96303	5.31635	2.02760
H	-3.34665	4.40401	2.67096
H	-3.52818	5.38129	1.20583
H	-5.38427	3.24551	-0.41694
H	-4.48118	3.68706	-1.88668
H	-4.50082	4.78214	-0.49710
H	0.20114	1.87125	1.97039
H	-1.61106	3.59556	3.78603
H	-0.24687	2.57108	4.26346
H	-1.71992	1.82181	3.60175
H	1.02890	3.97201	0.98392
H	1.22762	4.03673	2.75131
H	-0.07472	4.95431	1.98584
H	-2.52711	0.18257	-1.75746
H	-3.65771	2.59302	-3.32060
H	-3.17487	1.00338	-3.94468
H	-1.93440	2.09937	-3.29555
H	-4.71819	0.15056	-0.56178
H	-4.84654	-0.11793	-2.31307
H	-5.33715	1.44261	-1.63533
H	-5.37447	-3.64571	0.77993
H	-5.39852	-2.11323	1.66071
H	-4.47367	-3.49220	2.30083
H	-4.56834	-4.65969	-0.81820
H	-3.08545	-4.96595	-1.73143
H	-4.26861	-3.78352	-2.33187
H	-1.80167	-0.10830	2.10000
H	-3.70808	-1.98502	3.64397
H	-2.51240	-0.84354	4.28253
H	-1.96646	-2.30626	3.42767
H	-3.86470	0.98738	1.27934
H	-3.88895	0.88761	3.05545
H	-4.89090	-0.22154	2.10561
H	-0.32265	-1.96098	-2.14052
H	0.21471	-4.11964	-1.09253
H	0.28097	-4.23063	-2.86815
H	-1.08883	-4.94743	-1.99837
H	-2.55551	-3.42153	-3.68331
H	-1.12239	-2.58126	-4.30876
H	-2.41426	-1.64231	-3.53260
H	-0.10521	0.04604	1.41852

[Ru(IMe$_2$iPr$_2$)4(η^1-OOH)]$^+$

Energy = -2408.67225847
Enthalpy 0K = -2407.492676
Enthalpy 298K = -2407.421721
Free Energy 298K = -2407.592066

N	1.74262	-2.50537	0.94514
C	1.57634	-1.49497	-0.00379

N	2.67595	-1.68042	-0.84372
C	3.46174	-2.77617	-0.44246
C	2.87972	-3.29222	0.69073
Ru	-0.01189	-0.01393	-0.06885
O	0.34059	-0.11944	-2.04432
O	-0.65098	0.35455	-3.06860
C	3.00176	-0.80573	-2.00739
C	4.38720	-0.14424	-1.90675
C	4.72261	-3.25121	-1.11021
C	3.39428	-4.41764	1.54460
C	0.80882	-2.70997	2.07731
C	1.48732	-2.57957	3.45389
C	-1.57630	1.49829	0.05919
N	-1.62274	2.54009	0.99217
C	-2.74093	3.37086	0.80669
C	-3.44121	2.84920	-0.25454
N	-2.73915	1.70901	-0.68370
C	-0.64194	2.68748	2.09543
C	0.11133	4.02798	2.04499
C	-3.20954	0.80717	-1.76873
C	-3.35841	1.53533	-3.11685
C	-4.67765	3.41807	-0.89349
C	-3.05603	4.62290	1.57738
C	-1.49693	-1.54461	0.00004
N	-2.44366	-1.74218	1.01281
C	-3.25281	-2.86753	0.76588
C	-2.82205	-3.40517	-0.42448
N	-1.75567	-2.60037	-0.86936
C	-2.54728	-0.85207	2.19714
C	-3.83317	-0.00566	2.20978
C	-4.34604	-3.37935	1.66172
C	-3.38550	-4.59136	-1.15567
C	-0.93192	-2.85255	-2.08100
C	-0.05720	-4.11281	-1.95718
C	1.49781	1.53045	-0.01620
N	1.68100	2.60212	-0.88088
C	2.78555	3.39120	-0.51179
C	3.31637	2.82542	0.62441
N	2.52597	1.69871	0.91469
C	0.79039	2.86466	-2.04685
C	0.08846	4.23154	-1.96553
C	3.24912	4.63790	-1.21218
C	4.46966	3.33235	1.44449
C	2.72160	0.78693	2.06968
C	4.01767	-0.03673	1.97075
C	-2.36848	-1.58233	3.54218
C	-1.77127	-2.86556	-3.37577
C	-4.47766	0.01680	-1.39765
C	-1.25200	2.42810	3.48660
C	1.50257	2.65286	-3.39336
C	2.62201	1.49285	3.43521
C	2.78811	-1.52092	-3.35323
C	0.01714	-4.02406	1.95065
H	-4.89283	-4.18977	1.15336
H	-5.09105	-2.60731	1.92058
H	-3.95868	-3.79698	2.60876
H	-4.10317	-5.12303	-0.51006
H	-2.61381	-5.32385	-1.44691
H	-3.92917	-4.30084	-2.07306
H	-1.69111	-0.16538	2.05497
H	-3.26750	-2.14773	3.83210
H	-2.19039	-0.83564	4.33460
H	-1.51413	-2.27390	3.53133
H	-3.90809	0.63642	1.32214
H	-3.83550	0.64310	3.10143
H	-4.73675	-0.63293	2.26888
H	-0.25656	-1.97816	-2.10310
H	-2.33609	-3.80127	-3.51381
H	-1.10006	-2.77214	-4.24753
H	-2.49728	-2.03366	-3.40307
H	0.59610	-4.05652	-1.07316
H	0.59002	-4.18861	-2.84743
H	-0.64451	-5.04427	-1.90390
H	2.61601	-5.14544	1.82713
H	3.86654	-4.05791	2.47778
H	4.16837	-4.97502	0.99196
H	4.94678	-4.28294	-0.79192
H	5.60223	-2.63488	-0.84779
H	4.64339	-3.26379	-2.20856
H	0.09869	-1.87212	1.95793
H	-0.53914	-4.06375	1.00323
H	-0.70920	-4.10446	2.77615
H	0.66830	-4.90980	2.01256
H	2.13097	-3.44043	3.69075
H	0.71256	-2.53072	4.23757
H	2.09471	-1.66386	3.52343
H	2.24410	-0.01312	-1.94812
H	3.54790	-2.29062	-3.56635
H	2.84020	-0.77734	-4.16631
H	1.79198	-1.98604	-3.38875
H	4.51402	0.38170	-0.94767
H	4.46731	0.60925	-2.70839
H	5.22435	-0.84649	-2.04106
H	5.20177	2.54730	1.69765
H	4.14401	3.80048	2.39206
H	5.01364	4.10628	0.87852
H	2.60175	5.50950	-1.00260
H	3.29695	4.51801	-2.30637
H	4.26396	4.90270	-0.87198
H	1.86950	0.08966	1.97290
H	3.50694	2.11033	3.65344
H	2.55648	0.73088	4.23042
H	1.72937	2.13145	3.50650
H	4.06228	-0.60379	1.03096
H	4.06011	-0.75586	2.80585
H	4.91722	0.59436	2.04665
H	0.02416	2.08722	-1.95321
H	2.24449	3.43586	-3.62049
H	0.74955	2.66444	-4.19741
H	1.99625	1.67058	-3.42075
H	-0.43784	4.35545	-1.00556
H	-0.66615	4.28398	-2.76843
H	0.77080	5.08404	-2.10926
H	-4.09204	4.93593	1.36799
H	-2.40286	5.46908	1.29373
H	-2.97559	4.49467	2.66907

H	-5.14074	4.15593	-0.21778
H	-5.44277	2.65580	-1.11166
H	-4.45441	3.94255	-1.84055
H	0.08311	1.88277	1.88137
H	-1.95672	3.21476	3.79783
H	-0.44501	2.40416	4.23842
H	-1.77893	1.46360	3.52704
H	0.56753	4.18965	1.05721
H	0.92060	4.02381	2.79356
H	-0.53943	4.88328	2.28231
H	-2.37958	0.09929	-1.86663
H	-4.30958	-0.63014	-0.52475
H	-4.74751	-0.63267	-2.24807
H	-5.35019	0.65849	-1.19500
H	-4.26693	2.15440	-3.17211
H	-3.43418	0.78435	-3.92173
H	-2.47845	2.16044	-3.32765
H	-0.99489	-0.50741	-3.39016

$[Ru(^{i}Pr_2P(CH_2)_2P^{i}Pr_2)_2(\eta^2\text{-}O_2)H]^+$

Energy = -1377.74048359
Enthalpy 0K = -1376.868719
Enthalpy 298K = -1376.816952
Free Energy 298K = -1376.946563

C	-1.25198	4.70132	-0.72177
C	-1.44371	3.17743	-0.85611
P	-0.79718	2.11970	0.59815
C	0.70499	3.07118	1.19919
C	1.82858	2.96299	0.16632
P	2.14899	1.16221	-0.32923
C	2.77575	1.35459	-2.12369
C	3.62717	2.60484	-2.42317
C	-2.89239	2.81449	-1.22872
C	-2.00554	2.26670	2.06550
C	-1.33260	1.82854	3.38112
C	-2.62924	3.66463	2.25188
C	3.60532	0.67619	0.80844
C	3.25502	0.95681	2.28295
C	4.96336	1.31025	0.45584
C	3.44362	0.08156	-2.66788
Ru	0.00653	-0.01571	-0.20329
O	-0.27760	0.74360	-2.11293
O	0.27603	-0.54675	-2.21490
P	-2.14278	-1.18291	-0.46934
C	-2.82383	-0.92601	-2.25387
C	-2.51431	-2.10272	-3.19783
C	-3.57894	-0.93608	0.77773
C	-3.07605	-1.10226	2.22585
C	-1.80473	-3.03306	-0.30158
C	-0.74380	-3.32003	0.76461
P	0.76873	-2.20327	0.58399
C	1.60160	-2.37288	2.30084
C	0.75753	-1.77043	3.43544
C	-4.81614	-1.83289	0.57253
C	1.89720	-3.31440	-0.49750
C	3.37969	-2.91114	-0.46682
C	1.38552	-3.47639	-1.93944
C	-4.29746	-0.49849	-2.40379
C	1.98832	-3.82433	2.65812
H	0.01366	-0.01583	1.41174
H	3.15598	3.54644	-2.10043
H	3.28006	2.03920	2.49794
H	-1.43890	-2.33479	-3.22464
H	-2.81020	-1.81897	-4.22354
H	-3.81748	-0.69294	2.93468
H	1.33573	-1.78963	4.37549
H	3.78895	-2.84882	0.55484
H	0.43011	4.12174	1.39501
H	1.55116	3.49780	-0.75770
H	-0.41244	-4.37228	0.71969
H	1.00235	2.61848	2.15793
H	2.76216	3.42223	0.53456
H	-2.74465	-3.56604	-0.07996
H	-1.46459	-3.37754	-1.28888
H	-1.14454	-3.14437	1.77616
H	-0.79626	2.81914	-1.67767
H	-3.17032	3.33214	-2.16307
H	-3.00843	1.73622	-1.40857
H	-3.61783	3.12176	-0.45699
H	-1.56387	5.17478	-1.66966
H	-1.86502	5.14303	0.07854
H	-0.20301	4.99226	-0.55012
H	-2.80569	1.54742	1.81865
H	-2.10164	1.68136	4.15859
H	-0.77118	0.88584	3.28621
H	-0.64000	2.60319	3.75121
H	-3.24027	3.98557	1.39624
H	-3.28880	3.64550	3.13744
H	-1.86092	4.43337	2.43894
H	1.79838	1.45584	-2.63245
H	4.63048	2.55556	-1.97273
H	3.76538	2.67665	-3.51675
H	4.40927	-0.13765	-2.17852
H	2.77334	-0.78350	-2.56558
H	3.65170	0.21251	-3.74453
H	3.68182	-0.41651	0.66733
H	2.26105	0.57301	2.56413
H	4.00264	0.48364	2.94380
H	4.92768	2.41264	0.49711
H	5.72105	0.98460	1.19109
H	5.32378	1.01554	-0.54072
H	-2.17779	-0.08210	-2.56026
H	-3.08323	-3.01232	-2.93563
H	-4.42741	-0.03818	-3.39927
H	-4.98419	-1.35996	-2.36119
H	-4.63077	0.24359	-1.66013
H	-3.87498	0.11954	0.62049
H	-2.95733	-2.17087	2.47577
H	-2.11288	-0.60201	2.40320
H	-5.27736	-1.72996	-0.41703
H	-4.57520	-2.89787	0.73136
H	-5.58088	-1.56821	1.32467
H	2.52481	-1.77319	2.20116
H	0.47415	-0.72552	3.23659

```
H  -0.16648 -2.34731  3.61154
H   2.47593 -3.83108  3.64854
H   1.10285 -4.47812  2.73368
H   2.69452 -4.28020  1.94836
H   1.79919 -4.29179  0.01257
H   3.97176 -3.67066 -1.00747
H   3.55103 -1.94985 -0.97272
H   2.07400 -4.13713 -2.49553
H   0.38973 -3.94534 -1.97846
H   1.33115 -2.51221 -2.46643
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3. We assume that the chloride salt of $[Ru(I^{i}Pr_2Me_2)_4H]^+$ is formed initially. We made this assumption and carried out the metathesis by adding ten mole equivalents of $NaBAr_4^F$.

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