Supplementary Information

Novel stereoelectronic properties of 5-coordinate Ruthenium(0) nitrosyl complexes

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Methods

General: $Ru(NO)Cl_3 \cdot H_2O$ and bis(2-diisopropylphosphinoethyl)amine (10% in THF) were purchased from Strem Chemicals. NaBr and NaI were purchased from Merck Denmark. Deuterated solvents were purchased from Fluorochem. Ethanol, THF, diethyl ether and anhydrous acetone were purchased from VWR Denmark. Ethanol was dried by refluxing over magnesium/iodine under N_2 atmosphere overnight followed by trap-to-trap distillation followed by degassing by 3 cycles of freeze-pump-thaw and stored under N_2 over 3 Å molecular sieves (activated by microwave heating). Acetone was flushed with N_2 prior to use. THF and Et_2O were dried over aluminum oxide, purged with N_2 and stored inside an Ar filled glovebox. All manipulations were conducted using standard Schlenk techniques unless otherwise stated. $Ru^{15}NOCl_3$ used for ^{15}N-enriched samples were synthesized according to literature.[45] The complexes **1a** and **1b** were obtained *a priori.*[46]

(PNP)RuCl(NO) (**2**): To a red ethanolic solution (1 mL) of 70 mg (129 µmol) of **1** was added 17.6 mg (2 equiv.) NaOEt in 3 mL EtOH whereby the solution darkened. The dark red solution was stirred at 50 °C for 2 h, giving an intense dark green solution which was allowed to cool down to rt before all volatiles were removed *in vacuo*. The crude product was extracted three times with 1.5 mL THF by filtering through cannula. The combined extracts were dried *in vacuo* yielding the pure product as a green solid. Further handling of the extremely air sensitive compound was done in a glovebox where the product was dissolved in THF and subsequently left in the freezer at −30 °C for 3 days whereafter the mother liquor was decanted off and the crystals were washed with cold THF. An additional batch of crystals was isolated by reducing the volume of the mother liquor until precipitation set in followed by storing at −30 °C, decanting and washing with cold THF. Yield (crystals): 45% NMR DATA ^1H NMR (14.1 T C_6D_6): δ/ppm 3.05 (m, iPr1-CH, 2H), 2.44 (t, 3J = 11.6 Hz, NH, 1H) 2.28 (m, NCH_2a, 2H), 2.13 (m, iPr2-CH, 2H), 2.09 (m, NCH_2b, 2H), 1.62 (m, P-CH_2, 4H), 1.69 (m, iPr1-$CH_3$1, 6H), 1.18 (m, iPr1-$CH_3$2, 6H), 1.15 (m, iPr2-$CH_3$1, 6H) 1.06 (m, iPr2-$CH_3$2, 6H). ^{13}C NMR (18.8 T C_6D_6): δ/ppm 53.7 (broad, NCH_2) , 28.7 (t, $^1J(^{13}C\text{-}^{31}P)$ = 9.5 Hz, PCH_2), 26.5 (t, $^1J(^{13}C\text{-}^{31}P)$ = 8.8 Hz, iPr*2*-CH) 26.0 (t, $^1J(^{13}C\text{-}^{31}P)$ = 10.8 Hz, iPr*1*-CH), 21.0 (broad, iPr1-$CH_3$1), 19.8 (broad, iPr2-$CH_3$1), 17.3 (broad, iPr1-$CH_3$2), 19.3 (broad, iPr2-$CH_3$2). ^{31}P NMR (14.1 T C_6D_6): δ/ppm 71.2. ^{15}N NMR (18.8 T C_6D_6): δ/ppm 62.6 (Ru-$NCH_2$1), 429 (Ru-NO). ATR-FTIR: $\tilde{\nu}$/cm^{-1} 1630 (NO).

(PNP)RuBr(NO) (**3**): In in 3 mL EtOH was dissolved 120 mg (221 µmol) **1** and treated with 30 mg (442 µmol, 2 equiv.) NaOEt in 5 mL EtOH. The resulting dark red solution was stirred at 50 °C for 2 h and subsequently allowed to cool to rt. The tempered solution was filtered via cannula into a Schlenk flask loaded with 68 mg (661 µmol, 2.6 equiv.) NaBr. The head space atmosphere was carefully removed, and the suspension was stirred at rt for 24 h. All volatiles were removed in vacuo and the product was extracted 3 times with 4 mL THF using cannula filtration. By evaporation of the combined extracts, the extremely air sensitive compound **3** could be isolated as a brownish powder. Inside an Ar filled glovebox, the product was dissolved in THF and layered with Et_2O and left for crystallization at −30 °C for one week. The liquid phase was decanted, and the crystals were washed with cold THF. An additional amount of product was isolated by concentration until precipitation occurred followed by layering with Et_2O and storing at −30 °C for one week. Combined yield (crystals): 51% NMR DATA ^1H NMR (14.1 T C_6D_6): δ/ppm 3.18 (m, iPr1-CH, 2H), 2.51 (t, 3J = 11.6 Hz, NH, 1H) 2.31 (m, NCH_2a, 2H), 2.15 (m, iPr2-CH, 2H), 2.03 (m, NCH_2b, 2H), 1.72 (m, P-CH_2a, 2H), 1.68 (m, iPr1-$CH_3$1, 6H), 1.63 (m, P-CH_2b, 2H), 1.35 (m, iPr1-$CH_3$2, 6H), 1.17 (m, iPr2-$CH_3$1, 6H) 1.05 (m, iPr2-$CH_3$2, 6H). ^{13}C NMR (18.8 T C_6D_6): δ/ppm 54.0 (broad, NCH_2), 29.0 (t, $^1J(^{13}C\text{-}^{31}P)$ = 9.5 Hz, PCH_2), 27.0 (t, $^1J(^{13}C\text{-}^{31}P)$ = 8.8 Hz, iPr*1*-CH) 26.6 (t,

$^{1}J(^{13}C\text{-}^{31}P)$ = 10.8 Hz, iPr*2*-CH), 21.0 (broad, iPr1-$CH_3$1), 19.9 (broad, iPr2-$CH_3$1), 19.6 (broad, iPr2-$CH_3$2). 17.4 (broad, iPr1-$CH_3$2). ^{31}P NMR (14.1 T C_6D_6): δ/ppm 70.1. ^{15}N NMR (18.8 T C_6D_6): δ/ppm 60.3 (Ru-NCH_2), 415 (Ru-NO). ATR-FTIR: $\tilde{\nu}$/cm^{-1} 1643 (NO).

(PNP)RuI(NO) (**4**): Dissolved in 3 mL acetone 50 mg (106 µmol) of **2** was resulting in an intensely green solution. Upon addition of 19 mg (127 µmol, 1.2 equiv.) NaI in 3 mL acetone, the green solution changed color instantly to purple. The purple solution was stirred at rt for 30 min before the solvent was removed in vacuo. The crude product was extracted 3 times with 1 mL THF via cannula filtration. By evaporation of the combined extracts the extremely air sensitive compound **4** could be isolated as purple powder. Inside the glovebox, the product was dissolved in the minimum amount of THF and Et_2O was diffused into the solution at −30 °C over the course of 10 days whereupon high quality crystals precipitated as black rhombic blocks. Yield (crystals): 45% NMR DATA ^{1}H NMR (14.1 T Tol-d_8): δ/ppm 3.29 (m, iPr1-CH, 2H), 2.65 (t, 3J = 11.6 Hz, NH, 1H) 2.50 (m, NCH_2a, 2H), 2.23 (m, iPr2-CH, 2H), 2.00 (m, NCH_2b, 2H), 1.91 (m, P-CH_2a, 2H), 1.76 (m, P-CH_2b, 2H), 1.66 (m, iPr1-$CH_3$1, 6H), 1.19 (m, iPr1-$CH_3$2, 6H), 1.13 (m, iPr2-$CH_3$1, 6H) 1.09 (m, iPr2-$CH_3$2, 6H). ^{13}C NMR (18.8 T Tol-d_8): δ/ppm 54.4 (broad, NCH_2), 29.5 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 10.4 Hz, PCH_2), 29.3 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 11.8 Hz, iPr*1*-CH) 26.6 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 9.9 Hz, iPr2-CH), 20.9 (t, $^{2}J(^{13}C\text{-}^{31}P)$ = 3.1 Hz, iPr1-$CH_3$1), 19.9 (broad, iPr2-$CH_3$1), 19.8 (t, $^{2}J(^{13}C\text{-}^{31}P)$ = 1.0 Hz, iPr2-$CH_3$2). 17.2 t, $^{2}J(^{13}C\text{-}^{31}P)$ = 1.4 Hz, iPr1-$CH_3$2). ^{31}P NMR (14.1 T Tol-d_8): δ/ppm 69.1. ^{15}N NMR (18.8 T Tol-d_8): δ/ppm 56.0 (Ru-NCH_2), 416 (Ru-NO). ATR-FTIR: $\tilde{\nu}$/cm^{-1} 1646 (NO).

[(PNP)RuNO]BF_4 (**5**): In 4 mL EtOH was 100 mg (168.3 µmol) of **1b** dissolved and slowly treated with 22.9 mg (336.6 µmol, 2 equiv.) NaOEt in 4 mL EtOH at rt. The resulting dark red solution was heated to 55 °C and stirred at this temperature for 1 h where after the dark green solution was allowed to cool to rt. All volatiles were removed *in vacuo*. The crude product was washed with small amounts of toluene until the filtrates were only slightly colored (green). The pure, extremely air sensitive product was transferred to an argon filled glove box where the product was dissolved in THF and layered with Et_2O and left at −30 °C for 3 days. The mother liquor was decanted off and the high-quality crystals were dried in vacuo. An additional amount of product could be isolated by concentration of the mother liquor until precipitation followed by layering with Et_2O and leaving the solution at −30 °C for 5 days. Combined yield (crystals): 65% NMR DATA ^{1}H NMR (14.1 T THF-d_8): δ/ppm 2.99 (m, NCH_2a, 2H), 2.78 (m, iPr2-CH, 2H), 2.87 (m, iPr1-CH, 2H), 2.49 (t, 3J = 11.6 Hz, NH, 1H), 2.99 (m, NCH_2a, 2H), 2.78 (m, iPr2-CH, 2H), 2.60 (m, P-CH_2a, 2H), 2.46 (m, P-CH_2b, 2H), 2.21 (m, NCH_2b, 2H), 1.54 (m, iPr1-$CH_3$1, 6H), 1.52 (m, iPr2-$CH_3$1, 6H), 1.50 (m, iPr2-$CH_3$2, 6H) 1.46 (m, iPr1-$CH_3$2, 6H). ^{13}C NMR (18.8 T THF-d_8): δ/ppm 52.3 (dt, $^{2}J(^{13}C\text{-}^{31}P)$ = 4.7 Hz NCH_2), 22.0 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 10.2 Hz, PCH_2), 26.9 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 11.4 Hz, iPr*1*-CH) 26.0 (t, $^{1}J(^{13}C\text{-}^{31}P)$ = 12.8 Hz, iPr*2*-CH), 19.2 (t, $^{2}J(^{13}C\text{-}^{31}P)$ = 2.3 Hz, iPr2-$CH_3$2), 18.8 ($t^{2}J(^{13}C\text{-}^{31}P)$ = 2.1 Hz, iPr1-$CH_3$2), 18.3 (broad iPr1-$CH_3$1). 18.1 (broad, iPr2-$CH_3$1). ^{31}P NMR (14.1 T THF-d_8): δ/ppm 75.5. ^{15}N NMR (18.8 T THF-d_8): δ/ppm 56.9 (Ru-NCH2). ATR-FTIR: $\tilde{\nu}$/cm^{-1} 1737 (NO).

(PNP)RuNO (**6**): In 10 mL Et_2O, was 100 mg (191.1 µmol) of **5** and 21.5 mg KO^{t}Bu (191.6 µmol, 1 equiv.) suspended. The resulting dark red suspension was stirred at rt for 1 h and the mixture was subsequently filtered through a plug of Celite. The filtrate was evaporated in vacuo until dryness whereby the product was isolated as a reddish black powder. Single crystals suitable for X-ray diffraction analysis were obtained by saturating a mixture of Et_2O and pentane (1:1) with the titled compound and leaving the solution at −30 °C for ~25 days. Yield (crystals): 30% NMR DATA ^{1}H NMR

(14.1 T C_6D_6): δ/ppm 2.95 (m, NCH_2, 4H), 2.20 (m, iPr1-CH1, 4H), 1.86 (m, P-CH_2, 4H), 1.34 (m, iPr-$CH_3$1, 12H), 1.21 (m, iPr-$CH_3$2, 12H). ^{13}C NMR (18.8 T C_6D_6): δ/ppm 61.2 (t, $^1J(^{13}C\text{-}^{31}P$ = 8.3 NCH_2), 26.4 (t, $^1J(^{13}C\text{-}^{31}P)$ = 10.7 Hz, iPr*1*-CH), 24.1 (t, $^1J(^{13}C\text{-}^{31}P)$ = 9.5 Hz, PCH_2), 19.7 t, $^2J(^{13}C\text{-}^{31}P)$ = 3 Hz iPr-$CH_3$1), 18.4 (broad, iPr-$CH_3$2). ^{31}P NMR (14.1 T C_6D_6): δ/ppm 89.0. ^{15}N NMR (18.8 T C_6D_6): δ/ppm 388.9 (Ru-NO), 159.5 (Ru-NCH2). ATR-FTIR: $\tilde{\nu}$/cm^{-1} 1666 (NO).

Computational details

All DFT calculations were performed using the ORCA 5 software package.[47,48] All energies were converged to 10^{-6} atomic units using the identity approximation to speed up calculations.[49] Geometry-optimized structures and energies were calculated using the PBE0[50,51] and the hybrid TPSSh[52] functional with def2-SVP and def2-TZVPP basis sets respectively[53] together with Grimme's D4 methodology to account for dispersion forces,[54,55] as well as Weigend's def2/J auxiliary basis.[56] Specifically for geometry optimization, the def2-QZVP[53,56] basis set was employed on Ru, N and O atoms. Single-point energy calculations were achieved using the TPSSh/def2-TZVP methodology together with the NBO7 program to obtain natural population analysis (NPA).[57] The effective core potential (ECP) approximation was used to account for the 28 inner core electrons of the Ru and I atoms.[58,59] All vibrational frequencies were calculated under the harmonic oscillator approximation. No solvent model was employed in the calculations as all spectroscopic and crystallographic results did not suggest any non-negligible solvent-effect in solution phase.

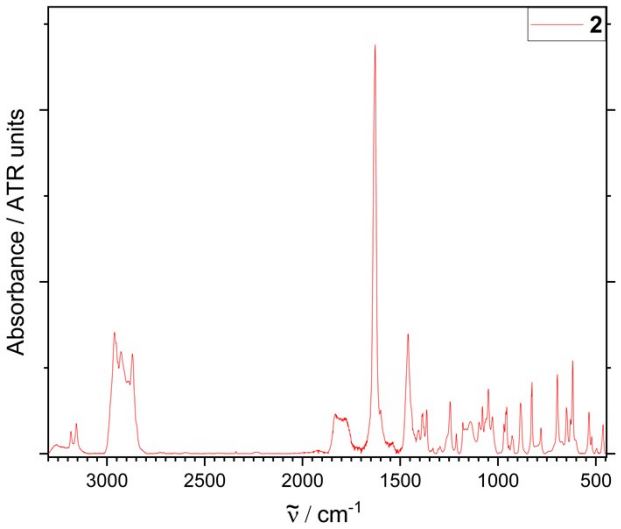
X-ray Crystallography

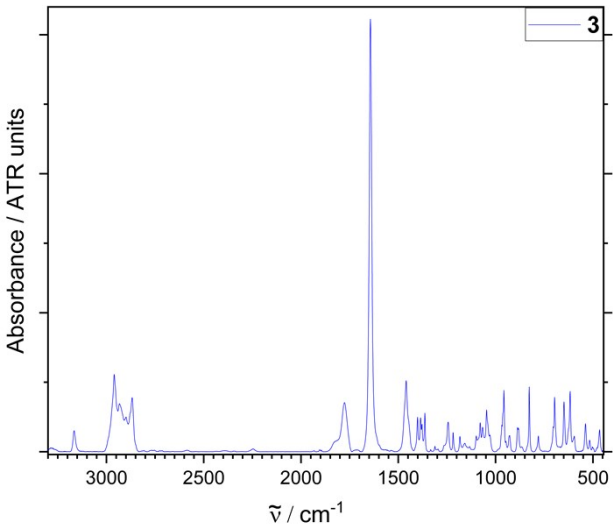
General: All crystal batches for X-ray diffraction analysis were immersed in polybutene oil (Aldrich, >90%) as protection against air. A suitable crystal was harvested with a MiTeGen cryo loop and mounted on a goniometer attached to a SuperNova Dual Source CCD-diffractometer. Data was collected at 120 K using CuKα radiation (**1b, 2, 5, 6**) or MoKα (**1a, 3, 4**). Using Olex2,[60] all structures were solved using SHELXT[61] structure solution program using Intrinsic Phasing and refined with SHELXL[62] refinement package using Least Squares minimization.

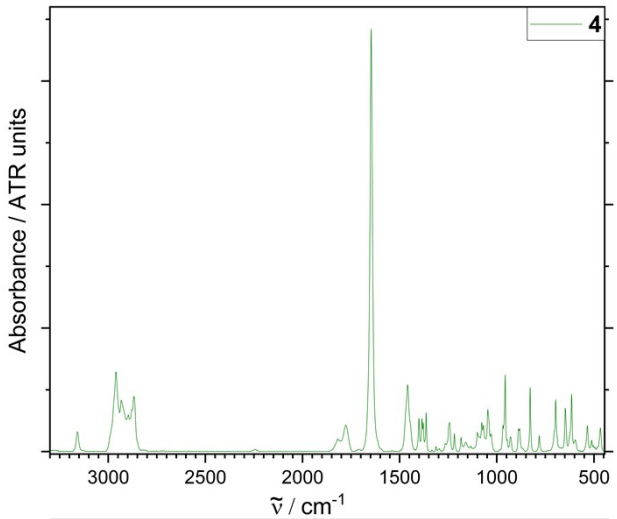
Attenuated-Total-Reflection Fourier Transform Infrared Spectroscopy

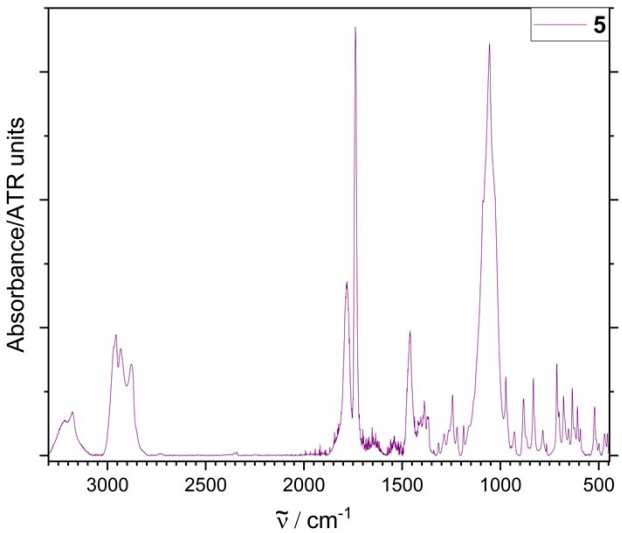
The attenuated-total-Reflectance (ATR) Fourier Transform infrared (FTIR) spectra were recorded on a VERTEX 80 vacuum FTIR spectrometer from Bruker Optics GmbH. The FTIR spectrometer was equipped with a Ge on KBr beam splitter, a liquid nitrogen cooled HgCDTe detector, a thermal global radiation source and a single-reflection germanium ATR accessory (IRIS) from PIKE Technologies Inc. Small traces of residual water vapor absorption from the interferometer were subtracted and the resulting absorption spectra were corrected for minor baseline drifts. Subsequently, extended ATR corrections were applied to account for the wavelength-dependent penetration depth of the infrared probe beam into the solid samples.

Below are the full ATR FTIR spectra of the complexes **2** – **6** shown









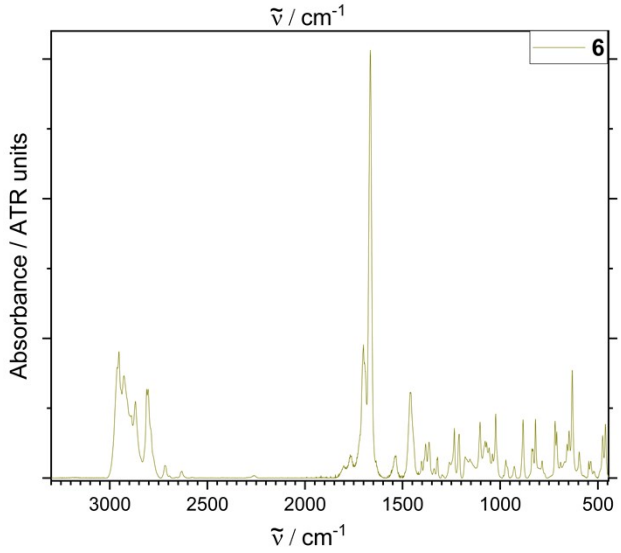


Table S1. Selected experimental and calculated (harmonic approximation) geometries, vibrational NO frequencies and experimental NMR data. Experimental data is expressed in bold. "*Syn"* and "*anti"* refer to the orientation with respect to the amine proton.

Measure	**1a**	**2**	**3**	**4**	**5**	**6**	X=F	X=OMe
ν(NO) / cm^{-1}								
exp.	**1838**	**1630**	**1643**	**1646**	**1737**	**1666**	-	-
calc.	-	1752	1756	1762	1867	1784	1741	1720
Ru-X / Å								
exp.	***syn:* 2.377** ***anti:* 2.366**	**2.5523**	**2.698**	**2.8637**	**-**	**-**	**-**	**-**
calc.	-	2.5767	2.725	2.9211	-	-	2.178	2.174
Ru-NO / Å								
exp.	**1.7536**	**1.727**	**1.752**	**1.737**	**1.719**	**1.752**	**-**	**-**
calc.	-	1.734	1.734	1.735	1.727	1.750	1.728	1.733
N-O / Å								
exp.	**1.134**	**1.191**	**1.173**	**1.185**	**1.172**	**1.187**	**-**	**-**
calc.	-	1.195	1.194	1.193	1.174	1.191	1.198	1.200
HN-Ru / Å								
exp.	**2.150**	**2.221**	**2.225**	**2.235**	**2.176**	**2.007**	**-**	**-**
calc.	-	2.285	2.289	2.291	2.197	2.019	2.276	2.314
Ru-N-O / °								
exp.	**178.039**	**172.9**	**174.28**	**174.2**	**177.56**	**179.89**	**-**	**-**
calc.	-	179.3	178.38	177.0	178.43	176.49	176.09	177.92
X-Ru-NO / °								
exp.	***syn:* 92.665** ***anti:* 85.724**	**141.041**	**138.149**	**135.716**	**-**	**-**	**-**	**-**
calc.	-	136.88	133.33	128.34	-	-	148.8	146.6
HN-Ru-X / °								
exp.	***syn:* 86.164** ***anti:* 85.724**	**79.616**	**79.945**	**82.328**	**-**	**-**	**-**	**-**
calc.	-	74.153	75.712	77.754	-	-	67.691	66.827
NMR δ / ppm:								
^{15}NH	**67.8**	**62.6**	**60.3**	**56.0**	**75.5**	**159.5**	-	-
^{31}P	**68.0**	**71.2**	**70.1**	**69.1**	**56.9**	**89.0**	-	-
^{1}H-N	**-**	**2.44**	**2.51**	**2.65**	**2.49**	**-**	-	-
^{15}NO	**373**	**429**	**415**	**416**	**-**	**388**		

NMR Spectroscopy:

The NMR spectra were measured using either a 18.8T Bruker Avance III or 14.1T Bruker Avance IIIHD spectrometer. The 18.8T system was mounted with a 5 mm TCI CryoProbe (Bruker) while the 14.1T system was mounted with a 5 mm RT BBFO probe (Bruker). All measurements were performed at 25^{o}C. Resonance assignment was performed using 2D ^{1}H-^{13}C HSQC, ^{1}H-^{13}C HMBC and ^{1}H-^{31}P HMBC spectra measured at 14.1 T, while ^{1}H-^{15}N HMBC spectra and 1D ^{13}C spectra were measured at 18.8 T. ^{1}H and ^{13}C Chemical shifts are reported relative to TMS, ^{31}P chemical shifts are reported relative to H_3PO_4 and ^{15}N chemical shifts are reported relative to liquid ammonia (for comparison with CH_3NO_2 subtract 380.2 ppm from the listed values).

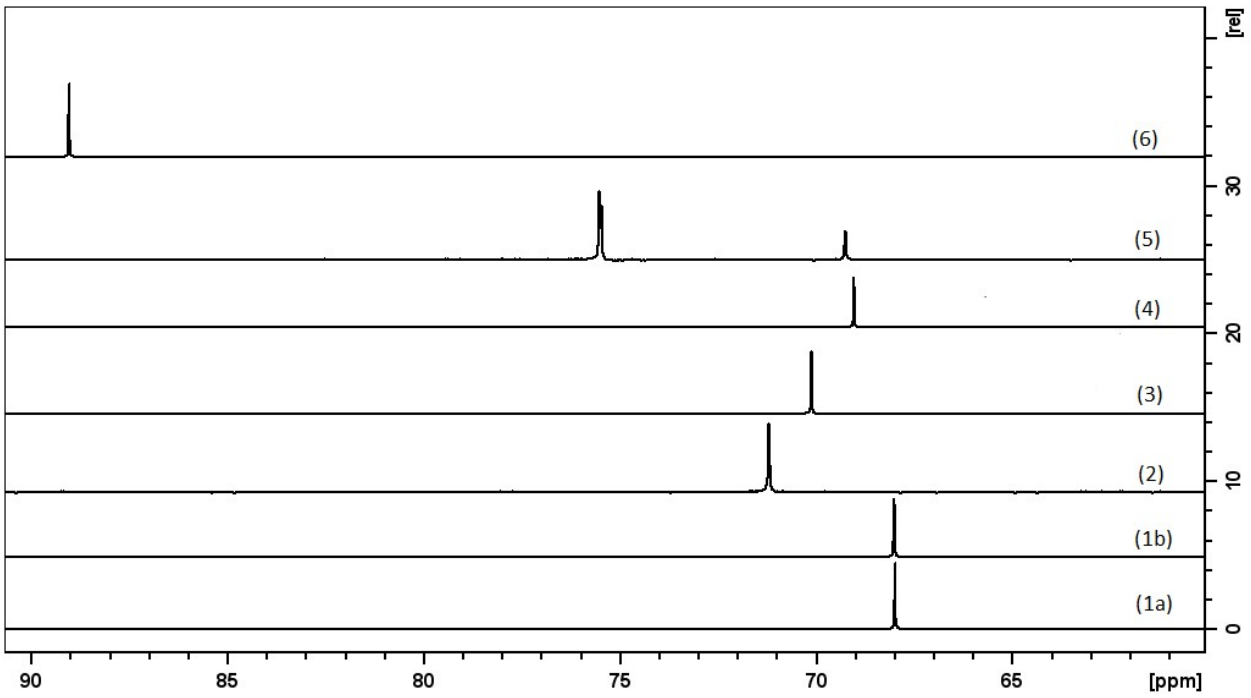


Figure S1: ^{31}P NMR spectra of all complexes indicated by number as they appear in the main text.

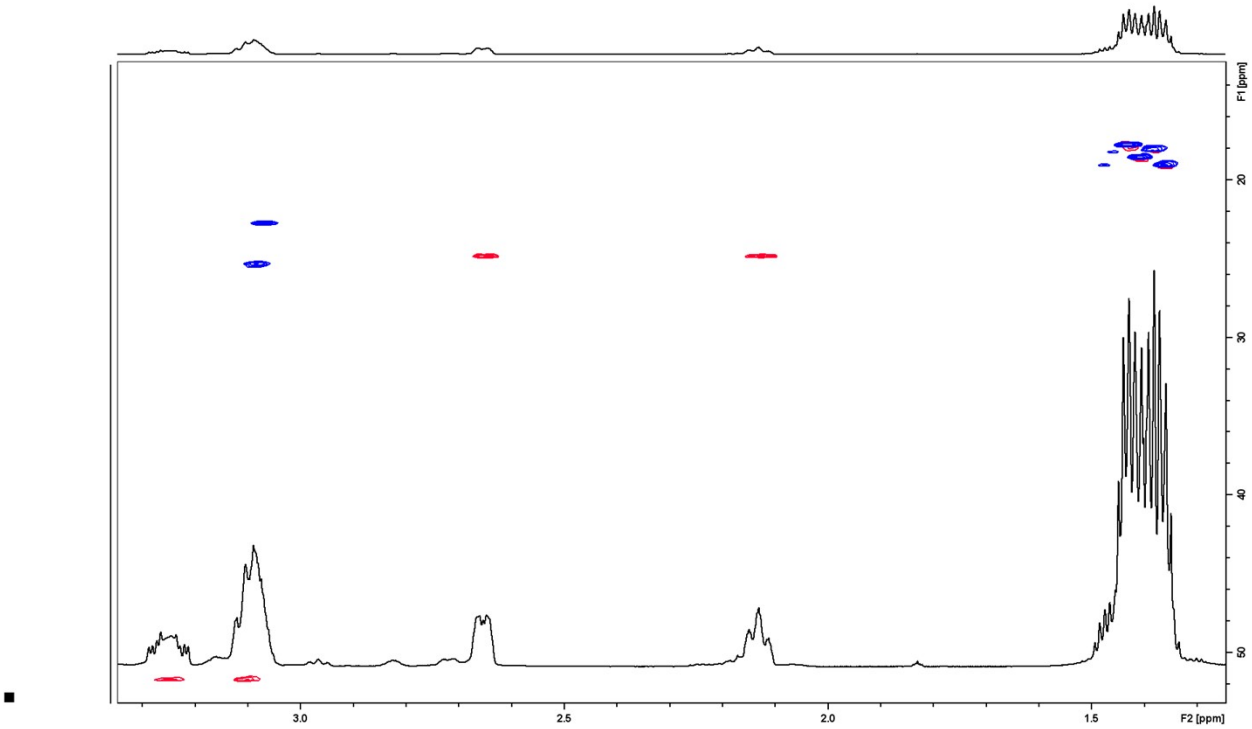


Figure S2: HSQC NMR spectrum of **1a** with ^{1}H spectrum attached for clarity.

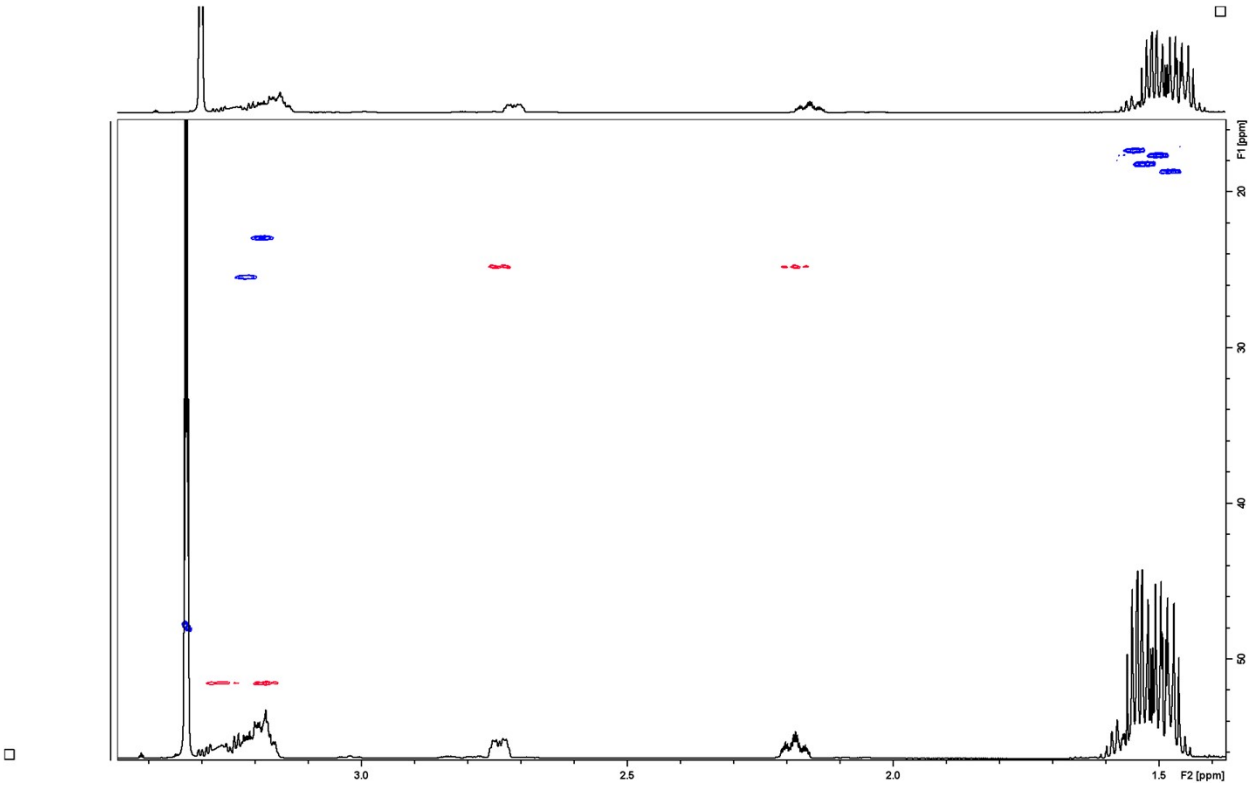


Figure S3: HSQC NMR spectrum of **1b** with ^{1}H NMR spectrum attached for clarity.

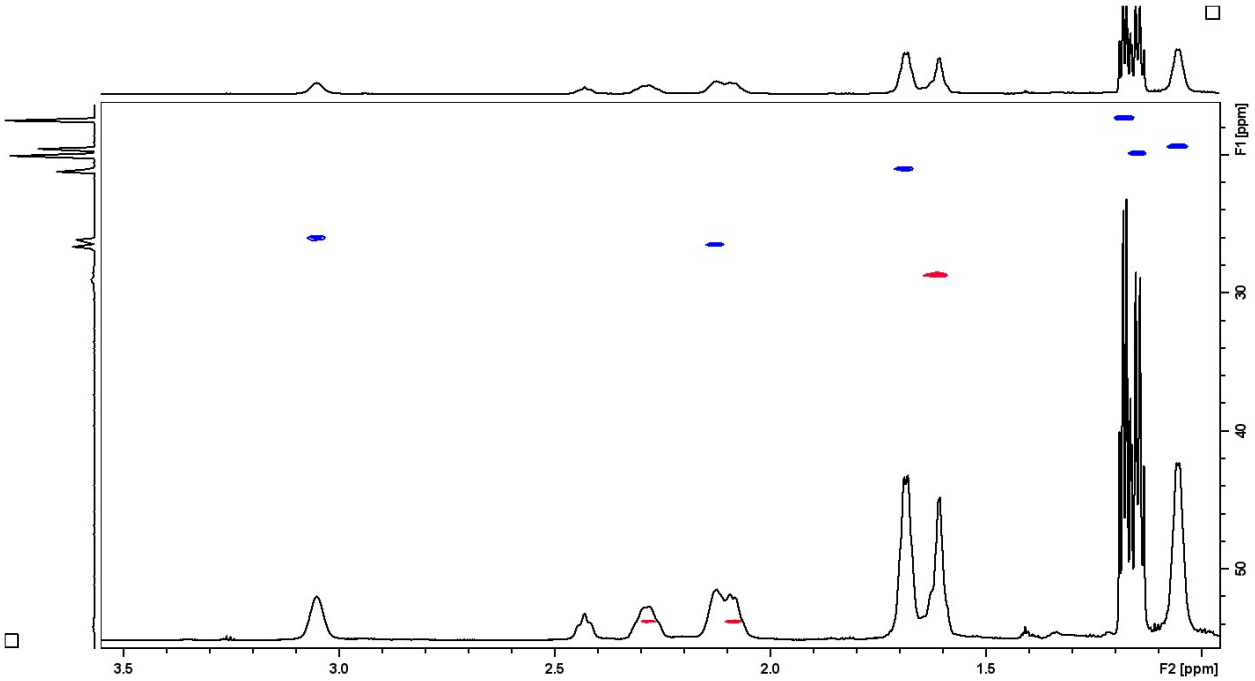


Figure S4: HSQC NMR spectrum of **2** with ^{1}H NMR spectrum attached for clarity.

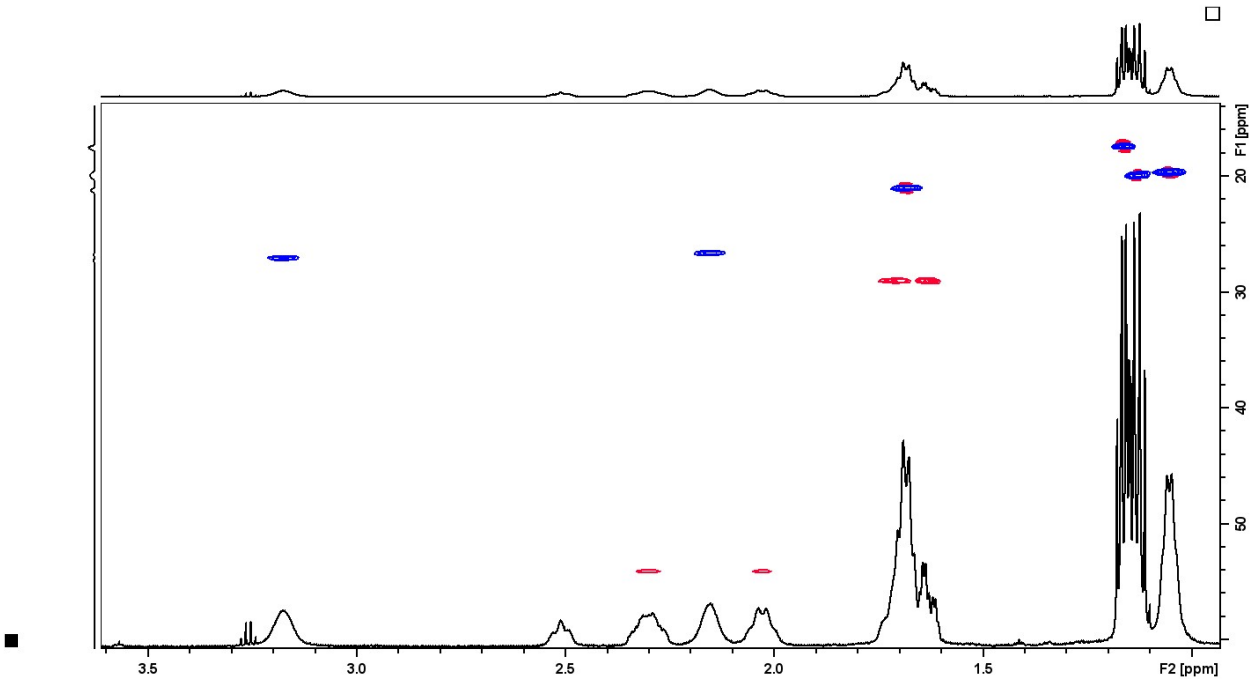


Figure S5: HSQC NMR spectrum of **3** with ^{1}H NMR spectrum attached for clarity.

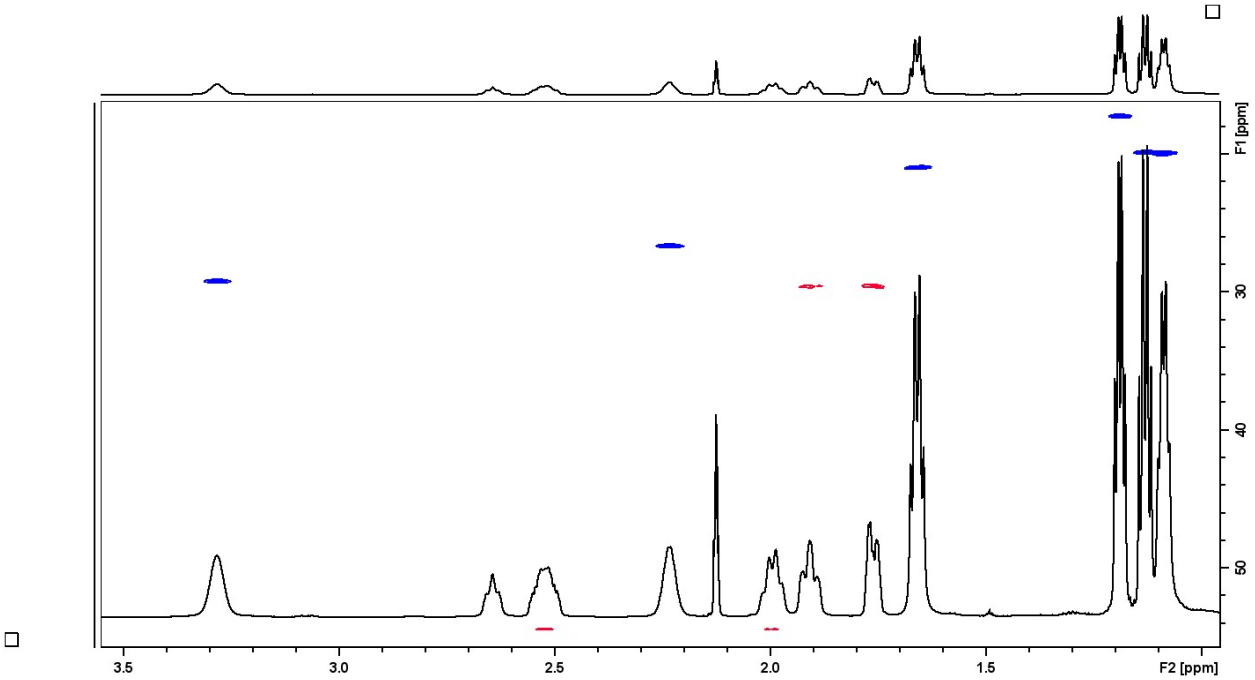


Figure S6: HSQC NMR spectrum of **4** with ^{1}H NMR spectrum attached for clarity.

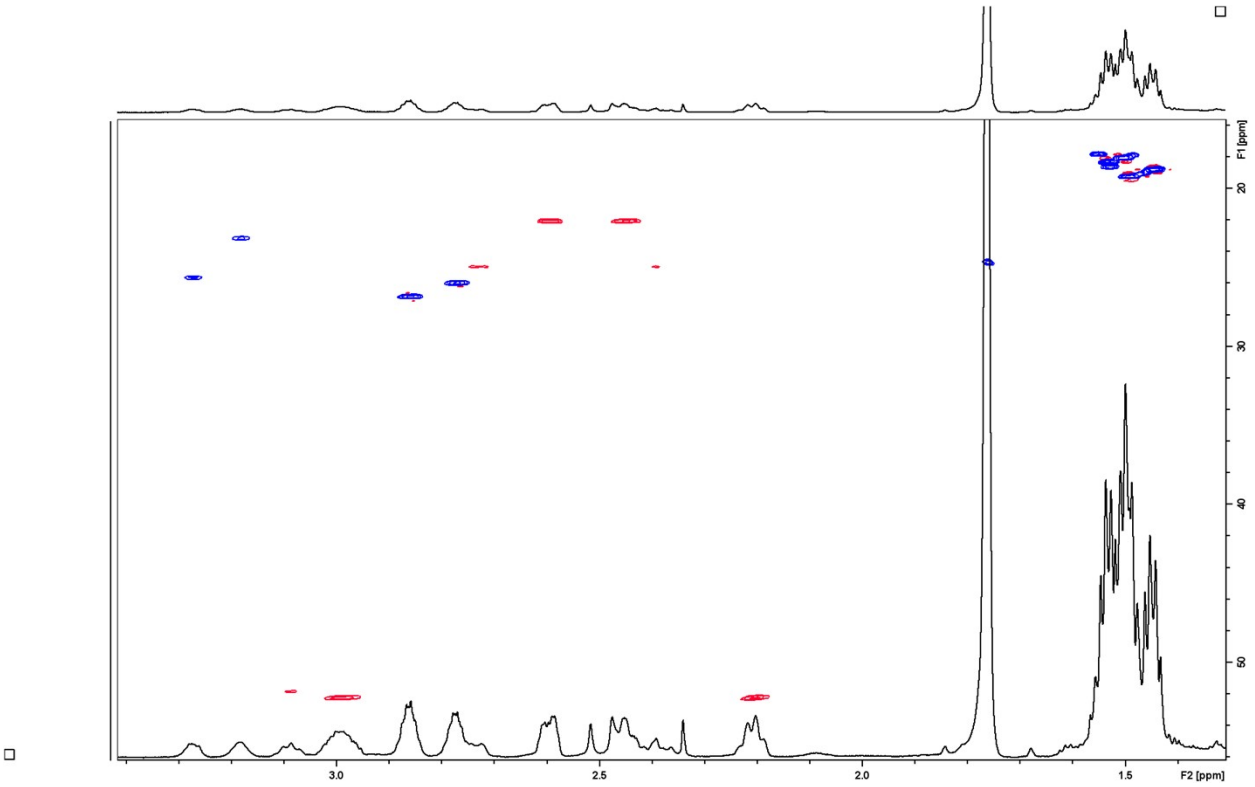


Figure S7: HSQC NMR spectrum of **5** with ^{1}H NMR spectrum attached for clarity.

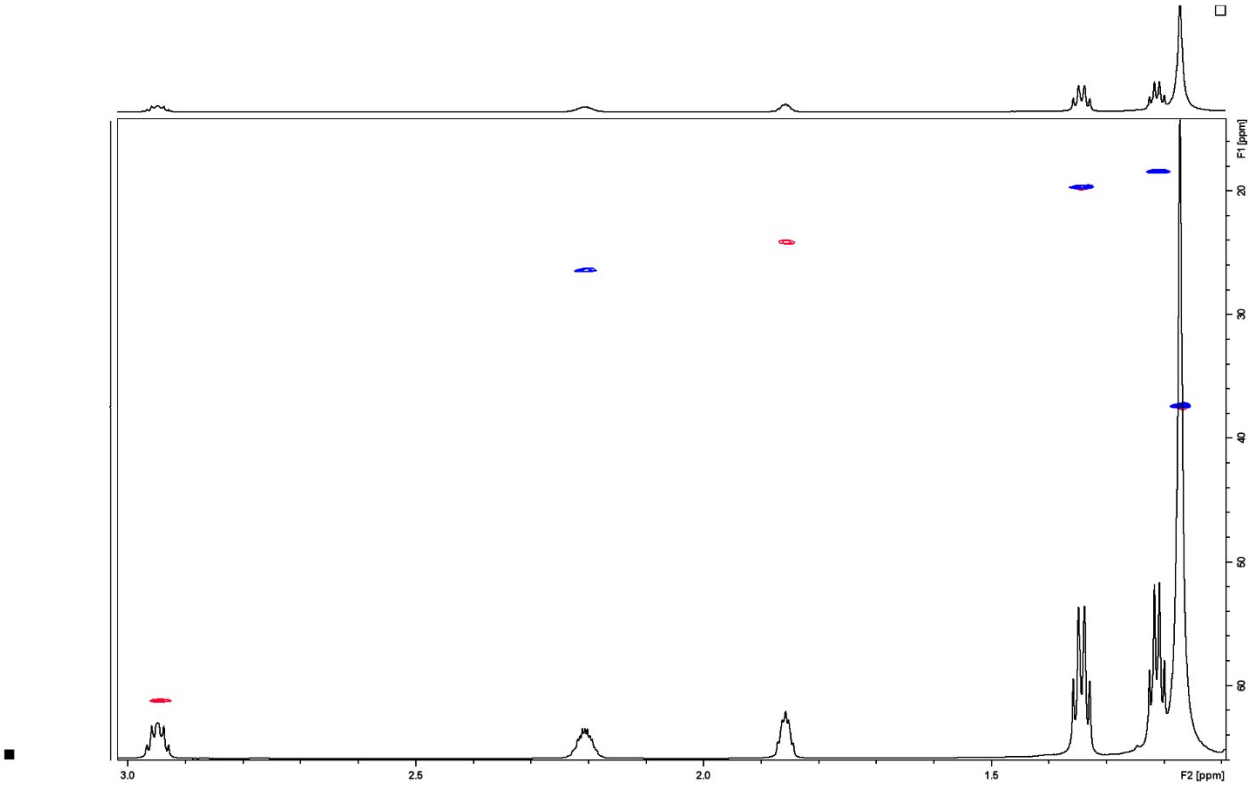
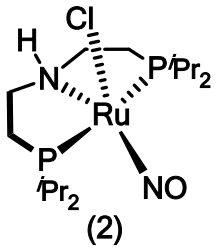


Figure S8: HSQC NMR spectrum of **6** with ^{1}H NMR spectrum attached for clarity.

DFT-optimised structures, xyz-coordinates

Table S2. Atom coordinates from DFT geometry optimization of **2**

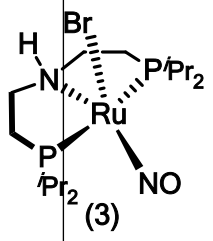
Ru	-3.8779663	5.8611499	6.6055191
P	-2.3574999	4.0685090	6.6511605
P	-4.9502949	7.9104565	7.0226401
N	-2.2831761	6.8087007	7.9405203
O	-4.9672571	5.4006630	3.9262215
N	-4.5153542	5.5899510	5.0161997
Cl	-4.4980669	5.2026828	9.0182356
C	-0.9962789	4.7081471	7.7820665
C	-1.4249161	3.5330672	5.0966591
C	-6.5316723	7.8671600	8.0541465
C	-4.2696493	1.9953747	7.0350329
C	-0.6895479	4.7230402	4.4607151
C	-3.7433260	8.7866729	8.1701219
C	-0.9370032	6.2385235	7.7485539
C	-5.2383644	9.1692598	5.6424061
C	-2.3534222	2.8512023	4.0786073
C	-3.9252115	9.4895961	4.9110437
C	-2.3150034	8.2831529	7.9424736
C	-2.8997215	2.4866169	7.5295551
C	-1.8374154	1.3804588	7.5795659
C	-7.5395017	6.8401415	7.5138953
C	-6.3191172	8.7004453	4.6543348
C	-7.1552435	9.2399539	8.3394297
H	-2.6815131	6.4535871	8.8389045
H	-1.2578714	4.3662192	8.8061238
H	-0.0095743	4.2686800	7.5276879
H	-0.6705663	2.7938216	5.4487044
H	-6.1268197	7.4360206	8.9963802
H	-4.2282965	1.5699132	6.0118026
H	-4.6484769	1.1987092	7.7096514
H	-5.0002686	2.8279389	7.0405309
H	-1.4013654	5.5342487	4.2025587
H	0.0884951	5.1484113	5.1264490
H	-0.1801402	4.3990268	3.5284836
H	-3.7959134	9.8896579	8.0589025
H	-4.0655815	8.5427977	9.2046247
H	-0.5547234	6.5984871	6.7714092
H	-0.2348745	6.6096923	8.5351188
H	-5.5954296	10.0897979	6.1574009
H	-1.7706335	2.5484603	3.1828009
H	-2.8312944	1.9387964	4.4845354
H	-3.1569841	3.5351565	3.7394999
H	-3.4778787	8.5696655	4.4808557
H	-4.1177221	10.2020934	4.0813056
H	-3.1713191	9.9595289	5.5747980
H	-1.6362979	8.6916722	8.7310680
H	-1.9255050	8.6302007	6.9634596



(2)

Table S3. Atom coordinates from DFT geometry optimization of **3**

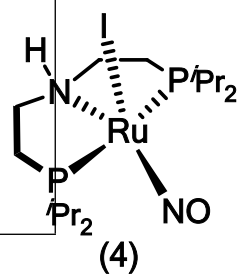
Ru	4.4863132	6.4360317	8.2097148
P	4.0477287	8.1773439	9.7302295
O	2.6866970	7.3487052	6.0880622
N	3.4055335	6.9661815	6.9614124
P	5.0165477	4.3419471	7.2742510
Br	7.1446785	6.8189228	8.6681337
C	5.1914483	9.6819495	9.7360461
H	6.1527452	9.1857453	9.9974339
N	4.8946367	5.2955401	10.1514820
H	5.9139527	3.5136443	10.2133282
C	4.2109313	5.8669289	11.3286589
H	3.1325528	5.6233165	11.2401676
H	4.5815126	5.3893198	12.2684051
C	4.7252152	3.8341517	10.0274496
H	5.1071095	3.3158410	10.9408160
H	3.6373286	3.6280736	9.9640799
C	6.5797842	4.1893310	6.2235652
H	7.3441842	4.4692029	6.9824557
C	4.4231534	7.3817356	11.3930361
H	3.8183963	7.8299340	12.2083430
H	5.4899053	7.6026927	11.6102926
C	5.4511757	3.3098170	8.7857931
H	6.5492834	3.4073320	8.9226301
H	5.2307216	2.2338209	8.6269025
C	3.6915344	3.3079701	6.4043843
H	4.1673080	2.3164333	6.2309559
C	2.2919712	8.8466876	9.9523507
H	2.3475631	9.5127796	10.8430000
C	1.8337222	9.6742222	8.7408172
H	2.4854101	10.5490267	8.5536412
H	1.8083435	9.0635725	7.8167475
H	0.8064847	10.0586452	8.9164395
C	4.8592335	10.7414539	10.7961829
H	3.9208928	11.2868648	10.5633182
H	4.7593538	10.3118899	11.8143135
H	5.6696980	11.5001716	10.8411631
C	1.3013275	7.7100829	10.2488391
H	1.3140336	6.9539414	9.4364863
H	1.5212223	7.1906346	11.2034615
H	0.2713104	8.1170463	10.3279547
C	5.3809207	10.2704849	8.3289235
H	5.6401306	9.4726263	7.6058283
H	4.4774106	10.7971900	7.9609606
H	6.2126079	11.0063244	8.3400263
C	6.6479542	5.2645643	5.1272825
H	5.9226088	5.0851696	4.3080801
H	6.4532634	6.2681185	5.5543992
H	-3.0674498	2.8918252	8.5521294
H	-0.8634531	1.7396474	7.9717870
H	-2.1747048	0.5591998	8.2474725
H	-1.6561494	0.9296862	6.5813669
H	-8.3560852	6.6921456	8.2516148
H	-8.0076499	7.1605102	6.5611411
H	-7.0420696	5.8639448	7.3507361
H	-7.3009773	8.5446458	5.1414571
H	-6.4605096	9.4662773	3.8625896
H	-6.0308372	7.7534259	4.1560393
H	-7.9765115	9.1377478	9.0805678
H	-6.4257681	9.9630976	8.7598751
H	-7.5975913	9.6948339	7.4287705



(3)

H	7.6622143	5.2752933	4.6756187
C	3.2897122	3.9106056	5.0481775
H	2.5199667	3.2707320	4.5669837
H	2.8564735	4.9238930	5.1650712
H	4.1428208	3.9848586	4.3463873
C	2.4627150	3.1135280	7.3058174
H	2.0345511	4.0924760	7.6060631
H	1.6793297	2.5447592	6.7615409
H	3.2545041	8.9357449	7.9846055
H	2.6969927	2.5445230	8.2279350
C	6.8709057	2.7750215	5.7029335
H	6.8501471	3.4093223	6.5061979
H	6.1518798	2.4628682	4.9172153
H	7.8830004	2.7399394	5.2463910

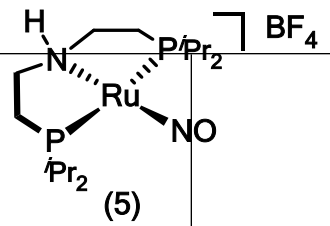
Table S4. Atom coordinates from DFT geometry optimization of 4



(4)

Ru	5.4338789	8.7153361	10.2952032
P	7.4980209	7.5796889	10.3000412
P	3.1247507	9.4857401	10.2555713
N	4.6843526	6.5776943	9.6231338
O	0.1690987	10.7645589	12.2515903
N	5.8603713	9.9072856	11.4822688
C	2.4423233	10.4563674	9.0316675
C	5.5852036	5.5441227	9.9902634
C	9.1370432	9.6229831	9.1655256
C	2.3862386	7.5826799	9.6132197
C	8.8652833	8.1114653	9.1054796
C	7.0373939	5.8804343	9.6453804
C	2.5547652	10.8342366	12.5116173
C	3.2047852	11.7900704	9.0874481
C	3.2743340	6.3928562	9.9812653
C	8.9485935	8.4668385	12.5905813
C	2.1910116	9.4821625	11.8772860
C	8.3680226	7.2004260	11.9396603
C	0.9177091	10.6339026	9.0695018
C	10.1463879	7.2671267	9.1746234
C	7.4332905	6.4649100	12.9119706
C	2.4160954	8.3323337	12.8709697
H	4.7424989	6.8038823	8.5920584
H	2.7310376	9.9704267	8.0721036
H	5.4702295	5.3704351	11.0793052
H	5.2745230	4.6046137	9.4720161
H	8.1917077	10.1949518	9.0869798
H	9.6539278	9.9267918	10.0983623
H	9.7867726	9.9198958	8.3157013
H	1.3521369	7.4296971	9.9853045
H	2.3312889	7.6862818	8.5086429
H	8.3538749	7.9233177	8.1340632
H	7.1635431	5.9296700	8.5429370
H	7.7226327	5.0941720	10.0245610
H	3.6304728	10.8862873	12.7726497
H	2.3243237	11.6906861	11.8496132
H	1.9767478	10.9750799	13.4494947
H	2.9821600	12.3708992	10.0053943
H	4.2982619	11.6192488	9.0373208
H	2.9190551	12.4204543	8.2194693
H	2.9092327	5.4688406	9.4707199
H	3.2406800	6.1991894	11.0726128

Table S5. Atom coordinates from DFT geometry optimization of **5**



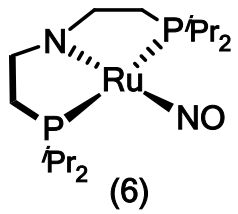
(5)

Ru	1.9964844	7.9905434	9.5783857
P	2.6206012	10.2748714	9.4000123
P	1.4147650	5.7310810	9.1181704
N	2.4622621	8.0016838	7.4309429
H	3.4702814	7.7628327	7.4890294
O	1.5497703	7.9817403	12.4447093
N	1.7122303	7.9805330	11.2820248
C	2.2983933	4.3311472	10.0129301
H	2.0249039	3.4067134	9.4567864
C	1.3027136	11.5846971	9.6959005
H	1.7692069	12.5457050	9.3836136
C	1.7944980	6.9230237	6.6329101
H	0.7274399	7.2073739	6.5296759
H	2.2242147	6.8944909	5.6069634
C	3.0767492	10.4169891	7.5851647
H	2.8464687	11.4237381	7.1860680
H	4.1775117	10.2881398	7.5078395
C	4.1441088	10.8519297	10.3444792
H	3.7990965	10.8216106	11.4019339
C	1.9388311	5.5691594	7.3247756
H	2.9952569	5.2300458	7.3011831
H	1.3425161	4.7966774	6.7973338
C	2.3549334	9.3427670	6.7713386
H	2.7664222	9.2845770	5.7390144
H	1.2750229	9.5726398	6.6810490
C	5.2860958	9.8332271	10.1954453
H	4.9499753	8.8050548	10.4407948
H	5.7041152	9.8252195	9.1664772
H	6.1198134	10.0974253	10.8773522
C	0.0645047	11.3261623	8.8227613
H	0.2850937	11.3853067	7.7376993
H	-0.3758112	10.3299533	9.0386712
H	-0.7093514	12.0921634	9.0341004
C	-0.7270497	3.8399199	8.7805457
H	-0.1801892	3.4346892	7.9048166
H	-0.4827545	3.2084532	9.6579782
H	-1.8094292	3.7068377	8.5762260
C	-0.4302377	5.3252130	9.0431969
H	-0.7399185	5.9095343	8.1464145
C	0.9392032	11.6628797	11.1876228
H	0.5024413	10.7099411	11.5493297
H	1.8063544	11.9114515	11.8312051
H	0.1804169	12.4565968	11.3451019
C	3.8228295	4.5240742	9.9529573
H	4.2210305	4.5353475	8.9183952
H	4.1247376	5.4696737	10.4491844
H	4.3245956	3.6872314	10.4806911
C	-1.2091369	5.8874449	10.2437556
H	-0.9537788	5.3698696	11.1897083

H	-1.0136275	6.9692373	10.3819090
H	-2.2979858	5.7531070	10.0797947
C	1.8121950	4.2044219	11.4668927
H	2.0187163	5.1250567	12.0491754
H	0.7298469	3.9855459	11.5411362
H	2.3496106	3.3718688	11.9650452
C	4.5836206	12.2846491	10.0038523
H	4.8988521	12.3804530	8.9440186
H	3.7937504	13.0367808	10.1977736
H	5.4578694	12.5653600	10.6269687

Table S6. Atom coordinates from DFT geometry optimization of **6**

Ru	-0.0555699	-0.3181043	-0.0577433
P	-0.8848422	0.4986832	-2.0849983
P	1.0270284	-0.5794270	1.9990217
N	0.9173097	1.4513660	-0.0471451
O	-1.6257771	-2.8021743	0.0074510
N	-0.9566334	-1.8178571	-0.0372197
C	0.6614297	2.5275684	-1.0034594
C	2.2023049	0.8658536	2.0051867
C	-0.6942838	-0.5429016	-3.6514749
C	0.1776777	2.0027929	-2.3615185
C	-1.0660825	0.1853835	-4.9519601
C	2.1112851	-2.1002997	2.2920899
C	-2.6720393	1.1049382	-2.1583305
C	0.7143216	-1.1555984	-3.7094298
C	1.6347360	1.9775849	1.1132637
C	0.0139926	-0.4333026	3.5857633
C	-0.9188162	-1.6451995	3.7451942
C	2.9565041	-2.3961100	1.0427066
C	2.9632912	-2.0385544	3.5688441
C	-3.6470554	-0.0774176	-2.0372566
C	-2.9242012	2.1500650	-1.0604663
C	-0.7784050	0.8831615	3.5880036
H	1.5950366	3.1264120	-1.1595556
H	-0.0836834	3.2607716	-0.5966537
H	2.4248399	1.2265477	3.0314291
H	3.1497999	0.4848383	1.5711264
H	-1.4150509	-1.3741798	-3.4846446
H	1.0454095	1.6543223	-2.9597175
H	-0.3437568	2.7864248	-2.9494343
H	-0.4013160	1.0553181	-5.1360944
H	-2.1127863	0.5498267	-4.9565643
H	-0.9537602	-0.4980010	-5.8205973
H	1.3652648	-2.9193251	2.3955749
H	-2.8016701	1.5879074	-3.1529073
H	0.9715660	-1.6534593	-2.7526614
H	1.4892993	-0.3846265	-3.9036710
H	0.7775220	-1.9003345	-4.5310525

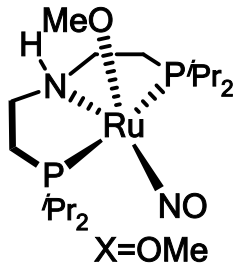


(6)

H	0.9776170	2.6513112	1.7232708
H	2.4770948	2.6325427	0.7730069
H	0.7429431	-0.4171151	4.4276744
H	-0.3666437	-2.6026872	3.8325874
H	-1.6105033	-1.7309869	2.8816565
H	-1.5343744	-1.5355665	4.6629235
H	3.7432262	-1.6276830	0.8887475
H	2.3260342	-2.4133448	0.1308241
H	3.4679502	-3.3765099	1.1462203
H	2.3543992	-1.9134726	4.4865745
H	3.6961075	-1.2048908	3.5305997
H	3.5464084	-2.9765255	3.6879319
H	-3.4931004	-0.6232693	-1.0835375
H	-3.5395734	-0.8068516	-2.8652580
H	-4.6956994	0.2877191	-2.0539969
H	-2.3010606	3.0575237	-1.1892631
H	-2.6994165	1.7235796	-0.0604040
H	-3.9874825	2.4706948	-1.0736445
H	-1.4440976	0.9368162	2.7010827
H	-0.1178291	1.7731890	3.5694196
H	-1.4048891	0.9526335	4.5024857

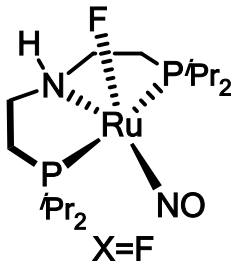
Table S7. Atom coordinates from DFT geometry optimization of **7**

C	-0.7507141	-2.1368412	0.4921739
Ru	-0.0425232	-0.1172696	0.0170440
P	2.1469326	-0.8464839	0.3654439
P	-2.2026478	0.6869650	0.3795868
N	-0.0202866	-0.0755148	2.3802210
O	0.2725322	0.8060228	-2.7489145
N	0.2122099	0.6225157	-1.5590609
C	-3.7158513	-0.3604210	-0.0921588
C	1.3428006	0.0705653	2.9183496
C	2.2637487	-2.9509668	-1.5590230
C	-2.3564577	0.7297305	2.2584354
C	2.6652179	-2.6103721	-0.1140599
C	2.3034193	-0.9139666	2.2432706
C	-2.7326214	2.6141083	-1.6517781
C	-3.6242328	-0.8770540	-1.5376307
C	-0.9872053	0.8924383	2.9261891
C	3.7595319	0.3272905	-1.6701985
C	-2.6544904	2.4590031	-0.1243250
C	3.6081972	0.2510946	-0.1424490
C	-5.0789629	0.2671504	0.2310139
C	4.1221069	-2.9793152	0.2017310
C	3.4718495	1.6575875	0.4612903
C	-1.6618297	3.4672939	0.4744275
H	-0.3561150	-1.0302503	2.5870712
H	-3.5690590	-1.2406716	0.5726346
H	1.6599421	1.1151614	2.7253407
H	1.3611815	-0.0790075	4.0273663
H	1.2249521	-2.6282232	-1.7677345
H	2.9254246	-2.4624891	-2.3022746
H	2.3320913	-4.0466259	-1.7276870
H	-3.0493310	1.5289533	2.5951978
H	-2.8126392	-0.2374500	2.5636956
H	2.0009349	-3.2049705	0.5521336
H	2.0529699	-1.9538362	2.5472357
H	3.3462904	-0.7270931	2.5741551
H	-1.7662174	2.3661533	-2.1350778
H	-3.5135584	1.9738936	-2.1059363
H	-2.9778192	3.6660482	-1.9107073
H	-3.8329528	-0.0813904	-2.2807977
H	-2.6145242	-1.2803753	-1.7498442
H	-4.3679220	-1.6851215	-1.7036368
H	-1.0890638	0.7851808	4.0354099
H	-0.5794057	1.9055664	2.7339304
H	3.9613686	-0.6604958	-2.1281852
H	2.8500844	0.7436991	-2.1473098
H	4.6108527	0.9915942	-1.9303231
H	-3.6619448	2.6460589	0.3115407
H	4.5111504	-0.2370686	0.2884169
H	-5.1545806	0.6089080	1.2840050
H	-5.2996713	1.1351730	-0.4240606



H	-5.8917145	-0.4730325	0.0683999	
H	4.8360949	-2.4408730	-0.4551718	
H	4.3997929	-2.7624699	1.2536946	
H	4.2886717	-4.0655475	0.0359675	
H	2.5132239	2.1232808	0.1510422	
H	3.5093663	1.6517656	1.5693620	
H	4.3042508	2.3038009	0.1099181	
H	-1.6868707	3.4841983	1.5826833	
H	-0.6254565	3.2285406	0.1564911	
H	-1.9070616	4.4931083	0.1262145	
H	-0.9377038	-2.6989419	-0.4485241	
H	-0.0418344	-2.7671922	1.0845532	
H	-1.7067194	-2.1841467	1.0692352	

Table S8. Atom coordinates from DFT geometry optimization of **8**

Ru	4.1933916	6.3566744	8.2143306	
P	3.9491759	8.1403407	9.7104382	
O	1.9384452	6.9333472	6.4429154	
N	2.8909995	6.7216451	7.1386297	
P	4.9146559	4.3410827	7.2664050	
F	6.3011414	6.5655147	8.7283449	
C	5.2955413	9.4523784	9.5679630	
N	4.7275926	5.2569877	10.1343766	
C	4.1257767	5.8361710	11.3428303	
C	4.6435372	3.7943414	10.0301141	
C	6.5641611	4.4599169	6.3617418	
C	4.3520973	7.3529690	11.3788037	
C	5.3766884	3.3036048	8.7751286	
C	3.7765746	3.2132264	6.2739857	
C	2.3044490	9.0114380	10.0080425	
C	1.8721933	9.8428095	8.7891005	
C	5.2575837	10.5381426	10.6508925	
C	1.2217887	7.9878170	10.3891534	
C	5.4047870	10.0214599	8.1440926	
C	6.5501514	5.5394759	5.2677555	
C	3.4054166	3.8329261	4.9165853	
C	2.5172430	2.8783500	7.0896343	
C	7.1369306	3.1198537	5.8803652	
H	6.1819809	8.7955722	9.7122609	
H	5.7134264	5.5992535	9.9910578	
H	3.0402592	5.6011705	11.3344333	

H	4.5535282	5.3715423	12.2660615	
H	5.0791539	3.3024893	10.9354180	
H	3.5698199	3.5126307	9.9925364	
H	7.1813359	4.8650104	7.1942759	
H	3.7729653	7.8194482	12.2020976	
H	5.4245351	7.5650172	11.5745639	
H	6.4723886	3.4225998	8.9126057	
H	5.1859703	2.2240249	8.6042612	
H	4.3550033	2.2767307	6.1019138	
H	2.4776983	9.6927343	10.8716847	
H	2.5874129	10.6545172	8.5553219	
H	1.7655879	9.2088582	7.8861302	
H	0.8865247	10.3155052	8.9863365	
H	4.3846038	11.2130295	10.5283392	
H	5.2206933	10.1195370	11.6778000	
H	6.1671278	11.1733002	10.5899311	
H	1.0745490	7.2485508	9.5755543	
H	1.4675489	7.4313052	11.3164534	
H	0.2551597	8.5061541	10.5633104	
H	5.3882207	9.2024093	7.3975792	
H	4.5839019	10.7275614	7.9046377	
H	6.3602529	10.5761404	8.0326715	
H	5.9854542	5.2237165	4.3668322	
H	6.0978684	6.4747250	5.6528340	
H	7.5889632	5.7616674	4.9439547	
H	2.7088032	3.1598512	4.3732264	
H	2.8961932	4.8093515	5.0449949	
H	4.2878220	3.9901827	4.2670219	
H	1.9506508	3.7995345	7.3371885	
H	1.8513305	2.2116360	6.5020234	
H	2.7504900	2.3559312	8.0394629	
H	7.1816689	2.3574028	6.6857079	
H	6.5449305	2.6939089	5.0431422	
H	8.1735074	3.2578381	5.5049922	

Representative orbital plots

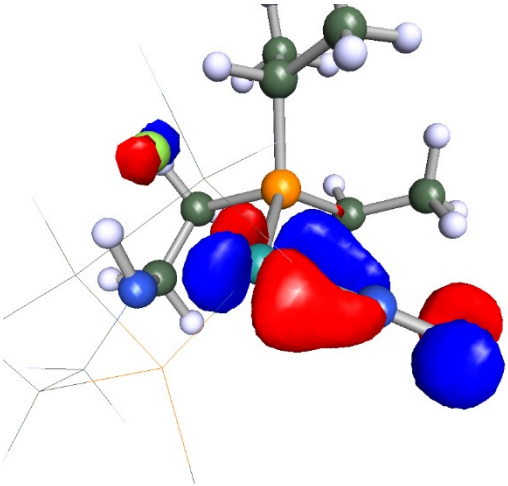


Figure S10: Plot of HOMO-3 orbital of the X=F compound.

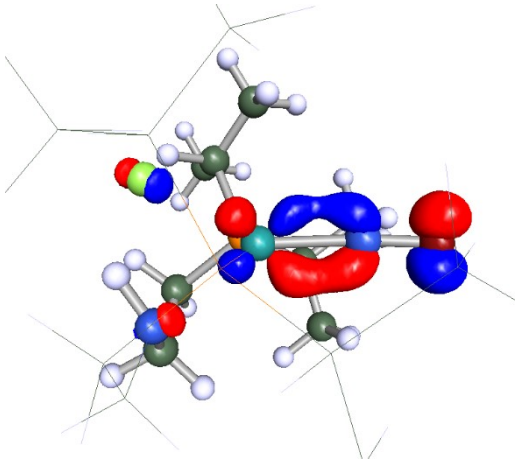


Figure S9: Plot of the HOMO-2 orbital of the X=F compound.

Table S10. Selected NPA charges for the compounds outlined in the main text.

Compound / Atom	X=F	X=OMe	**2**[a]	**3**	**4**	**5**	**6**
X	-0.73869	-0.86514	-0.66083	-0.64246	-0.61215		
$N_{nitrosyl}$	0.11607	0.11590	0.12880	0.13329	0.14066	0.26757	0.16533
$O_{nitrosyl}$	-0.32949	-0.33568	-0.31027	-0.30452	-0.29632	-0.20827	-0.30562
Ru	-0.00403	-0.02534	-0.09755	-0.11100	-0.12879	-0.17874	-0.18794

[a] only the complex cation was involved in the calculation.

Crystallographic details

Crystal data and structure refinement parameters for compounds **2-6** are summarized in the tables S11-15 below.

Table S11. Crystal data and structure refinement for Compound 2.

Identification code (**CCDC**)	exp_1817_autored (**2497985**)
Empirical formula	$C_{16}H_{37}ClN_2OP_2Ru$
Formula weight	471.93
Temperature/K	120.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	20.63369(18)
b/Å	10.63542(9)
c/Å	20.78902(19)
α/°	90
β/°	107.5461(10)
γ/°	90
Volume/Å^3	4349.85(7)
Z	8
ρcalcg/cm^3	1.441
μ/mm^{-1}	8.389
F(000)	1968.0
Crystal size/mm^3	0.2 × 0.1 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.222 to 153.44
Index ranges	$-25 \leq h \leq 21$, $-13 \leq k \leq 13$, $-25 \leq l \leq 26$
Reflections collected	73391
Independent reflections	9145 [R_{int} = 0.0479, R_{sigma} = 0.0226]
Data/restraints/parameters	9145/0/431
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0238, wR_2 = 0.0557
Final R indexes [all data]	R_1 = 0.0301, wR_2 = 0.0593
Largest diff. peak/hole / e Å^{-3}	0.46/-0.93

Table 12. Crystal data and structure refinement for Compound 3.

Identification code (**CCDC**)	exp_1930_autored (**2497986**)
Empirical formula	$C_{16}H_{37}BrN_2OP_2Ru$
Formula weight	516.39
Temperature/K	119.98(10)
Crystal system	monoclinic

Space group	$P2_1/n$
a/Å	11.6223(2)
b/Å	13.6476(2)
c/Å	14.3545(2)
α/°	90
β/°	98.602(2)
γ/°	90
Volume/Å^3	2251.25(6)
Z	4
ρ_{calc}g/cm^3	1.524
μ/mm^{-1}	2.619
F(000)	1056.0
Crystal size/mm^3	0.6 × 0.25 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.472 to 59.378
Index ranges	$-15 \leq h \leq 15$, $-18 \leq k \leq 18$, $-18 \leq l \leq 20$
Reflections collected	42954
Independent reflections	5925 [R_{int} = 0.0434, R_{sigma} = 0.0274]
Data/restraints/parameters	5925/0/216
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0279, wR_2 = 0.0662
Final R indexes [all data]	R_1 = 0.0358, wR_2 = 0.0702
Largest diff. peak/hole / e Å^{-3}	0.87/-0.77

Table 13. Crystal data and structure refinement for Compound 4.

Identification code (**CCDC**)	exp_1938_autored (**2497987**)
Empirical formula	$C_{16}H_{37}IN_2OP_2Ru$
Formula weight	563.38
Temperature/K	120.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.7122(3)
b/Å	13.6832(3)
c/Å	14.4336(3)
α/°	90
β/°	97.665(2)
γ/°	90

Volume/Å^3	2292.47(9)
Z	4
ρ_{calc}g/cm^3	1.632
μ/mm^{-1}	2.176
F(000)	1128.0
Crystal size/mm^3	0.8 × 0.5 × 0.45
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.602 to 59.376
Index ranges	-15 ≤ h ≤ 16, -17 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	44558
Independent reflections	6088 [R_{int} = 0.0540, R_{sigma} = 0.0359]
Data/restraints/parameters	6088/0/216
Goodness-of-fit on F^2	1.175
Final R indexes [I>=2σ (I)]	R_1 = 0.0305, wR_2 = 0.0578
Final R indexes [all data]	R_1 = 0.0500, wR_2 = 0.0682
Largest diff. peak/hole / e Å^{-3}	1.51/-0.92

Comments for the **Compound 4** structure: Higher residual density near the ruthenium atom and a high K value reflect data quality limitations. It results from crystal quality and absorption effects typical of structures containing heavy atoms and does not indicate deficiencies or other errors in the structural model.

Table 14. Crystal data and structure refinement for Compound 5.

Identification code (**CCDC**)	exp_1875f3 (**2497988**)
Empirical formula	$C_{16}H_{37}BF_4N_2OP_2Ru$
Formula weight	523.29
Temperature/K	119.99(14)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.4356(3)
b/Å	11.3117(4)
c/Å	24.7627(8)
α/°	90
β/°	92.207(4)
γ/°	90
Volume/Å^3	2361.13(14)
Z	4
ρ_{calc}g/cm^3	1.472
μ/mm^{-1}	7.015
F(000)	1080.0

Crystal size/mm^3	0.09 × 0.025 × 0.009
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.144 to 152.896
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 13, -30 ≤ l ≤ 31
Reflections collected	12527
Independent reflections	4919 [R_{int} = 0.0392, R_{sigma} = 0.0428]
Data/restraints/parameters	4919/0/252
Goodness-of-fit on F^2	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0630, wR_2 = 0.1385
Final R indexes [all data]	R_1 = 0.0731, wR_2 = 0.1436
Largest diff. peak/hole / e Å^{-3}	2.88/-0.98

Table 15. Crystal data and structure refinement for Compound 6.

Identification code (**CCDC**)	exp_1858 (**2497989**)
Empirical formula	$C_{16}H_{36}N_2OP_2Ru$
Formula weight	435.48
Temperature/K	120.0(1)
Crystal system	Triclinic
Space group	P-1
a/Å	7.5893(2)
b/Å	13.3916(4)
c/Å	21.8997(5)
α/°	97.055(2)
β/°	98.855(2)
γ/°	106.400(2)
Volume/Å^3	2077.01(10)
Z	4
ρ_{calc}g/cm^3	1.393
μ/mm^{-1}	7.582
F(000)	912.0
Crystal size/mm^3	0.1 × 0.02 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.99 to 153.962
Index ranges	-9 ≤ h ≤ 9, -16 ≤ k ≤ 14, -27 ≤ l ≤ 25
Reflections collected	21660
Independent reflections	8643 [R_{int} = 0.0298, R_{sigma} = 0.0340]
Data/restraints/parameters	8643/0/413
Goodness-of-fit on F^2	1.034

Final R indexes [I>=2σ (I)]	R_1 = 0.0299, wR_2 = 0.0764
Final R indexes [all data]	R_1 = 0.0368, wR_2 = 0.0808
Largest diff. peak/hole / e $Å^{-3}$	0.87/-1.05