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1. General procedure

All manipulations were carried out by using standard Schlenk technique or a nitrogen filled glovebox (O_2/H_2O < 0.1 ppm). All the reactions were performed in Schlenk tubes with grease free PTFE-valves. The solvent 1,2,3,4-Tetrafluorobenzene (TFB, $C_6F_4H_2$, from Fluorochem) was stirred over a few days over calcium hydride (CaH_2) and distilled. The distillate was stirred over $Ag^+[Al(OR^F)_4]^-$ and condensed to remove traces of less fluorinated benzenes. This leads to a minor contamination of R^FOH, which does not affect the reactions. *n*-pentane was dried using a Grubbs apparatus. TFB and *n*-pentane were stored over 3 Å molar sieves. Iodine (I_2, Acros) was sublimed under static vacuum before use. Triruthenium dodecacarbonyl (Sigma Aldrich), 9,10-Dichlorooctafluoroanthrace (Sigma Aldrich) and triosmium dodecacarbonyl (ABCR) were bought from commercial sources. $Ag^+[WCA]^-$ and $[NO]^+[WCA]^-$ were synthezised according to literature procedures.[1]

Vibrational Spectroscopy

FTIR spectra were recorded inside a glovebox with a Bruker ALPHA equipped with QuickSnap Eco ATR module and ZnSe crystal. The spectra were measured at RT in the range of 4000-550 cm^{-1} with 32 scans and a resolution of 2 cm^{-1}. The data were processed with the Bruker OPUS 7.5 software package and, if not stated otherwise, a baseline correction with 3 iterations was performed. FT Raman spectra were recorded with a VERTEX 70 with Bruker RAM II Modul (1064 nm exciting line of a Nd-YAG laser) and liquid nitrogen cooled Ge detector. The samples were flame-sealed in soda-lime glass Pasteur pipettes and were measured at RT in the range of 4000-80 cm^{-1} with up to 10,000 scans and a resolution of 4 cm^{-1}. The data were processed with the Bruker OPUS 7.5 software package. The graphical representations were created with OriginPro 2021.

NMR Spectroscopy

NMR spectra were recorded at RT either on a Bruker Avance II Widebore 400 MHz, Bruker Avance III HD 300 MHz or Bruker Avance DPX 200 MHz. The samples were dissolved with 4FB (0.6 ml) in a 5 mm thick-walled NMR tube with J. Young PTFE valve. The spectra were calibrated by using the ^1H signal of the solvent 4FB (δ = 6.97 ppm, rel. to Tetramethylsilane). The field corrections of other nuclei were adjusted accordingly. Typically, small impurities of $HOC(CF_3)_3$ were detected in the ^{19}F NMR at –76.0 ppm. The MestReNova software package was used for measuring, processing and creation of the graphical representations of the spectra. ^1H and ^{13}C NMR spectra are referenced against TMS and ^{19}F NMR spectra against $CFCl_3$.

EPR Spectroscopy

The continuous wave (cw) EPR spectrum of a solution of $[\mathbf{6}]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$ in TFB was recorded at the X-band (9.75 GHz) on a Bruker EMXnano benchtop EPR spectrometer at room temperature. The modulation frequency was set to 100 kHz and the modulation amplitude to 0.01 mT at a microwave power of 1 mW (20 dB). After data acquisition, the spectrum was baseline-corrected, frequency-corrected to 9.75 GHz and field-corrected using a carbon fibre standard with g = 2.002644.[2] The numerical simulation of the experimental spectrum using EasySpin functions in MATLAB yielded g = 2.0065.[3] The hyperfine coupling constants were calculated with DFT by using the ORCA program package version 4.0.[4] The structure was optimised using B3LYP/def2-TZVP and the hyperfine coupling constants were then calculated at the B3LYP/EPR-II (6-31G** for Cl) level of theory.

Single Crystal X-ray Diffraction

The data were collected on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using mirror optics as monochromator and a Bruker PHOTON III detector. Single crystals were selected at RT under perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG), mounted on CryoLoops with a diameter of 0.1 to 0.2 mm and shock-cooled using an Oxford Cryostream 800 low temperature device. The data were gathered at 100(2) K using Mo K_α radiation

(λ = 0.71073 Å). All data were integrated with SAINT (version 8.38A) and a multi-scan absorption correction using SADABS or TWINABS was applied. The structures were solved by direct methods using SHELXT[5] and refined by full-matrix least-squares methods against F^2 by SHELXL-2018/3[6] using the GUI software ShelXle.[7] Disordered moieties were refined using bond lengths restraints and displacement parameter restraints and were modelled with the program DSR.[8] The gathered data were finalized with the tool FinalCif.[9] The graphical representations of the crystal structures were generated with Mercury (version 4.0).[10] Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[11] Copies of the data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Powder X-ray Diffraction

Powder diffractograms were recorded on a STOE STADI P powder diffractometer with Mo $K_{\alpha1}$ radiation (λ = 0.709300 Å), Ge-(111) monochromator and Mythen 1K detector at 100(10) K. The samples were sealed in a 0.5 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) with silicon grease. Data acquisition, processing, and the calculation of powder diffractograms from single-crystal data was performed using the STOE WinXPOW® package.

Computational Details

Geometry optimizations were performed with the TURBOMOLE software[12] (v7.2 or v7.5) using the DFT functionals B3LYP[13] with the def2-TZVPP[14] basis set, the resolution-of-identity (RI) approximation,[15] dispersion correction (D3BJ),[16] a fine integration grid (m4 or 5 for NMR chemical shift calculations) and the default SCF convergence criteria (10^{-6} a.u.). All structures were checked for proper spin occupancies and imaginary frequencies with the integrated *EIGER* and *AOFORC*[17] modules. IR and Raman spectra were simulated on B3LYP(D3BJ)/def2-TZVPP level with a scaling factor of 0.968 for all TMCCs, the spectra for the other molecules were simulated without scaling factor. QTAIM-charges were calculated with MultiWFN.[18] The EDA-NOCV analyses where carried out with the ADF software package.[19]

2. Experimental

$[Ru_4N(CO)_{13}]^+[Al(OC(CF_3)_3)_4]^-$ abbreviated as $[2]^+[Al(OR^F)_4]^-$

$[NO]^+[Al(OC(CF_3)_3)_4]^-$ (100 mg, 100 µmol, 1.0 eq.) and $Ru_3(CO)_{12}$ (63 mg, 100 µmol, 1.0 eq.) were filled in a Schlenk-tube. 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to a brown solution, which was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days leads to some red crystals, which have been identified as $[Ru_4N(CO)_{13}]^+[Al(OC(CF_3)_3)_4]^-$ with scXRD and IR. The bulk product was an undefined mixture. The synthesis was not optimized and no yield was determined.

IR (ATR, in cm^{-1}): ν 2042 (m), 2031 (m), 1513 (vw), 1522 (vw), 1351 (vw), 1297 (w), 1274 (m), 1239 (s), 1208 (vs), 1167 (m), 1046 (vw), 968 (vs), 831 (vw), 805 (vw), 756 (vw), 745 (vw), 726 (s), 682 (vw), 617 (vw), 607 (vw), 585 (vw), 561 (vw).

$[Ag\{Ru_3(CO)_{12}\}_2]^+[Al(OC(CF_3)_3)_4]^-$ abbreviated as $[3a]^+[Al(OR^F)_4]^-$

$Ag^+[Al(OC(CF_3)_3)_4]^-$ (50 mg, 47 µmol, 1.0 eq.) and $Ru_3(CO)_{12}$ (59 mg, 93 µmol, 2.0 eq.) were filled in a Schlenk-tube and 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to an orange solution. The mixture was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days led to red crystals in 92 % yield, which were identified as $[Ag\{Ru_3(CO)_{12}\}_2]^+[Al(OC(CF_3)_3)_4]^-$ *via* scXRD.

$[Ag\{Ru_3(CO)_{12}\}_2]^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ abbreviated as $[3a]^+[F\{Al(OR^F)_3\}_2]^-$

The reaction was performed analogously to $[\mathbf{3a}]^+[Al(OR^F)_4]^-$ but $Ag^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ was used instead of $Ag^+[Al(OC(CF_3)_3)_4]^-$.

IR (ATR, in cm^{-1}): ν 2130 (w), 2084 (vs), 2068 (s), 2052 (s), 2034 (m), 2017 (vs), 1353 (w), 1301 (m), 1278 (s), 1243 (vs), 1214 (vs), 1176 (m), 862 (w), 974 (vs), 728 (vs), 639 (w), 584 (s), 567 (s), 558 (vs).

Raman (1064 nm, in cm^{-1}): ν 2140 (w), 2119 (vw), 2092 (vw), 2062 (w), 2028 (w), 2011 (vw), 753 (vw), 595 (vw), 573 (vw), 518 (vw), 457 (vw), 424 (vw), 372 (vw), 303 (vw), 268 (vw), 171 (vs), 148 (m), 102 (vs), 87 (vs).

$[Ag\{Os_3(CO)_{12}\}_2]^+[Al(OC(CF_3)_3)_4]^-$ abbreviated as $[3b]^+[Al(OR^F)_4]^-$

$Ag^+[Al(OC(CF_3)_3)_4]^-$ (27 mg, 25 µmol, 1.0 eq.) and $Os_3(CO)_{12}$ (45 mg, 50 µmol, 2.0 eq.) were filled in a Schlenk-tube and 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to an orange solution. Slow diffusion over the course of two days leads to red crystals in 87 % yield, which were identified as $[Ag\{Ru_3(CO)_{12}\}_2]^+[Al(OC(CF_3)_3)_4]^-$ *via* scXRD, the structure had however severe disorders and is therefore not uploaded to the CCDC.

$[Ag\{Os_3(CO)_{12}\}_2]^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ abbreviated as $[3b]^+[F\{Al(OR^F)_3\}_2]^-$

The reaction was performed analogously to $[\mathbf{3b}]^+[Al(OR^F)_4]^-$ but $Ag^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ was used instead of $Ag^+[Al(OC(CF_3)_3)_4]^-$.

IR (ATR, in cm^{-1}): ν 2138 (w), 2091 (s), 2062 (s), 2055 (vs), 2041 (s), 2012 (s), 2003 (vs), 1353 (vw), 1266 (s), 1241 (vs), 1216 (vs), 1177 (m), 972 (vs), 852 (vw), 727 (vs), 692 (vw), 599 (m), 579 (w), 570 (w).

Raman (1064 nm, in cm^{-1}): ν 2149 (w), 2092 (vw), 2064 (w), 2030 (vw), 2012 (vw), 1998 (vw), 752 (vw), 539 (vw), 486 (w), 460 (vw), 323 (vw), 145 (s), 107 (vs), 85 (m).

$[Ru(CO)_5I]^+[Al(OC(CF_3)_3)_4]^-$ and $[Ru_2(CO)_6I_3]^+[Al(OC(CF_3)_3)_4]^-$ abbreviated as $[4]^+[Al(OR^F)_4]^-$ and $[5]^+[Al(OR^F)_4]^-$

$Ag^+[Al(OC(CF_3)_3)_4]^-$ (130 mg, 120 µmol, 1.0 eq.) and I_2 (28 mg, 120 µmol, 1.0 eq.) were filled in a Schlenk tube. 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture at −20 °C. $Ru_3(CO)_{12}$ (75 mg, 120 µmol, 1.0 eq.) was added to the solution leading to a red solution and a white precipitate. The mixture was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days leads to some red crystals, which were identified as $[Ru(CO)_5I]^+[Al(OC(CF_3)_3)_4]^-$ and $[Ru_2(CO)_6I_3]^+[Al(OC(CF_3)_3)_4]^-$. The synthesis was not optimized and no yield was determined.

$[C_{14}F_8Cl_2]^{+\cdot}[F\{Al(OC(CF_3)_3)_3\}_2]^-$ abbreviated as $[6]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$

9,10-dichlorooctafluoroanthracene (30 mg, 81 µmol, 1.2 eq.) and $[NO]^+[F\{Al(OC(CF_3)_3)_2\}_2]^-$ (100 mg, 66 µmol, 1.0 eq.) were filled in a Schlenk tube. 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to an immediate colour change and gas evolution. The green solution was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days leads to analytically pure dark green crystals of $[C_{14}F_8Cl_2]^{+\cdot}[F\{Al(OC(CF_3)_3)_3\}_2]^-$, which are suitable for scXRD (100 mg, 53 µmol, 80 %).

IR (ATR, in cm^{-1}): ν 1602 (w), 1573 (vw), 1500 (vw), 1467 (s), 1406 (vw), 1355 (w), 1299 (m), 1276 (s), 1243 (vs), 1204 (vs), 1173 (vs), 1100 (m), 1087 (m), 970 (vs), 858 (m), 726 (vs), 637 (m), 567 (w).

Raman (1064 nm, in cm^{-1}): ν 1594 (vw), 1570 (vw), 1543 (vw), 1390 (vs), 1187 (vw), 1594 (vw), 1570 (vw), 1543 (vw), 1021 (vw), 982 (vw), 856 (vw), 371 (vw), 326 (vw), 294 (vw), 250 (vw).

^{19}F-NMR (188 MHz, 1,2,3,4-Tetraflurobenzene) δ = −75.9 (s, C**F**$_3$) ppm.

$[Ru_3(CO)_{14}]^{2+}[Al(OC(CF_3)_3)_4]^-_2$ abbreviated as $[7a]^{2+}[Al(OR^F)_4]^-_2$

9,10-dichlorooctafluoroanthracene (88 mg, 240 µmol, 2.4 eq.) and $[NO]^+[Al(OC(CF_3)_3)_4]^-$ (200 mg, 200 µmol, 2.0 eq.) were filled in a Schlenk tube. 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to an immediate colour change and gas evolution. The solution was frozen (−78 °C) and $Ru_3(CO)_{12}$ (63 mg, 100 µmol, 1.0 eq.) was added. The Schlenk tube was evacuated and CO was added (1-2 atm.). The solution was brought to room temperature under vigorous stirring and the intense green colour vanished. The clear brownish solution was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days leads to analytically pure colourless/light yellow crystals of $[Ru_3(CO)_{14}]^{2+}[Al(OC(CF_3)_3)_4]^-_2\cdot C_6F_4H_2$, which are suitable for scXRD (210 mg, 88 µmol, 88 %).

^{13}C-NMR (50 MHz, 1,2,3,4-Tetraflurobenzene) δ = 195.1 (s, 4C, **C**O$_{cen}$), 185.0 (s, 8C, **C**O$_{eq}$), 171.5 (s, 2C, **C**O$_{ax}$), 121.3 (q, **C**F$_3$) ppm.

^{19}F-NMR (188 MHz, 1,2,3,4-Tetraflurobenzene) δ = −76.1 (s, C**F**$_3$) ppm.

IR (ATR, in cm^{-1}): ν 2171 (w), 2134 (vw), 2115 (s), 2056 (w), 1351 (vw), 1326 (vw), 1274 (m), 1296 (w), 1213 (vs), 1172 (w), 1045 (w), 969 (vs), 833 (vw), 805 (vw), 755 (vw), 744 (vw), 727 (s), 682 (vw), 615 (vw), 576 (vw), 558 (s).

Raman (1064 nm, in cm^{-1}): ν 2195 (m), 2147 (vs), 2139 (s), 2112 (w), 2092 (w).

$[Ru_3(CO)_{14}]^{2+}[F\{Al(OC(CF_3)_3)_3\}_2]^-_2$ abbreviated as $[7a]^{2+}[F\{Al(OR^F)_3\}_2]^-_2$

The reaction was performed analogously to $[\mathbf{7a}]^{2+}[Al(OR^F)_4]^-_2$ but $[NO]^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ was used instead of $[NO]^+[Al(OC(CF_3)_3)_4]^-$. No yield was determined and the product was only analysed *via* scXRD.

$[Os_3(CO)_{14}]^{2+}[Al(OC(CF_3)_3)_4]^-_2$ abbreviated as $[\mathbf{7b}]^{2+}[Al(OR^F)_4]^-_2$

9,10-dichlorooctafluoroanthracene (94 mg, 250 µmol, 2.4 eq.) and $[NO]^+[Al(OC(CF_3)_3)_4]^-$ (210 mg, 210 µmol, 2.0 eq.) were filled in a Schlenk tube. 1,2,3,4-Tetrafluorobenzene (2 mL) was added to the mixture leading to an immediate colour change and gas evolution. The solution was frozen (−78 °C) and $Os_3(CO)_{12}$ (96 mg, 105 µmol, 1.0 eq.) was added. The Schlenk tube was evacuated and CO was added (1-2 atm.). The solution was brought to room temperature under vigorous stirring and the intense green colour vanished. The clear brownish solution was layered with *n*-pentane (20 mL). Slow diffusion over the course of two days leads to analytically pure colourless/light yellow crystals of $[Os_3(CO)_{14}]^{2+}[Al(OC(CF_3)_3)_4]^-_2 \cdot C_6F_4H_2$, which are suitable for scXRD (230 mg, 75 µmol, 72 %).

^{13}C-NMR (50 MHz, 1,2,3,4-Tetraflurobenzene) δ = 176.8 (s, 4C, **C**O_{cen}), 163.8 (s, 8C, *eq*-**C**O_{eq}), 121.3 (q, **C**F_3) ppm.

^{19}F-NMR (188 MHz, 1,2,3,4-Tetraflurobenzene) δ = −76.1 (s, C**F$_3$**) ppm.

IR (ATR, in cm^{-1}): ν 2179 (w), 2112 (s), 2138 (vw), 2038 (m), 2084 (w), 1511 (w), 1352 (vw), 1296 (w), 1273 (m), 1238 (s), 1212 (vs), 1172 (m), 1045 (vw), 969 (vs), 832 (vw), 805 (vw), 744 (vw), 727 (vs), 682 (vw), 629 (vw), 566 (s).

Raman (1064 nm, in cm^{-1}): ν 2201 (m), 2136 (vs), 2108 (vw), 2083 (w), 167 (w), 113 (s), 91 (vs).

$[Os_3(CO)_{14}]^{2+}[F\{Al(OC(CF_3)_3)_3\}_2]^-_2$ abbreviated as $[\mathbf{7b}]^{2+}[F\{Al(OR^F)_3\}_2]^-_2$

The reaction was performed analogously to $[\mathbf{7b}]^{2+}[Al(OR^F)_4]^-_2$ but $[NO]^+[F\{Al(OC(CF_3)_3)_3\}_2]^-$ was used instead of $[NO]^+[Al(OC(CF_3)_3)_4]^-$. No yield was determined and the product was only analysed *via* scXRD.

3. Shift of the Bond Lengths upon Deelectronation

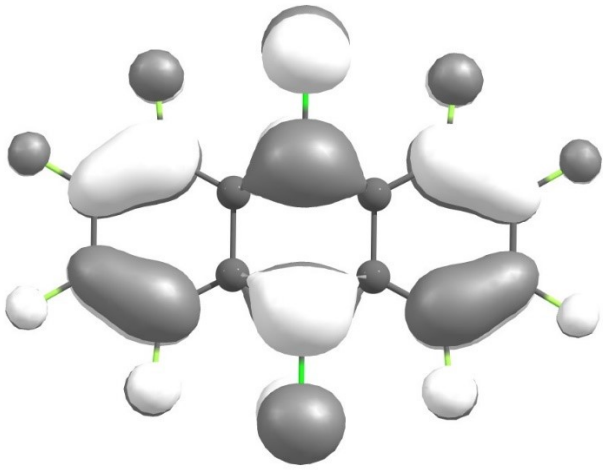


Figure S 1: SOMO of [**6**]$^{+\cdot}$ (B3LYP(D3BJ)/def2-TZVPP).

Table S 1: Calculated and experimental bond lengths of neutral, monocationic and dicationic anthracene^{Hal}.

	scXRD^0	Calc.^{0}	scXRD$^+$	Calc.$^+$
d(C-Cl)$_{ax.}$ [Å]	1.735(3)	1.735	1.701(3)	1.703
d(C-F)$_{ortho}$ [Å]	1.351	1.335	1.323	1.318
d(C-F)$_{meta}$ [Å]	1.339	1.330	1.335	1.312
d(C$_1$-C$_2$)$_{avg.}$ [Å]	1.402	1.407	1.420	1.420
d(C$_2$-C$_2$) [Å]	1.460(4)	1.453	1.450(3)	1.448
d(C$_2$-C$_3$)$_{avg.}$ [Å]	1.427	1.428	1.419	1.416
d(C$_3$-C$_4$)$_{avg.}$ [Å]	1.343	1.362	1.378	1.386
d(C$_4$-C$_4$)$_{avg.}$ [Å]	1.398(5)	1.406	1.381(4)	1.390

4. Absence of Nitrosyl-Ligands in [**2**]$^+$

Nitrosyl and carbonyl ligands are difficult to differentiate *via* scXRD. Because the treatment of monometallic TCMs with nitrosyl salts often yields heteroleptic carbonyl/nitrosyl complexes, the presence of a nitrosyl ligand is not unlikely and has to be ruled out carefully.

Possible reaction-sequence:

$4\ Ru_3(CO)_{12} + 3\ [NO]^+ \rightarrow 3\ [Ru_3(CO)_{11}(NO)]^+ + 3\ CO + Ru_3(CO)_{12} \rightarrow 3\ CO_2 + [NRu_3(CO)_9]^+ + 6\ CO + Ru_3(CO)_{12} \rightarrow [NRu_4(CO)_{13}]^+ + 3\ CO_2 + 6\ CO$

The positive charge gets introduced with the nitrosyl ligand. The reductive carbonylation of the nitrosyl ligand (probably bridging) abstracts the oxygen atom from the nitrosyl ligand, but does not change the overall charge of the fragments. A further reaction with $[NO]^+$ would result in a multicationic charge. Because the reaction does not proceed stoichiometrically, the possible presence of nitrogen monoxide $NO^{\cdot}$ has to be respected. Terminal nitrosyl ligands are leading to vibrational bands between ca. 1950-1750 cm^{-1}. The IR-spectrum of the mixture shows no bands in this region (DFT calculations show, that terminal nitrosyl ligands would have a bent geometry; the ligands in the scXRD are linearly bound). The IR spectrum displays however vibrational bands at 1523 and 1513 cm^{-1}, which are attributed tetrafluorobenzene here, but could hide a band of a bridging nitrosyl ligand, which could be in the crystallographically analysed molecule. Because the scXRD shows 12 terminal and just one bridging ligand around the $\{NRu_4\}^+$-core, the complex seen in the scXRD could be either $[NRu_4(CO)_{12}(\mu_2\text{-}CO)]^+$ or $[NRu_4(CO)_{12}(\mu_2\text{-}NO)]^{+\cdot}$. The ligand is however not symmetrically bridging in both crystallographically independent complex cations. This structural aspect is the most prominent difference in the DFT-optimized structures of these complexes (Table S 2). Due to the *semi* bridging geometry of the relevant ligand, we are sure, that compound [**2**]$^+$ does not bear any nitrosyl ligands.

Table S 2: Comparison of the experimental bond lengths of the bridging ligand in [**2**]$^+$ with the DFT optimized structures of $[NRu_4(CO)_{12}(\mu_2\text{-}CO)]^+$ and $[NRu_4(CO)_{12}(\mu_2\text{-}NO)]^{+\cdot}$ (B3LYP(B3BJ)/def2-TZVPP).

	Longer Ru-C/N	Shorter Ru-C/N	diff
[**2**]$^+$ (N1)	2.425	2.013	0.412
[**2**]$^+$ (N2)	2.343	2.049	0.294
$[NRu_4(CO)_{13}]^+$	2.568	1.993	0.575
$[NRu_4(CO)_{12}(\mu_2\text{-}NO)]^+$	2.126	2.125	0.001

5. NMR spectra

$[Ru_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2$ in 1,2,3,4-Tetrafluorobenzene

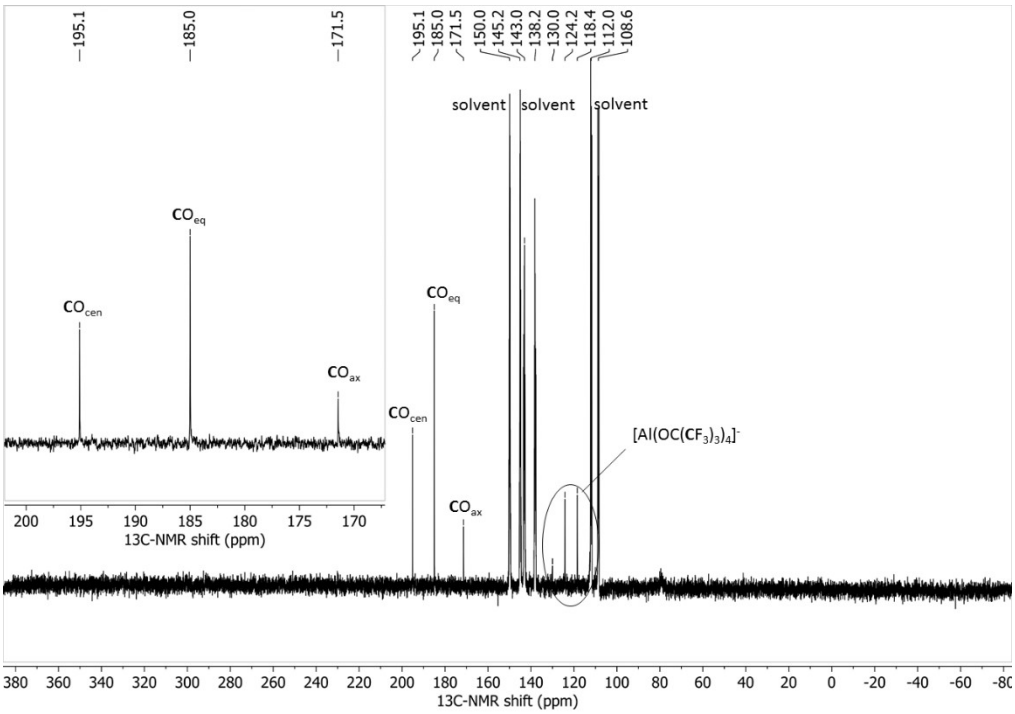


Figure S 2: ^{13}C NMR spectrum of [**7a**]$^{2+}$[Al(OR^F)$_4$]$^-_2$ in 1,2,3,4-Tetrafluorobenzene.

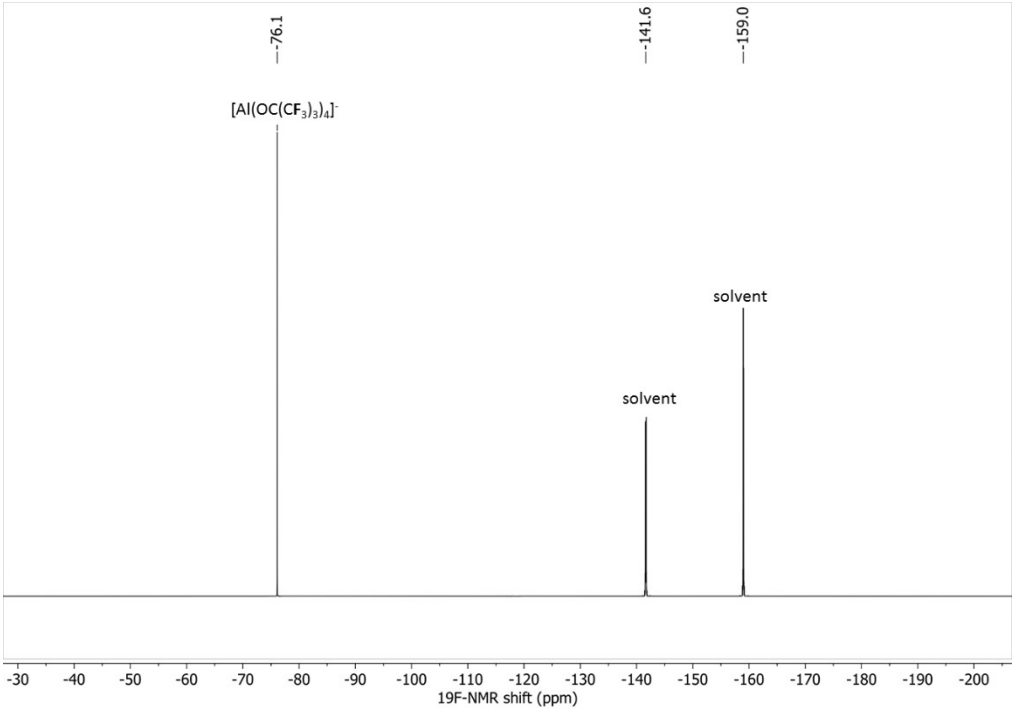


Figure S 3: ^{19}F NMR spectrum of [**7a**]$^{2+}$[Al(OR^F)$_4$]$^-_2$ in 1,2,3,4-Tetrafluorobenzene.

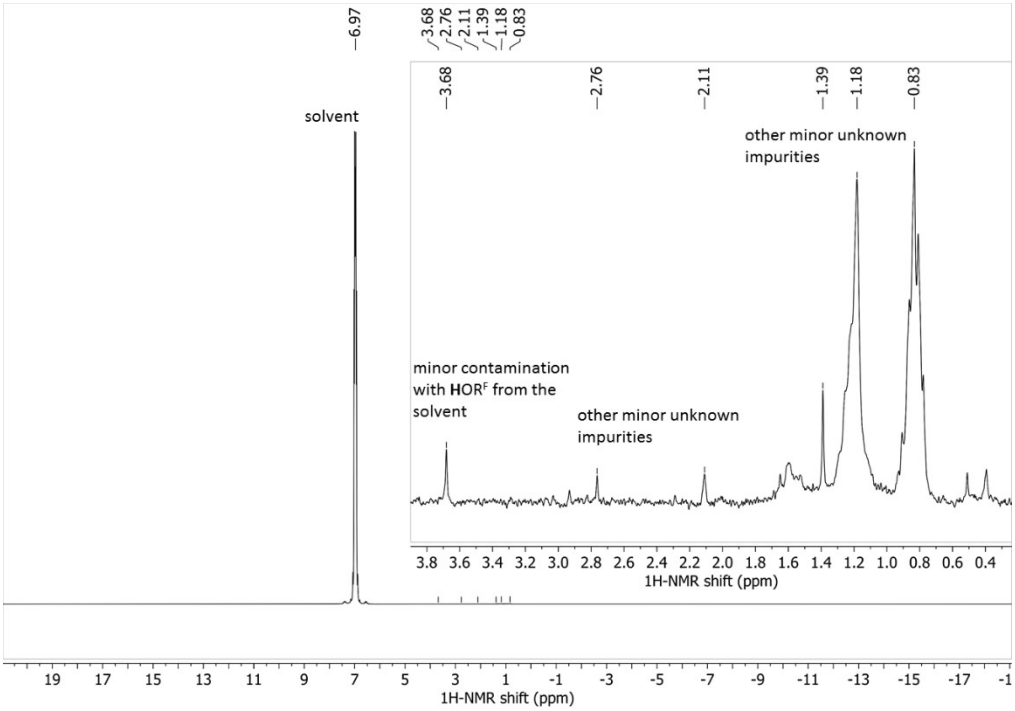


Figure S 4: ^{1}H NMR spectrum of [**7a**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ in 1,2,3,4-Tetrafluorobenzene.

$[Os_3(CO)_{14}]^{2+}[Al(OR^F)_4]^{-}_2$ in 1,2,3,4-Tetrafluorobenzene

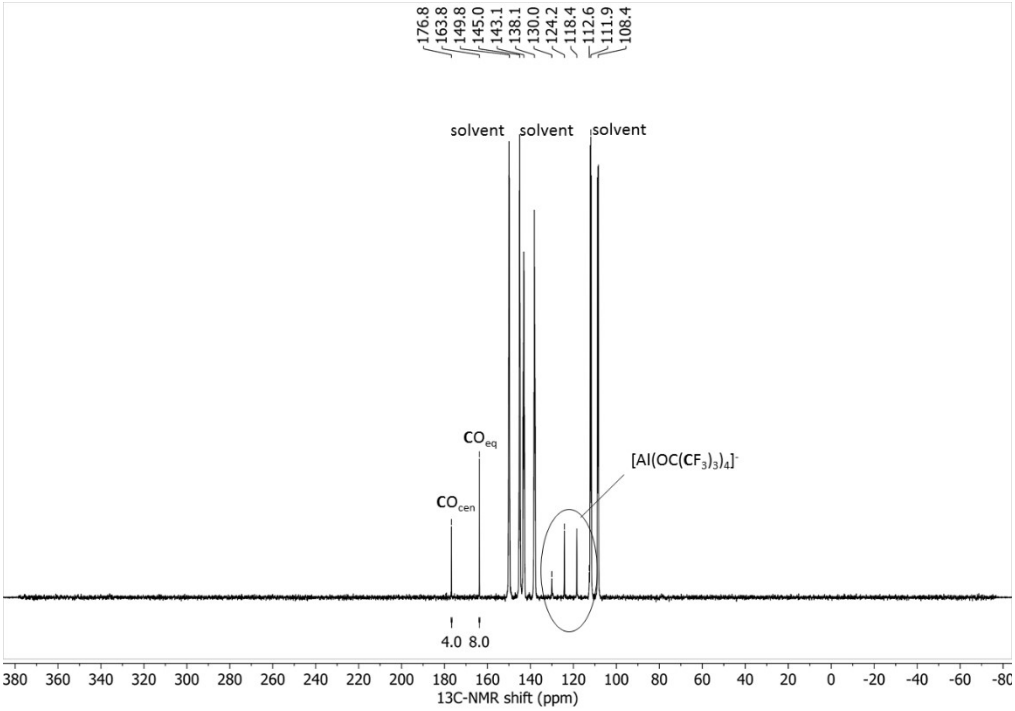


Figure S 5: ^{13}C NMR spectrum of [**7b**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ in 1,2,3,4-Tetrafluorobenzene.

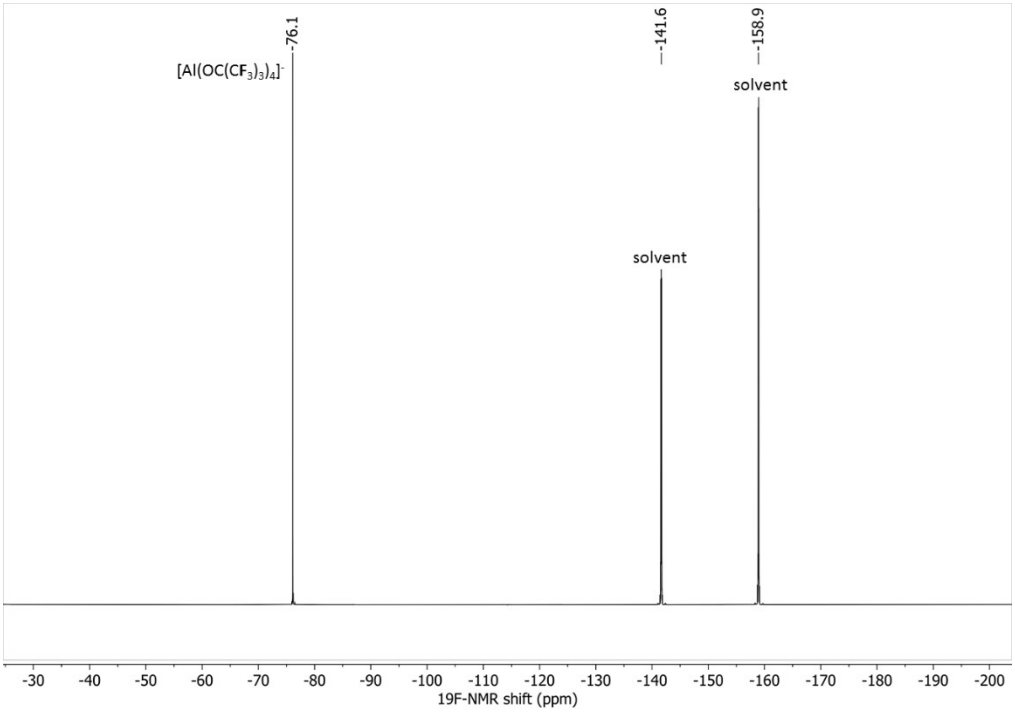


Figure S 6: ^{19}F NMR spectrum of [**7b**]$^{2+}$[Al(OR^{F})$_4$]$^{-}{}_2$ in 1,2,3,4-Tetrafluorobenzene.

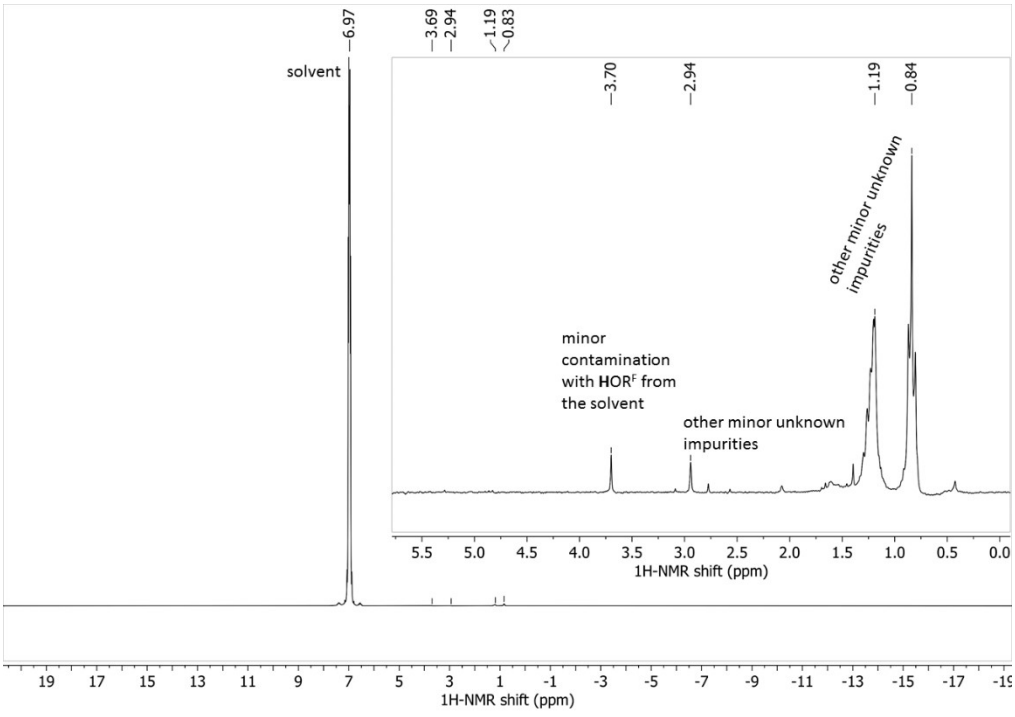


Figure S 7: ^{1}H NMR spectrum of [**7b**]$^{2+}$[Al(OR^{F})$_4$]$^{-}{}_2$ in 1,2,3,4-Tetrafluorobenzene.

$[C_{14}F_8Cl_2]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$ in 1,2,3,4-Tetrafluorobenzene

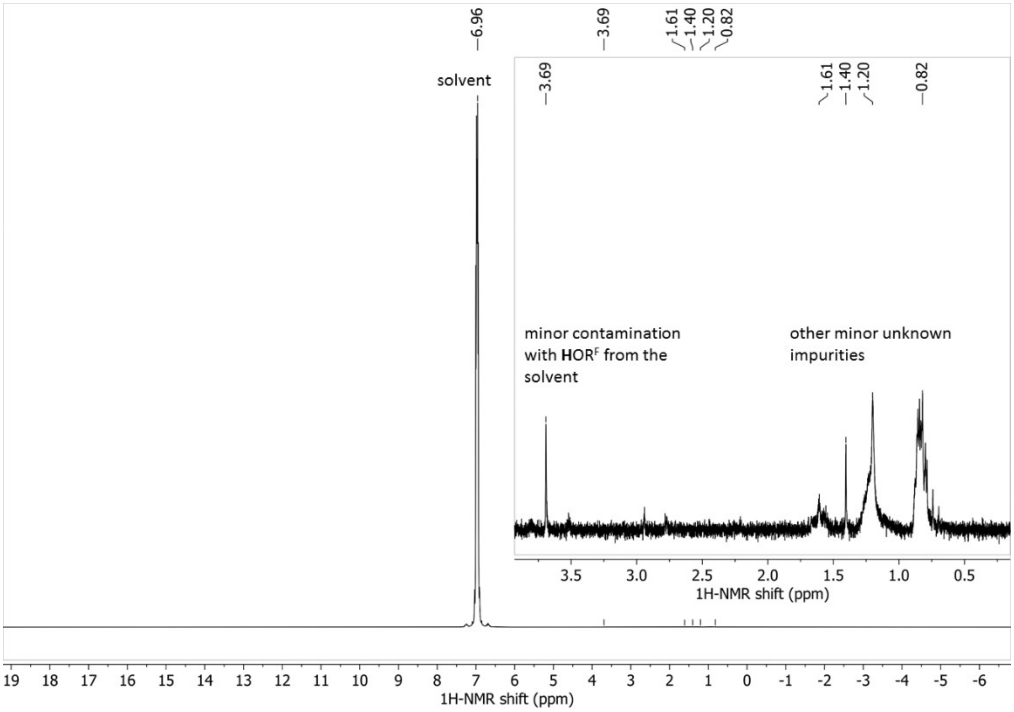


Figure S 8: ^{1}H NMR spectrum of [**6**]$^{+\cdot}$[F{Al(OR^F)$_3$}$_2$]$^-$ in 1,2,3,4-Tetrafluorobenzene.

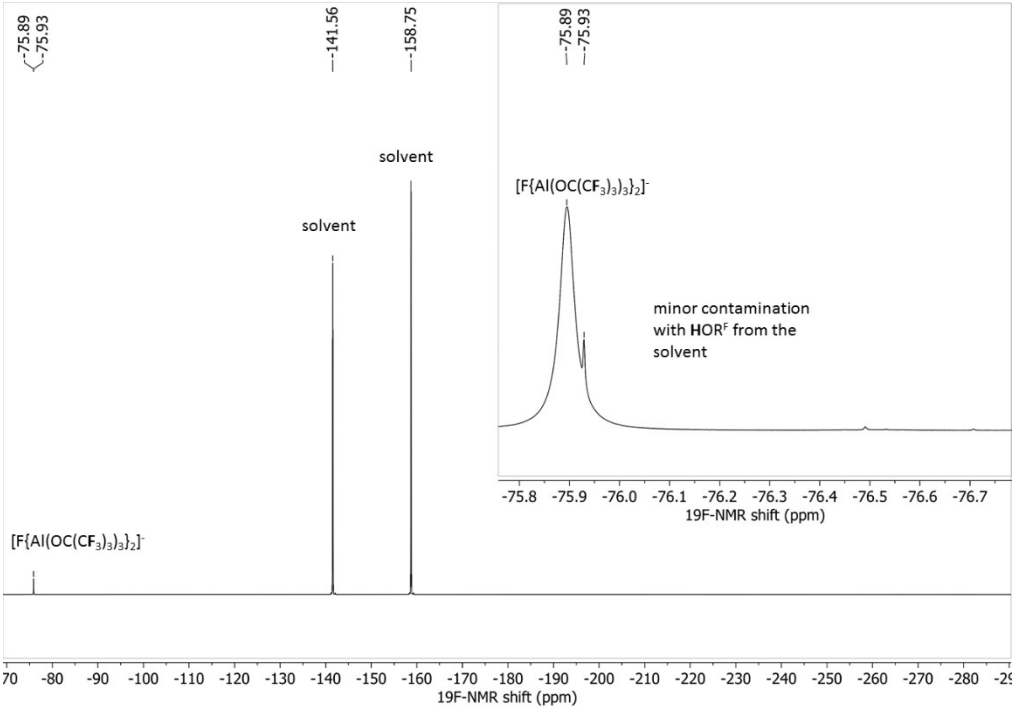


Figure S 9: ^{19}F NMR spectrum of [**6**]$^{+\cdot}$[F{Al(OR^F)$_3$}$_2$]$^-$ in 1,2,3,4-Tetrafluorobenzene.

6. Vibrational Spectroscopy

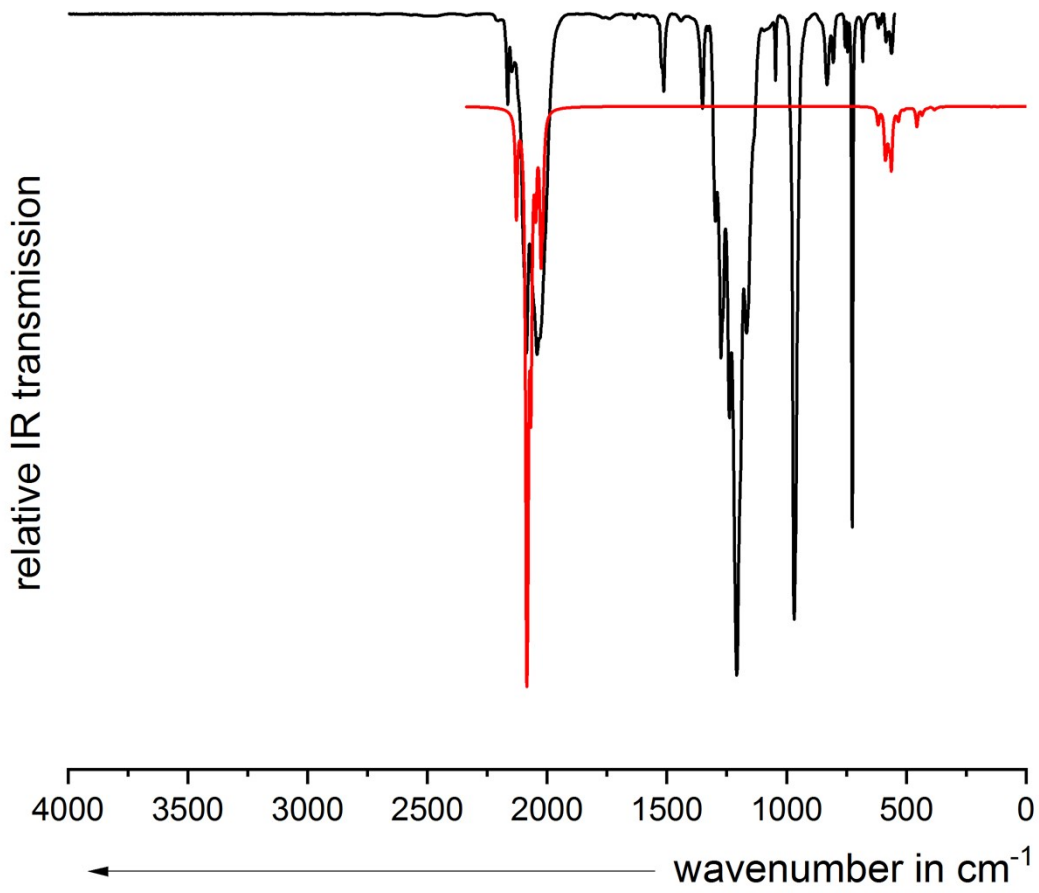


Figure S 10: IR spectrum of the reaction mixture containing [**2**]$^+$[Al(OR^F)$_4$]$^-$ (**black**) and the calculated IR spectrum of C_2 symmetric [**2**]$^+$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

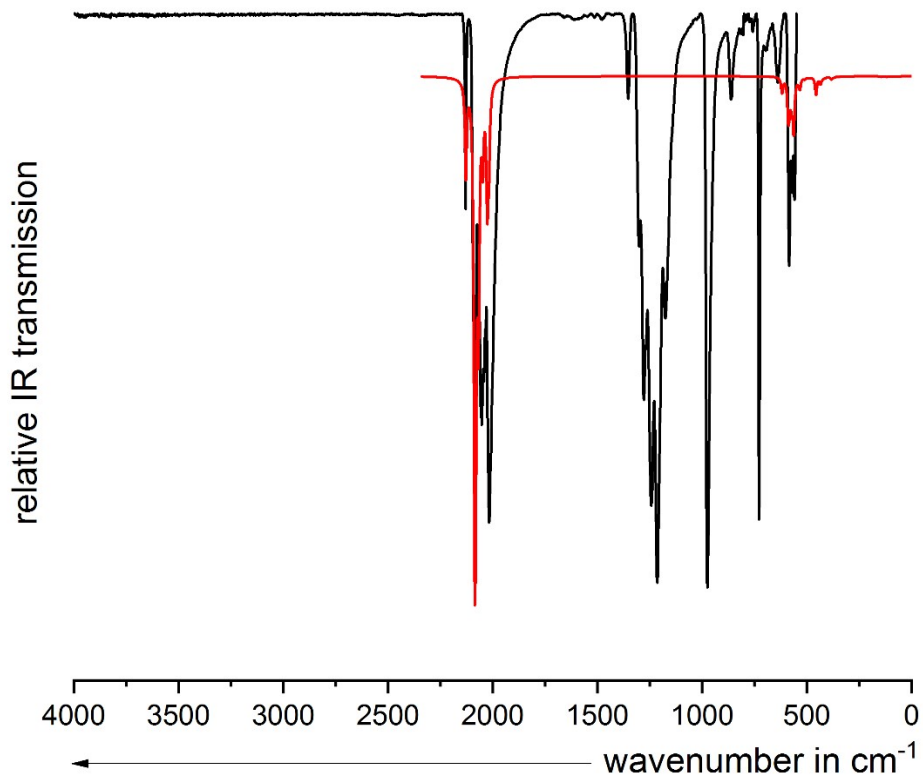


Figure S 11: IR spectrum of a dried 1,2,3,4-Tetrafluorobenzene solution [**3a**]$^+$[F{Al(OR^F)$_3$}$_2$]$^-$ (**black**) and the calculated IR spectrum of C_2 symmetric [**3a**]$^+$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

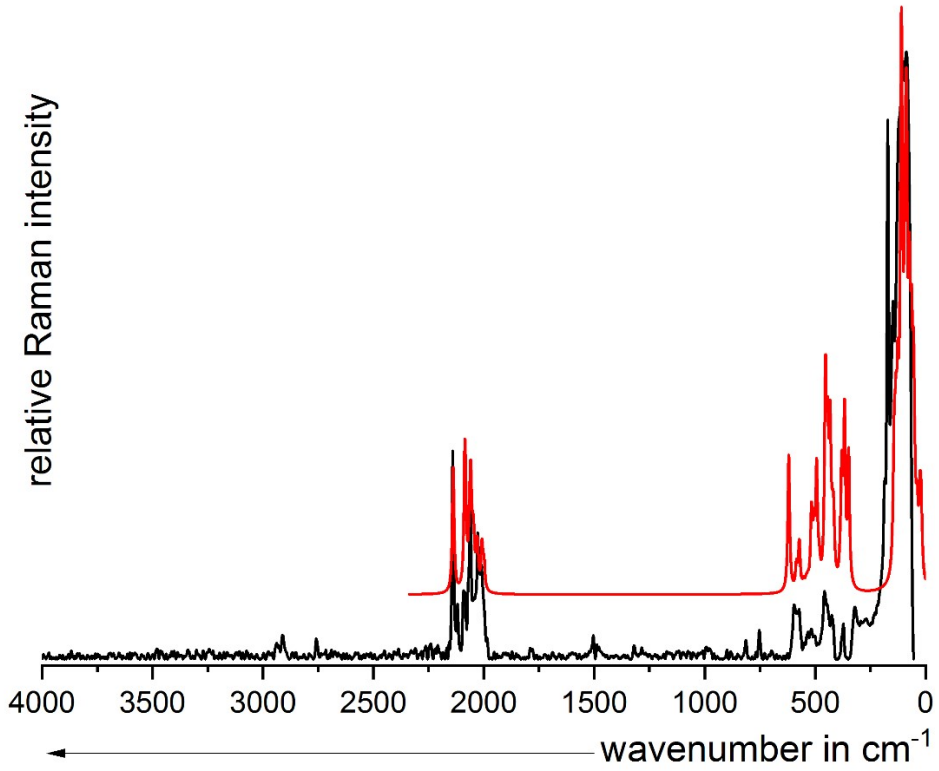


Figure S 12: Raman spectrum of a dried 1,2,3,4-Tetrafluorobenzene solution [**3a**]$^+$[F{Al(OR^F)$_3$}$_2$]$^-$ (**black**) and the calculated Raman spectrum of C_2 symmetric [**3a**]$^+$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

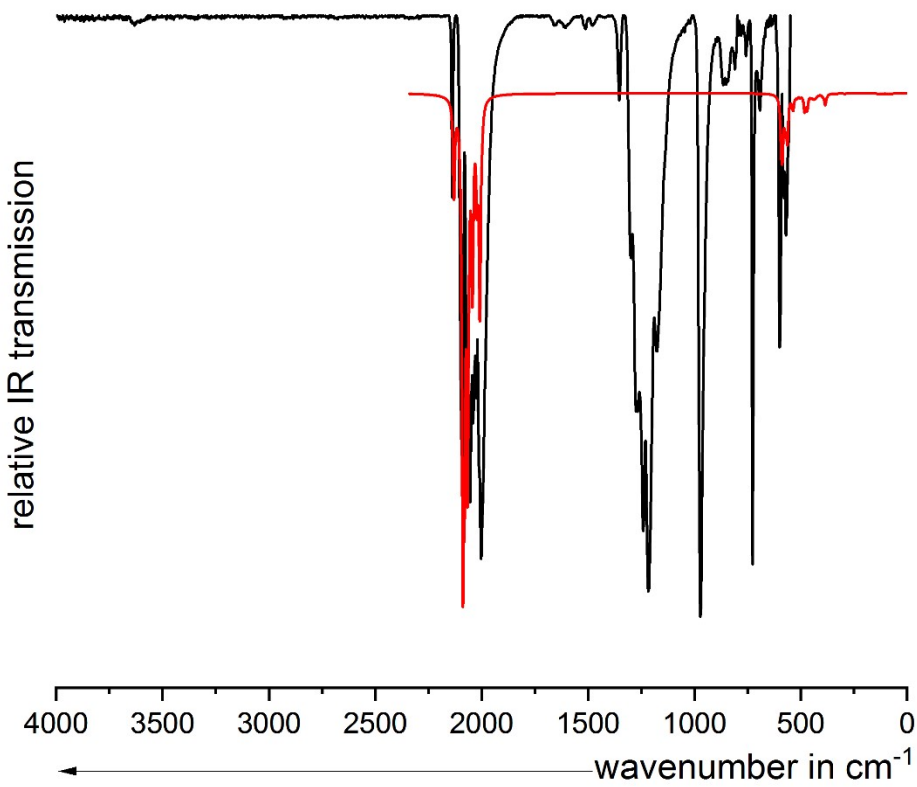


Figure S 13: IR spectrum of a dried 1,2,3,4-Tetrafluorobenzene solution with [**3b**]$^{+}$[F{Al(OR^{F})$_3$}$_2$]$^{-}$ (**black**) and the calculated IR spectrum of C_1 symmetric [**3b**]$^{+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

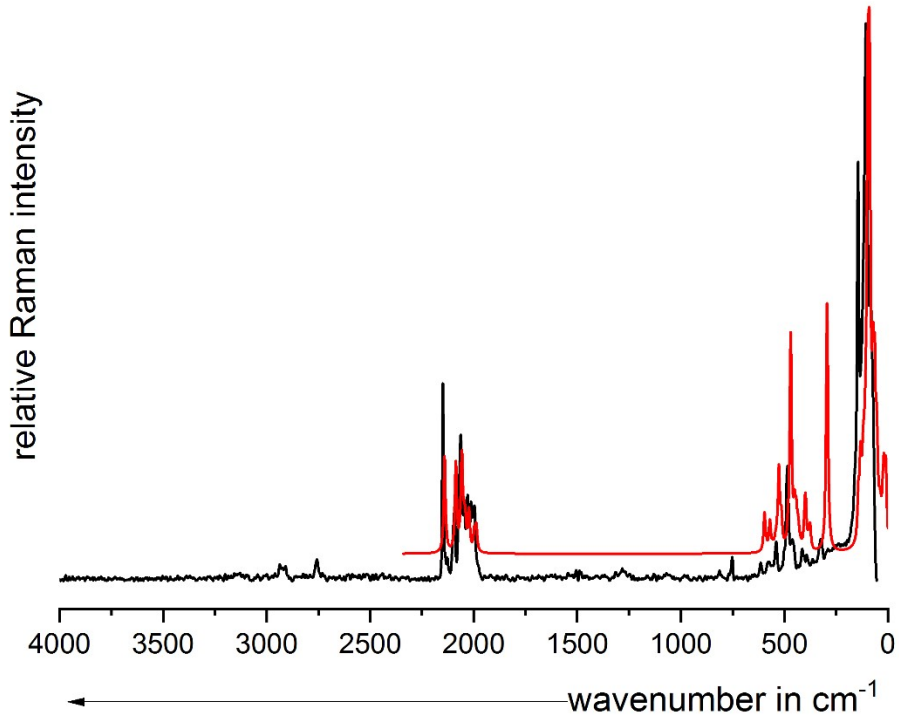


Figure S 14: Raman spectrum of a dried 1,2,3,4-Tetraflurobenzene solution of [**3b**]$^{+}$[F{Al(OR^{F})$_3$}$_2$]$^{-}$ (**black**) and the calculated Raman spectrum of C_1 symmetric [**3b**]$^{+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

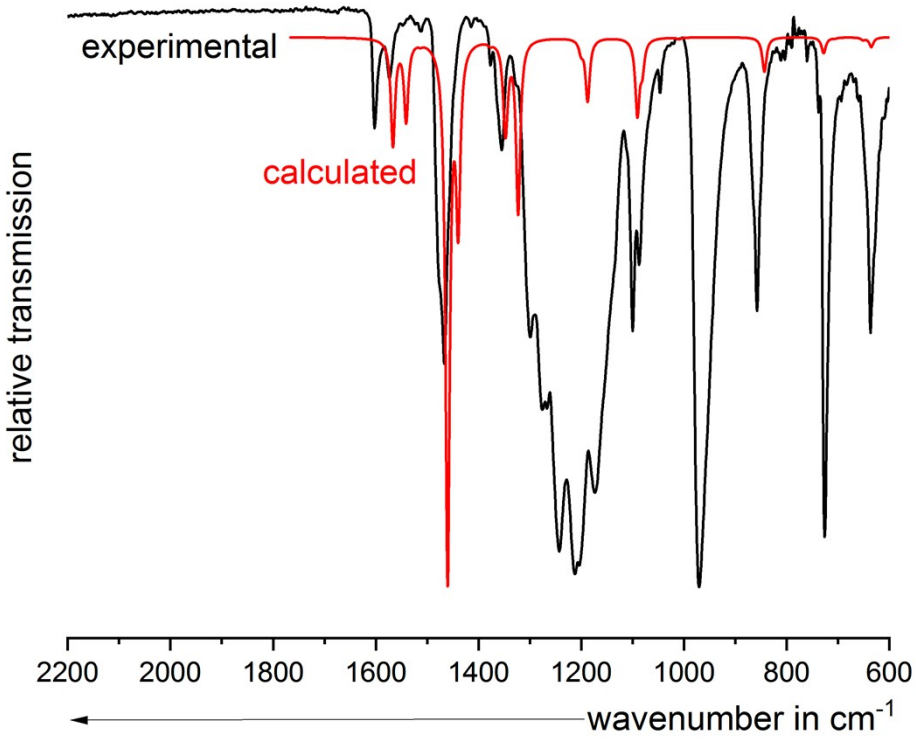


Figure S 15: IR spectrum of crystalline $[\mathbf{6}]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$ (**black**) and the calculated IR spectrum of C_2 symmetric $[\mathbf{6}]^{+\cdot}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

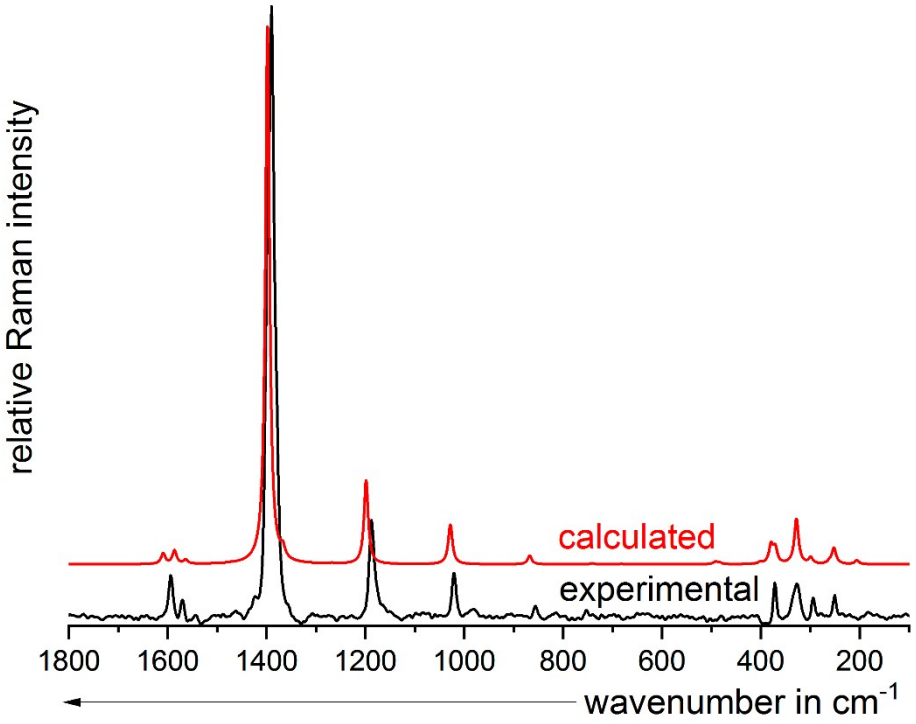


Figure S 16: Raman spectrum of crystalline $[\mathbf{6}]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$ (**black**) and the calculated Raman spectrum of C_2 symmetric $[\mathbf{6}]^{+\cdot}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

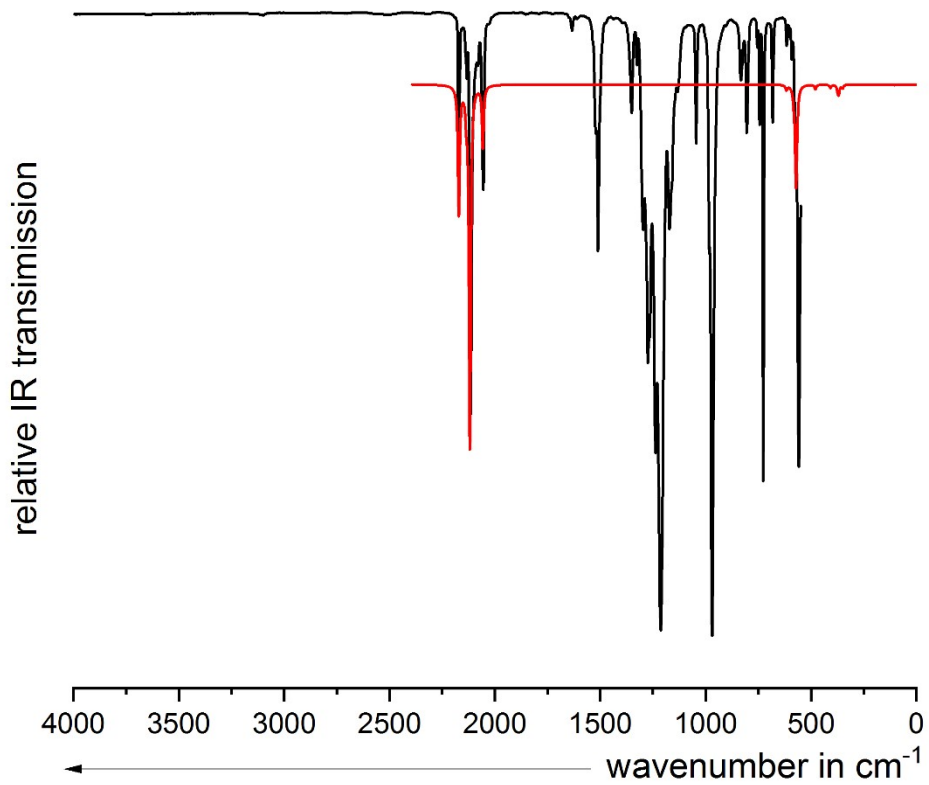


Figure S 17: IR spectrum of crystalline [**7a**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ (**black**) and the calculated IR spectrum of D_{4h} symmetric [**7a**]$^{2+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

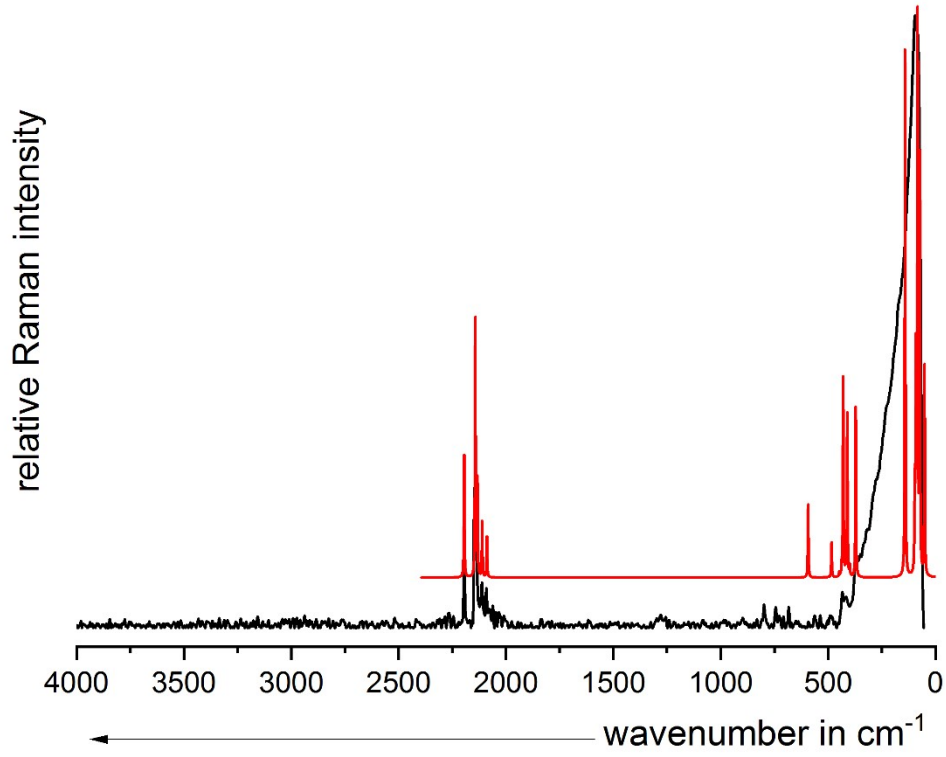


Figure S 18: Raman spectrum of crystalline [**7a**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ (**black**) and the calculated Raman spectrum of D_{4h} symmetric [**7a**]$^{2+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

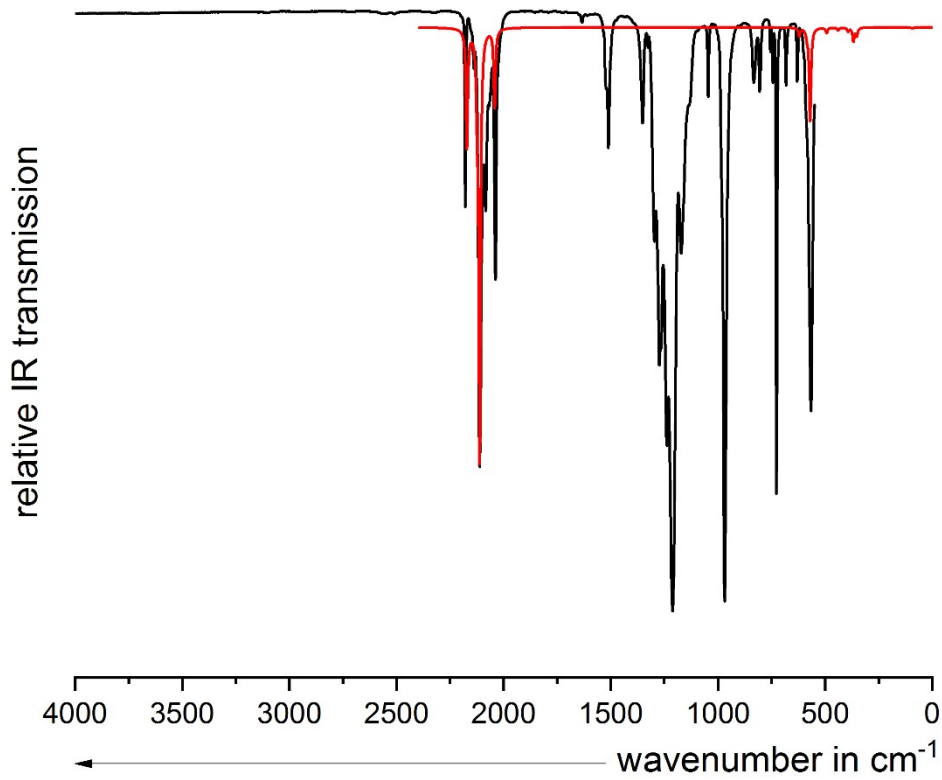


Figure S 19: IR spectrum of a dried 1,2,3,4-Tetraflurobenzene-solution of [**7b**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ (**black**) and the calculated IR spectrum of D_{4h} symmetric [**7b**]$^{2+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

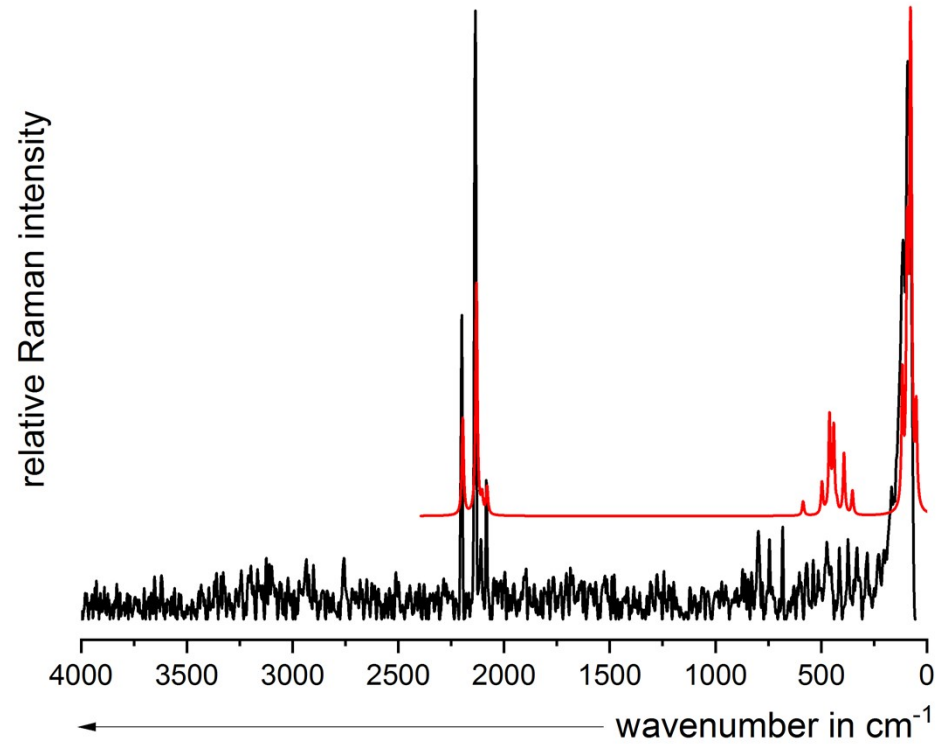


Figure S 20: Raman spectrum of crystalline [**7b**]$^{2+}$[Al(OR^{F})$_4$]$^{-}_2$ (**black**) and the calculated Raman spectrum of D_{4h} symmetric [**7b**]$^{2+}$ at the B3LYP(B3BJ)/def2-TZVPP level of theory (**red**).

7. Vibrational Modes of the 50 VE Trimetal Tetradecacarbonyls

Table S 3: Comparison of the experimentally obtained data of $[Ru_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2$ with DFT calculated values (B3LYP/def2-TZVPP, scaling factor for vibrational frequencies set to 0.968 according to M. A. Duncan et al.[20]).

	exp. $Ru(CO)_5$	calcd. $Ru(CO)_5$ (D_{3h})	exp. $[Ru_3(CO)_{14}]^{2+}$ $[Al(OC(CF_3)_3)_4]^-_2$	calcd. $[Ru_3(CO)_{14}]^{2+}$ (D_{4h})	exp. $[Ru(CO)_6]^{2+}$ $[SbF_6]^-_2$	calcd. $[Ru(CO)_6]^{2+}$ (O_h)
IR ν(CO) in cm^{-1}	2002	2005 (E')	2173	2171 (A_{2u})	2198	2206 (T_{1u})
	2037	2040 (A''_2)	2139	2136 (A_{2u})		
			2114	2119 (E_u)		
			2058	2058 (E_u)		
Raman ν(CO) in cm^{-1}		2005 (E')	2194	2195 (A_{1g})	2252	2260 (E_g)
		2030 (A'_1)	2146	2143 (A_{1g})	2219	2223 (A_{1g})
		2118(A'_1)	2138	2133 (B_{2g})		
			2113	2111 (E_g & A_{1g})		
			2092	2089 (B_{1g})		
d(M-CO)$_{ax.}$ in Å		1.955	1.999(1)	1.985	2.024	2.037
avg. d(M-CO)$_{eq\text{-}ter.}$ in Å		1.958	1.981	1.984		
avg. d(M-CO)$_{eq\text{-}cen.}$ in Å			1.964	1.960		
d(M-M) in Å			2.896	2.970		
^{13}C-shift in ppm	200.4		195.1			
			185.0			
			171.5		168.8	

Table S 4: Comparison of the experimentally obtained data of $[Os_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2$ with DFT calculated values (B3LYP/def2-TZVPP, scaling factor for vibrational frequencies set to 0.968 according to M. A. Duncan et al.[20].

	exp. $Os(CO)_5$	calcd. $Os(CO)_5$ (D_{3h})	$[Os_3(CO)_{14}]^{2+}$ $[Al(OC(CF_3)_3)_4]^-_2$	calcd. $[Os_3(CO)_{14}]^{2+}$	exp. $[Os(CO)_6]^{2+}$ $[SbF_6]^-_2$	calcd. $[Os(CO)_6]^{2+}$ (O_h)
IR ν(CO)	1993	1993 (E')	2179	2172 (A_{2u})	2189	2195 (T_{1u})
	2035	2035 (A''_2)	2127	2124 (A_{2u})		
			2109	2112 (E_u)		
			2042	2043 (E_u)		
Raman ν(CO)		1993 (E')	2200	2195 (A_{1g})	2258	2260 (E_g)
		2023 (A'_1)	2136	2130 (A_{1g} & B_{2g})	2214	2215 (A_{1g})
		2117 (A'_1)	2109	2104 (E_g & A_{1g})		
			2084	2081 (B_{1g})		
d(M-CO)$_{ax.}$ in Å		1.977	1.983(4)	1.985	2.022	2.049
avg. d(M-CO)$_{eq\text{-}ter.}$ in Å		1.964	1.983	2.000		
avg. d(M-CO)$_{eq\text{-}cen.}$ in Å			1.964	1.975		
d(M-M) in Å			2.913	3.002		
^{13}C-shift in ppm	182.6		176.8			
			163.8			
			not observed		150.6	

8. Determination of the force constants

For the determination of the force constants the Cotton-Kraihanzel-approximation is used:[21]

The central -$M(CO)_4$- fragment of $[M_3(CO)_{14}]^{2+}$ is approximated as *trans*-$M(CO)_4L_2$. The force constant $k_{cen,eq}$ can be easily determined with the mode 10 (see manuscript):

$$k_{cen,eq} = \frac{\lambda}{\mu}$$

The both -$M(CO)_5$ fragments are approximated as $M(CO)_5L$ fragments. This interaction is here approximated as zero due to the long distance between the two terminal fragments (>5 Å). The mode 6 gives the force constant $k_{out,eq}$:

$$k_{out,eq} = \frac{\lambda}{\mu}$$

Because the interaction between the carbonyl-ligands in the -$M(CO)_5$ fragments ($k_{out\text{-}out}$) is needed for the calculation of $k_{out,ax}$, this is calculated before:

$$k_{out,eq\,-\,out,eq} = -\frac{\left(\frac{\lambda}{\mu} - k_{out,eq}\right)}{2}$$

This gives finally $k_{out,ax}$:

$$k_{out,ax} = \mu^{-1}\left(\lambda + \frac{4\mu^2 k_{out,eq\,-\,out,eq}^{\;2}}{\mu\, k_{out,eq} + 4\,\mu\, k_{out,eq\,-\,out,eq} - \lambda}\right)$$

9. pXRD

$[\mathbf{6}]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$

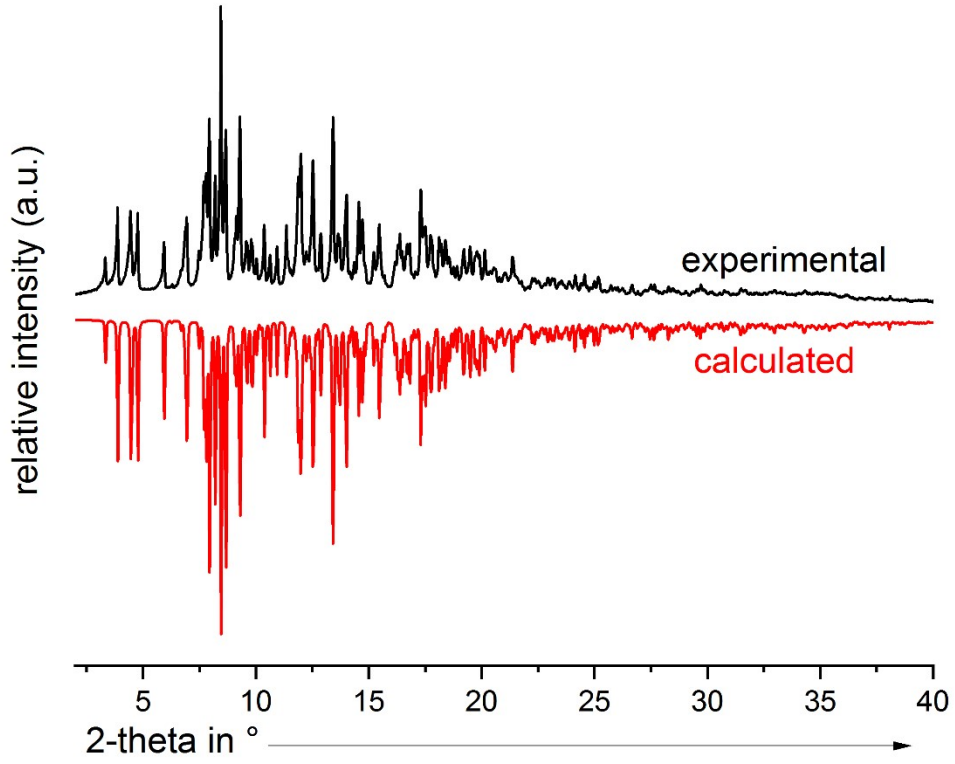


Figure S 21: Measured pXRD data of the bulk material of $[anthracene^{Hal}]^{+\cdot}[Al(OR^F)_4]^-$ at 100 K (**black**) and the calculated powder diffraction pattern, simulated with the respective single crystal data (**red**).

$[\mathbf{7a/7b}]^{2+}[Al(OR^F)_4]^-_2 \cdot x\ C_6F_4H_2$ (x < 2)

The pXRD shows, that the $[\mathbf{7a}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$ is not phase-pure. Because the same material was used for the NMR-spectroscopy, which showed no significant impurities, we expected, that the phase decomposes under vacuum, because the co-crystallized 1,2,3,4-Tetrafluorobenzene (bp. = 95 °C) evaporates. When the experiment is repeated with a longer vacuum exposure, the crystalline phase is even more decomposed, which validates the theory. The effect is even more pronounced at $[\mathbf{7b}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$.

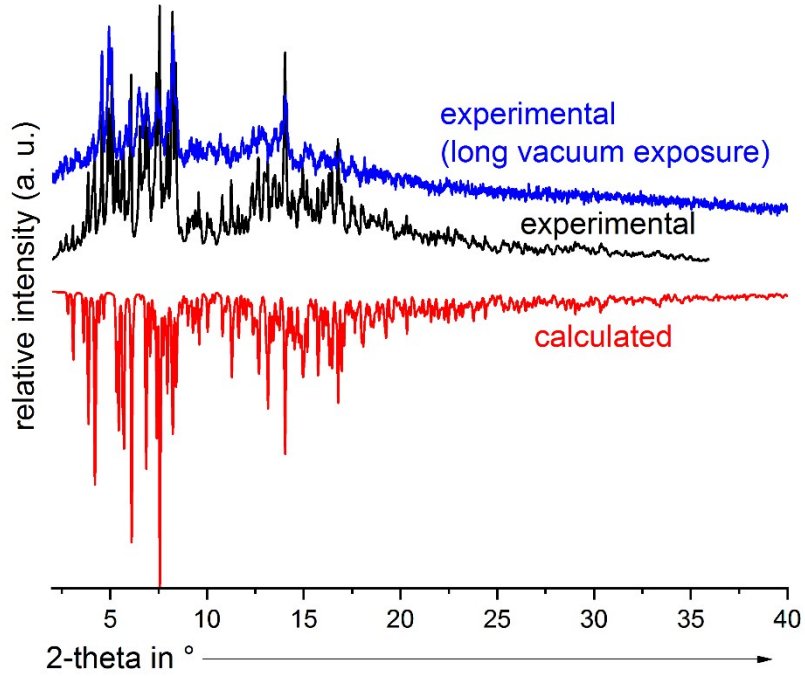


Figure S 22: Measured pXRD data of the bulk material of $[Ru_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$ at 100 K with a short drying period (**black**) + a long drying period in the high-vacuum (**blue**) and the calculated powder diffraction pattern, simulated with the respective single crystal data (**red**).

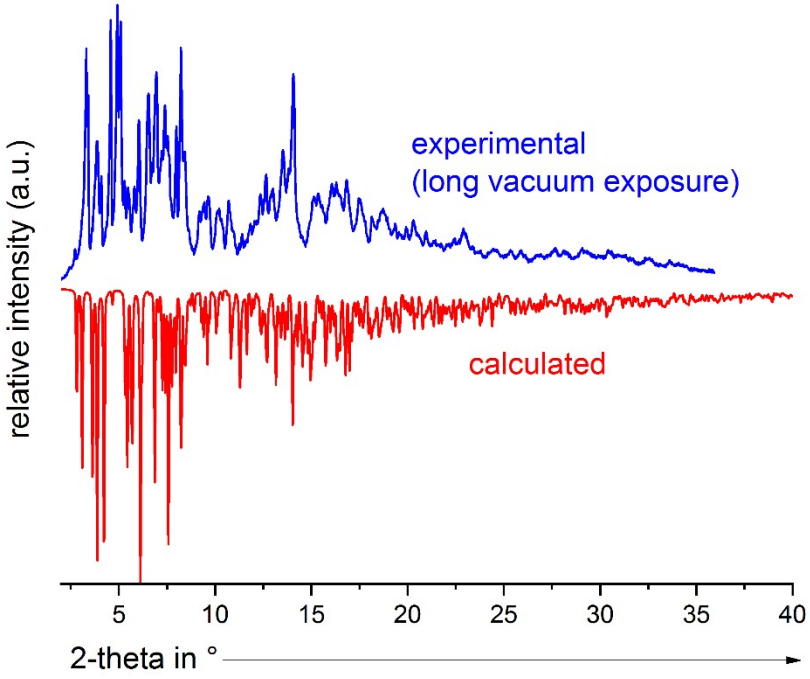


Figure S 23: Measured pXRD data of the bulk material of $[Os_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$ at 100 K with a long drying period in the high-vacuum (**blue**) and the calculated powder diffraction pattern, simulated with the respective single crystal data (**red**).

10. EPR-Spectroscopy

The isotropic hyperfine coupling constants obtained from DFT calculations at the B3LYP/EPR-II level of theory are shown in Figure S 24. For the simulation of the continuous wave EPR spectrum shown in the main text using EasySpin functions in MATLAB, the computed hyperfine coupling constants of the eight fluorine atoms were divided into two groups, each consisting of four fluorine atoms. The DFT values were used as the starting values for the fit of the experimental spectrum: Initially, the hyperfine coupling constants were assumed to be 6 MHz for the fluorine atoms in β-position and 21 MHz for the fluorine atoms in α-position and an isotropic hyperfine coupling constant of 5 MHz was assumed for each of the two chlorine atoms. During the fitting procedure of the experimental cw EPR spectrum, the hyperfine coupling constants were only adjusted by applying an identical scaling factor to all values computed by DFT. The best fit was obtained for hyperfine coupling constants of 5.82 MHz and 20.37 MHz for the two groups of fluorine atoms and 4.85 MHz for the two chlorine atoms (scaling factor of 0.97). The excellent agreement with the experimental data confirms the assignment of the hyperfine couplings and the accuracy of the calculated spin density.

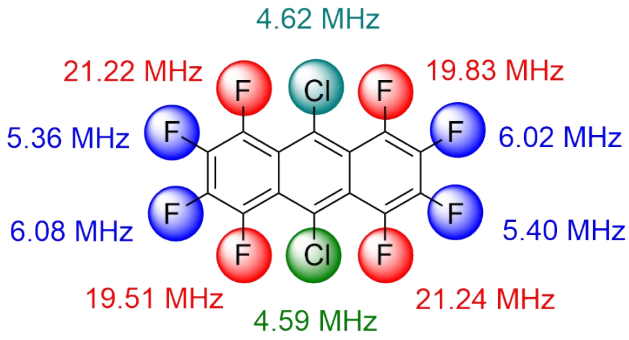


Figure S 24: Assignment of the hyperfine coupling constants using DFT at the B3LYP/EPR-II (6-31G** for Cl) level of theory.

11. Cyclic Voltammetry

Cyclic voltammetry was performed in a setup with a platinum working electrode, platinum mesh counter electrode and a platinum quasi-reference electrode. The measurements were done with a 10 mM solution of **6** in 1,2-Difluorobenzene and 1,2,3,4-Tetraflurobenzene. $[NBu_4]^+[Al(OR^F)_4]^-$ was used as conducting salt in 100 mM solution and $[Fc]^+[Al(OR^F)_4]^-$ (10 mM) + Fc (10 mM) as internal reference. The half-wave potential is almost independent from the scan rate ν (Table S 1 + Table S 2). The redox reaction is electrochemically reversible under the given conditions, because the anodic peak current is I_{ac} is proportional to the square-root of the scan rate $\nu^{1/2}$ (Figure S 11 + Figure S 12).

Table S 6: Half-wave potentials of **6** in 1,2-Difluorobenzene vs. $Fc^{0/+}$ and anodic peak currents at different scan rates.

υ in mV s^{-1}	$E_{1/2}$ in V	I_{ac} in µA
20	1.419	10.78
50	1.419	15.47
100	1.417	20.39

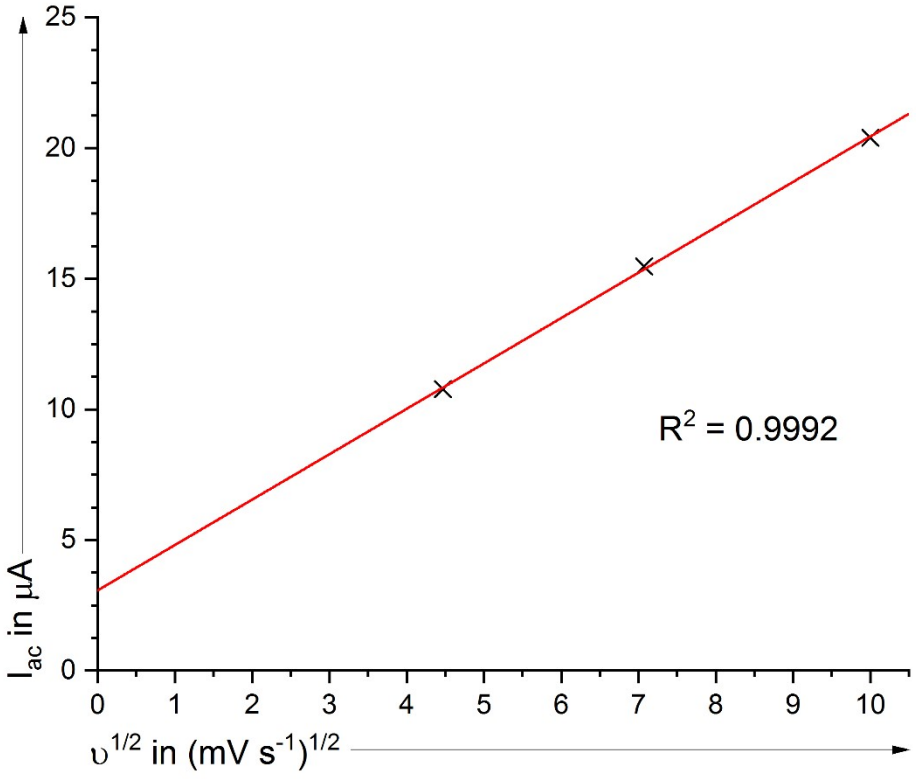


Figure S 25: Linear fit of the anodic peak current I_{ac} against the square root of the scan rate $\upsilon^{1/2}$ of **6** in 1,2-Difluorobenzene.

Table S 7: Half-wave potentials of **6** vs. $Fc^{0/+}$ in 1,2,3,4-Tetrafluorobenzene and anodic peak currents at different scan rates.

υ in mV s^{-1}	$E_{1/2}$ in V	I_{ac} in µA
20	1.419	6.201
50	1.417	9.349
100	1.419	12.62
200	1.419	17.04
500	1.422	25.53
1000	1.425	34.39

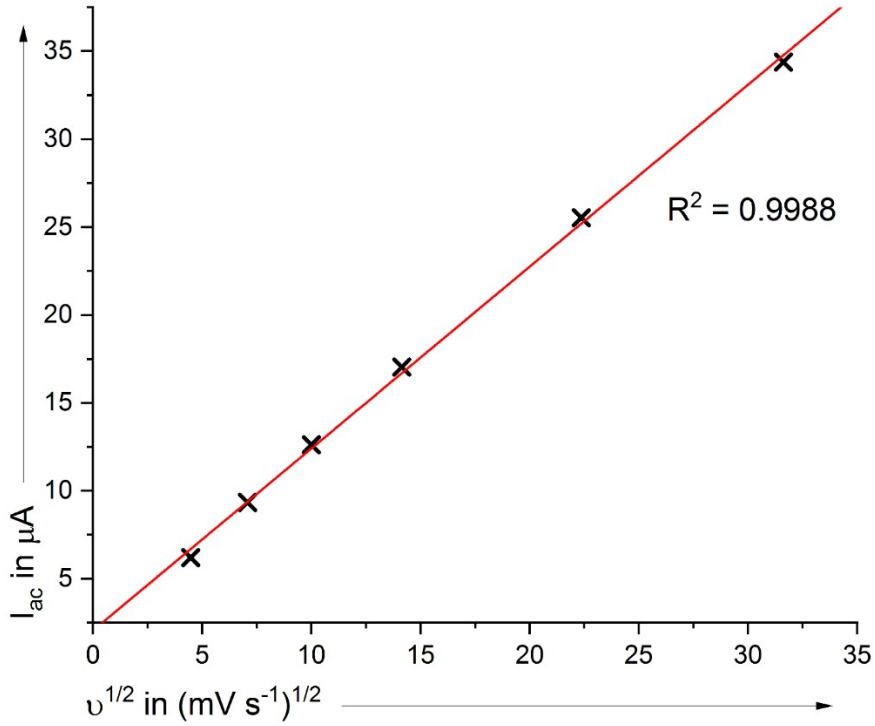


Figure S 26: Linear fit of the anodic peak current I_{ac} against the square root of the scan rate $\upsilon^{1/2}$ of **6** in 1,2,3,4-Tetrafluorobenzene.

12. EDA-NOCV

Table S 8: EDA-NOCV results of the $[Ag\{M_3(CO)_{12}\}_2]^+$ (M = Ru, Os) complexes using the fragments Ag^+ and $\{[M_3(CO)_{12}]_2\}$ at the BP86-D3(BJ)/TZ2P level. Values are given in kcal/mol.

Energies	Orbital interaction	$Ag^+ + \{[Ru_3(CO)_{12}]_2\}$	$Ag^+ + \{[Os_3(CO)_{12}]_2\}$
ΔE_{int}		−118.45	−123.68
ΔE_{Pauli}		130.54	131.94
ΔE_{disp}		−7.89	−11.13
ΔE_{elstat}		−123.80	−124.68
ΔE_{orb}		−117.30	−119.87
$\Delta E_{orb(1)}$	[TMC] → Ag^+ (s) ← [TMC] σ-donation	−45.17	−44.98
$\Delta E_{orb(2)}$	[TMC] → Ag^+ (p_σ) ← [TMC] σ-donation	−15.02	−16.07
$\Delta E_{orb(3)}$	[TMC] → Ag^+ (p_π) ← [TMC] π-donation	−10.68	−10.99
$\Delta E_{orb(4)}$	[TMC] → Ag^+ (p_π) ← [TMC] π-donation	−7.35	−7.88
$\Delta E_{orb(5)}$	[TMC] ← Ag^+ (p_σ) → [TMC] σ-backdonation	−5.28	−5.94
$\Delta E_{orb(6)}$		−3.95	−4.80
$\Delta E_{orb(7)}$		−4.37	−3.75
$\Delta E_{orb(8)}$		−3.31	−3.57
$\Delta E_{orb(9)}$		−2.35	−2.36
$\Delta E_{orb(rest)}$		−19.80	−19.51

Table S 9: EDA-NOCV results of the $[M_3(CO)_{14}]^{2+}$ (M = Ru, Os) complexes using the fragments $[Ru(CO)_4]^{\cdot\cdot} + \{[Ru(CO)_5]_2\}^{2+\cdot\cdot}$ at the BP86-D3(BJ)/TZ2P level. Values are given in kcal/mol.

Energies	Orbital interaction	$[Ru(CO)_4]^{\cdot\cdot} + \{[Ru(CO)_5]_2\}^{2+\cdot\cdot}$		$[Os(CO)_4]^{\cdot\cdot} + \{[Os(CO)_5]_2\}^{2+\cdot\cdot}$	
ΔE_{int}		−124.91		−138.02	
ΔE_{Pauli}		136.87		140.72	
ΔE_{disp}		−33.70		−34.41	
ΔE_{elstat}		−106.54		−114.38	
ΔE_{orb}		−124.91		−129.96	
$\Delta E_{orb(1)}$	covalent metal-metal bonding	−35.37	−19.67	−40.73	−21.86
$\Delta E_{orb(2)}$	donation of neighbouring carbonyls	−10.58	−44.53	−11.91	−44.17
$\Delta E_{orb(rest)}$		−5.84	−5.60	−5.75	−5.58

13. QTAIM Results

$[Os_3(CO)_{14}]^{2+}$

Normalization factor of the integral of electron density is 0.999842

The atomic charges after normalization and atomic volumes:

1	(Os)	Charge:	0.989859	Volume:	106.723 Bohr^3
2	(Os)	Charge:	0.667593	Volume:	110.746 Bohr^3
3	(O)	Charge:	-1.082865	Volume:	127.505 Bohr^3
4	(O)	Charge:	-1.099051	Volume:	128.098 Bohr^3
5	(O)	Charge:	-1.085804	Volume:	129.370 Bohr^3
6	(O)	Charge:	-1.089490	Volume:	128.851 Bohr^3
7	(O)	Charge:	-1.099167	Volume:	127.871 Bohr^3
8	(O)	Charge:	-1.118869	Volume:	132.023 Bohr^3
9	(O)	Charge:	-1.119974	Volume:	131.323 Bohr^3
10	(C)	Charge:	1.112415	Volume:	70.825 Bohr^3
11	(C)	Charge:	1.075248	Volume:	65.996 Bohr^3
12	(C)	Charge:	1.061842	Volume:	67.067 Bohr^3
13	(C)	Charge:	1.063778	Volume:	65.419 Bohr^3
14	(C)	Charge:	1.068485	Volume:	64.479 Bohr^3
15	(C)	Charge:	0.997766	Volume:	63.299 Bohr^3
16	(C)	Charge:	0.992029	Volume:	62.271 Bohr^3
17	(Os)	Charge:	0.989859	Volume:	106.723 Bohr^3
18	(O)	Charge:	-1.082877	Volume:	127.505 Bohr^3
19	(O)	Charge:	-1.099050	Volume:	128.098 Bohr^3
20	(O)	Charge:	-1.085804	Volume:	129.370 Bohr^3
21	(O)	Charge:	-1.089489	Volume:	128.851 Bohr^3
22	(O)	Charge:	-1.099166	Volume:	127.871 Bohr^3
23	(O)	Charge:	-1.118865	Volume:	132.023 Bohr^3
24	(O)	Charge:	-1.119975	Volume:	131.323 Bohr^3
25	(C)	Charge:	1.112425	Volume:	70.825 Bohr^3
26	(C)	Charge:	1.075248	Volume:	65.996 Bohr^3
27	(C)	Charge:	1.061842	Volume:	67.067 Bohr^3
28	(C)	Charge:	1.063777	Volume:	65.419 Bohr^3
29	(C)	Charge:	1.068485	Volume:	64.479 Bohr^3
30	(C)	Charge:	0.997763	Volume:	63.299 Bohr^3
31	(C)	Charge:	0.992031	Volume:	62.271 Bohr^

Table S 10: Addition of the QTAIM-charges of the atoms into fragments.

Os core				
	0.989859			
	0.667593			
	0.989859			
Σ	**2.647311**			
$CO_{out,ax}$	C		O	
10	1.112415	3	-1.082865	
25	1.112425	18	-1.082877	
Σ	**2.22484**		**-2.165742**	**0.059098**
average	**1.11242**		**-1.082871**	**0.029549**
$CO_{out,eq}$	C		O	
11	1.075248	4	-1.099051	
12	1.061842	5	-1.085804	
13	1.063778	6	-1.08949	
14	1.068485	7	-1.099167	
26	1.075248	19	-1.09905	
27	1.061842	20	-1.085804	
28	1.063777	21	-1.089489	
29	1.068485	22	-1.099166	
Σ	**8.538705**		**-8.747021**	**-0.208316**
average	**1.06733813**		**-1.09337763**	**-0.0260395**
$CO_{cen,eq}$	C		O	
15	0.997766	8	-1.118869	
16	0.992029	9	-1.119974	
30	0.997763	23	-1.118865	
31	0.992031	24	-1.119975	
Σ	**3.979589**		**-4.477683**	**-0.498094**
average	**0.99489725**		**-1.11942075**	**-0.1245235**
Test	Test Sum		**$Os(CO)_5$**	**0.91525**
1.999999	1.999999		**$Os(CO)_4$**	**0.169499**

$[Ru_3(CO)_{14}]^{2+}$

Normalization factor of the integral of electron density is 0.999792

The atomic charges after normalization and atomic volumes:

1	(Ru)	Charge:	0.850674	Volume:	98.113 Bohr^3
2	(Ru)	Charge:	0.610090	Volume:	102.253 Bohr^3
3	(C)	Charge:	1.143366	Volume:	72.778 Bohr^3
4	(C)	Charge:	1.093758	Volume:	67.039 Bohr^3
5	(O)	Charge:	-1.088244	Volume:	127.764 Bohr^3
6	(O)	Charge:	-1.102432	Volume:	128.521 Bohr^3
7	(O)	Charge:	-1.102370	Volume:	128.281 Bohr^3
8	(O)	Charge:	-1.098883	Volume:	129.021 Bohr^3
9	(O)	Charge:	-1.093207	Volume:	129.623 Bohr^3
10	(O)	Charge:	-1.124845	Volume:	130.967 Bohr^3
11	(O)	Charge:	-1.122831	Volume:	131.940 Bohr^3
12	(C)	Charge:	1.086975	Volume:	65.361 Bohr^3
13	(C)	Charge:	1.094211	Volume:	66.278 Bohr^3
14	(C)	Charge:	1.090743	Volume:	68.265 Bohr^3
15	(C)	Charge:	1.035782	Volume:	63.002 Bohr^3
16	(C)	Charge:	1.032259	Volume:	64.074 Bohr^3
17	(Ru)	Charge:	0.850674	Volume:	98.113 Bohr^3
18	(C)	Charge:	1.143380	Volume:	72.778 Bohr^3
19	(C)	Charge:	1.093753	Volume:	67.039 Bohr^3
20	(O)	Charge:	-1.088258	Volume:	127.764 Bohr^3
21	(O)	Charge:	-1.102427	Volume:	128.521 Bohr^3
22	(O)	Charge:	-1.102373	Volume:	128.281 Bohr^3
23	(O)	Charge:	-1.098881	Volume:	129.021 Bohr^3
24	(O)	Charge:	-1.093207	Volume:	129.623 Bohr^3
25	(O)	Charge:	-1.124844	Volume:	130.967 Bohr^3
26	(O)	Charge:	-1.122831	Volume:	131.940 Bohr^3
27	(C)	Charge:	1.086978	Volume:	65.361 Bohr^3
28	(C)	Charge:	1.094210	Volume:	66.278 Bohr^3
29	(C)	Charge:	1.090742	Volume:	68.265 Bohr^3
30	(C)	Charge:	1.035781	Volume:	63.002 Bohr^3
31	(C)	Charge:	1.032259	Volume:	64.074 Bohr^3

Table S 11: Addition of the QTAIM-charges of the atoms into fragments.

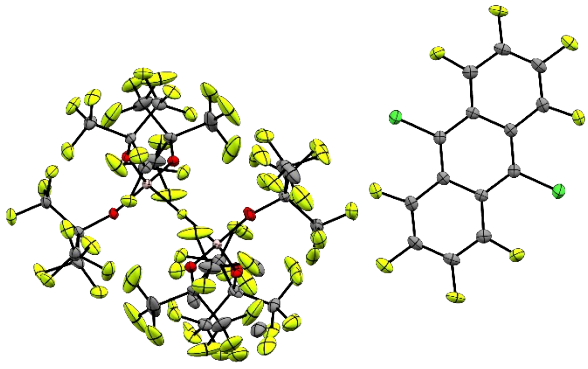
Ru core				
	0.850674			
	0.61009			
	0.850674			
	2.311438			
CO-achse	C		O	
3	1.143366	5	-1.088244	
18	1.14338	20	-1.088258	
Σ	**2.286746**		**-2.176502**	**0.110244**
average	**1.143373**		**-1.088251**	**0.055122**
CO-equa	C		O	
C4	1.093758	O6	-1.102432	
C12	1.086975	O7	-1.10237	
C13	1.094211	O8	-1.098883	
C14	1.090743	O9	-1.093207	
C19	1.093753	O21	-1.102427	
C27	1.086978	O22	-1.102373	
C28	1.09421	O23	-1.098881	
C29	1.090742	O24	-1.093207	
Σ	**8.73137**		**-8.79378**	**-0.06241**
average	**1.09142125**		**-1.0992225**	**-0.00780125**
CO-cent	C		O	
C15	1.035782	O10	-1.124845	
C16	1.032259	O11	-1.122831	
C30	1.035781	O25	-1.124844	
C31	1.032259	O26	-1.122831	
Σ	**4.136081**		**-4.495351**	**-0.35927**
average	**1.03402025**		**-1.12383775**	**-0.0898175**
Test	Test Sum		**$Ru(CO)_5$**	**0.874591**
2.000002	2.000002		**$Ru(CO)_4$**	**0.25082**

14. scXRD-Data

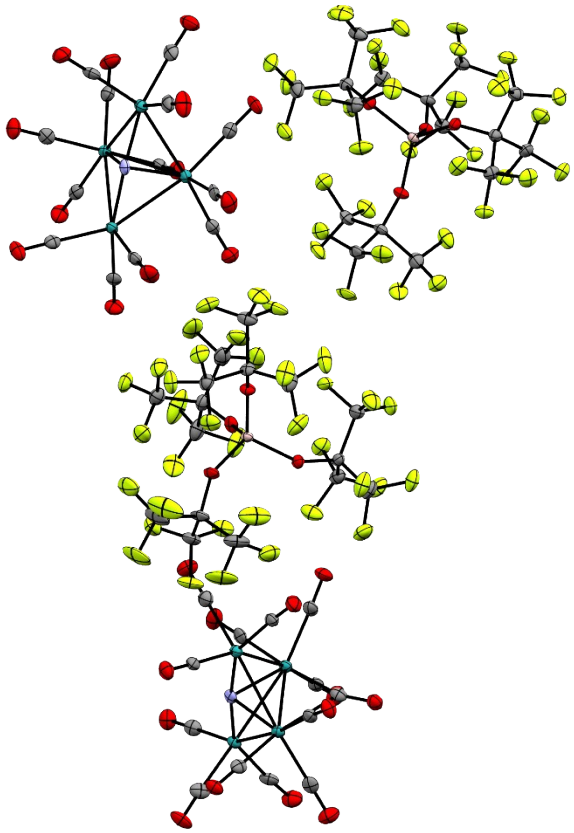
$[C_{14}F_8Cl_2]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$

Table S 12: Crystal data and structure refinement for $[anthracene^{Hal}]^{+\cdot}[F\{Al(OR^F)_3\}_2]^-$.

CCDC number 2151155



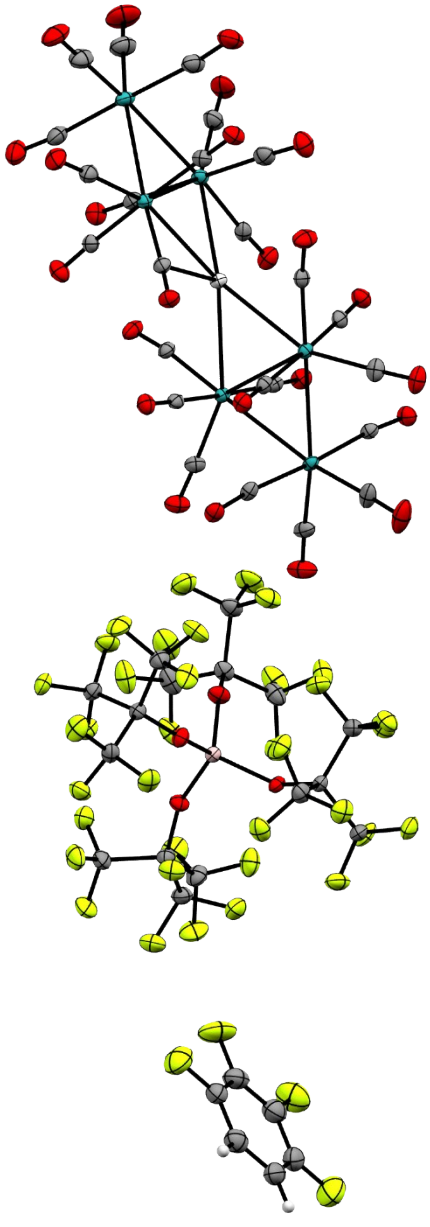
Empirical formula	$C_{38}Al_2Cl_2F_{63}O_6$
Formula weight	1874.24
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	14.514(9)
b [Å]	10.566(6)
c [Å]	18.161(11)
α [°]	90
β [°]	98.81(3)
γ [°]	90
Volume [Å^3]	2752(3)
Z	2
ρ_{calc} [gcm^{-3}]	2.262
μ [mm^{-1}]	0.414
F(000)	1806
Crystal size [mm^3]	0.23×0.21×0.12
Crystal colour	blue
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.35 to 54.20 (0.78 Å)
Index ranges	-18 ≤ h ≤ 18 -13 ≤ k ≤ 13 -23 ≤ l ≤ 23
Reflections collected	28399
Independent reflections	6071 R_{int} = 0.0272 R_{sigma} = 0.0225
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	6071/4354/757
Goodness-of-fit on F^2	1.072
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0421 wR_2 = 0.0993
Final *R* indexes [all data]	R_1 = 0.0542 wR_2 = 0.1061
Largest peak/hole [eÅ^{-3}]	1.02/-0.54



$[NRu_4(CO)_{13}]^+[Al(OR^F)_4]^-$

CCDC number	2151474
Empirical formula	$C_{29}AlF_{36}NO_{17}Ru_4$
Formula weight	1749.56
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	15.639(14)
b [Å]	15.156(14)

c [Å]	41.36(4)
α [°]	90
β [°]	95.87(2)
γ [°]	90
Volume [Å^3]	9752(15)
Z	8
ρ_{calc} [gcm^{-3}]	2.383
μ [mm^{-1}]	1.440
F(000)	6640
Crystal size [mm^3]	0.23×0.17×0.05
Crystal colour	red
Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	1.98 to 56.04 (0.76 Å)
Index ranges	-20 ≤ h ≤ 20 -19 ≤ k ≤ 16 -54 ≤ l ≤ 54
Reflections collected	135688
Independent reflections	23163 R_{int} = 0.1000 R_{sigma} = 0.0867
Completeness to Θ = 25.242°	99.9 %
Data / Restraints / Parameters	23163/19111/1966
Goodness-of-fit on F^2	1.005
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0436 wR_2 = 0.0740
Final *R* indexes [all data]	R_1 = 0.0889 wR_2 = 0.0867
Largest peak/hole [eÅ^{-3}]	0.81/-1.03



$[Ag\{Ru_3(CO)_{12}\}_2]^+[Al(OR^F)_4]^-\cdot C_6F_4H_2$

Table S 13: Crystal data and structure refinement for $[Ag\{Ru_3(CO)_{12}\}_2]^+[Al(OR^F)_4]^-\cdot C_6F_4H_2$.

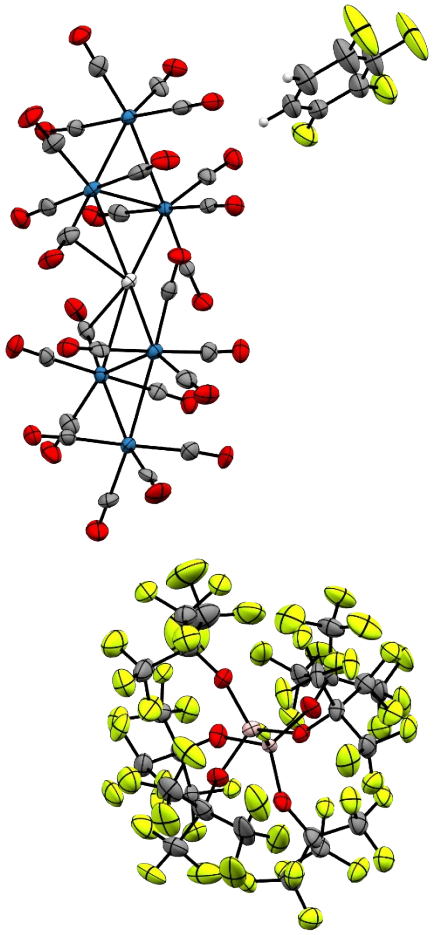
CCDC number	2151852
Empirical formula	$C_{46}H_2AgAlF_{40}O_{28}Ru_6$
Formula weight	2503.75
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	12.349(6)
b [Å]	12.385(4)
c [Å]	23.041(10)
α [°]	90.85(2)
β [°]	94.031(10)
γ [°]	93.152(13)
Volume [Å^3]	3509(3)
Z	2

ρ_{calc} [gcm^{-3}]	2.369
μ [mm^{-1}]	1.728
F(000)	2372
Crystal size [mm^3]	0.24×0.15×0.05
Crystal colour	red
Crystal shape	needle
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.29 to 66.43 (0.65 Å)
Index ranges	-18 ≤ h ≤ 19
	-19 ≤ k ≤ 18
	-35 ≤ l ≤ 35
Reflections collected	206219
Independent reflections	26616
	R_{int} = 0.0858
	R_{sigma} = 0.0574
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	26616/7259/1444
Goodness-of-fit on F^2	1.070
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0495
	wR_2 = 0.0955
Final *R* indexes [all data]	R_1 = 0.0723
	wR_2 = 0.1053
Largest peak/hole [eÅ^{-3}]	1.15/-2.02

$[Ag\{Os_3(CO)_{12}\}_2]^+[F\{Al(OR^F)_3\}_2]^-\cdot 1.5\ C_6F_4H_2$

Table S 14: Crystal data and structure refinement for $[Ag\{Os_3(CO)_{12}\}_2]^+[F\{Al(OR^F)_3\}_2]^-\cdot 1.5\ C_6F_4H_2$.

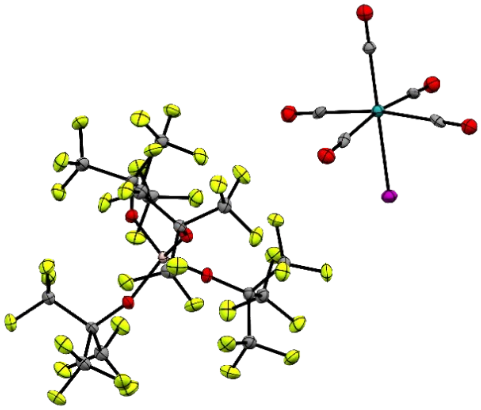
CCDC number	2151840
Empirical formula	$C_{57}H_3AgAl_2F_{61}O_{30}Os_6$
Formula weight	3629.62
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	20.504(4)
b [Å]	17.810(3)
c [Å]	25.217(8)
α [°]	90
β [°]	107.09(2)
γ [°]	90
Volume [Å^3]	8802(4)
Z	4
ρ_{calc} [gcm^{-3}]	2.739
μ [mm^{-1}]	9.070
F(000)	6652
Crystal size [mm^3]	0.14×0.12×0.05
Crystal colour	colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)



2Θ range [°]	2.84 to 54.29 (0.78 Å)
Index ranges	-26 ≤ h ≤ 26
	-22 ≤ k ≤ 22
	-32 ≤ l ≤ 31
Reflections collected	158056
Independent reflections	19471
	R_{int} = 0.0589
	R_{sigma} = 0.0323
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	19471/27525/2368
Goodness-of-fit on F^2	1.124
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0420
	wR_2 = 0.0881
Final *R* indexes [all data]	R_1 = 0.0587
	wR_2 = 0.0965
Largest peak/hole [eÅ^{-3}]	1.52/-1.93

$[Ru(CO)_5I]^+[Al(OR^F)_4]^-$

Table S 15: Crystal data and structure refinement for $[Ru(CO)_5I]^{+}[Al(OR^F)_4]^-$.

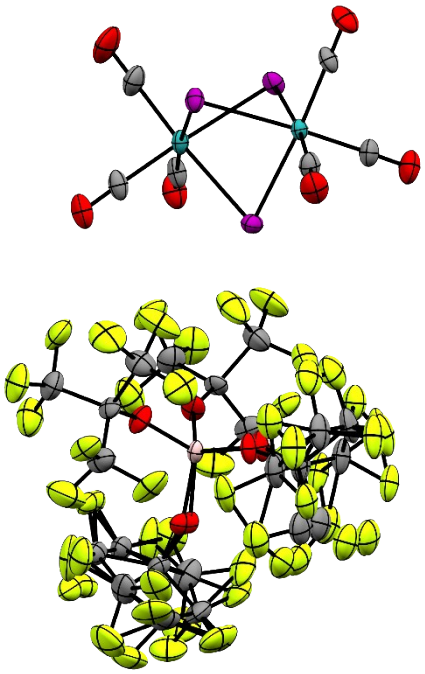


CCDC number	2151510
Empirical formula	$C_{21}AlF_{36}IO_9Ru$
Formula weight	1335.16
Temperature [K]	100(2)
Crystal system	tetragonal
Space group (number)	$P4/n$ (85)
a [Å]	13.7680(16)
b [Å]	13.7680(16)
c [Å]	9.5388(12)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	1808.2(5)
Z	2
ρ_{calc} [gcm^{-3}]	2.452
μ [mm^{-1}]	1.547
F(000)	1264
Crystal size [mm^3]	0.18×0.10×0.05
Crystal colour	yellow
Crystal shape	needle
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.96 to 63.05 (0.68 Å)
Index ranges	-20 ≤ h ≤ 20
	-20 ≤ k ≤ 20
	-13 ≤ l ≤ 14
Reflections collected	134767
Independent reflections	3025
	R_{int} = 0.0816
	R_{sigma} = 0.0163
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	3025/306/160
Goodness-of-fit on F^2	1.073
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0250
	wR_2 = 0.0648
Final *R* indexes [all data]	R_1 = 0.0288
	wR_2 = 0.0676
Largest peak/hole [eÅ^{-3}]	0.84/-0.98

$[Ru_2(CO)_6I_3]^+[Al(OR^F)_4]^-$

Table S 16: Crystal data and structure refinement for $[Ru_2(CO)_6I_3]^+[Al(OR^F)_4]^-$.

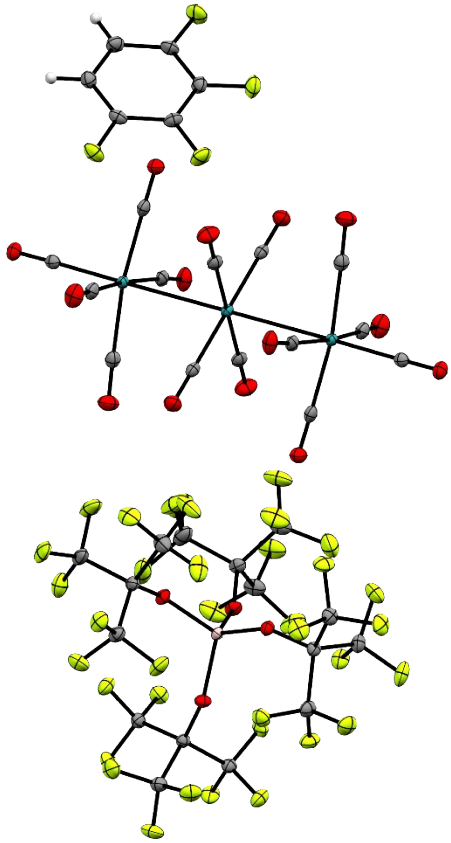
CCDC number	2153977
Empirical formula	$C_{22}AlF_{36}I_3O_{10}Ru_2$
Formula weight	1718.04
Temperature [K]	109(2)
Crystal system	orthorhombic
Space group (number)	$Pnma$ (62)
a [Å]	18.581(3)
b [Å]	13.756(2)
c [Å]	16.816(3)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	4298.3(13)
Z	4
ρ_{calc} [gcm^{-3}]	2.655
μ [mm^{-1}]	3.083
F(000)	3184
Crystal size [mm^3]	0.11×0.09×0.07
Crystal colour	yellow
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.27 to 66.40 (0.65 Å)
Index ranges	-27 ≤ h ≤ 28 -19 ≤ k ≤ 21 -25 ≤ l ≤ 25
Reflections collected	182411
Independent reflections	8508 R_{int} = 0.0509 R_{sigma} = 0.0179
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	8508/12323/1110
Goodness-of-fit on F^2	1.193
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0528 wR_2 = 0.1077
Final *R* indexes [all data]	R_1 = 0.0604 wR_2 = 0.1107
Largest peak/hole [eÅ^{-3}]	1.51/-1.51



$[Ru_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$

Table S 17: Crystal data and structure refinement $[Ru_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$.

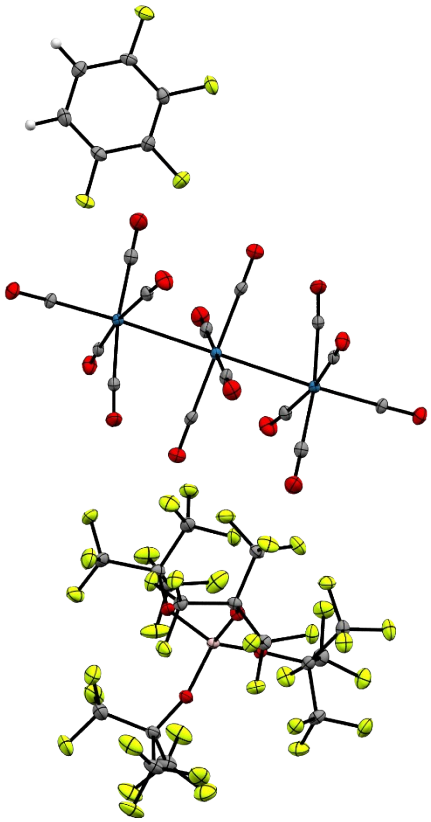
CCDC number	2150901
Empirical formula	$C_{58}H_4Al_2F_{80}O_{22}Ru_3$
Formula weight	2929.78
Temperature [K]	106(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	11.298(4)
b [Å]	14.164(6)
c [Å]	15.698(5)
α [°]	71.621(10)
β [°]	71.685(18)
γ [°]	73.388(12)
Volume [Å^3]	2213.9(14)
Z	1
ρ_{calc} [gcm^{-3}]	2.197
μ [mm^{-1}]	0.763
F(000)	1406
Crystal size [mm^3]	0.12×0.11×0.07
Crystal colour	colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.82 to 56.73 (0.75 Å)
Index ranges	-15 ≤ h ≤ 15
	-18 ≤ k ≤ 18
	-20 ≤ l ≤ 20
Reflections collected	201036
Independent reflections	11068
	R_{int} = 0.0544
	R_{sigma} = 0.0155
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	11068/0/745
Goodness-of-fit on F^2	1.017
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0192
	wR_2 = 0.0453
Final *R* indexes [all data]	R_1 = 0.0217
	wR_2 = 0.0463
Largest peak/hole [eÅ^{-3}]	0.49/-0.55



$[Os_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$

Table S 18: Crystal data and structure refinement $[Os_3(CO)_{14}]^{2+}[Al(OR^F)_4]^-_2 \cdot 2\ C_6F_4H_2$.

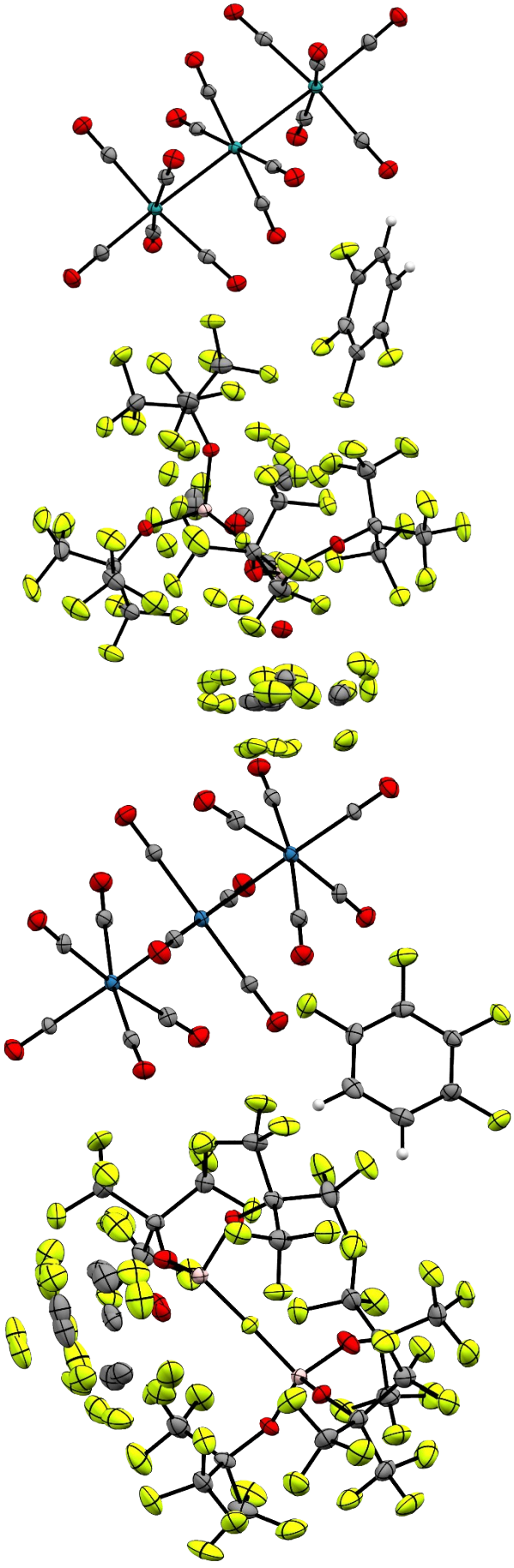
CCDC number	2150925
Empirical formula	$C_{58}H_4Al_2F_{80}O_{22}Os_3$
Formula weight	152.25
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.283(3)
b [Å]	14.143(3)
c [Å]	15.714(3)
α [°]	71.674(9)
β [°]	71.730(7)
γ [°]	73.486(9)
Volume [Å^3]	2211.8(8)
Z	1
ρ_{calc} [gcm^{-3}]	2.400
μ [mm^{-1}]	4.556
F(000)	1502
Crystal size [mm^3]	0.252×0.081×0.029
Crystal colour	colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.82 to 61.30 (0.70 Å)
Index ranges	-15 ≤ h ≤ 16
	-18 ≤ k ≤ 20
	0 ≤ l ≤ 22
Reflections collected	13532
Independent reflections	13532
	R_{int} = 0.0544
	R_{sigma} = 0.0526
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	13532/3053/745
Goodness-of-fit on F^2	1.000
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0411
	wR_2 = 0.0665
Final *R* indexes [all data]	R_1 = 0.0604
	wR_2 = 0.0713
Largest peak/hole [eÅ^{-3}]	1.19/-2.39



$[Ru_3(CO)_{14}]^{2+}[F\{Al(OR^F)_3\}_2]^-_2 \cdot C_6F_4H_2$

Table S 19: Crystal data and structure refinement $[Ru_3(CO)_{14}]^{2+}[F\{Al(OR^F)_3\}_2]^-_2 \cdot C_6F_4H_2$.

CCDC number	2159967
Empirical formula	$C_{68}H_2Al_4F_{114}O_{26}Ru_3$
Formula weight	3811.83
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	11.819(3)
b [Å]	12.940(3)
c [Å]	19.477(5)
α [°]	102.636(12)
β [°]	103.912(17)
γ [°]	92.736(17)
Volume [Å^3]	2805.5(12)
Z	1
ρ_{calc} [gcm^{-3}]	2.256
μ [mm^{-1}]	0.689
F(000)	1828
Crystal size [mm^3]	0.231×0.134×0.115
Crystal colour	colourless
Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.24 to 64.21 (0.67 Å)
Index ranges	-17 ≤ h ≤ 17 -19 ≤ k ≤ 19 -29 ≤ l ≤ 28
Reflections collected	227209
Independent reflections	19545 R_{int} = 0.0779 R_{sigma} = 0.0343
Completeness to Θ = 25.242°	99.1 %
Data / Restraints / Parameters	19545/10839/1265
Goodness-of-fit on F^2	1.032
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0382 wR_2 = 0.0869
Final *R* indexes [all data]	R_1 = 0.0513 wR_2 = 0.0962
Largest peak/hole [eÅ^{-3}]	0.88/-0.81



$[Os_3(CO)_{14}]^{2+}[F\{Al(OR^F)_3\}_2]^-_2 \cdot C_6F_4H_2$

Table S 20: Crystal data and structure refinement $[Os_3(CO)_{14}]^{2+}[F\{Al(OR^F)_3\}_2]^-_2 \cdot C_6F_4H_2$.

CCDC number	2151836
Empirical formula	$C_{68}H_2Al_4F_{114}O_{26}Os_3$
Formula weight	4079.22
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	11.810(4)
b [Å]	12.939(2)
c [Å]	19.507(5)
α [°]	102.689(9)
β [°]	103.941(14)
γ [°]	92.667(9)
Volume [Å^3]	2806.9(13)
Z	1
ρ_{calc} [gcm^{-3}]	2.413
μ [mm^{-1}]	3.677
F(000)	1924
Crystal size [mm^3]	0.103×0.080×0.071
Crystal colour	white
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.24 to 64.18 (0.67 Å)
Index ranges	-15 ≤ h ≤ 17
	-19 ≤ k ≤ 19
	-29 ≤ l ≤ 28
Reflections collected	86130
Independent reflections	19196
	R_{int} = 0.0673
	R_{sigma} = 0.0590
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	19196/8318/1142
Goodness-of-fit on F^2	1.003
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0415
	wR_2 = 0.0901
Final *R* indexes [all data]	R_1 = 0.0672
	wR_2 = 0.1020
Largest peak/hole [eÅ^{-3}]	2.00/-2.13

15. DFT

$[NRu_4(CO)_{12}(\mu_2\text{-}NO)]^+$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

N	0.1055038	0.6716612	0.3803071
C	2.1827995	2.4394233	-1.0973169
O	-1.6463413	0.9431299	4.0361398
Ru	-0.6168509	0.2073810	-1.5961090
O	2.3327399	3.4774906	-1.5306034
Ru	0.4324857	-1.3849855	0.9307298
Ru	-1.6940651	0.5101912	1.0251659
O	2.9012629	-3.1773637	0.5146872
O	-3.4637628	-0.4503456	-2.5673319
Ru	1.8864146	0.7179888	-0.3304804
O	3.9922525	-0.6760052	-2.0940926
C	1.9997650	-2.5072495	0.6632567
C	-2.5975498	2.1599007	0.7078924
C	-0.8735504	2.0509467	-1.9838240
O	1.4216143	-0.5489225	3.6743691
C	3.1031674	1.0426529	1.1024579
O	-3.1024272	3.1585372	0.5190005
O	-4.2820071	-1.1596723	1.0428770
O	-1.0214982	3.1527721	-2.2005825
C	-3.3583513	-0.5023054	1.0757905
O	3.8002397	1.2508697	1.9734253
C	-1.6835413	0.7694952	2.9152889
C	1.0539760	-0.8703373	2.6524100
C	-2.4210215	-0.2042205	-2.1986839
C	3.2601545	-0.1165560	-1.4327790
N	-0.2864917	-1.8128191	-1.0231320
O	-0.4471039	-2.8112561	-1.5856969
O	-1.4970116	-3.4334444	2.1799133
C	-0.7956492	-2.6701454	1.7224622
O	0.9376086	-0.1886571	-4.2243928
C	0.3772388	-0.0381548	-3.2511487

SCF energy GEOOPT = -1924.433691867 H

$[NRu_4(CO)_{12}(\mu_2\text{-}CO)]^+$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: cs

Cartesian coordinates in Ångström:

N	0.3063936	-0.7836687	0.0000000
C	-0.6092413	-2.2813562	2.5924277
O	3.0142188	-1.7315061	-2.7752733
Ru	-1.6204877	0.2199349	0.0000000
O	-1.1352551	-3.2203300	2.9519239
Ru	1.1447010	1.0957348	0.0000000
Ru	0.2850068	-0.7218109	-1.9305131
O	1.6118789	3.0270784	2.3597964
O	-3.2969712	0.8461951	-2.5158691
Ru	0.2850068	-0.7218109	1.9305131
O	-0.1663324	0.9083282	4.5052114
C	1.4309912	2.3037482	1.5056728
C	-0.6092413	-2.2813562	-2.5924277
C	-2.3966692	-1.5866970	0.0000000
O	4.0344598	0.2758713	0.0000000
C	1.9849795	-1.3513834	2.4864827
O	-1.1352551	-3.2203300	-2.9519239
O	-0.1663324	0.9083282	-4.5052114
O	-2.8653498	-2.6121268	0.0000000
C	0.0149839	0.2671907	-3.5883642
O	3.0142188	-1.7315061	2.7752733
C	1.9849795	-1.3513834	-2.4864827
C	2.9488240	0.6082322	0.0000000
C	-2.6541599	0.6157062	-1.6116296
C	0.0149839	0.2671907	3.5883642
C	-1.1893576	2.1659620	0.0000000

O	-1.3350526	3.2932790	0.0000000
O	1.6118789	3.0270784	-2.3597964
C	1.4309912	2.3037482	-1.5056728
O	-3.2969712	0.8461951	2.5158691
C	-2.6541599	0.6157062	1.6116296

SCF energy GEOOPT = -1907.864596087 H
ZPE = 304.9 kJ/mol
FREEH energy = 402.75 kJ/mol
FREEH entropy = 0.98869 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a"	30.28	0.00372	YES	YES
8	a"	33.88	0.00017	YES	YES
9	a'	37.00	0.00763	YES	YES
10	a'	39.13	0.08426	YES	YES
11	a"	47.83	0.09296	YES	YES
12	a"	58.27	0.43180	YES	YES
13	a'	62.02	0.15351	YES	YES
14	a'	64.88	0.51978	YES	YES
15	a"	67.15	0.35152	YES	YES
16	a'	69.47	0.08997	YES	YES
17	a"	71.46	0.12201	YES	YES
18	a"	77.78	0.00891	YES	YES
19	a'	78.16	0.20635	YES	YES
20	a'	79.64	0.11887	YES	YES
21	a"	80.19	0.12092	YES	YES
22	a'	83.10	0.24152	YES	YES
23	a"	86.70	0.90054	YES	YES
24	a'	90.34	0.28086	YES	YES
25	a"	90.82	0.06019	YES	YES
26	a'	91.83	0.02545	YES	YES
27	a'	93.65	0.21807	YES	YES
28	a"	95.42	0.03486	YES	YES
29	a"	95.70	0.51591	YES	YES
30	a'	96.92	0.04071	YES	YES
31	a"	99.92	0.00469	YES	YES
32	a'	123.27	0.15035	YES	YES
33	a'	136.02	0.20988	YES	YES
34	a"	139.11	0.03435	YES	YES
35	a'	165.49	0.09800	YES	YES
36	a'	171.00	1.04472	YES	YES
37	a"	174.44	17.41513	YES	YES
38	a'	236.34	0.33566	YES	YES
39	a'	347.79	10.24511	YES	YES
40	a"	360.64	0.35731	YES	YES
41	a"	372.46	11.28255	YES	YES
42	a'	374.77	18.92598	YES	YES
43	a"	382.34	11.92759	YES	YES
44	a'	385.67	5.98985	YES	YES
45	a'	406.47	13.54368	YES	YES
46	a"	406.93	0.51164	YES	YES
47	a'	410.54	6.36984	YES	YES
48	a"	410.75	11.81746	YES	YES
49	a"	414.22	0.29505	YES	YES
50	a'	415.66	18.85549	YES	YES
51	a'	421.21	3.31206	YES	YES
52	a"	423.43	2.28290	YES	YES
53	a'	426.31	13.44826	YES	YES
54	a"	427.99	2.22129	YES	YES
55	a'	431.37	12.91427	YES	YES
56	a"	440.00	0.32171	YES	YES
57	a'	450.32	2.38129	YES	YES
58	a"	451.70	3.63590	YES	YES
59	a'	452.40	1.56069	YES	YES
60	a"	452.84	1.98399	YES	YES
61	a'	461.19	2.05016	YES	YES
62	a"	467.22	14.79884	YES	YES

63	a'	470.54	6.01843	YES	YES
64	a'	477.09	13.17981	YES	YES
65	a'	514.92	70.78085	YES	YES
66	a"	516.78	0.04633	YES	YES
67	a'	534.96	14.76025	YES	YES
68	a"	539.64	38.25460	YES	YES
69	a'	542.19	13.97641	YES	YES
70	a'	546.48	11.82843	YES	YES
71	a"	550.74	19.93350	YES	YES
72	a"	567.24	28.06113	YES	YES
73	a"	575.78	110.93215	YES	YES
74	a'	576.28	266.49017	YES	YES
75	a"	583.72	48.58028	YES	YES
76	a'	583.85	74.85025	YES	YES
77	a'	594.68	52.25314	YES	YES
78	a'	598.17	12.62312	YES	YES
79	a'	634.66	117.39948	YES	YES
80	a"	811.92	16.85133	YES	YES
81	a'	2096.55	109.70101	YES	YES
82	a'	2106.06	233.89288	YES	YES
83	a"	2107.46	6.03749	YES	YES
84	a"	2111.68	7.29919	YES	YES
85	a'	2112.80	358.00531	YES	YES
86	a'	2127.96	501.73344	YES	YES
87	a"	2128.10	18.80426	YES	YES
88	a"	2133.31	307.10137	YES	YES
89	a'	2148.36	1434.55358	YES	YES
90	a'	2154.87	1351.48678	YES	YES
91	a"	2170.78	2102.79688	YES	YES
92	a'	2181.77	975.32180	YES	YES
93	a'	2210.76	162.65827	YES	YES

$Ru(CO)_5$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: d3h

Cartesian coordinates in Ångström:

Ru	-0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.9546691
C	0.0000000	0.0000000	-1.9546691
C	0.9788860	-1.6954802	0.0000000
C	0.9788860	1.6954802	0.0000000
C	-1.9577719	0.0000000	0.0000000
O	1.5490571	-2.6830457	0.0000000
O	0.0000000	0.0000000	3.0900179
O	0.0000000	0.0000000	-3.0900179
O	1.5490571	2.6830457	0.0000000
O	-3.0981143	0.0000000	0.0000000

SCF energy GEOOPT = -661.6659126117 H
ZPE = 106.3 kJ/mol
FREEH energy = 139.02 kJ/mol
FREEH entropy = 0.46596 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e'	42.98	0.15783	YES	YES
8	e'	42.98	0.15783	YES	YES
9	e"	84.97	0.00000	NO	YES
10	e"	84.97	0.00000	NO	YES
11	a2"	87.76	0.69532	YES	NO
12	e'	90.19	0.08748	YES	YES
13	e'	90.19	0.08748	YES	YES
14	e"	332.77	0.00000	NO	YES
15	e"	332.77	0.00000	NO	YES
16	a2'	338.83	0.00000	NO	NO
17	e'	372.41	48.52942	YES	YES

```
    18        e'            372.41        48.52942       YES     YES
    19        a2"           405.18        28.44086       YES     NO
    20        a1'           418.08         0.00000       NO      YES
    21        e'            449.70         0.32464       YES     YES
    22        e'            449.70         0.32464       YES     YES
    23        a1'           451.47         0.00000       NO      YES
    24        e"            509.98         0.00000       NO      YES
    25        e"            509.98         0.00000       NO      YES
    26        a2"           541.17       112.43898       YES     NO
    27        e'            616.12       113.15155       YES     YES
    28        e'            616.12       113.15155       YES     YES
    29        e'           2070.70      1305.48032       YES     YES
    30        e'           2070.70      1305.48032       YES     YES
    31        a1'          2097.55         0.00000       NO      YES
    32        a2"          2107.17      1460.88685       YES     NO
    33        a1'          2187.76         0.00000       NO      YES
$end
$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.           a.u.        bohr**2/sr
#                                                                T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    e'     42.98   YES       -0.000000     0.054761 0.34018D-13 0.25514D-13
    8    e'     42.98   YES       -0.000000     0.054761 0.34018D-13 0.25514D-13
    9    e"     84.97   YES        0.000000     0.087405 0.23976D-13 0.17982D-13
   10    e"     84.97   YES        0.000000     0.087405 0.23976D-13 0.17982D-13
   11    a2"    87.76   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   12    e'     90.19   YES       -0.000000     0.043992 0.54422D-14 0.40816D-14
   13    e'     90.19   YES       -0.000000     0.043992 0.54422D-14 0.40816D-14
   14    e"    332.77   YES        0.000000     0.011880 0.42732D-16 0.32049D-16
   15    e"    332.77   YES        0.000000     0.011880 0.42732D-16 0.32049D-16
   16    a2'   338.83   NO         0.000000     0.000000 0.11959D-34 0.89689D-35
   17    e'    372.41   YES       -0.000000     0.024808 0.15675D-15 0.11756D-15
   18    e'    372.41   YES       -0.000000     0.024808 0.15675D-15 0.11756D-15
   19    a2"   405.18   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   20    a1'   418.08   YES        0.052936     0.046134 0.71987D-14 0.34145D-15
   21    e'    449.70   YES       -0.000000     0.035107 0.23654D-15 0.17741D-15
   22    e'    449.70   YES       -0.000000     0.035107 0.23654D-15 0.17741D-15
   23    a1'   451.47   YES        0.054861     0.058458 0.71125D-14 0.48903D-15
   24    e"    509.98   YES        0.000000     0.017682 0.49879D-16 0.37409D-16
   25    e"    509.98   YES        0.000000     0.017682 0.49879D-16 0.37409D-16
   26    a2"   541.17   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   27    e'    616.12   YES        0.000000     0.007716 0.72218D-17 0.54163D-17
   28    e'    616.12   YES       -0.000000     0.007716 0.72218D-17 0.54163D-17
   29    e'   2070.70   YES        0.000000     0.316402 0.16619D-14 0.12464D-14
   30    e'   2070.70   YES        0.000000     0.316402 0.16619D-14 0.12464D-14
   31    a1'  2097.55   YES        0.034091     0.465470 0.37100D-14 0.26242D-14
   32    a2"  2107.17   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   33    a1'  2187.76   YES       -0.111721     0.205014 0.26878D-14 0.46439D-15
```

$Os(CO)_5$

```
Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: d3h

Cartesian coordinates in Ångström:
Os   -0.0000000    0.0000000   -0.0000000
C     0.0000000    0.0000000    1.9767761
C     0.0000000    0.0000000   -1.9767761
C     0.9821736   -1.7011745    0.0000000
C     0.9821736    1.7011745    0.0000000
C    -1.9643472    0.0000000    0.0000000
O     1.5535885   -2.6908941    0.0000000
O     0.0000000    0.0000000    3.1132914
O     0.0000000    0.0000000   -3.1132914
O     1.5535885    2.6908941    0.0000000
O    -3.1071769    0.0000000    0.0000000
```

SCF energy GEOOPT = -657.4622115622 H
ZPE =   107.2 kJ/mol
FREEH energy =   139.41 kJ/mol
FREEH entropy =   0.46775 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e'	40.29	0.26200	YES	YES
8	e'	40.29	0.26200	YES	YES
9	e"	87.47	0.00000	NO	YES
10	e"	87.47	0.00000	NO	YES
11	a2"	88.46	0.41107	YES	NO
12	e'	88.66	0.00386	YES	YES
13	e'	88.66	0.00386	YES	YES
14	e"	354.50	0.00000	NO	YES
15	e"	354.50	0.00000	NO	YES
16	a2'	371.34	0.00000	NO	NO
17	e'	395.98	63.41617	YES	YES
18	e'	395.98	63.41617	YES	YES
19	a2"	400.89	47.23878	YES	NO
20	e'	454.36	0.16832	YES	YES
21	e'	454.36	0.16832	YES	YES
22	a1'	456.17	0.00000	NO	YES
23	a1'	478.15	0.00000	NO	YES
24	e"	510.52	0.00000	NO	YES
25	e"	510.52	0.00000	NO	YES
26	a2"	554.08	97.30998	YES	NO
27	e'	605.70	95.81025	YES	YES
28	e'	605.70	95.81025	YES	YES
29	e'	2059.18	1387.10787	YES	YES
30	e'	2059.18	1387.10787	YES	YES
31	a1'	2089.42	0.00000	NO	YES
32	a2"	2102.11	1546.03946	YES	NO
33	a1'	2186.83	0.00000	NO	YES

$end
$raman spectrum

# mode	symmetry	wave number cm**(-1)	selection rule	derivative of isotropic polarizability a.u.	derivative of polarizability anisotropy a.u.	raman scattering cross sections bohr**2/sr T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
7	e'	40.29	YES	0.000000	0.054767	0.38523D-13	0.28892D-13
8	e'	40.29	YES	0.000000	0.054767	0.38523D-13	0.28892D-13
9	e"	87.47	YES	0.000000	0.089854	0.24019D-13	0.18014D-13
10	e"	87.47	YES	0.000000	0.089854	0.24019D-13	0.18014D-13
11	a2"	88.46	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
12	e'	88.66	YES	-0.000000	0.043554	0.55048D-14	0.41286D-14
13	e'	88.66	YES	-0.000000	0.043554	0.55048D-14	0.41286D-14
14	e"	354.50	YES	0.000000	0.000123	0.41282D-20	0.30961D-20
15	e"	354.50	YES	0.000000	0.000123	0.41282D-20	0.30961D-20
16	a2'	371.34	NO	0.000000	0.000000	0.17011D-34	0.12759D-34
17	e'	395.98	YES	-0.000000	0.045506	0.48061D-15	0.36046D-15
18	e'	395.98	YES	-0.000000	0.045506	0.48061D-15	0.36046D-15
19	a2"	400.89	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
20	e'	454.36	YES	0.000000	0.036956	0.25813D-15	0.19360D-15
21	e'	454.36	YES	-0.000000	0.036956	0.25813D-15	0.19360D-15
22	a1'	456.17	YES	0.045020	0.060166	0.49647D-14	0.51015D-15
23	a1'	478.15	YES	0.064982	0.055388	0.88660D-14	0.40338D-15
24	e"	510.52	YES	0.000000	0.006979	0.77590D-17	0.58193D-17
25	e"	510.52	YES	0.000000	0.006979	0.77590D-17	0.58193D-17
26	a2"	554.08	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
27	e'	605.70	YES	-0.000000	0.007455	0.69093D-17	0.51820D-17
28	e'	605.70	YES	-0.000000	0.007455	0.69093D-17	0.51820D-17

29	e'	2059.18	YES	-0.000000	0.287554	0.13890D-14	0.10418D-14
30	e'	2059.18	YES	-0.000000	0.287554	0.13890D-14	0.10418D-14
31	a1'	2089.42	YES	0.034813	0.450214	0.35227D-14	0.24755D-14
32	a2"	2102.11	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
33	a1'	2186.83	YES	-0.113261	0.210224	0.27797D-14	0.48876D-15

$[Ru_3(CO)_{14}]^{2+}$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: d4h

Cartesian coordinates in Ångström:

Ru	0.0000000	0.0000000	-2.9715497
Ru	-0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	-6.0802738
O	2.1926223	-2.1926223	-2.7420687
O	3.0914122	0.0000000	0.0000000
O	-2.1926223	-2.1926223	-2.7420687
O	2.1926223	2.1926223	-2.7420687
C	1.9600803	-0.0000000	0.0000000
O	-2.1926223	2.1926223	-2.7420687
C	-0.0000000	-1.9600803	0.0000000
O	0.0000000	-3.0914122	0.0000000
C	1.3989130	-1.3989130	-2.8258967
C	0.0000000	0.0000000	-4.9570337
C	-1.3989130	1.3989130	-2.8258967
C	-1.3989130	-1.3989130	-2.8258967
C	1.3989130	1.3989130	-2.8258967
Ru	0.0000000	0.0000000	2.9715497
O	0.0000000	0.0000000	6.0802738
O	-2.1926223	2.1926223	2.7420687
O	-3.0914122	0.0000000	0.0000000
O	2.1926223	2.1926223	2.7420687
O	-2.1926223	-2.1926223	2.7420687
C	-1.9600803	0.0000000	0.0000000
O	2.1926223	-2.1926223	2.7420687
C	0.0000000	1.9600803	0.0000000
O	0.0000000	3.0914122	0.0000000
C	-1.3989130	1.3989130	2.8258967
C	0.0000000	0.0000000	4.9570337
C	1.3989130	-1.3989130	2.8258967
C	1.3989130	1.3989130	2.8258967
C	-1.3989130	-1.3989130	2.8258967

SCF energy GEOOPT = -1871.141115223 H
ZPE = 314.5 kJ/mol
FREEH energy = 413.57 kJ/mol
FREEH entropy = 0.98279 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a1u	24.17	0.00000	NO	NO
8	eu	34.82	0.09321	YES	NO
9	eu	34.82	0.09321	YES	NO
10	a2g	41.38	0.00000	NO	NO
11	eg	52.27	0.00000	NO	YES
12	eg	52.27	0.00000	NO	YES
13	eu	63.40	0.74643	YES	NO
14	eu	63.40	0.74643	YES	NO
15	b2u	73.81	0.00000	NO	NO
16	b2g	74.65	0.00000	NO	YES
17	eg	75.56	0.00000	NO	YES
18	eg	75.56	0.00000	NO	YES
19	b1u	76.80	0.00000	NO	NO
20	a1g	84.39	0.00000	NO	YES
21	eu	86.72	0.72623	YES	NO
22	eu	86.72	0.72623	YES	NO
23	eu	92.99	0.33714	YES	NO

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    24        eu             92.99         0.33714       YES     NO
    25        eg             93.09         0.00000       NO      YES
    26        eg             93.09         0.00000       NO      YES
    27        b1g            93.27         0.00000       NO      YES
    28        b2u            94.85         0.00000       NO      NO
    29        b2g            95.66         0.00000       NO      YES
    30        a2u            97.18         1.57554       YES     NO
    31        eg             99.38         0.00000       NO      YES
    32        eg             99.38         0.00000       NO      YES
    33        eu            100.70         0.43283       YES     NO
    34        eu            100.70         0.43283       YES     NO
    35        a2u           106.24         6.54365       YES     NO
    36        a1g           142.48         0.00000       NO      YES
    37        a2u           174.98         0.00139       YES     NO
    38        a2g           350.26         0.00000       NO      NO
    39        a1u           350.41         0.00000       NO      NO
    40        a2g           361.40         0.00000       NO      NO
    41        eg            361.77         0.00000       NO      YES
    42        eg            361.77         0.00000       NO      YES
    43        eu            362.16        18.47424       YES     NO
    44        eu            362.16        18.47424       YES     NO
    45        a2u           380.95         5.92914       YES     NO
    46        eu            381.18        45.14729       YES     NO
    47        eu            381.18        45.14729       YES     NO
    48        a1g           382.69         0.00000       NO      YES
    49        eg            384.42         0.00000       NO      YES
    50        eg            384.42         0.00000       NO      YES
    51        eu            386.27        18.54243       YES     NO
    52        eu            386.27        18.54243       YES     NO
    53        b1u           411.51         0.00000       NO      NO
    54        b2g           411.91         0.00000       NO      YES
    55        a2u           421.61        34.43429       YES     NO
    56        a1g           423.80         0.00000       NO      YES
    57        b1g           433.18         0.00000       NO      YES
    58        a1g           443.54         0.00000       NO      YES
    59        eg            451.33         0.00000       NO      YES
    60        eg            451.33         0.00000       NO      YES
    61        b2g           462.95         0.00000       NO      YES
    62        b1u           464.23         0.00000       NO      NO
    63        b2u           494.96         0.00000       NO      NO
    64        eu            495.22        22.65124       YES     NO
    65        eu            495.22        22.65124       YES     NO
    66        eg            499.57         0.00000       NO      YES
    67        eg            499.57         0.00000       NO      YES
    68        b1g           501.82         0.00000       NO      YES
    69        b2u           502.28         0.00000       NO      NO
    70        b2g           515.85         0.00000       NO      YES
    71        eg            584.69         0.00000       NO      YES
    72        eg            584.69         0.00000       NO      YES
    73        eu            584.84        79.91601       YES     NO
    74        eu            584.84        79.91601       YES     NO
    75        a2u           590.27       976.09580       YES     NO
    76        eu            600.44        53.28793       YES     NO
    77        eu            600.44        53.28793       YES     NO
    78        a1g           612.41         0.00000       NO      YES
    79        a2u           637.13        49.91096       YES     NO
    80        eu           2125.54       321.10794       YES     NO
    81        eu           2125.54       321.10794       YES     NO
    82        b1g          2158.01         0.00000       NO      YES
    83        a1g          2180.08         0.00000       NO      YES
    84        eg           2180.85         0.00000       NO      YES
    85        eg           2180.85         0.00000       NO      YES
    86        eu           2188.94      1884.25428       YES     NO
    87        eu           2188.94      1884.25428       YES     NO
    88        b1u          2201.68         0.00000       NO      NO
    89        b2g          2203.56         0.00000       NO      YES
    90        a2u          2206.62       234.37572       YES     NO
    91        a1g          2214.13         0.00000       NO      YES
    92        a2u          2243.22      1342.01810       YES     NO
    93        a1g          2267.28         0.00000       NO      YES
$end
$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.          a.u.        bohr**2/sr
```

#						T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
7	a1u	24.17	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
8	eu	34.82	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
9	eu	34.82	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
10	a2g	41.38	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
11	eg	52.27	YES	0.000000	0.053347	0.22215D-13	0.16661D-13
12	eg	52.27	YES	0.000000	0.053347	0.22215D-13	0.16661D-13
13	eu	63.40	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
14	eu	63.40	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
15	b2u	73.81	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
16	b2g	74.65	YES	0.000000	0.032620	0.42456D-14	0.31842D-14
17	eg	75.56	YES	0.000000	0.087250	0.29696D-13	0.22272D-13
18	eg	75.56	YES	0.000000	0.087250	0.29696D-13	0.22272D-13
19	b1u	76.80	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
20	a1g	84.39	YES	0.050300	0.103428	0.12446D-12	0.25499D-13
21	eu	86.72	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
22	eu	86.72	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
23	eu	92.99	NO	0.000000	0.000000	0.10404D-32	0.78029D-33
24	eu	92.99	NO	0.000000	0.000000	0.12754D-32	0.95655D-33
25	eg	93.09	YES	0.000000	0.025807	0.17672D-14	0.13254D-14
26	eg	93.09	YES	0.000000	0.025807	0.17672D-14	0.13254D-14
27	b1g	93.27	YES	0.000000	0.091404	0.22090D-13	0.16568D-13
28	b2u	94.85	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
29	b2g	95.66	YES	0.000000	0.052235	0.68879D-14	0.51659D-14
30	a2u	97.18	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
31	eg	99.38	YES	0.000000	0.044894	0.47458D-14	0.35593D-14
32	eg	99.38	YES	0.000000	0.044894	0.47458D-14	0.35593D-14
33	eu	100.70	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
34	eu	100.70	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
35	a2u	106.24	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
36	a1g	142.48	YES	-0.049066	0.155997	0.63513D-13	0.22544D-13
37	a2u	174.98	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
38	a2g	350.26	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
39	a1u	350.41	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
40	a2g	361.40	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
41	eg	361.77	YES	0.000000	0.005394	0.77445D-17	0.58084D-17
42	eg	361.77	YES	0.000000	0.005394	0.77445D-17	0.58084D-17
43	eu	362.16	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
44	eu	362.16	NO	0.000000	0.000000	0.30370D-35	0.22777D-35
45	a2u	380.95	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
46	eu	381.18	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
47	eu	381.18	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
48	a1g	382.69	YES	-0.041851	0.157110	0.10847D-13	0.45240D-14
49	eg	384.42	YES	0.000000	0.049991	0.60656D-15	0.45492D-15
50	eg	384.42	YES	0.000000	0.049991	0.60656D-15	0.45492D-15
51	eu	386.27	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
52	eu	386.27	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
53	b1u	411.51	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
54	b2g	411.91	YES	0.000000	0.051442	0.57880D-15	0.43410D-15
55	a2u	421.61	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
56	a1g	423.80	YES	-0.078056	0.050425	0.14900D-13	0.39972D-15
57	b1g	433.18	YES	0.000000	0.051170	0.53122D-15	0.39841D-15
58	a1g	443.54	YES	0.088181	0.055767	0.17744D-13	0.45688D-15
59	eg	451.33	YES	0.000000	0.035091	0.23506D-15	0.17630D-15
60	eg	451.33	YES	0.000000	0.035091	0.23506D-15	0.17630D-15
61	b2g	462.95	YES	0.000000	0.034481	0.21859D-15	0.16394D-15
62	b1u	464.23	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
63	b2u	494.96	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
64	eu	495.22	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
65	eu	495.22	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
66	eg	499.57	YES	0.000000	0.073804	0.89554D-15	0.67165D-15
67	eg	499.57	YES	0.000000	0.073804	0.89554D-15	0.67165D-15
68	b1g	501.82	YES	0.000000	0.006384	0.66564D-17	0.49923D-17
69	b2u	502.28	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
70	b2g	515.85	YES	0.000000	0.008379	0.11015D-16	0.82612D-17
71	eg	584.69	YES	0.000000	0.007144	0.66772D-17	0.50079D-17
72	eg	584.69	YES	0.000000	0.007144	0.66772D-17	0.50079D-17
73	eu	584.84	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
74	eu	584.84	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
75	a2u	590.27	NO	0.000000	0.000000	0.00000D+00	0.00000D+00

76	eu	600.44	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
77	eu	600.44	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
78	a1g	612.41	YES	-0.042436	0.134128	0.46807D-14	0.16512D-14
79	a2u	637.13	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
80	eu	2125.54	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
81	eu	2125.54	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
82	b1g	2158.01	YES	0.000000	0.352308	0.18845D-14	0.14134D-14
83	a1g	2180.08	YES	0.015981	0.046944	0.75374D-16	0.24539D-16
84	eg	2180.85	YES	0.000000	0.294708	0.12885D-14	0.96636D-15
85	eg	2180.85	YES	0.000000	0.294708	0.12885D-14	0.96636D-15
86	eu	2188.94	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
87	eu	2188.94	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
88	b1u	2201.68	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
89	b2g	2203.56	YES	0.000000	0.556377	0.44880D-14	0.33660D-14
90	a2u	2206.62	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
91	a1g	2214.13	YES	0.138357	0.846588	0.13370D-13	0.77107D-14
92	a2u	2243.22	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
93	a1g	2267.28	YES	-0.256021	0.030899	0.10040D-13	0.97371D-17

$[Os_3(CO)_{14}]^{2+}$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: d4h

Cartesian coordinates in Ångström:

Os	0.0000000	0.0000000	-3.0027593
Os	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	-6.1131312
O	2.2043293	-2.2043293	-2.7585071
O	3.1088335	0.0000000	0.0000000
O	-2.2043293	-2.2043293	-2.7585071
O	2.2043293	2.2043293	-2.7585071
C	1.9753861	0.0000000	0.0000000
O	-2.2043293	2.2043293	-2.7585071
C	-0.0000000	-1.9753861	0.0000000
O	0.0000000	-3.1088335	0.0000000
C	1.4109064	-1.4109064	-2.8596346
C	0.0000000	0.0000000	-4.9877032
C	-1.4109064	1.4109064	-2.8596346
C	-1.4109064	-1.4109064	-2.8596346
C	1.4109064	1.4109064	-2.8596346
Os	0.0000000	0.0000000	3.0027593
O	0.0000000	0.0000000	6.1131312
O	-2.2043293	2.2043293	2.7585071
O	-3.1088335	-0.0000000	0.0000000
O	2.2043293	2.2043293	2.7585071
O	-2.2043293	-2.2043293	2.7585071
C	-1.9753861	0.0000000	0.0000000
O	2.2043293	-2.2043293	2.7585071
C	-0.0000000	1.9753861	0.0000000
O	-0.0000000	3.1088335	0.0000000
C	-1.4109064	1.4109064	2.8596346
C	0.0000000	0.0000000	4.9877032
C	1.4109064	-1.4109064	2.8596346
C	1.4109064	1.4109064	2.8596346
C	-1.4109064	-1.4109064	2.8596346

SCF energy GEOOPT = -1858.544241910 H
ZPE = 316.7 kJ/mol
FREEH energy = 414.93 kJ/mol
FREEH entropy = 0.98946 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a1u	22.85	0.00000	NO	NO
8	eu	32.54	0.16002	YES	NO
9	eu	32.54	0.16002	YES	NO
10	a2g	38.88	0.00000	NO	NO

11	eg	52.12	0.00000	NO	YES
12	eg	52.12	0.00000	NO	YES
13	eu	60.50	0.66426	YES	NO
14	eu	60.50	0.66426	YES	NO
15	b2u	69.86	0.00000	NO	NO
16	b2g	75.03	0.00000	NO	YES
17	b1u	76.36	0.00000	NO	NO
18	eg	76.62	0.00000	NO	YES
19	eg	76.62	0.00000	NO	YES
20	a1g	81.27	0.00000	NO	YES
21	eu	87.83	0.61080	YES	NO
22	eu	87.83	0.61080	YES	NO
23	eu	90.43	0.02519	YES	NO
24	eu	90.43	0.02519	YES	NO
25	eg	91.60	0.00000	NO	YES
26	eg	91.60	0.00000	NO	YES
27	a2u	92.05	4.25784	YES	NO
28	b1g	94.99	0.00000	NO	YES
29	b2u	95.78	0.00000	NO	NO
30	b2g	96.46	0.00000	NO	YES
31	eg	98.20	0.00000	NO	YES
32	eg	98.20	0.00000	NO	YES
33	eu	98.74	0.01475	YES	NO
34	eu	98.74	0.01475	YES	NO
35	a2u	101.18	4.83092	YES	NO
36	a1g	119.68	0.00000	NO	YES
37	a2u	141.46	0.06955	YES	NO
38	eu	363.54	39.40685	YES	NO
39	eu	363.54	39.40685	YES	NO
40	eg	363.87	0.00000	NO	YES
41	eg	363.87	0.00000	NO	YES
42	a2g	365.67	0.00000	NO	NO
43	a1u	365.97	0.00000	NO	NO
44	a2g	377.40	0.00000	NO	NO
45	eu	379.80	66.40964	YES	NO
46	eu	379.80	66.40964	YES	NO
47	eg	404.00	0.00000	NO	YES
48	eg	404.00	0.00000	NO	YES
49	a1g	405.19	0.00000	NO	YES
50	a2u	405.26	23.16852	YES	NO
51	eu	405.47	6.06237	YES	NO
52	eu	405.47	6.06237	YES	NO
53	b1u	439.06	0.00000	NO	NO
54	b2g	439.42	0.00000	NO	YES
55	a2u	453.37	27.31657	YES	NO
56	a1g	455.09	0.00000	NO	YES
57	b1g	463.17	0.00000	NO	YES
58	eg	467.79	0.00000	NO	YES
59	eg	467.79	0.00000	NO	YES
60	a1g	475.75	0.00000	NO	YES
61	b2g	495.92	0.00000	NO	YES
62	b1u	497.18	0.00000	NO	NO
63	b2u	503.45	0.00000	NO	NO
64	b1g	503.99	0.00000	NO	YES
65	eu	508.95	25.51592	YES	NO
66	eu	508.95	25.51592	YES	NO
67	eg	512.58	0.00000	NO	YES
68	eg	512.58	0.00000	NO	YES
69	b2g	517.18	0.00000	NO	YES
70	b2u	534.62	0.00000	NO	NO
71	a2u	588.51	755.11874	YES	NO
72	eg	588.51	0.00000	NO	YES
73	eg	588.51	0.00000	NO	YES
74	eu	588.64	71.07035	YES	NO
75	eu	588.64	71.07035	YES	NO
76	eu	603.43	32.39831	YES	NO
77	eu	603.43	32.39831	YES	NO
78	a1g	604.75	0.00000	NO	YES
79	a2u	640.51	78.48412	YES	NO
80	eu	2109.78	379.33325	YES	NO
81	eu	2109.78	379.33325	YES	NO
82	b1g	2149.10	0.00000	NO	YES
83	eg	2173.31	0.00000	NO	YES
84	eg	2173.31	0.00000	NO	YES
85	a1g	2175.94	0.00000	NO	YES
86	eu	2181.76	2059.94565	YES	NO

```
    87        eu           2181.76      2059.94565       YES     NO
    88        a2u          2194.09       579.80876       YES     NO
    89        b1u          2198.16         0.00000       NO      NO
    90        b2g          2200.21         0.00000       NO      YES
    91        a1g          2201.21         0.00000       NO      YES
    92        a2u          2243.54      1143.27589       YES     NO
    93        a1g          2267.89         0.00000       NO      YES
$end
$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.           a.u.         bohr**2/sr
#                                                                 T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    a1u    22.85   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    8    eu     32.54   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    9    eu     32.54   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   10    a2g    38.88   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   11    eg     52.12   YES        0.000000     0.043460 0.14825D-13 0.11119D-13
   12    eg     52.12   YES        0.000000     0.043460 0.14825D-13 0.11119D-13
   13    eu     60.50   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   14    eu     60.50   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   15    b2u    69.86   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   16    b2g    75.03   YES       -0.000000     0.032532 0.41830D-14 0.31373D-14
   17    b1u    76.36   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   18    eg     76.62   YES        0.000000     0.079543 0.24050D-13 0.18037D-13
   19    eg     76.62   YES        0.000000     0.079543 0.24050D-13 0.18037D-13
   20    a1g    81.27   YES       -0.045130     0.089429 0.10533D-12 0.20439D-13
   21    eu     87.83   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   22    eu     87.83   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   23    eu     90.43   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   24    eu     90.43   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   25    eg     91.60   YES        0.000000     0.022901 0.14334D-14 0.10751D-14
   26    eg     91.60   YES        0.000000     0.022901 0.14334D-14 0.10751D-14
   27    a2u    92.05   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   28    b1g    94.99   YES        0.000000     0.093640 0.22422D-13 0.16816D-13
   29    b2u    95.78   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   30    b2g    96.46   YES        0.000000     0.055177 0.75696D-14 0.56772D-14
   31    eg     98.20   YES        0.000000     0.062444 0.93833D-14 0.70375D-14
   32    eg     98.20   YES        0.000000     0.062444 0.93833D-14 0.70375D-14
   33    eu     98.74   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   34    eu     98.74   NO         0.000000     0.000000 0.11410D-35 0.85575D-36
   35    a2u   101.18   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   36    a1g   119.68   YES        0.023588     0.092184 0.24837D-13 0.10727D-13
   37    a2u   141.46   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   38    eu    363.54   NO         0.000000     0.000000 0.13395D-33 0.89409D-34
   39    eu    363.54   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   40    eg    363.87   YES        0.000000     0.061417 0.99533D-15 0.74649D-15
   41    eg    363.87   YES        0.000000     0.061417 0.99533D-15 0.74649D-15
   42    a2g   365.67   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   43    a1u   365.97   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   44    a2g   377.40   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   45    eu    379.80   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   46    eu    379.80   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   47    eg    404.00   YES        0.000000     0.032800 0.24226D-15 0.18170D-15
   48    eg    404.00   YES        0.000000     0.032800 0.24226D-15 0.18170D-15
   49    a1g   405.19   YES       -0.030404     0.117962 0.54511D-14 0.23397D-14
   50    a2u   405.26   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   51    eu    405.47   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   52    eu    405.47   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   53    b1u   439.06   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   54    b2g   439.42   YES        0.000000     0.055332 0.60808D-15 0.45606D-15
   55    a2u   453.37   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   56    a1g   455.09   YES        0.072786     0.015093 0.11281D-13 0.32214D-16
   57    b1g   463.17   YES        0.000000     0.056798 0.59270D-15 0.44452D-15
   58    eg    467.79   YES        0.000000     0.031314 0.17753D-15 0.13315D-15
   59    eg    467.79   YES        0.000000     0.031314 0.17753D-15 0.13315D-15
   60    a1g   475.75   YES       -0.079484     0.027053 0.12682D-13 0.96944D-16
   61    b2g   495.92   YES        0.000000     0.026939 0.12060D-15 0.90447D-16
   62    b1u   497.18   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
```

63	b2u	503.45	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
64	b1g	503.99	YES	0.000000	0.004983	0.40298D-17	0.30224D-17
65	eu	508.95	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
66	eu	508.95	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
67	eg	512.58	YES	0.000000	0.086688	0.11900D-14	0.89248D-15
68	eg	512.58	YES	0.000000	0.086688	0.11900D-14	0.89248D-15
69	b2g	517.18	YES	0.000000	0.008433	0.11115D-16	0.83361D-17
70	b2u	534.62	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
71	a2u	588.51	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
72	eg	588.51	YES	0.000000	0.002702	0.94619D-18	0.70964D-18
73	eg	588.51	YES	0.000000	0.002702	0.94619D-18	0.70964D-18
74	eu	588.64	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
75	eu	588.64	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
76	eu	603.43	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
77	eu	603.43	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
78	a1g	604.75	YES	0.021175	0.073989	0.13108D-14	0.51164D-15
79	a2u	640.51	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
80	eu	2109.78	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
81	eu	2109.78	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
82	b1g	2149.10	YES	0.000000	0.351011	0.18877D-14	0.14158D-14
83	eg	2173.31	YES	0.000000	0.198875	0.59125D-15	0.44344D-15
84	eg	2173.31	YES	0.000000	0.198875	0.59125D-15	0.44344D-15
85	a1g	2175.94	YES	0.007062	0.056541	0.56028D-16	0.35747D-16
86	eu	2181.76	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
87	eu	2181.76	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
88	a2u	2194.09	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
89	b1u	2198.16	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
90	b2g	2200.21	YES	0.000000	0.562591	0.46044D-14	0.34533D-14
91	a1g	2201.21	YES	0.131753	0.827957	0.12801D-13	0.74718D-14
92	a2u	2243.54	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
93	a1g	2267.89	YES	-0.275461	0.076347	0.11680D-13	0.59410D-16

$[Ru(CO)_6]^{2+}$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: oh

Cartesian coordinates in Ångström:

Ru	-0.0000000	-0.0000000	0.0000000
C	-0.0000000	2.0368877	-0.0000000
C	0.0000000	-2.0368877	0.0000000
C	-0.0000000	0.0000000	2.0368877
C	2.0368877	0.0000000	0.0000000
C	0.0000000	-0.0000000	-2.0368877
O	0.0000000	0.0000000	3.1520648
O	-0.0000000	3.1520648	0.0000000
O	0.0000000	-3.1520648	-0.0000000
O	3.1520648	0.0000000	-0.0000000
O	-0.0000000	-0.0000000	-3.1520648
C	-2.0368877	-0.0000000	0.0000000
O	-3.1520648	-0.0000000	0.0000000

SCF energy GEOOPT = -774.3069275394 H
ZPE = 133.6 kJ/mol
FREEH energy = 172.53 kJ/mol
FREEH entropy = 0.49054 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	t2u	77.68	0.00000	NO	NO
8	t2u	77.68	0.00000	NO	NO
9	t2u	77.68	0.00000	NO	NO
10	t2g	91.72	0.00000	NO	YES
11	t2g	91.72	0.00000	NO	YES
12	t2g	91.72	0.00000	NO	YES
13	t1u	106.89	0.54598	YES	NO
14	t1u	106.89	0.54598	YES	NO
15	t1u	106.89	0.54598	YES	NO

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    16        t1u           320.71        15.29841       YES     NO
    17        t1u           320.71        15.29841       YES     NO
    18        t1u           320.71        15.29841       YES     NO
    19        t1g           333.02         0.00000       NO      NO
    20        t1g           333.02         0.00000       NO      NO
    21        t1g           333.02         0.00000       NO      NO
    22        eg            366.03         0.00000       NO      YES
    23        eg            366.03         0.00000       NO      YES
    24        a1g           386.73         0.00000       NO      YES
    25        t2g           475.48         0.00000       NO      YES
    26        t2g           475.48         0.00000       NO      YES
    27        t2g           475.48         0.00000       NO      YES
    28        t2u           499.53         0.00000       NO      NO
    29        t2u           499.53         0.00000       NO      NO
    30        t2u           499.53         0.00000       NO      NO
    31        t1u           577.27        90.74924       YES     NO
    32        t1u           577.27        90.74924       YES     NO
    33        t1u           577.27        90.74924       YES     NO
    34        t1u          2278.85       435.64559       YES     NO
    35        t1u          2278.85       435.64559       YES     NO
    36        t1u          2278.85       435.64559       YES     NO
    37        eg           2296.85         0.00000       NO      YES
    38        eg           2296.85         0.00000       NO      YES
    39        a1g          2334.79         0.00000       NO      YES
$end
$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.          a.u.        bohr**2/sr
#                                                                T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    t2u    77.68   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    8    t2u    77.68   NO         0.000000     0.000000 0.55182D-34 0.41386D-34
    9    t2u    77.68   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   10    t2g    91.72   YES        0.000000     0.075735 0.15639D-13 0.11729D-13
   11    t2g    91.72   YES        0.000000     0.075735 0.15639D-13 0.11729D-13
   12    t2g    91.72   YES        0.000000     0.075735 0.15639D-13 0.11729D-13
   13    t1u   106.89   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   14    t1u   106.89   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   15    t1u   106.89   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   16    t1u   320.71   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   17    t1u   320.71   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   18    t1u   320.71   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   19    t1g   333.02   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   20    t1g   333.02   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   21    t1g   333.02   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   22    eg    366.03   YES        0.000000     0.004914 0.63139D-17 0.47354D-17
   23    eg    366.03   YES        0.000000     0.004914 0.63139D-17 0.47354D-17
   24    a1g   386.73   YES        0.038822     0.000000 0.40782D-14 0.00000D+00
   25    t2g   475.48   YES        0.000000     0.012299 0.26739D-16 0.20054D-16
   26    t2g   475.48   YES        0.000000     0.012299 0.26739D-16 0.20054D-16
   27    t2g   475.48   YES        0.000000     0.012299 0.26739D-16 0.20054D-16
   28    t2u   499.53   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   29    t2u   499.53   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   30    t2u   499.53   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   31    t1u   577.27   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   32    t1u   577.27   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   33    t1u   577.27   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   34    t1u  2278.85   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   35    t1u  2278.85   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   36    t1u  2278.85   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
   37    eg   2296.85   YES       -0.000000     0.461391 0.28104D-14 0.21078D-14
   38    eg   2296.85   YES        0.000000     0.461391 0.28104D-14 0.21078D-14
   39    a1g  2334.79   YES       -0.184766     0.000000 0.48821D-14 0.19847D-30
```

$[Os(CO)_6]^{2+}$

```
Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: oh
```

Cartesian coordinates in Ångström:

Os	0.0000000	0.0000000	0.0000000
C	0.0000000	2.0487891	-0.0000000
C	-0.0000000	-2.0487891	0.0000000
C	-0.0000000	-0.0000000	2.0487891
C	2.0487891	-0.0000000	0.0000000
C	-0.0000000	0.0000000	-2.0487891
O	0.0000000	-0.0000000	3.1650797
O	0.0000000	3.1650797	0.0000000
O	-0.0000000	-3.1650797	0.0000000
O	3.1650797	-0.0000000	0.0000000
O	0.0000000	0.0000000	-3.1650797
C	-2.0487891	0.0000000	-0.0000000
O	-3.1650797	0.0000000	-0.0000000

SCF energy GEOOPT = -770.1136460220 H
ZPE = 134.5 kJ/mol
FREEH energy = 172.97 kJ/mol
FREEH entropy = 0.49105 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	t2u	78.95	0.00000	NO	NO
8	t2u	78.95	0.00000	NO	NO
9	t2u	78.95	0.00000	NO	NO
10	t2g	93.67	0.00000	NO	YES
11	t2g	93.67	0.00000	NO	YES
12	t2g	93.67	0.00000	NO	YES
13	t1u	102.82	0.00310	YES	NO
14	t1u	102.82	0.00310	YES	NO
15	t1u	102.82	0.00310	YES	NO
16	t1u	322.11	37.01062	YES	NO
17	t1u	322.11	37.01062	YES	NO
18	t1u	322.11	37.01062	YES	NO
19	t1g	347.41	0.00000	NO	NO
20	t1g	347.41	0.00000	NO	NO
21	t1g	347.41	0.00000	NO	NO
22	eg	393.40	0.00000	NO	YES
23	eg	393.40	0.00000	NO	YES
24	a1g	419.35	0.00000	NO	YES
25	t2g	481.82	0.00000	NO	YES
26	t2g	481.82	0.00000	NO	YES
27	t2g	481.82	0.00000	NO	YES
28	t2u	521.21	0.00000	NO	NO
29	t2u	521.21	0.00000	NO	NO
30	t2u	521.21	0.00000	NO	NO
31	t1u	576.66	84.60866	YES	NO
32	t1u	576.66	84.60866	YES	NO
33	t1u	576.66	84.60866	YES	NO
34	t1u	2266.91	559.55988	YES	NO
35	t1u	2266.91	559.55988	YES	NO
36	t1u	2266.91	559.55988	YES	NO
37	eg	2288.31	0.00000	NO	YES
38	eg	2288.31	0.00000	NO	YES
39	a1g	2334.26	0.00000	NO	YES

$end
$raman spectrum

# mode	symmetry	wave number cm**(-1)	selection rule	derivative of isotropic polarizability a.u.	derivative of polarizability anisotropy a.u.	raman scattering cross sections bohr**2/sr T,T	II,II
1		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00

7	t2u	78.95	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
8	t2u	78.95	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
9	t2u	78.95	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
10	t2g	93.67	YES	0.000000	0.080183	0.16867D-13 0.12650D-13
11	t2g	93.67	YES	0.000000	0.080183	0.16867D-13 0.12650D-13
12	t2g	93.67	YES	0.000000	0.080183	0.16867D-13 0.12650D-13
13	t1u	102.82	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
14	t1u	102.82	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
15	t1u	102.82	NO	0.000000	0.000000	0.12067D-35 0.90503D-36
16	t1u	322.11	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
17	t1u	322.11	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
18	t1u	322.11	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
19	t1g	347.41	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
20	t1g	347.41	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
21	t1g	347.41	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
22	eg	393.40	YES	-0.000000	0.004540	0.48314D-17 0.36236D-17
23	eg	393.40	YES	0.000000	0.004540	0.48314D-17 0.36236D-17
24	a1g	419.35	YES	0.044059	0.000000	0.46503D-14 0.62335D-30
25	t2g	481.82	YES	0.000000	0.012740	0.28139D-16 0.21104D-16
26	t2g	481.82	YES	0.000000	0.012740	0.28139D-16 0.21104D-16
27	t2g	481.82	YES	0.000000	0.012740	0.28139D-16 0.21104D-16
28	t2u	521.21	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
29	t2u	521.21	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
30	t2u	521.21	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
31	t1u	576.66	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
32	t1u	576.66	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
33	t1u	576.66	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
34	t1u	2266.91	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
35	t1u	2266.91	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
36	t1u	2266.91	NO	0.000000	0.000000	0.00000D+00 0.00000D+00
37	eg	2288.31	YES	0.000000	0.509414	0.34553D-14 0.25915D-14
38	eg	2288.31	YES	-0.000000	0.509414	0.34553D-14 0.25915D-14
39	a1g	2334.26	YES	-0.190087	0.000000	0.51701D-14 0.39714D-30

$[Ru(CO)_5I]^+$

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: c4v

Cartesian coordinates in Ångström:

I	0.0000000	0.0000000	-2.7982790
Ru	0.0000000	-0.0000000	-0.0455790
O	-0.0000000	-3.1096726	-0.3252698
O	0.0000000	0.0000000	3.0467970
C	0.0000000	-1.9945407	-0.2058014
C	0.0000000	0.0000000	1.9213457
O	0.0000000	3.1096726	-0.3252698
C	0.0000000	1.9945407	-0.2058014
O	3.1096726	-0.0000000	-0.3252698
C	1.9945407	0.0000000	-0.2058014
O	-3.1096726	0.0000000	-0.3252698
C	-1.9945407	-0.0000000	-0.2058014

SCF energy GEOOPT = -959.1573105631 H
ZPE = 112.8 kJ/mol
FREEH energy = 150.52 kJ/mol
FREEH entropy = 0.51242 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e	62.55	1.06564	YES	YES
8	e	62.55	1.06564	YES	YES
9	b1	74.50	0.00000	NO	YES
10	e	85.54	0.08530	YES	YES
11	e	85.54	0.08530	YES	YES

12	b2	92.74	0.00000	NO	YES
13	e	101.20	0.80085	YES	YES
14	e	101.20	0.80085	YES	YES
15	a1	103.26	1.13715	YES	YES
16	a1	191.81	1.90886	YES	YES
17	e	338.58	21.96700	YES	YES
18	e	338.58	21.96700	YES	YES
19	a2	345.53	0.00000	NO	NO
20	e	384.60	2.32621	YES	YES
21	e	384.60	2.32621	YES	YES
22	b1	395.35	0.00000	NO	YES
23	a1	398.13	3.13557	YES	YES
24	a1	410.22	0.16482	YES	YES
25	b1	483.61	0.00000	NO	YES
26	b2	494.89	0.00000	NO	YES
27	e	504.63	6.53408	YES	YES
28	e	504.63	6.53408	YES	YES
29	e	579.01	69.22085	YES	YES
30	e	579.01	69.22085	YES	YES
31	a1	588.93	157.17852	YES	YES
32	a1	2198.10	476.41380	YES	YES
33	e	2220.56	721.36720	YES	YES
34	e	2220.56	721.36720	YES	YES
35	b1	2241.32	0.00000	NO	YES
36	a1	2280.96	73.16201	YES	YES

Anthracene[Hal]

Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: c2h

Cartesian coordinates in Ångström:

C	0.7017848	-0.0198348	-3.6749582
C	-0.7017848	0.0198348	-3.6749582
C	-1.3887363	0.0614971	-2.5002764
C	-0.7237612	0.0663536	-1.2313360
C	0.7237612	-0.0663536	-1.2313360
C	1.3887363	-0.0614971	-2.5002764
C	1.3970561	-0.1768662	0.0000000
C	-1.3970561	0.1768662	0.0000000
C	-0.7237612	0.0663536	1.2313360
C	0.7237612	-0.0663536	1.2313360
C	1.3887363	-0.0614971	2.5002764
C	-1.3887363	0.0614971	2.5002764
C	-0.7017848	0.0198348	3.6749582
C	0.7017848	-0.0198348	3.6749582
F	1.3434914	-0.0066994	4.8392254
F	2.7185195	-0.0492949	2.6146688
F	-1.3434914	0.0066994	4.8392254
F	-2.7185195	0.0492949	2.6146688
Cl	3.0870371	-0.5750228	0.0000000
Cl	-3.0870371	0.5750228	0.0000000
F	2.7185195	-0.0492949	-2.6146688
F	1.3434914	-0.0066994	-4.8392254
F	-1.3434914	0.0066994	-4.8392254
F	-2.7185195	0.0492949	-2.6146688

SCF energy GEOOPT = -2252.472358433 H
ZPE = 284.8 kJ/mol
FREEH energy = 333.53 kJ/mol
FREEH entropy = 0.58631 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	bu	-17.86	0.00000	YES	NO
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	au	19.58	0.00127	YES	NO
9	ag	40.31	0.00000	NO	YES
10	bu	58.08	0.04289	YES	NO

```
    11        bg             87.06         0.00000       NO      YES
    12        ag            152.10         0.00000       NO      YES
    13        au            153.41         0.05563       YES     NO
    14        bu            157.68         1.49156       YES     NO
    15        bu            164.87         0.42605       YES     NO
    16        bg            198.51         0.00000       NO      YES
    17        bg            236.61         0.00000       NO      YES
    18        ag            251.18         0.00000       NO      YES
    19        au            256.38         0.03104       YES     NO
    20        bg            261.94         0.00000       NO      YES
    21        au            292.10         0.27809       YES     NO
    22        ag            296.51         0.00000       NO      YES
    23        bu            313.52         2.65593       YES     NO
    24        ag            320.24         0.00000       NO      YES
    25        bu            328.27         5.33642       YES     NO
    26        bg            337.58         0.00000       NO      YES
    27        ag            348.10         0.00000       NO      YES
    28        bu            350.52         1.22760       YES     NO
    29        au            354.49         0.57951       YES     NO
    30        au            371.11         7.95302       YES     NO
    31        ag            371.39         0.00000       NO      YES
    32        bg            420.47         0.00000       NO      YES
    33        ag            446.53         0.00000       NO      YES
    34        au            458.90         1.11020       YES     NO
    35        ag            487.88         0.00000       NO      YES
    36        bg            498.10         0.00000       NO      YES
    37        bu            537.70         0.85604       YES     NO
    38        bu            573.19         0.65720       YES     NO
    39        au            639.66        63.08170       YES     NO
    40        au            650.21        27.15268       YES     NO
    41        bg            664.57         0.00000       NO      YES
    42        ag            683.19         0.00000       NO      YES
    43        bg            684.64         0.00000       NO      YES
    44        bu            691.43         1.53469       YES     NO
    45        bu            716.15        54.64981       YES     NO
    46        au            722.58         2.00867       YES     NO
    47        ag            753.74         0.00000       NO      YES
    48        bg            788.37         0.00000       NO      YES
    49        ag            849.56         0.00000       NO      YES
    50        bu            856.78        88.72765       YES     NO
    51        bg           1003.57         0.00000       NO      YES
    52        ag           1012.98         0.00000       NO      YES
    53        bu           1086.27       132.74687       YES     NO
    54        au           1096.09       310.77760       YES     NO
    55        ag           1165.68         0.00000       NO      YES
    56        bu           1199.61       145.32682       YES     NO
    57        au           1201.37        16.58651       YES     NO
    58        bg           1230.89         0.00000       NO      YES
    59        au           1238.38        14.80301       YES     NO
    60        au           1347.41        10.36485       YES     NO
    61        ag           1361.09         0.00000       NO      YES
    62        bg           1366.65         0.00000       NO      YES
    63        bu           1374.90       267.62900       YES     NO
    64        ag           1412.83         0.00000       NO      YES
    65        bu           1463.11       226.45397       YES     NO
    66        au           1525.00       948.29325       YES     NO
    67        ag           1534.02         0.00000       NO      YES
    68        bg           1562.81         0.00000       NO      YES
    69        au           1593.69        73.86058       YES     NO
    70        ag           1616.74         0.00000       NO      YES
    71        bg           1683.11         0.00000       NO      YES
    72        bu           1696.35       164.46929       YES     NO
$end
$raman spectrum
# mode symmetry wave  selection  derivative of  derivative of     raman
#              number   rule       isotropic   polarizability   scattering
#                                polarizability   anisotropy   cross sections
#             cm**(-1)               a.u.          a.u.        bohr**2/sr
#                                                              T,T        II,II
    1    bu    -17.86   NO         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
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8	au	19.58	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
9	ag	40.31	YES	-0.000613	0.022397	0.64905D-14	0.48271D-14
10	bu	58.08	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
11	bg	87.06	YES	0.000000	0.027914	0.23382D-14	0.17536D-14
12	ag	152.10	YES	-0.000364	0.013168	0.19267D-15	0.14327D-15
13	au	153.41	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
14	bu	157.68	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
15	bu	164.87	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
16	bg	198.51	YES	0.000000	0.075477	0.39767D-14	0.29825D-14
17	bg	236.61	YES	0.000000	0.057166	0.17042D-14	0.12781D-14
18	ag	251.18	YES	0.027811	0.059415	0.57860D-14	0.12525D-14
19	au	256.38	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
20	bg	261.94	YES	0.000000	0.120796	0.64498D-14	0.48373D-14
21	au	292.10	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
22	ag	296.51	YES	-0.023862	0.034595	0.27572D-14	0.32553D-15
23	bu	313.52	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
24	ag	320.24	YES	0.041820	0.062247	0.75685D-14	0.93393D-15
25	bu	328.27	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
26	bg	337.58	YES	0.000000	0.022675	0.15224D-15	0.11418D-15
27	ag	348.10	YES	-0.025207	0.052906	0.28092D-14	0.59287D-15
28	bu	350.52	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
29	au	354.49	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
30	au	371.11	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
31	ag	371.39	YES	-0.033018	0.047571	0.37157D-14	0.43409D-15
32	bg	420.47	YES	0.000000	0.062371	0.82506D-15	0.61880D-15
33	ag	446.53	YES	-0.009614	0.033478	0.41902D-15	0.16302D-15
34	au	458.90	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
35	ag	487.88	YES	-0.045995	0.052376	0.45177D-14	0.35018D-15
36	bg	498.10	YES	0.000000	0.058064	0.55668D-15	0.41751D-15
37	bu	537.70	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
38	bu	573.19	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
39	au	639.66	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
40	au	650.21	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
41	bg	664.57	YES	0.000000	0.065301	0.46388D-15	0.34791D-15
42	ag	683.19	YES	0.015113	0.052233	0.55383D-15	0.21391D-15
43	bg	684.64	YES	0.000000	0.054181	0.30596D-15	0.22947D-15
44	bu	691.43	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
45	bu	716.15	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
46	au	722.58	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
47	ag	753.74	YES	-0.000636	0.039011	0.13848D-15	0.10355D-15
48	bg	788.37	YES	0.000000	0.027467	0.64126D-16	0.48095D-16
49	ag	849.56	YES	0.047616	0.106367	0.28063D-14	0.64672D-15
50	bu	856.78	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
51	bg	1003.57	YES	0.000000	0.015869	0.14976D-16	0.11232D-16
52	ag	1012.98	YES	0.028586	0.124758	0.14516D-14	0.68442D-15
53	bu	1086.27	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
54	au	1096.09	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
55	ag	1165.68	YES	-0.112202	0.282185	0.10433D-13	0.28160D-14
56	bu	1199.61	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
57	au	1201.37	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
58	bg	1230.89	YES	0.000000	0.002695	0.31393D-18	0.23545D-18
59	au	1238.38	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
60	au	1347.41	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
61	ag	1361.09	YES	-0.338851	0.551386	0.58409D-13	0.83462D-14
62	bg	1366.65	YES	0.000000	0.093162	0.31550D-15	0.23663D-15
63	bu	1374.90	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
64	ag	1412.83	YES	-0.045843	0.446279	0.76540D-14	0.51313D-14
65	bu	1463.11	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
66	au	1525.00	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
67	ag	1534.02	YES	-0.118581	0.406372	0.96180D-14	0.36842D-14
68	bg	1562.81	YES	0.000000	0.554221	0.88374D-14	0.66281D-14
69	au	1593.69	NO	0.000000	0.000000	0.00000D+00	0.00000D+00
70	ag	1616.74	YES	0.158656	0.449715	0.13131D-13	0.41031D-14
71	bg	1683.11	YES	0.000000	0.301210	0.22778D-14	0.17083D-14
72	bu	1696.35	NO	0.000000	0.000000	0.00000D+00	0.00000D+00

[Anthracene^{Hal}]$^{+\cdot}$

Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: cs

Cartesian coordinates in Ångström:

C	0.6968884	0.1531083	-3.6925913
C	-0.7013152	0.1320171	-3.6925546
C	-1.3957681	0.0082202	-2.4886893

C	-0.7251881	-0.1130040	-1.2401142
C	0.7283844	-0.0910720	-1.2401274
C	1.3948808	0.0501979	-2.4887932
C	1.4175180	-0.2229164	0.0000000
C	-1.4099716	-0.2657679	0.0000000
C	-0.7251881	-0.1130040	1.2401142
C	0.7283844	-0.0910720	1.2401274
C	1.3948808	0.0501979	2.4887932
C	-1.3957681	0.0082202	2.4886893
C	-0.7013152	0.1320171	3.6925546
C	0.6968884	0.1531083	3.6925913
F	1.3543480	0.3008522	4.8277278
F	2.7140764	0.1460665	2.5886032
F	-1.3630284	0.2597445	4.8276364
F	-2.7172673	0.0646056	2.5882661
Cl	3.0775389	-0.6197259	0.0000000
Cl	-3.0571070	-0.7130622	0.0000000
F	2.7140764	0.1460665	-2.5886032
F	1.3543480	0.3008522	-4.8277278
F	-1.3630284	0.2597445	-4.8276364
F	-2.7172673	0.0646056	-2.5882661

SCF energy GEOOPT = -2253.077486613 H
ZPE = 278.8 kJ/mol
FREEH energy = 330.59 kJ/mol
FREEH entropy = 0.61776 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a"	27.20	0.00000	YES	YES
8	a'	31.75	0.12078	YES	YES
9	a'	44.44	0.01916	YES	YES
10	a'	74.30	0.00106	YES	YES
11	a"	85.30	0.00594	YES	YES
12	a'	137.63	0.03426	YES	YES
13	a"	140.47	0.00000	YES	YES
14	a'	146.30	1.57553	YES	YES
15	a'	157.77	0.09499	YES	YES
16	a"	200.40	0.29659	YES	YES
17	a"	222.22	0.00000	YES	YES
18	a"	245.74	0.01018	YES	YES
19	a'	246.59	0.90056	YES	YES
20	a"	251.05	0.00000	YES	YES
21	a"	282.44	2.45555	YES	YES
22	a'	285.06	0.15634	YES	YES
23	a'	302.60	2.99655	YES	YES
24	a'	312.85	2.27889	YES	YES
25	a"	317.07	0.00000	YES	YES
26	a'	326.48	0.00220	YES	YES
27	a'	342.13	0.50238	YES	YES
28	a"	348.64	4.65352	YES	YES
29	a'	362.88	0.06287	YES	YES
30	a'	371.28	0.08405	YES	YES
31	a"	381.34	2.93940	YES	YES
32	a"	382.19	0.00043	YES	YES
33	a"	438.97	1.53521	YES	YES
34	a'	461.38	1.61833	YES	YES
35	a'	473.14	0.00003	YES	YES
36	a"	475.55	0.00000	YES	YES
37	a'	523.76	0.42206	YES	YES
38	a'	576.83	0.00687	YES	YES
39	a"	616.67	0.00000	YES	YES
40	a"	634.95	25.67378	YES	YES
41	a"	651.81	5.94838	YES	YES
42	a"	661.39	0.00000	YES	YES
43	a'	665.09	0.00139	YES	YES
44	a'	678.52	0.15740	YES	YES
45	a"	690.29	0.00000	YES	YES
46	a'	706.95	3.01249	YES	YES

```
    47        a'            727.75        41.65241       YES     YES
    48        a"            771.43         0.00000       YES     YES
    49        a'            842.92        84.96128       YES     YES
    50        a'            845.29         6.41340       YES     YES
    51        a"            994.24         0.00000       YES     YES
    52        a'           1009.24         4.02967       YES     YES
    53        a'           1080.65        70.00230       YES     YES
    54        a"           1090.51       194.60336       YES     YES
    55        a'           1170.93         1.38821       YES     YES
    56        a'           1186.70       165.12425       YES     YES
    57        a"           1199.28        31.05291       YES     YES
    58        a"           1232.10         0.00002       YES     YES
    59        a"           1321.47       443.89279       YES     YES
    60        a'           1342.46        17.37933       YES     YES
    61        a"           1345.46       119.27106       YES     YES
    62        a'           1348.04       127.72724       YES     YES
    63        a"           1366.22         0.00016       YES     YES
    64        a'           1376.16         7.89150       YES     YES
    65        a'           1438.61       455.40838       YES     YES
    66        a"           1459.12         0.20601       YES     YES
    67        a"           1459.68      1409.24688       YES     YES
    68        a'           1512.62         4.95717       YES     YES
    69        a"           1540.29         0.66510       YES     YES
    70        a"           1540.37       209.97502       YES     YES
    71        a'           1555.70         1.31987       YES     YES
    72        a'           1566.07       277.49678       YES     YES
 $end
 $raman spectrum
 # mode symmetry wave  selection  derivative of  derivative of     raman
 #              number   rule       isotropic   polarizability   scattering
 #                                polarizability   anisotropy   cross sections
 #             cm**(-1)                a.u.          a.u.        bohr**2/sr
 #                                                                   T,T        II,II
    1            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    2            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    3            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    4            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    5            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    6            0.00    -         0.000000     0.000000 0.00000D+00 0.00000D+00
    7    a"     27.20   YES        0.000000     0.007604 0.15891D-14 0.11918D-14
    8    a'     31.75   YES       -0.001211     0.035647 0.26190D-13 0.19391D-13
    9    a'     44.44   YES        0.000004     0.010415 0.11543D-14 0.86571D-15
   10    a'     74.30   YES        0.013634     0.047276 0.17413D-13 0.67471D-14
   11    a"     85.30   YES        0.000000     0.009226 0.26525D-15 0.19894D-15
   12    a'    137.63   YES        0.000014     0.005631 0.41626D-16 0.31217D-16
   13    a"    140.47   YES        0.000000     0.004755 0.28634D-16 0.21476D-16
   14    a'    146.30   YES        0.010163     0.024584 0.20828D-14 0.53448D-15
   15    a'    157.77   YES       -0.000007     0.022213 0.51010D-15 0.38257D-15
   16    a"    200.40   YES        0.000000     0.076076 0.39761D-14 0.29821D-14
   17    a"    222.22   YES        0.000000     0.022155 0.28383D-15 0.21287D-15
   18    a"    245.74   YES        0.000000     0.036660 0.65880D-15 0.49410D-15
   19    a'    246.59   YES        0.076269     0.198224 0.51052D-13 0.14365D-13
   20    a"    251.05   YES        0.000000     0.081191 0.31210D-14 0.23408D-14
   21    a"    282.44   YES        0.000000     0.023582 0.21786D-15 0.16339D-15
   22    a'    285.06   YES       -0.052262     0.098288 0.15590D-13 0.27969D-14
   23    a'    302.60   YES        0.054356     0.061714 0.13012D-13 0.10033D-14
   24    a'    312.85   YES        0.000230     0.014263 0.68006D-16 0.50855D-16
   25    a"    317.07   YES        0.000000     0.051884 0.87865D-15 0.65899D-15
   26    a'    326.48   YES        0.000013     0.039748 0.49270D-15 0.36952D-15
   27    a'    342.13   YES        0.085539     0.187111 0.34030D-13 0.76159D-14
   28    a"    348.64   YES        0.000000     0.014628 0.60287D-16 0.45215D-16
   29    a'    362.88   YES        0.120754     0.290959 0.65897D-13 0.16824D-13
   30    a'    371.28   YES       -0.000164     0.017326 0.76887D-16 0.57607D-16
   31    a"    381.34   YES        0.000000     0.070990 0.12382D-14 0.92863D-15
   32    a"    382.19   YES        0.000000     0.013241 0.42929D-16 0.32197D-16
   33    a"    438.97   YES        0.000000     0.055696 0.61704D-15 0.46278D-15
   34    a'    461.38   YES       -0.000101     0.042872 0.33965D-15 0.25472D-15
   35    a'    473.14   YES       -0.044301     0.065710 0.46999D-14 0.57659D-15
   36    a"    475.55   YES        0.000000     0.086612 0.13257D-14 0.99430D-15
   37    a'    523.76   YES       -0.000030     0.003657 0.20535D-17 0.15390D-17
   38    a'    576.83   YES        0.019102     0.044531 0.81219D-15 0.19842D-15
   39    a"    616.67   YES        0.000000     0.003198 0.12388D-17 0.92911D-18
   40    a"    634.95   YES        0.000000     0.054452 0.34444D-15 0.25833D-15
   41    a"    651.81   YES        0.000000     0.068054 0.51808D-15 0.38856D-15
   42    a"    661.39   YES        0.000000     0.008094 0.71767D-17 0.53825D-17
   43    a'    665.09   YES       -0.000016     0.005657 0.34778D-17 0.26081D-17
```

44	a'	678.52	YES	0.001188	0.064535	0.44139D-15	0.32979D-15
45	a"	690.29	YES	0.000000	0.021611	0.48104D-16	0.36078D-16
46	a'	706.95	YES	0.000019	0.035227	0.12349D-15	0.92620D-16
47	a'	727.75	YES	0.000020	0.017310	0.28599D-16	0.21449D-16
48	a"	771.43	YES	0.000000	0.004429	0.17204D-17	0.12903D-17
49	a'	842.92	YES	-0.000067	0.011401	0.10025D-16	0.75161D-17
50	a'	845.29	YES	-0.070978	0.250225	0.91589D-14	0.36055D-14
51	a"	994.24	YES	0.000000	0.091478	0.50474D-15	0.37855D-15
52	a'	1009.24	YES	0.107806	0.362206	0.15445D-13	0.58015D-14
53	a'	1080.65	YES	0.000016	0.011801	0.73945D-17	0.55458D-17
54	a"	1090.51	YES	0.000000	0.053685	0.15089D-15	0.11316D-15
55	a'	1170.93	YES	0.254974	0.761339	0.61379D-13	0.20353D-13
56	a'	1186.70	YES	0.000117	0.017677	0.14327D-16	0.10740D-16
57	a"	1199.28	YES	0.000000	0.008147	0.29911D-17	0.22433D-17
58	a"	1232.10	YES	0.000000	0.162933	0.11454D-14	0.85905D-15
59	a"	1321.47	YES	0.000000	0.077983	0.23389D-15	0.17542D-15
60	a'	1342.46	YES	0.153518	0.545947	0.21098D-13	0.83741D-14
61	a"	1345.46	YES	0.000000	0.149164	0.83039D-15	0.62279D-15
62	a'	1348.04	YES	0.000404	0.012669	0.60397D-17	0.44785D-17
63	a"	1366.22	YES	0.000000	0.040771	0.60459D-16	0.45344D-16
64	a'	1376.16	YES	-0.730170	2.908748	0.51947D-12	0.22798D-12
65	a'	1438.61	YES	-0.000107	0.055441	0.10236D-15	0.76764D-16
66	a"	1459.12	YES	0.000000	0.117410	0.44789D-15	0.33592D-15
67	a"	1459.68	YES	0.000000	0.112211	0.40883D-15	0.30662D-15
68	a'	1512.62	YES	0.049561	0.479747	0.78624D-14	0.52647D-14
69	a"	1540.29	YES	0.000000	0.582752	0.10029D-13	0.75215D-14
70	a"	1540.37	YES	0.000000	0.066891	0.13212D-15	0.99092D-16
71	a'	1555.70	YES	-0.148888	0.238180	0.88799D-14	0.12342D-14
72	a'	1566.07	YES	0.000198	0.005102	0.75887D-18	0.55966D-18

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