Supporting Information

Mixed Precious-Group Metal-Organic Frameworks:

Case Study of the HKUST-1 Analogue $[Ru_xRh_{3-x}(BTC)_2]$

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Experimental Details

General considerations

Trimesic acid (Sigma-Aldrich), $RuCl_3 \cdot x\ H_2O$ (Precious Metals Online), $Rh_2(OAc)_4$ (Sigma-Aldrich) and HPLC-grade acetone and ethanol (VWR Chemicals) were purchased commercially and used without further purification. Ultra-pure water was obtained using a Milli-Q purification system (18.2 MΩ cm^{-1}). Technical dichloromethane was purified using a MBraun SPS-800. $Ru_2(OAc)_4Cl$ was synthesized following literature procedures.[1] Desolvated MOFs were handled in a glovebox using argon (>99.996%; Westfalen).

Instrumentation

Powder X-Ray diffraction

All diffraction patterns were collected on a PANalytical Empyrean equipped with a Cu X-ray tube (λ = 0.154 nm) operated at 45 kV and 40 mA in a 2Θ range of 5-50° in steps of 0.0065651° (2Θ) with 6.3025 s/step. The incident beam was focussed on the sample through a focusing beam mirror with a 1/16° divergence slit and a nickel beta filter (0.2 mm). A PIXcel1D detector was used in receiving mode with a 1/8° anti-scatter slit and 0.04 rad soller slits. The activated samples were filled in borosilicate capillaries of 0.5 mm inner diameter and mounted onto a capillary spinner.

Elemental Analysis & ICP-MS

Determination of the elemental composition was performed together with the microanalytical laboratories of the chemistry department at the Technical University of Munich. Determination of C, H, N and S was carried out with a Hekatech EuroEA elemental analyser. Ru and Rh were initially determined after digestion of activated MOF samples in sulfuric acid at up to 200 °C with both atomic absorption spectroscopy (AAS) as well as inductively coupled plasma – mass spectrometry detection (ICP-MS). Those digestions at ambient pressure turned out to provide underestimated metal contents. This was potentially due to formation of volatile ruthenium oxide and chloride species.[2, 3]

1. R. W. Mitchell, A. Spencer and G. Wilkinson, *J. Chem. Soc., Dalton Trans.*, 1973, DOI: 10.1039/DT9730000846, 846-854.
2. Y. D. Kim, H. Over, G. Krabbes and G. Ertl, *Top. Catal.*, 2000, **14**, 95-100.
3. M. Binnewies, R. Glaum, M. Schmidt and P. Schmidt, *Chemical Vapor Transport Reactions*, 2012.

Thus, microwave-assisted digestions were developed, and quantitative analysis was performed using ICP-MS:

Microwave assisted sample digestion

Prior to quantitative measurements, all samples were digested adding a mixture of 1 mL HCl (30% (w/w), suprapur, Merck, Darmstadt, Germany) and 8 mL HNO_3 (65% (w/w), suprapur, Merck) to 1 to 3 mg of the Ru and Rh containing sample. All samples were weighted under inert gas to avoid hygroscopic mass effects. Samples and reagents were filled in a PTFE liner fixed in a closed pressure vessel. The digestion was performed in an ETHOS.lab microwave system (MLS, Leutkirch, Germany). After subjecting the samples to the digestion process including a ramp time of 10 min to 240 °C

followed by 30 min holding this temperature and a cooling step for another 120 min, clear orange solutions were obtained. These solutions were filled up to 50 mL using ultra-pure water (UPW) with a resistivity of 18.2 MΩ cm^{-1} provided by a Milli-Q-Gradient-System (Millipore GmbH, Billerica, MA, USA). For quantification, all digests were diluted 1:200 in a 1.625% HNO_3 (w/w) solution.

Quantification of Ru and Rh in digested samples

Quantitative analysis of Ru and Rh in the digested samples was carried out using an Agilent 7900 ICP-Q-MS (Agilent, Santa Clara, CA, USA) equipped with a collision cell technique (CCT) and an autosampler SPS4 (Agilent). Argon 4.8 was used as plasma gas. ^{101}Ru and ^{103}Rh were chosen as target masses to avoid potential isobaric interferences and measured in triplicate. ^{115}In was used as internal standard by adding traces of a stock solution containing 400 µg L^{-1} In (in 1.625% HNO_3 (w/w), Merck) *via* a Y-connecting tubing to the sample immediately before nebulization. Integration time for detection of ^{101}Ru and ^{103}Rh was set to 0.1 s, whereby ^{101}Ru was measured in He-CCT and ^{103}Rh in high-energy He-CCT to overcome polyatomic interferences. For calibration, solutions containing simultaneously Ru and Rh in a range of 1 to 50 µg L^{-1} (in 1.625% HNO_3) were prepared from the stock solution Periodic Table Mix II (Sigma Aldrich, St. Louis, MO, USA). UPW was used for all kinds of dilutions, HNO_3 (65% (w/w), suprapur) was used for acidification. All calibration solutions were measured under the same conditions as used for the samples.

Calculation of the sum formula

Based on determined elemental contents and assuming oxygen to complete the 100 wt-%, sum formulas were calculated and normalized to three metal atoms per repeating unit. The GRG-nonlinear solver function implemented in Microsoft Excel was used for compositional fittings assuming acetate and BTC as exclusive organic framework components. It should be mentioned, that other efforts to determine organic ligand ratios (BTC to acetate) have not been successful as typical sample digestions in diluted acids were not quantitative.

MAS-NMR spectroscopy

Magic angle spinning-NMR spectra were recorded on a Bruker Avance 300 with measurement frequencies of 300.130 MHz (^{1}H) and 75.468 MHz (^{13}C) in 4 mm ZrO_2 rotors at ambient temperature with D1 = 2 s. Sample tubes were rotated with 15 kHz. Proton spectra were recorded with single pulse technique (250 ppm spectral width, each 200 scans), ^{13}C spectra with cross polarisation (CPMAS) (0%, 50%, 100% Rh sample with 84,104; 30,440 and 9,800 scans respectively). Adamantane was used as external (secondary) reference with 2.00 ppm (^{1}H) / 29.472 ppm (^{13}C) chemical shift versus tetramethylsilane.

HR-TEM with EDS mapping

Samples were measured by High Resolution Transmission Electron Microscope (HRTEM) Titan G2 (FEI) with image corrector on accelerating voltage 80 kV. Images were taken with BM UltraScan CCD camera (Gatan). Energy Dispersive Spectroscopy (EDS) was performed in Scanning TEM (STEM) mode by Super-X system with four silicon drift detectors (Bruker). STEM images were taken with HAADF detector 3000 (Fishione). Spectra acquisition time was set to 600 s.

X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectra were recorded on a *Leybold-Heraeus* LHS 10 spectrometer using a non-monochromatized Al K_α source (1486.7 eV). The powder samples were pressed into cavities and measured as pellets. Sample preparation and transfer into the XPS spectrometer were carried out under argon atmosphere. All spectra were recorded in an ultra-high vacuum chamber at a pressure below 5×10^{-8} mbar. The analyzer was operated at a constant pass energy of 100 eV leading to an

energy resolution with a full width at half-maximum (FWHM) of ~1.1 eV. In addition, a constant pass energy of 20 eV was used for the Ru 3d/C 1s region to gain spectral resolution (~0.8 eV FWHM). The energy scale of the spectra was corrected for sample charging by using the O 1s main signal (531 eV). Core level spectra were deconvoluted by using Doniach-Sunjic functions and linear background subtraction. To quantify the molar Rh/Ru ratio the Rh 3d and the Ru $3p_{3/2}$ signals were integrated due the overlap of Ru 3d and C 1s. Depth profiling was carried out by removing the top layers of the samples using Ar ion sputtering and subsequent XPS measurements. For sputtering, a *Leybold-Heraeus* IQE 12 ion gun was operated at an Ar ion current of 0.6 µA and a kinetic energy of 2 kV leading to a sputtering rate of ~ 1 Å/min.

Nitrogen and carbon dioxide sorption measurements

Sorption experiments were conducted using a Micromeritics 3Flex with 50 to 80 mg of desolvated sample. Prior to the measurement each sample was additionally degassed at 150°C for >10h. Nitrogen isotherms were recorded at 77K, CO_2 isotherms at 195K respectively. The BET surface area was calculated using data points in the relative pressure range of 0.01 to 0.1 in the adsorption branch with the Rouquerol consistency criteria taken into account.

Fourier-transform infrared spectroscopy

FT-IR spectra were recorded from finely ground activated powder samples under argon atmosphere in a glovebox using a Bruker ALPHA FTIR spectrometer equipped with a Pt attenuated total reflectance (ATR) unit at room temperature in the range of 400 to 4000 cm^{-1} with a resolution of 2 cm^{-1} and 24 scans per measurement. A pyroelectric deuterated L-alanine doped triglycine sulfate (RT-DLaTGS) detector was used.

Raman spectroscopy

Raman spectroscopy was measured with an inVia Reflex Raman System with an optical microscope (Leica DM2700M, 50x magnification) coupled to a Renishaw R04 Raman spectrometer with 532 nm laser wavelength (Laser: RL532C, Class 3B) with activated samples filled into Borosilicate glass capillaries (0.5 mm inner diameter) under argon atmosphere. A Renishaw 266n10 detector was used. All samples were measured with 10 s exposure time, 5 % laser power and 10 accumulations (exception 0%Rh sample: 10s exposure, 1% laser Power, 10 accumulations).

Solid-state UV / Vis spectroscopy

Absorption spectra were recorded with a Shimadzu UV3600Plus UV VIS NIR spectrophotometer from 300 to 800 nm. The system is equipped with halogen and deuterium lamps. R-928 photomultiplier tube (UV & VIS <700 nm) and InGaAs photodiode (VIS >700 nm) were used to detect the light. Automatic change of the lamp and the integrated detector occurred at 395 nm and 700 nm respectively. Samples were pressed between two optical glass plates and boundaries sealed with Teflon® grease under argon.

DFT calculations of Ru- and Rh-paddle-wheel complexes

All calculations have been performed with the Gaussian 16 suite of software[4]. The level of theory included the use of the hybrid DFT functional B3LYP together with the basis set 6-31+G** for C,H,O, Cl.[5,6] Ru and Rh have been described by the Stuttgart-Dresden97-ECP[7].

All structures have been optimized until no negative frequencies haven been calculated by frequency analysis. Frequencies calculation have been also used to determine unscaled frequencies and IR and Raman intensities. UV-VIS spectra of selected singlet state compounds have been calculated by time-dependent DFT[8] taking into account the three most probable electon transitions to singlet and triplet excited states.

4. Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

5. a) A.D. Becke, *J. Chem. Phys*. **1993**, 98, 5648-5652; b) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; c) S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200-1211; d) P.J. Stephens, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, *J.Phys.Chem.* **1994**, 98, 11623-11627.

6. a) W.J. Hehre, R. Ditchfield and J.A. Pople, J. Chem. Phys. **1972**, *56,* 2257-2261 (1972); b) T. Clark, J. Chandrasekhar, G. W. Spitznagel, and P. v. R. Schleyer, *J. Comp. Chem.*, **1983**, *4*, 294-301; c) M.M. Francl, W.J. Petro, W.J. Hehre, J.S. Binkley, M.S. Gordon, D.J. DeFrees and J.A. Pople, *J. Chem. Phys.* **1982**, *77*, 3654-3665.

7. a) A. Bergner, M. Dolg, W. Kuechle, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *80*,1431-1441 ; b) M. Kaupp, P. v. R. Schleyer, H. Stoll, H. Preuss, *J. Chem. Phys.* **1991**, *94*, 1360-1366; c) M. Dolg, H. Stoll, H. Preuss, R.M. Pitzer, *J. Phys. Chem.* **1993**, *97*, 5852-5859.

8. a) R. E. Stratmann, G. E. Scuseria, M. J. Frisch, *J. Chem. Phys.*, **1998**, *109*, 8218-24. b) F. Furche and R. Ahlrichs, *J. Chem. Phys.*, **2002**, *117*, 7433-7447.

Thermogravimetric analysis

Thermal stability of the materials was determined with a Mettler Toledo TGA/DSC 1 in aluminium oxide pans (70 µL with lid) with sample amounts of 1 to 5 mg. Samples of activated materials were taken under inert conditions in a glovebox and transferred to the measurement chamber in screw capped vials immediately prior to the measurement. The following thermal program was applied using synthetic air (20 mL min^{-1}, Westfalen, 80% N_2; 20% O_2): At 30 °C isothermal equilibration (15 min), ramp from 30 °C to 700 °C with 10 K min^{-1}, at 700 °C isothermal equilibration (15 min).

Additional information

Composition

Table S 1: Comparison of total metal contents determined by TG analysis and ICP-MS after digestion.

Sample	TGA residue (metal oxide) [%]	M_{total} (TGA) [%]	M_{total} (ICP) [%]
0 % Rh	48.2	38.9	38.9
5 % Rh	47.7	38.5	37.5
10 % Rh	48.3	39.0	38.2
20 % Rh	47.9	38.7	35.7
50 % Rh	49.9	40.4	39.6
75 % Rh	49.4	40.0	40.2
95 % Rh	48.3	39.2	41.0
100 % Rh	49.6	40.2	40.5

MAS-NMR spectroscopy

To confirm the findings of elemental analysis fittings regarding organic constituents, MAS-NMR was performed with 0%, 50% and 100% Rh samples. Ruthenium containing samples did not produce spectra with valuable information due to paramagnetism of the Ru_2 cores. However, the obtained spectra for 100% Rh sample (pure Rh-BTC) reveal some interesting information. In the ^{1}H-NMR spectrum, two singlets at 1.88 ppm and 8.74 ppm appear together with a set of rotation side bands shifted by the rotational frequency (15 kHz). Unambiguously, the set of signals centred at 1.88 ppm can be assigned to acetate protons while the one centred at 8.74 ppm originates from aromatic BTC protons. Total signal integration (including rotational side bands) indicates a molar BTC to acetate ratio (≈1.4) which is in accordance with the calculated composition based on EA values (≈1.3). The ^{13}C-NMR spectrum shows mainly three independent singlets. These signals can be assigned to carboxylate (182.4 ppm), aromatic (130.5 ppm) and aliphatic (19.4 ppm) carbon atoms representing BTC and acetate as framework constituents. Due to cross-polarization excitation, a quantitative comparison based on ^{13}C-NMR is not suitable. Low intensity signals (191.2; 174.2; 163.2 ppm) may be attributed to traces of carboxylates bound differently.

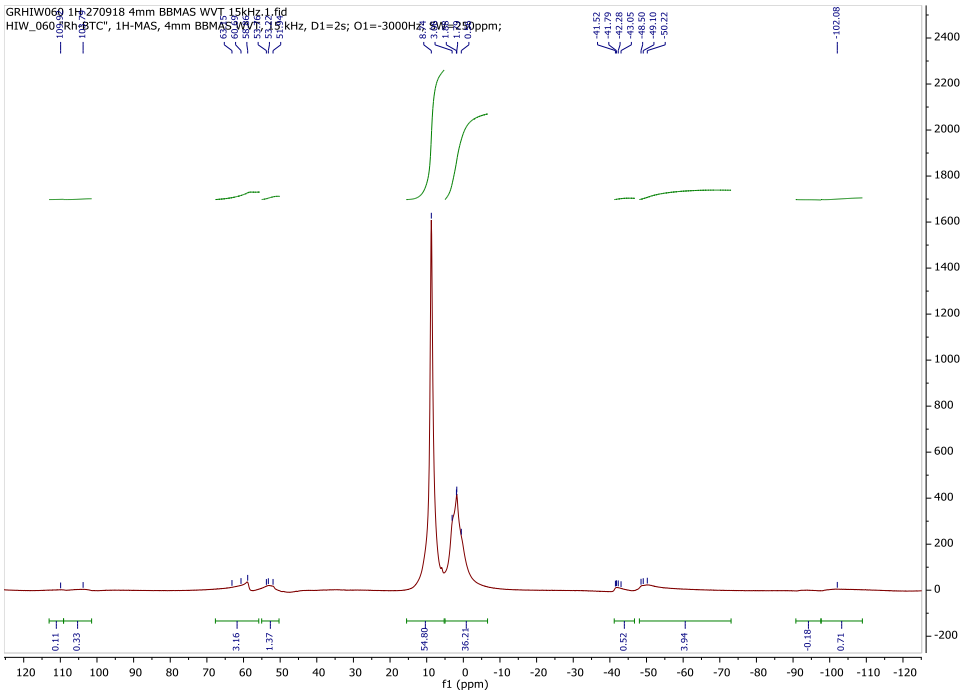

Figure S 1: Proton MAS-NMR spectrum of 100% Rh sample with signal integration.

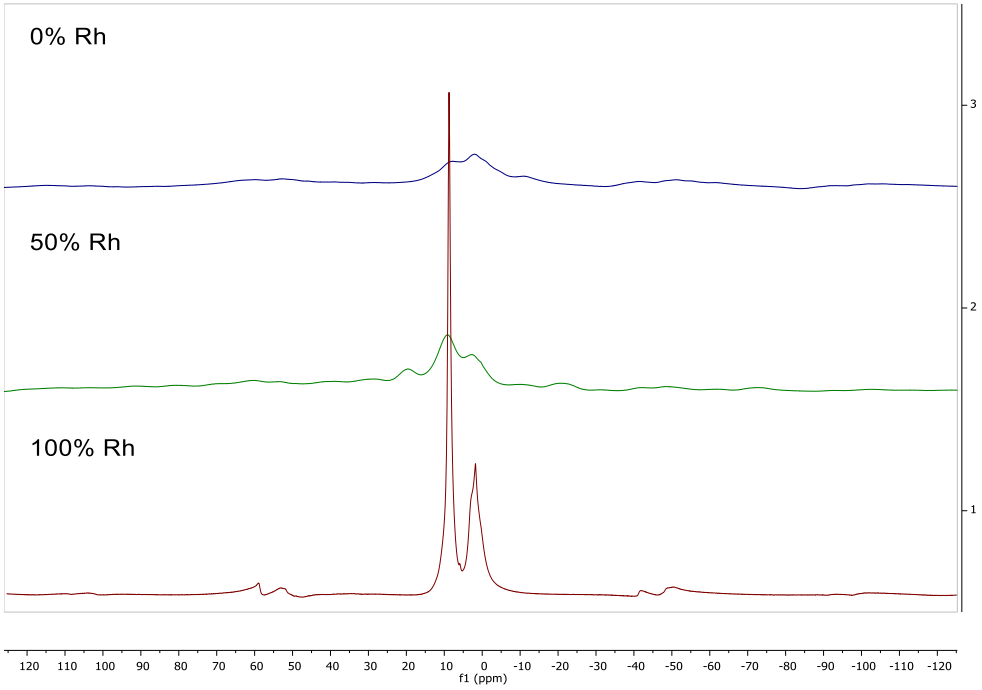

Figure S 2: Proton MAS-NMR spectra of 0%, 50% and 100% Rh samples.

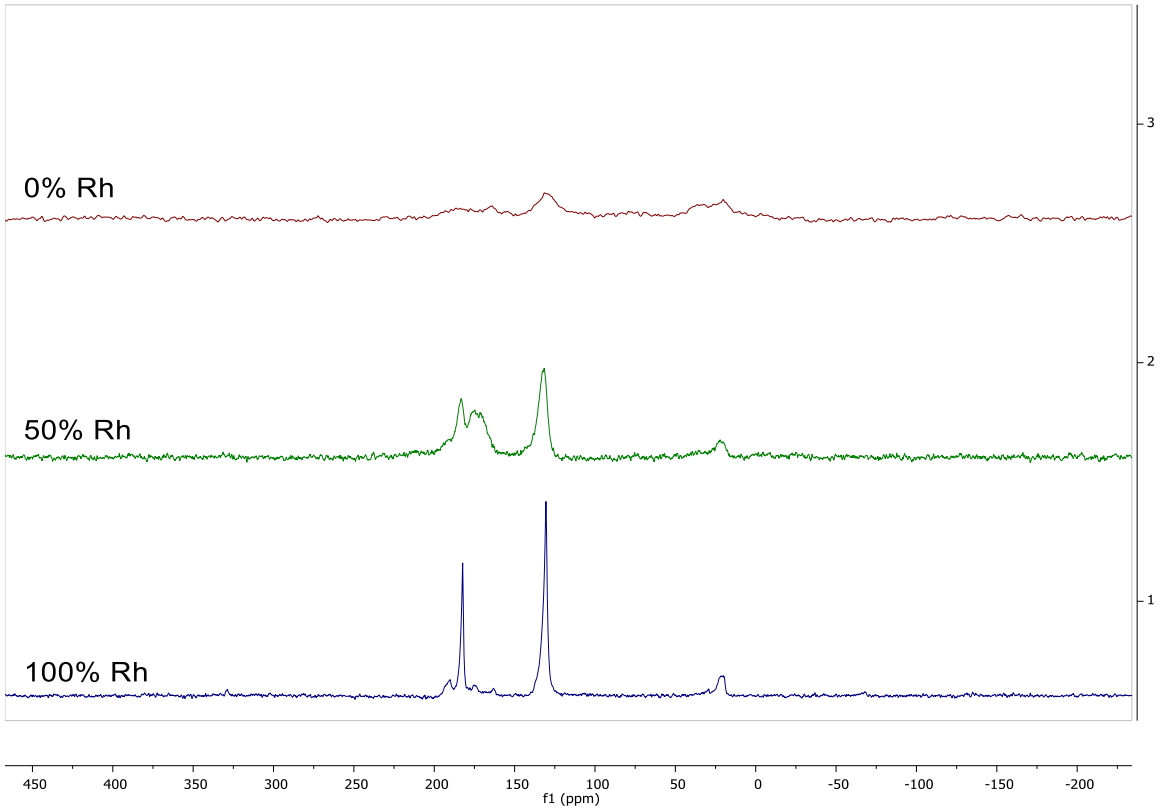

Figure S 3: ^{13}C-MAS-NMR spectra of 0, 50 and 100% Rh samples. Cross polarization was used.

HR-TEM-based elemental mapping

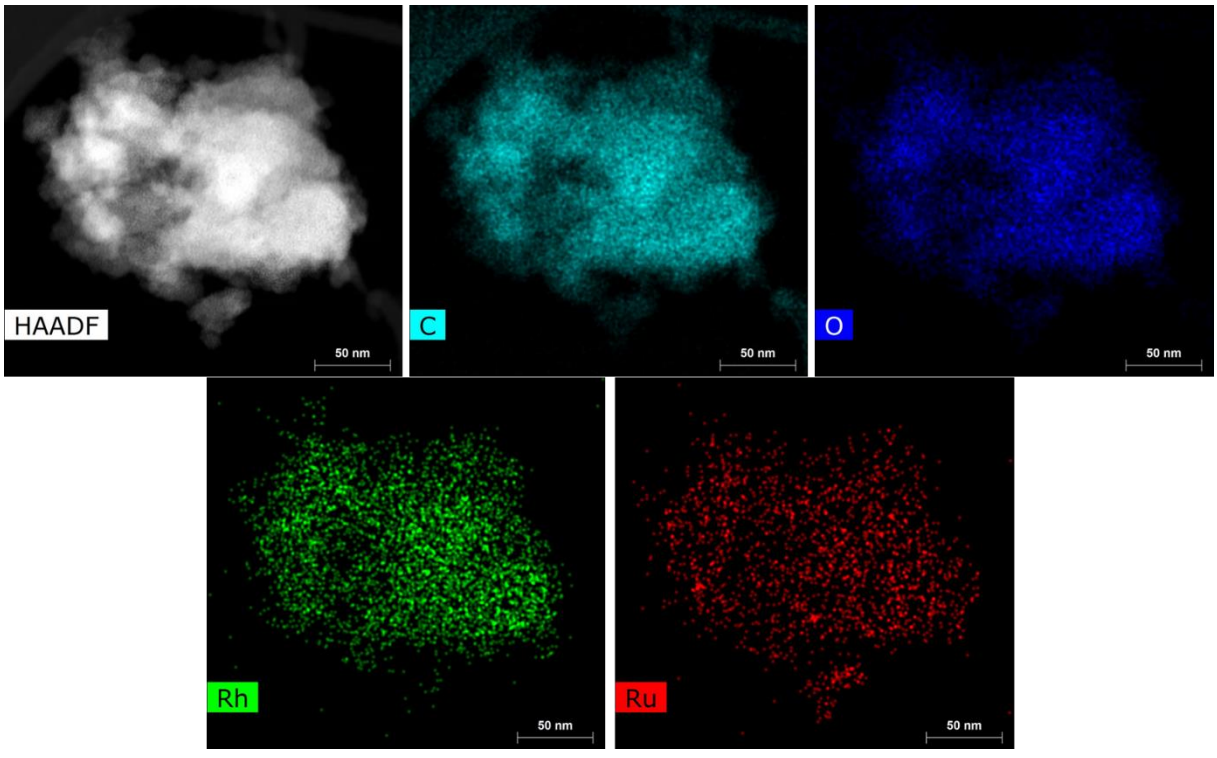

Figure S 4: HR-STEM images of representative particle of 75% Rh sample: From left to right: HAADF image and elemental mapping for C, O, Ru and Rh (map1).

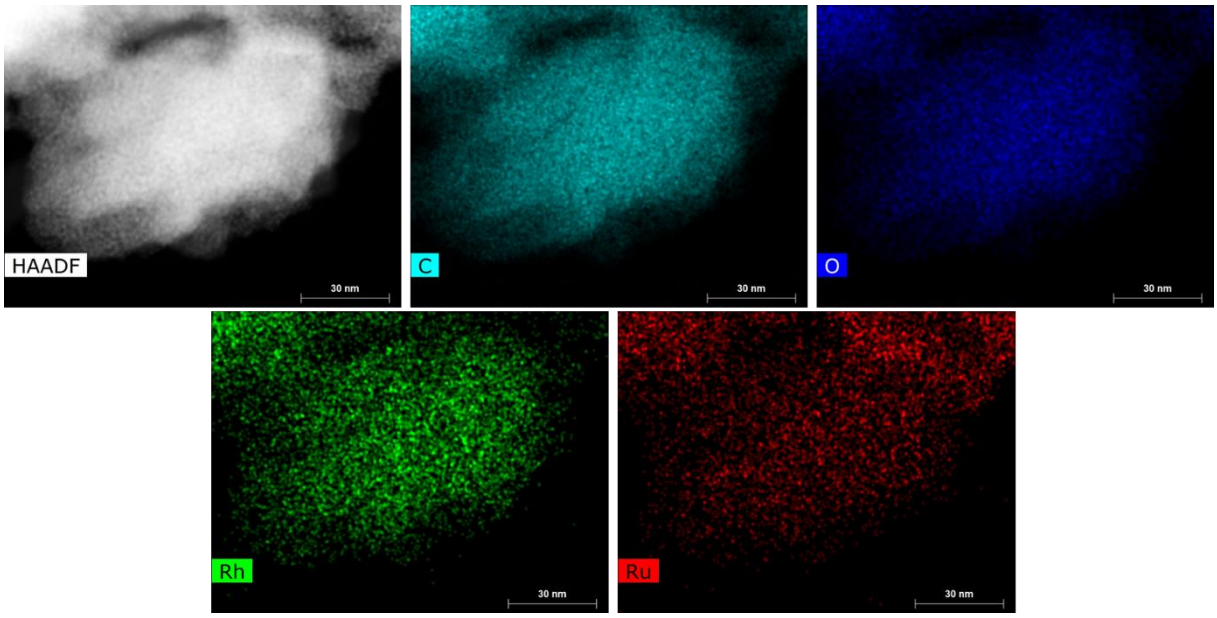

Figure S 5: HR-STEM images of representative particle of 75% Rh sample: From left to right: HAADF image and elemental mapping for C, O, Ru and Rh (map2).

HR-TEM images

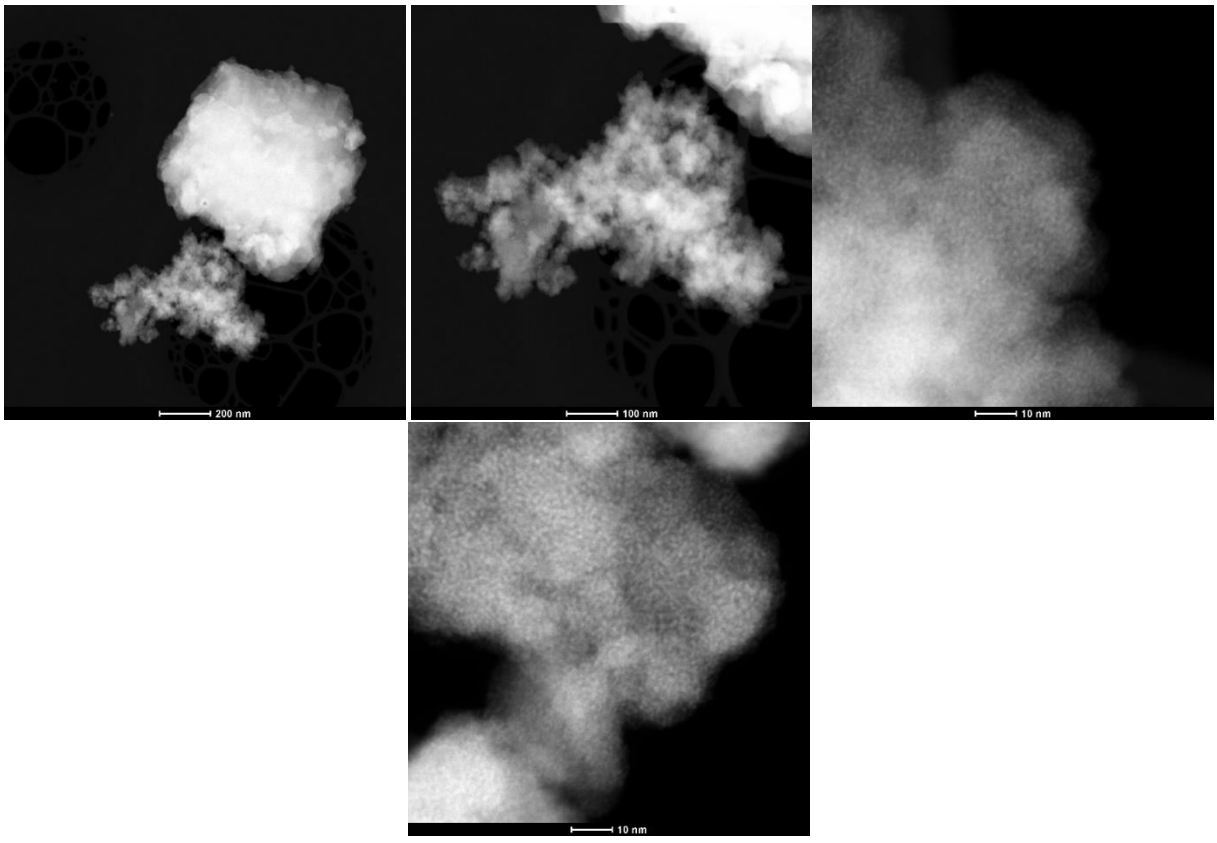

Figure S 6: HAADF-TEM images of 50% Rh sample.

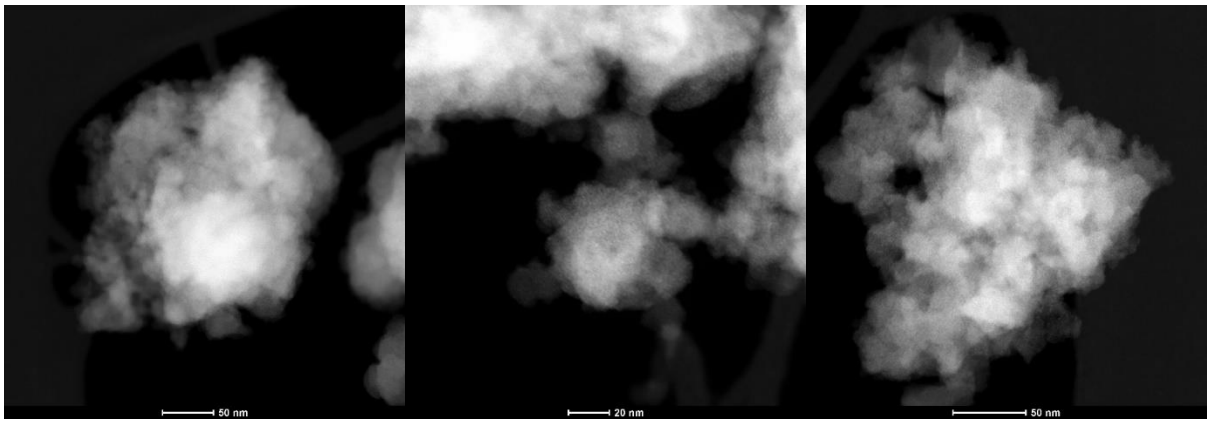

Figure S 7: HAADF-TEM images of 75% Rh sample.

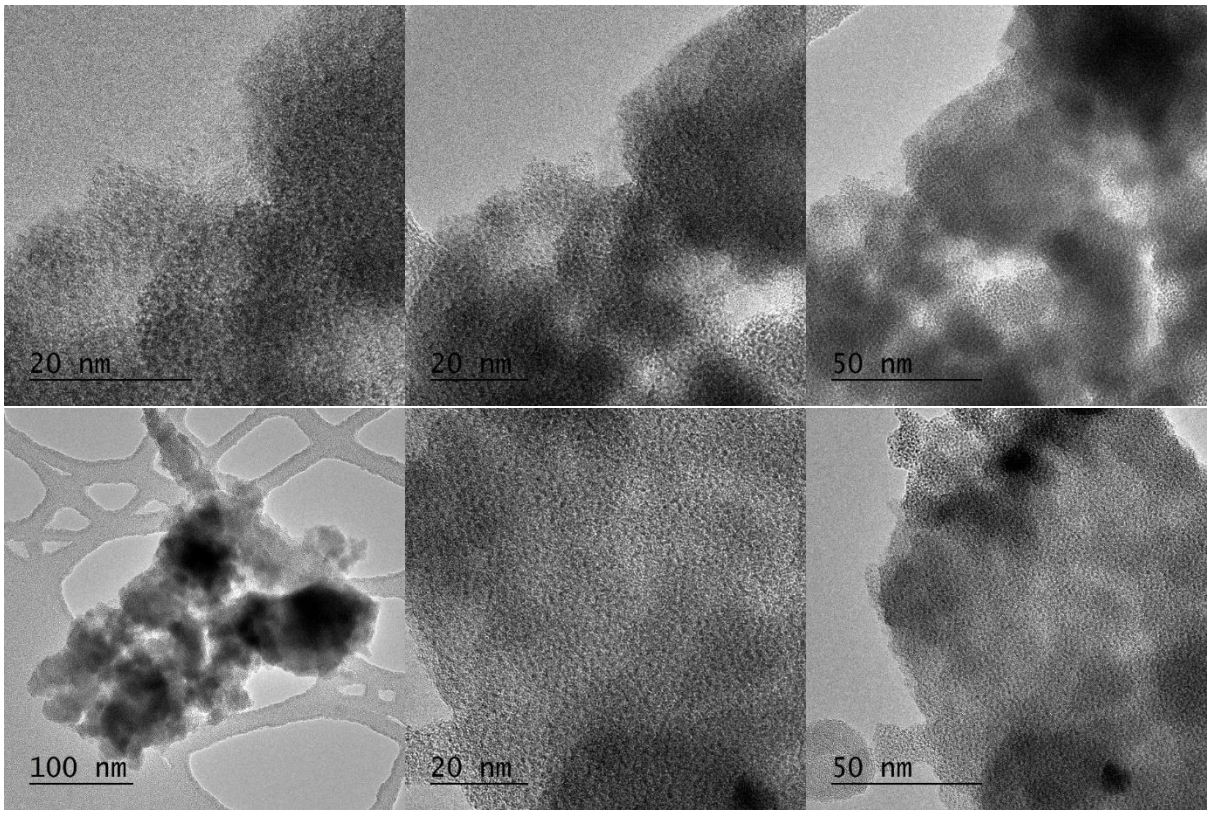

Figure S 8: HR-TEM images of 50% Rh sample.

XPS

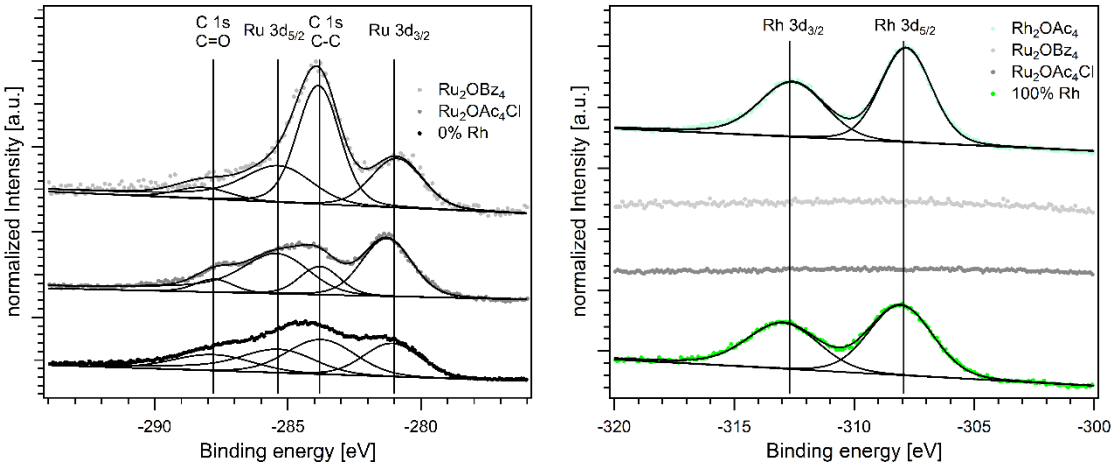

Figure S 9: Left: XP spectra showing Ru 3d and C 1s region of Ru-BTC and Ru containing reference substances. Right: XP spectra showing Rh 3d region of Rh-BTC and Rh-containing and Rh-free reference compounds.

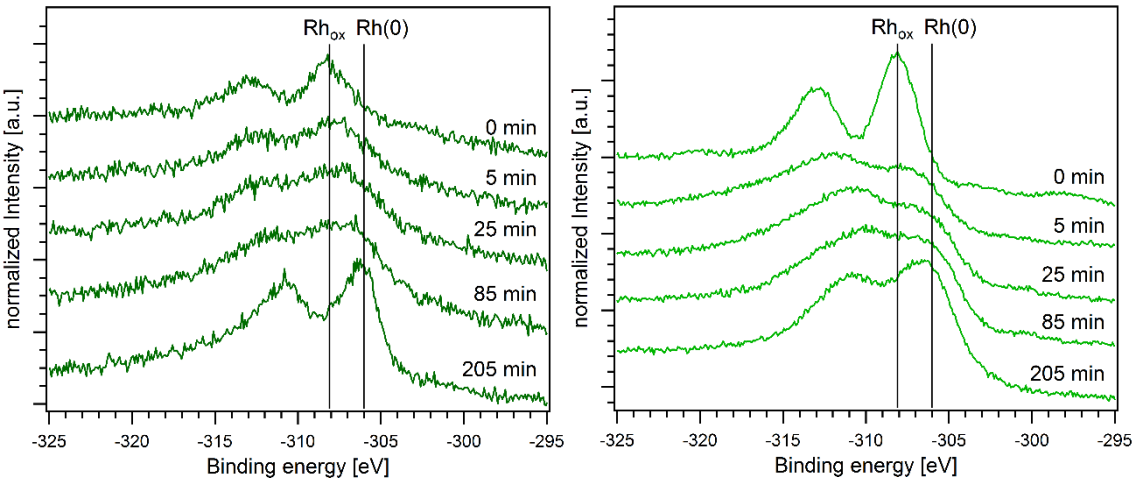

Figure S 10: XP spectra of Rh 3d peaks indicating sputter-induced metalation: Left: 20%Rh sample; Right: 75%Rh sample.

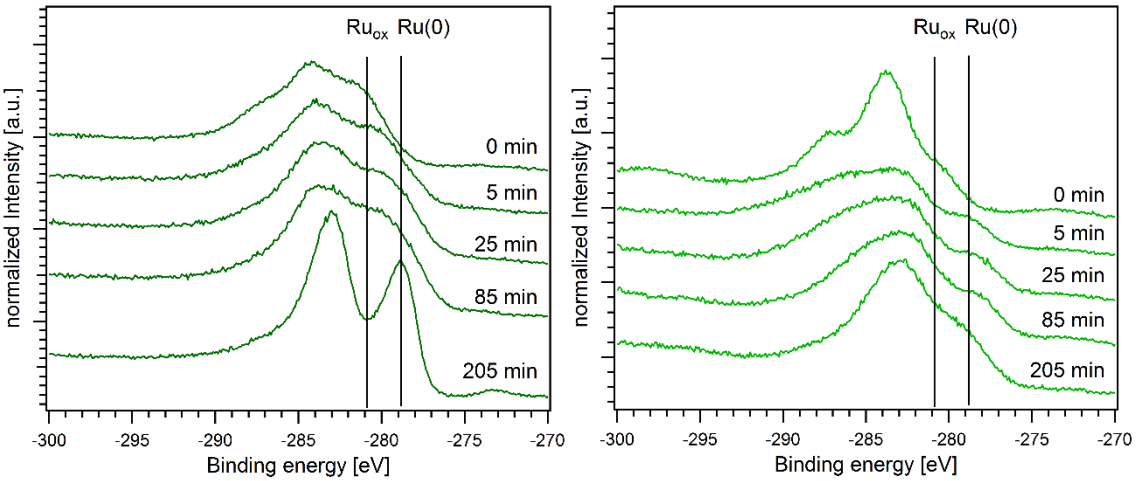

Figure S 11: XP spectra of Ru 3d peaks indicating sputter-induced metalation: Left: 20%Rh sample; Right: 75%Rh sample.

Table S 2: Found Rh content of selected MPG-MOFs related to the total metal content based on XPS.

Sample	Found Rh : M_{total} ratio
0% Rh	0%
20% Rh	21±2%
50% Rh	45±3%
75% Rh	75±2%
100% Rh	100%

Table S 3: Depth profiling of 20% Rh and 75% Rh samples and found Rh contents related to the total metal content

Overall sputtering time	Found Rh : M_{total} ratio	
	20% Rh sample	75% Rh sample
0 min	21±2%	75±2%
5 min	22±2%	76±2%
25 min	21±2%	75±2%
85 min	24±4%	75±2%
205 min	24±4%	76±2%

Sorption experiments

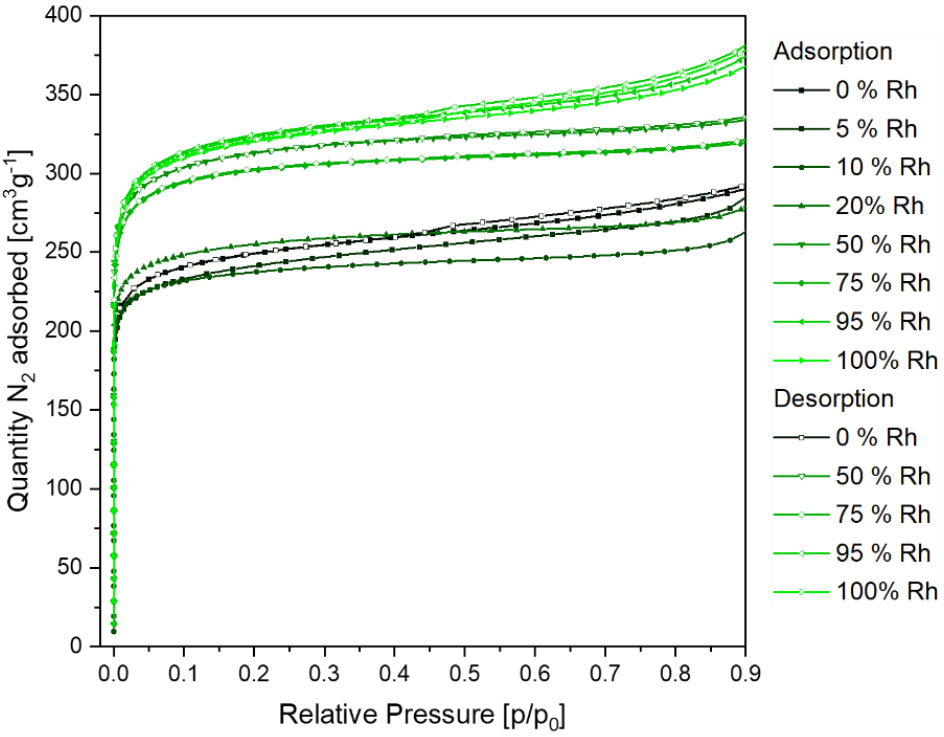

Figure S 12: Nitrogen sorption isotherms showing both adsorption and desorption branches. Isotherms were recorded at 77K. Closed symbols represent data points from adsorption branch, open symbols represent data points from desorption branch.

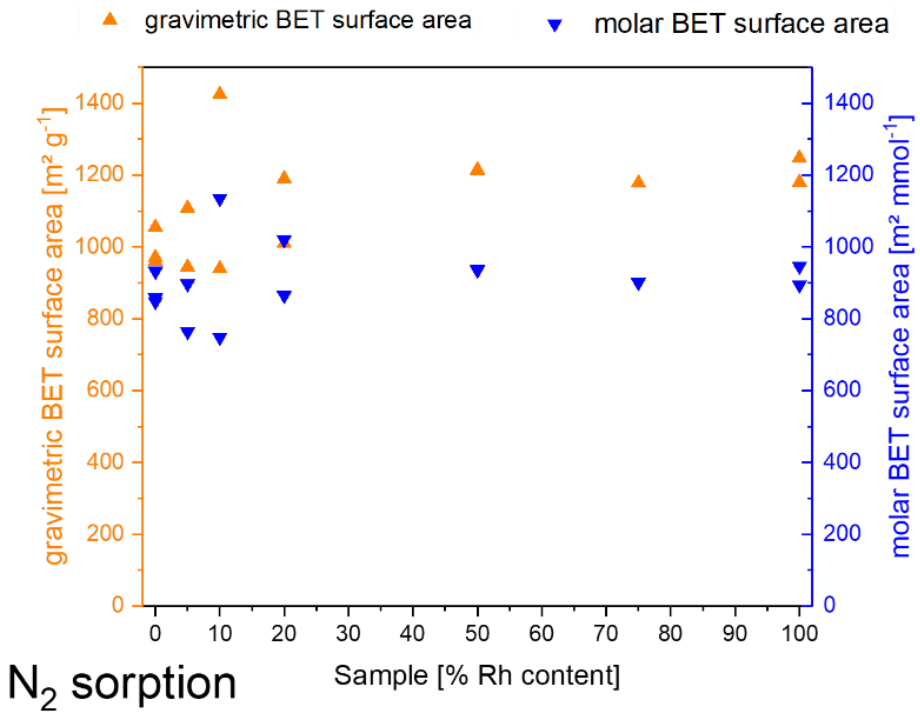

Figure S 13: Trend of gravimetric and molar BET surface areas of samples from different batches. Data was obtained with nitrogen as sorptive at 77 K.

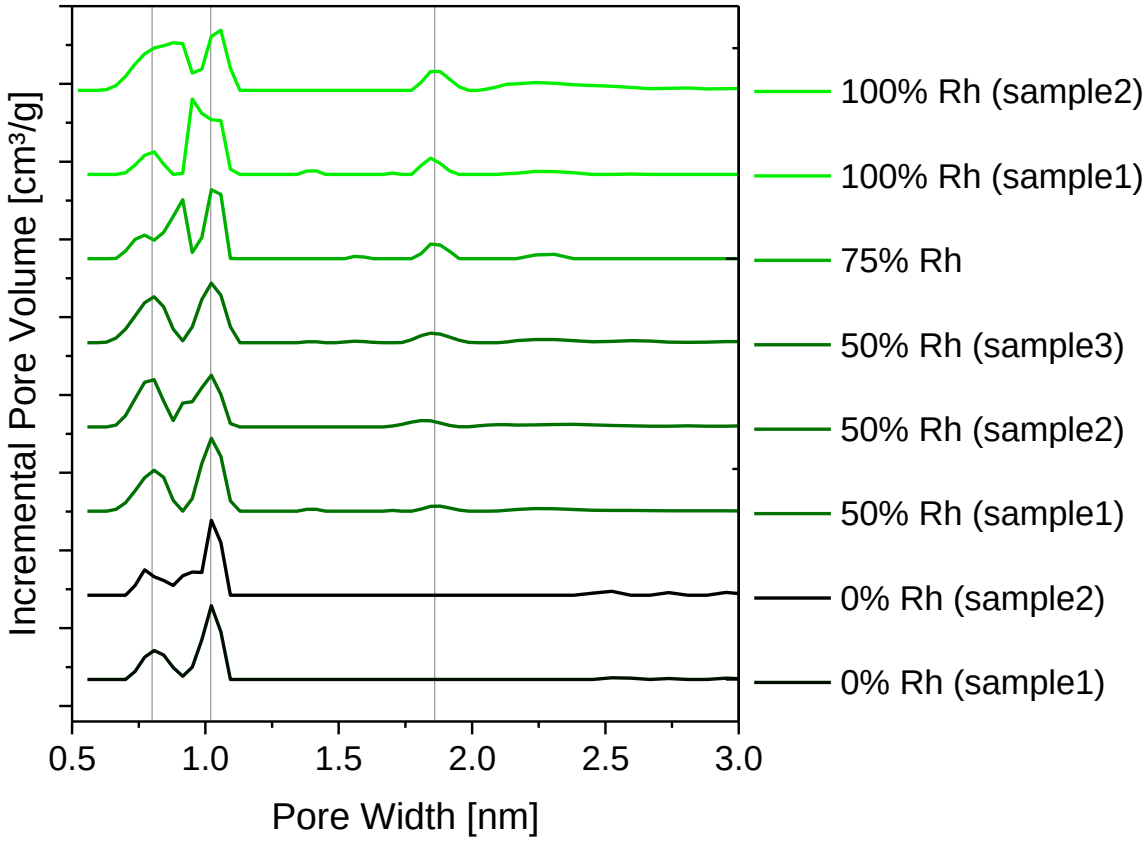

Figure S 14: DFT-based pore size distribution of different RuRh-BTC samples calculated from adsorption branches of sorption experiments. Broadening of pore size distribution and evolution of mesopore fractions occur upon Rh increase. Absolute pore size values might be shifted due to the chosen parameters (cylindrical pores on a silicon oxide substrate)

Vibrational spectroscopy

Table S 4: Experimental vibration frequencies in RuRh-MPG-MOFs and calculated modes based on the following model compounds: [a] $[Rh_2(OBz)_4(H_2O)_2]$, [b] $[Rh_2(H_2BTC)_4]$, [c] $[Rh_2(OBz)_4Cl_2]^{2-}$, [d] $[Rh_2(OBz)_4Cl]^-$, [e] $[Rh_2(OAc)_4]$, [f] $[Rh_2(OAc)_3(OBz)]$, [g] cis-$[Rh_2(OAc)_2(OBz)_2]$, [h] trans-$[Rh_2(OAc)_2(OBz)_2]$, [i] $[Rh_2(OAc)(OBz)_3]$.

Experimental frequencies [cm^{-1}]		Calculated frequencies [cm^{-1}]		Assigned vibration mode
IR mode	Raman mode	IR mode	Raman mode	
		1767[b]	1767[b]	$\nu_{as}(COOH)_{free\ acid}$
1687	1688			$\nu_{as}(COO)_{\ low\ coord}$
1622	1606	1622[b], 1627[d], 1604[e], 1609[f], 1612[i]	1611[b],	$\nu_{as}(COO) + \delta_{ip}(C\text{-}H_{arom})$
		1617[a]	1617[a]	$\nu_{as}(COO) + \nu_s(C{=}C_{arom})$
1577		1575		$\nu_{as}(COO) + \nu_s(C{=}C_{arom})$
	1503		1508[a], 1511[e], 1510[f]	$\nu_{as}(COO)$
	1452		1453[b]	$\nu_s(COO) + \delta_{ip}(C\text{-}H_{arom})$
1448		1446[b]		$\delta_{ip}(C\text{-}H_{arom})$
		1457[e]		$\delta(C\text{-}H_{OAc})$
1438		1439[e], 1434[i], 1425[i]		$\delta(C\text{-}H_{OAc})$
	1383	1395[a]	1395, 1411[a]	$\nu_s(COO)$
1366		1351[b]		$\nu_s(COO)$
1115		1176[a], 1151[b], 1113[b]	1141[a]	$\delta_{ip}(C\text{-}H_{arom})$
	1003		997[a]	$\nu_s(C{=}C_{arom})$
939		942[b]		$\delta_{oop}(C\text{-}H_{arom})$
	845		852, 859[a], 845[f]	$\delta_{ip}(COO)$
	792		804[a]	$\delta_{oop}(COO\ \&C\text{-}H_{arom})$
732-738		712[a], 740[b]		$\delta_{oop}(C\text{-}R_{arom})$
		685[e]		$\delta_{ip}(COO)$
523		515[a], 521[c], 524[c], 515[g]	515[c]	$\nu_{as}(ORhO)$
		529[b]		$\delta(C{=}C_{arom}) + \nu_{as}(ORhO)$
	375		357[c]	$\nu(Rh\text{-}Rh\text{-}Cl)$
			357[f], 358[g], 357[i]	$\nu_s(ORhO)$
	333		345[a], 318, 346[e], 340[f], 344[h]	$\nu(Rh\text{-}Rh)$
	278			$\nu(Rh\text{-}Cl)$
			245[d]	$\nu(Rh\text{-}Rh\text{-}Cl)$
	250 (Rh-BTC)		225[c]	$\nu_s(Rh\text{-}Rh) + \delta_{oop}(COO)$
	150			$\nu(Rh\text{-}Rh)$
			148[c]	$\nu_s(Rh\text{-}Cl)_2$
			148[e], 150[f], 149[g], 152[i]	$\delta(PW)$

FT-IR spectroscopy

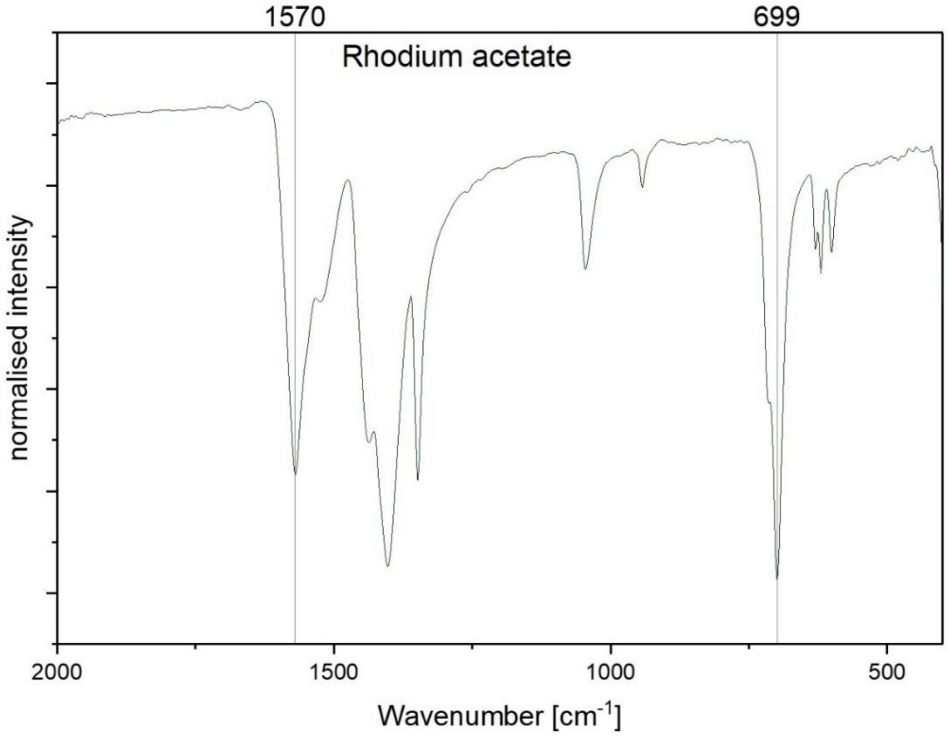

Figure S 15: FT-IR spectrum of dirhodium tetraacetate.

SS-UV / VIS spectroscopy

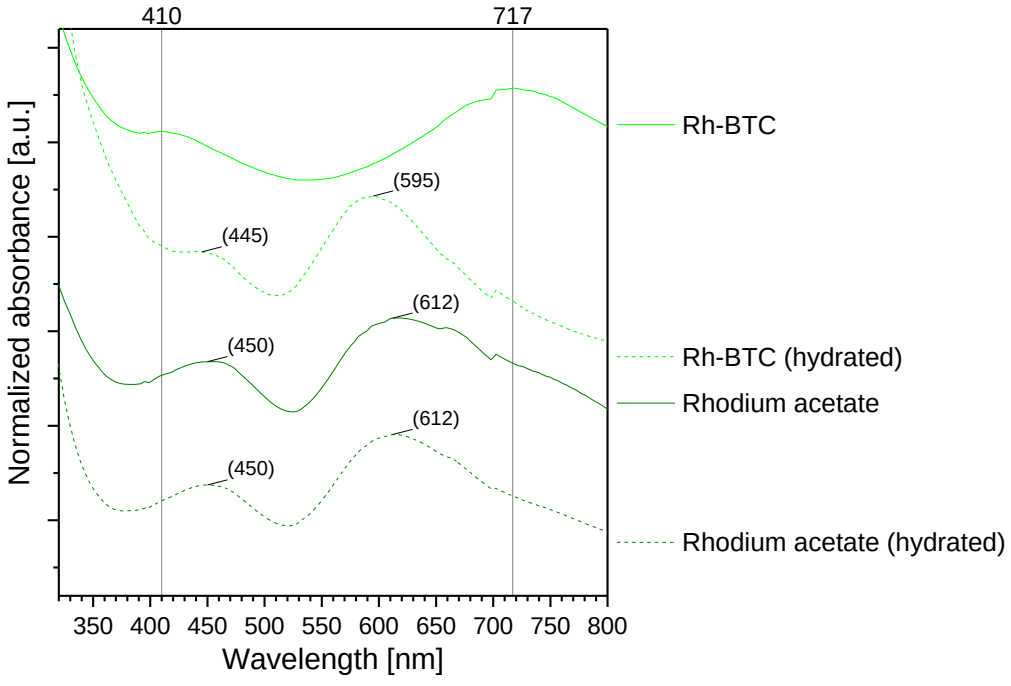

Figure S 16: SS-UV / VIS spectra of activated Rh-BTC and after rehydration in comparison with Rhodium acetate.

Table S 5: Comparison of optical properties between experimental and theoretical results (this work) and the literature from different dirhodium tetracarboxylates. [a] experimental result, this work; [b] theoretical result, this work; [c] experimental result from Kitchens et al.

Compound	Wavelength band **I** [nm]	Wavelength band **II** [nm]
Rh-BTC activated[a]	410	717
Rh-BTC rehydrated[a]	445	595
$[Rh_2(OAc)_4]$[a]	450	612
$[Rh_2(OAc)_4(H_2O)_2]$[a]	450	612
$[Rh_2(OBz)_4(H_2O)_2]$[b] (singlet)		601
$[Rh_2(OBz)_4(H_2O)_2]$[b] (triplet)		1230
$[Rh_2(OBz)_4]$[b] (singlet)		916
$[Rh_2(OBz)_4]$[b] (triplet)		1025
$[Rh_2(OBz)_4Cl_2]^{2-}$ [b] (singlet)		620
$[Rh_2(OBz)_4Cl]^-$ [b] (singlet)		677
$[Rh_2(OAc)_4]$[b] (singlet)		910
$[Rh_2(OAc)_3(OBz)_1]$[b] (singlet)		912
cis-$[Rh_2(OAc)_2(OBz)_2]$[b] (singlet)		913
Trans-$[Rh_2(OAc)_2(OBz)_2]$[b] (singlet)		914
$[Rh_2(OAc)_1(OBz)_3]$[b] (singlet)		914
$[Rh_2(OAc)_4]$[c]	442	617
$[Rh_2(OAc)_4(H_2O)_2]$[c]	441	584
$[Rh_2(OAc)_4(NH_3)_2]$[c]	442	528

Calculated vibration modes of selected model compounds

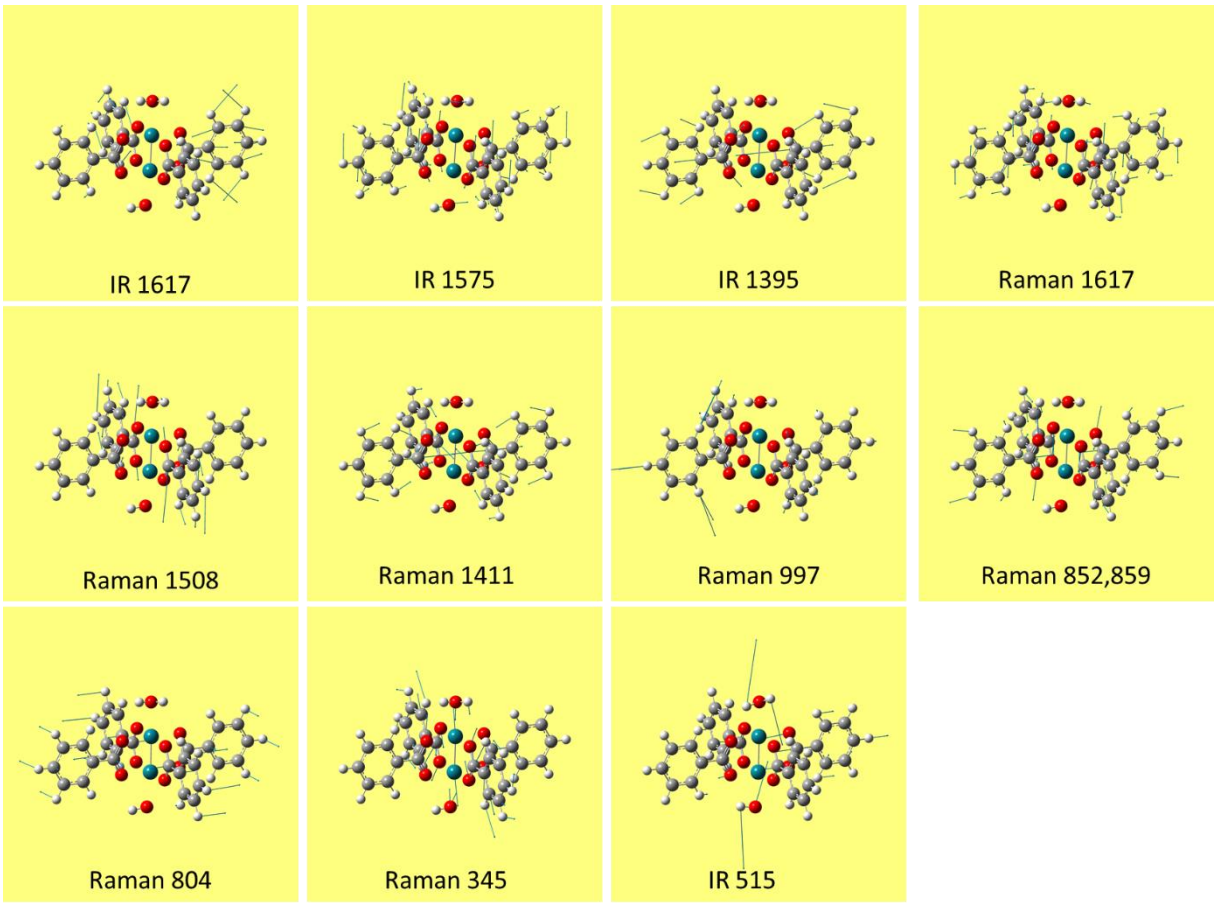

Figure S 17: Most prominent calculated vibrational modes of $[Rh_2(OBz)_4(H_2O)_2]$.

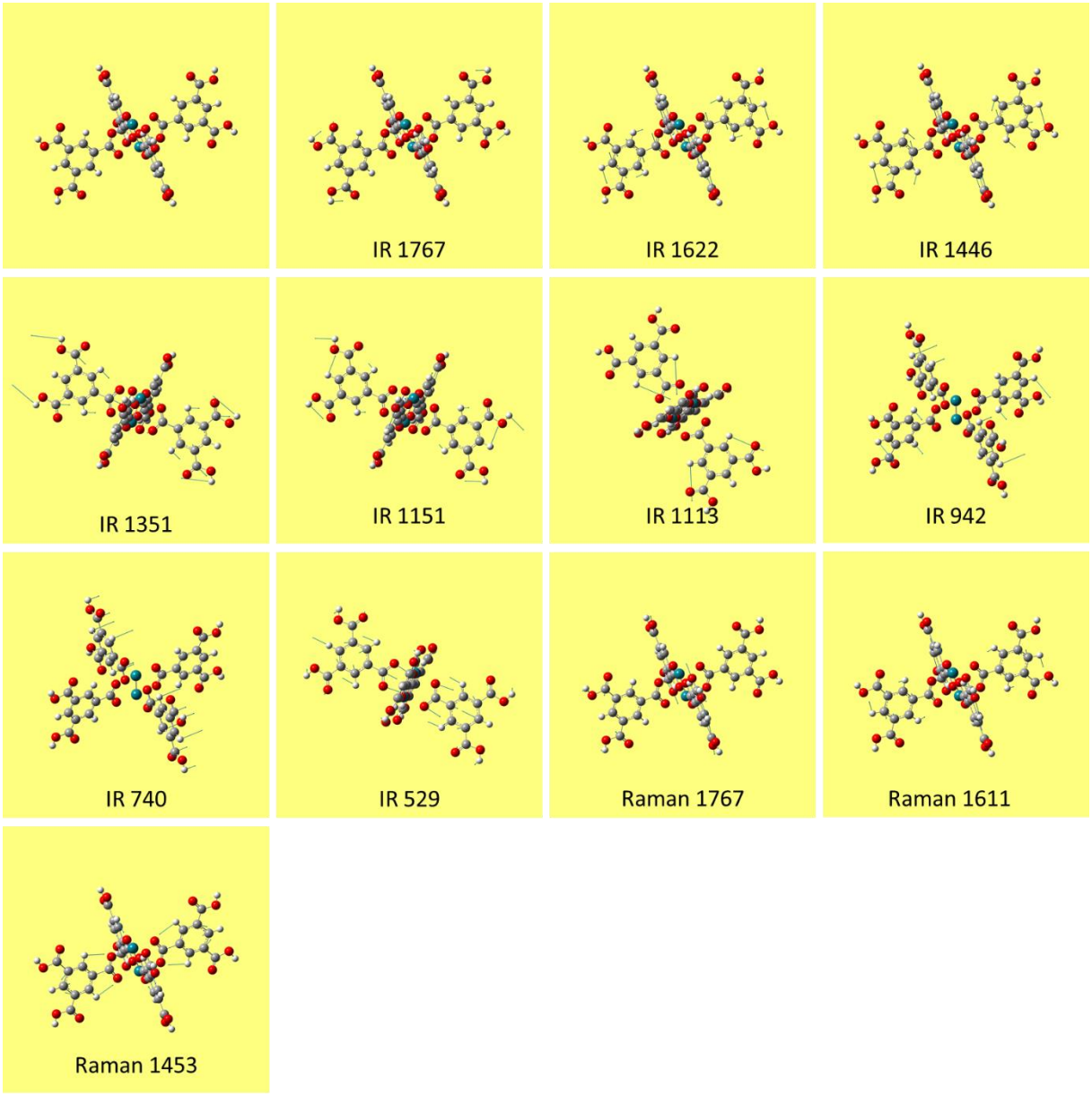

Figure S 18: Most prominent calculated vibrational modes of $[Rh_2(H_2BTC)_4]$.

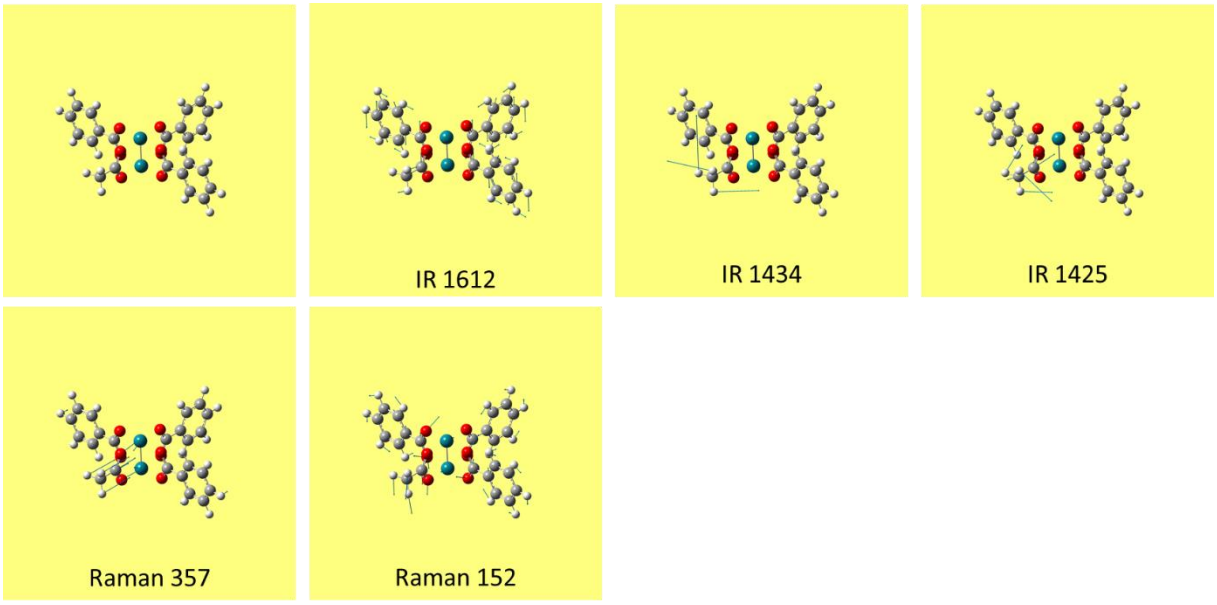

Figure S 19: Most prominent calculated vibrational modes of [$Rh_2(OBz)_3(OAc)$].

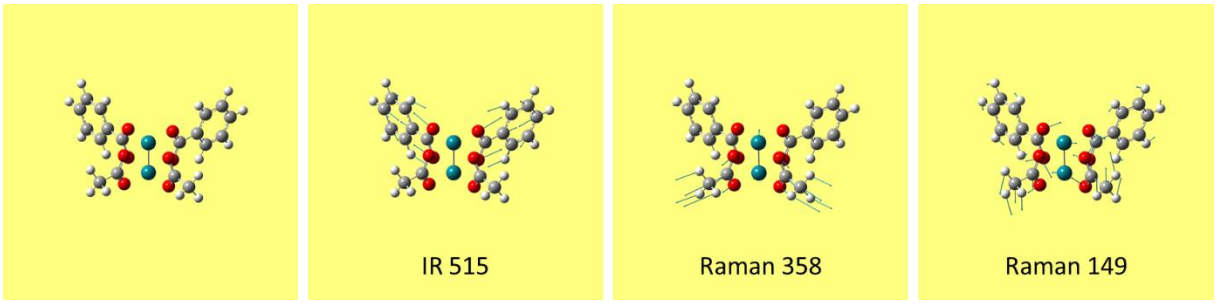

Figure S 20: Most prominent calculated vibrational modes of cis-[$Rh_2(OBz)_2(OAc)_2$].

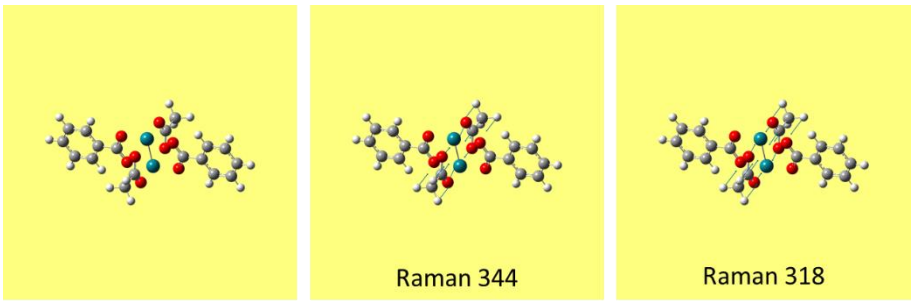

Figure S 21: Most prominent calculated vibrational modes of trans-[$Rh_2(OBz)_2(OAc)_2$].

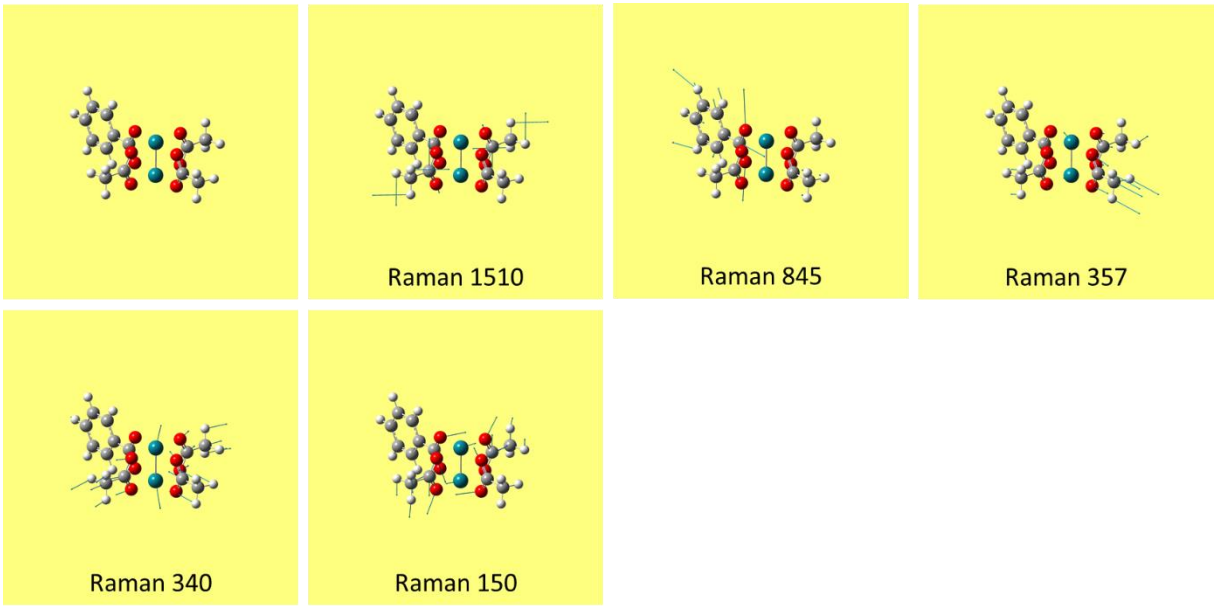

Figure S 22: Most prominent calculated vibrational modes of [$Rh_2(OBz)(OAc)_3$].

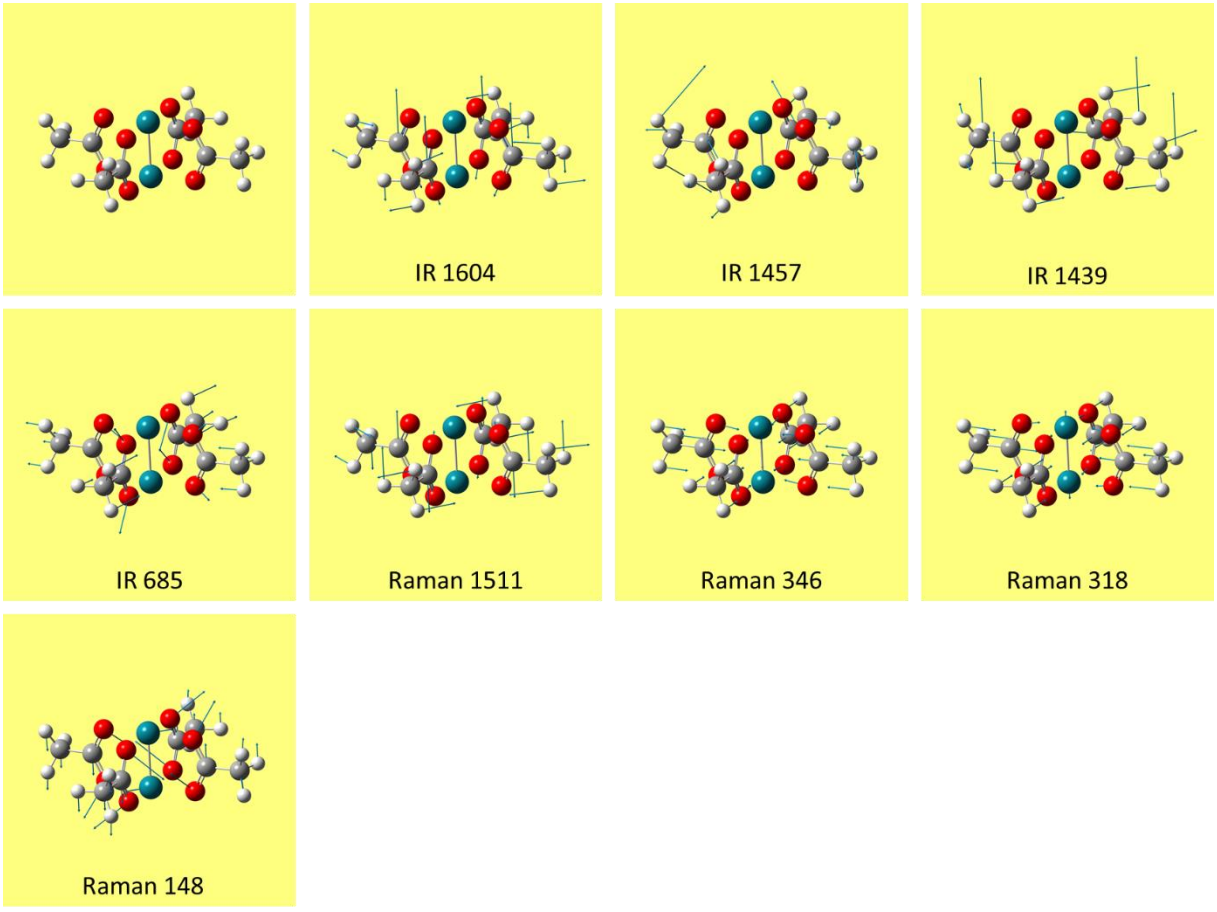

Figure S 23: Most prominent calculated vibrational modes of [$Rh_2(OAc)_4$].

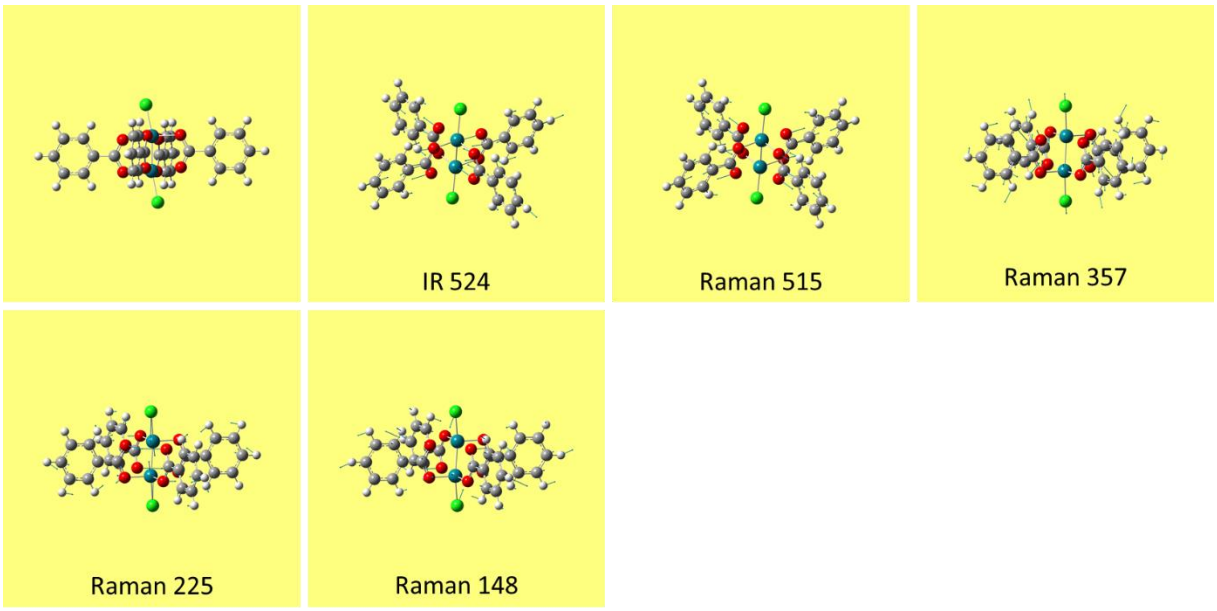

Figure S 24: Most prominent calculated vibrational modes of $[Rh_2(OBz)_4CL_2]^{2-}$.

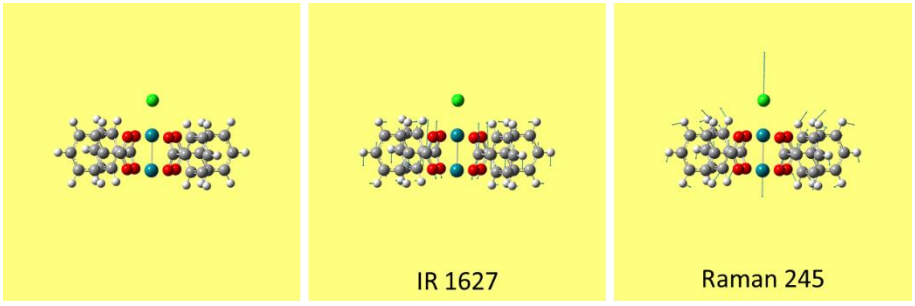

Figure S 25: Most prominent calculated vibrational modes of $[Rh_2(OBz)_4Cl]^{-}$.

Calculated molecules for the comparison of vibrational and UV/VIS spectra

Geometries and energies

$[Rh_2(OBz)_4(H_2O)_2]$ (singlet)

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.863670	6.328446	-0.049415
2	6	0	-2.561080	5.715196	1.170524
3	6	0	-1.986406	4.444238	1.190181
4	6	0	-1.709466	3.778066	-0.012294
5	6	0	-2.013857	4.396048	-1.234147
6	6	0	-2.589397	5.666629	-1.250528
7	6	0	-1.093569	2.414807	0.001859
8	8	0	-0.854186	1.888338	1.142127
9	45	0	-0.011569	0.001451	1.203582
10	8	0	0.045219	0.193758	3.588471
11	8	0	-0.850695	1.875089	-1.125223
12	45	0	-0.006639	-0.009389	-1.203581
13	8	0	0.175927	-0.095563	-3.588470
14	8	0	1.885016	0.832811	-1.133073
15	6	0	2.416419	1.081374	0.000084
16	6	0	3.781576	1.693595	0.000064
17	6	0	4.460808	1.904462	1.208828
18	6	0	5.734037	2.474180	1.207455
19	6	0	6.336748	2.840703	-0.000024
20	6	0	5.662296	2.633773	-1.207461
21	6	0	4.390478	2.060925	-1.208747
22	8	0	1.877211	0.850175	1.133216
23	8	0	0.838279	-1.895232	-1.142190
24	6	0	1.072056	-2.424233	-0.001920
25	6	0	1.681110	-3.790562	0.012220
26	6	0	1.941740	-4.428225	1.234083
27	6	0	2.509651	-5.702236	1.250458
28	6	0	2.821699	-6.347069	0.049329
29	6	0	2.563197	-5.713992	-1.170622
30	6	0	1.994468	-4.440364	-1.190270
31	8	0	0.830569	-1.883895	1.125155
32	8	0	-1.884869	-0.858659	-1.134240
33	6	0	-2.423794	-1.084556	-0.000048
34	6	0	-3.788350	-1.696739	-0.000018
35	6	0	-4.405305	-2.041686	1.211325
36	6	0	-5.677277	-2.614470	1.209409
37	6	0	-6.341427	-2.843564	0.000087
38	6	0	-5.729164	-2.499201	-1.209285
39	6	0	-4.456125	-1.928781	-1.211307
40	8	0	-1.896601	-0.832527	1.134169
41	1	0	3.982825	1.615008	2.137727
42	1	0	3.856437	1.896175	-2.137590
43	1	0	6.256345	2.632119	2.146533
44	1	0	6.127325	2.919142	-2.146574
45	1	0	7.327770	3.285669	-0.000061
46	1	0	1.693195	-3.915425	2.156516
47	1	0	1.788061	-3.938470	-2.128783
48	1	0	2.708467	-6.192423	2.199054
49	1	0	2.804260	-6.213057	-2.104753
50	1	0	3.264006	-7.339254	0.063732
51	1	0	-3.877301	-1.858704	2.140484
52	1	0	-3.968644	-1.655789	-2.140528
53	1	0	-6.150410	-2.882514	2.149638

54	1	0	-6.243843	-2.674942	-2.149472
55	1	0	-7.332447	-3.288789	0.000131
56	1	0	-1.747730	3.956843	2.128687
57	1	0	-1.796172	3.869367	-2.156555
58	1	0	-2.773598	6.227100	2.104638
59	1	0	-2.824565	6.140473	-2.199112
60	1	0	-3.311964	7.317940	-0.063826
61	1	0	1.102439	0.141956	-3.736666
62	1	0	0.838206	0.728368	3.737348
63	1	0	-0.704195	0.770604	3.793438
64	1	0	0.109557	-1.039144	-3.792523

HF=-2055.2282792

$[Rh_2(OBz)_4(H_2O)_2]$ (triplet)

Charge=0, Multiplicity=3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.977156	0.111825	-0.165867
2	6	0	6.308462	0.167578	1.061018
3	6	0	4.914482	0.141144	1.098272
4	6	0	4.179303	0.060253	-0.093239
5	6	0	4.853705	0.007820	-1.322530
6	6	0	6.247680	0.032198	-1.356385
7	6	0	2.685974	0.033333	-0.064496
8	8	0	2.102791	0.032892	1.072321
9	45	0	-0.009058	0.011360	1.232447
10	8	0	0.983055	-0.315980	3.635019
11	8	0	2.080360	0.010424	-1.184381
12	45	0	0.009124	0.011464	-1.232527
13	8	0	-0.981449	-0.323733	-3.634492
14	8	0	-0.001435	-2.066266	-1.136158
15	6	0	0.007225	-2.648942	0.000008
16	6	0	0.011571	-4.145053	-0.000023
17	6	0	-0.135990	-4.850971	1.203033
18	6	0	-0.134468	-6.245818	1.201182
19	6	0	0.019778	-6.945060	-0.000049
20	6	0	0.169925	-6.244904	-1.201267
21	6	0	0.163272	-4.850072	-1.203091
22	8	0	0.012516	-2.066283	1.136185
23	8	0	-2.102842	0.021892	-1.072217
24	6	0	-2.685998	0.018921	0.064613
25	6	0	-4.179458	0.037258	0.093355
26	6	0	-4.853562	-0.019934	1.322596
27	6	0	-6.247657	-0.003728	1.356438
28	6	0	-6.977566	0.072459	0.165960
29	6	0	-6.309189	0.132985	-1.060871
30	6	0	-4.915077	0.114693	-1.098116
31	8	0	-2.080258	-0.000625	1.184489
32	8	0	0.009183	2.074082	-1.137430
33	6	0	-0.007193	2.654588	-0.000127
34	6	0	-0.011696	4.149597	-0.000137
35	6	0	-0.055407	4.852677	1.212891
36	6	0	-0.060080	6.247572	1.210417
37	6	0	-0.020300	6.946946	-0.000154
38	6	0	0.023794	6.247816	-1.210717
39	6	0	0.027695	4.852919	-1.213173
40	8	0	-0.020107	2.073991	1.137155
41	1	0	-0.256383	-4.296926	2.127028
42	1	0	0.280454	-4.295322	-2.127075
43	1	0	-0.253873	-6.787378	2.134961
44	1	0	0.292516	-6.785737	-2.135055

45	1	0	0.022967	-8.031354	-0.000059
46	1	0	-4.274312	-0.075072	2.237385
47	1	0	-4.388885	0.166615	-2.044326
48	1	0	-6.764729	-0.048810	2.310342
49	1	0	-6.873569	0.196066	-1.986519
50	1	0	-8.063407	0.086595	0.194043
51	1	0	-0.085942	4.296058	2.142885
52	1	0	0.061636	4.296492	-2.143163
53	1	0	-0.094810	6.788953	2.151318
54	1	0	0.055184	6.789391	-2.151624
55	1	0	-0.023653	8.033381	-0.000160
56	1	0	4.388017	0.189323	2.044527
57	1	0	4.274769	-0.050074	-2.237348
58	1	0	6.872485	0.233293	1.986701
59	1	0	6.764987	-0.009190	-2.310330
60	1	0	8.062895	0.132337	-0.193958
61	1	0	-0.865818	-1.280895	-3.709147
62	1	0	0.872754	-1.273604	3.711689
63	1	0	1.855389	-0.190593	3.230791
64	1	0	-1.854464	-0.202408	-3.230494

HF=-2055.1797223

$[Rh_2(H_2BTC)_4]$

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.880995	4.928438	0.000058
2	6	0	-4.386301	4.429072	-1.211395
3	6	0	-3.401303	3.434697	-1.211222
4	6	0	-2.908436	2.937103	0.000047
5	6	0	-3.401360	3.434631	1.211323
6	6	0	-4.386350	4.429010	1.211508
7	6	0	-1.856365	1.875053	0.000045
8	8	0	-1.445428	1.460114	-1.133673
9	45	0	0.000034	-0.000002	-1.195222
10	8	0	-1.445398	1.460152	1.133778
11	45	0	0.000003	0.000026	1.195216
12	8	0	-1.460129	-1.445401	1.133722
13	6	0	-1.875025	-1.856370	-0.000005
14	6	0	-2.937110	-2.908410	-0.000002
15	6	0	-3.434818	-3.401166	-1.211272
16	6	0	-4.429205	-4.386150	-1.211445
17	6	0	-4.928499	-4.880918	0.000010
18	6	0	-4.428973	-4.386368	1.211458
19	6	0	-3.434555	-3.401416	1.211272
20	8	0	-1.460087	-1.445441	-1.133731
21	8	0	1.445427	-1.460128	1.133668
22	6	0	1.856389	-1.875043	-0.000050
23	6	0	2.908430	-2.937122	-0.000049
24	6	0	3.401270	-3.434741	-1.211322
25	6	0	4.386245	-4.429134	-1.211501
26	6	0	4.880948	-4.928498	-0.000048
27	6	0	4.386324	-4.429054	1.211403
28	6	0	3.401355	-3.434652	1.211223
29	8	0	1.445465	-1.460099	-1.133783
30	8	0	1.460137	1.445440	1.133722
31	6	0	1.875063	1.856392	-0.000002
32	6	0	2.937138	2.908434	-0.000004
33	6	0	3.434659	3.401365	-1.211278
34	6	0	4.429069	4.386326	-1.211461
35	6	0	4.928515	4.880951	-0.000011

36	6	0	4.429150	4.386254	1.211442
37	6	0	3.434765	3.401269	1.211268
38	8	0	1.460141	1.445436	-1.133727
39	1	0	-3.053959	-3.023692	-2.153026
40	1	0	-3.053490	-3.024138	2.153021
41	1	0	-5.697547	-5.642609	0.000015
42	1	0	3.023858	-3.053812	-2.153073
43	1	0	3.024010	-3.053657	2.152974
44	1	0	5.642645	-5.697542	-0.000047
45	1	0	3.053655	3.024026	-2.153027
46	1	0	3.053847	3.023851	2.153020
47	1	0	5.697560	5.642646	-0.000014
48	1	0	-3.023894	3.053772	-2.152975
49	1	0	-3.023994	3.053651	2.153071
50	1	0	-5.642704	5.697469	0.000062
51	6	0	4.926111	4.878357	2.527803
52	8	0	4.529901	4.486256	3.607093
53	8	0	5.886586	5.829408	2.409269
54	1	0	6.143652	6.084043	3.311176
55	6	0	4.925936	4.878512	-2.527826
56	8	0	4.529928	4.486197	-3.607112
57	8	0	5.886316	5.829661	-2.409299
58	1	0	6.143401	6.084268	-3.311208
59	6	0	-4.878532	4.925879	2.527873
60	8	0	-4.486313	4.529777	3.607160
61	8	0	-5.829729	5.886212	2.409348
62	1	0	-6.084387	6.143246	3.311258
63	6	0	-4.878424	4.926013	-2.527755
64	8	0	-4.486247	4.529879	-3.607046
65	8	0	-5.829624	5.886342	-2.409220
66	1	0	-6.084280	6.143386	-3.311127
67	6	0	-4.926254	-4.878164	-2.527804
68	8	0	-4.530097	-4.486013	-3.607096
69	8	0	-5.886802	-5.829143	-2.409269
70	1	0	-6.143943	-6.083701	-3.311177
71	6	0	-4.925754	-4.878635	2.527824
72	8	0	-4.529732	-4.486332	3.607110
73	8	0	-5.886099	-5.829821	2.409301
74	1	0	-6.143135	-6.084473	3.311212
75	6	0	4.878345	-4.926093	-2.527863
76	8	0	4.486201	-4.529923	-3.607152
77	8	0	5.829443	-5.886524	-2.409332
78	1	0	6.084073	-6.143590	-3.311240
79	6	0	4.878515	-4.925919	2.527766
80	8	0	4.486346	-4.529770	3.607054
81	8	0	5.829648	-5.886316	2.409237
82	1	0	6.084312	-6.143345	3.311146

HF=3411.0011819

$[Rh_2(OBz)_4Cl_2]^{2-}$

Charge=-2, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.000652	0.000114	3.885340
2	8	0	-1.417688	1.520315	1.137845
3	6	0	-1.800154	1.930608	-0.000080
4	8	0	-1.417494	1.520286	-1.137984
5	6	0	-2.829139	3.034280	-0.000216
6	6	0	-3.309187	3.549346	-1.212204
7	6	0	-3.309754	3.549085	1.211661
8	6	0	-4.261847	4.570863	-1.210961
9	1	0	-2.921468	3.133812	-2.136802
10	6	0	-4.262407	4.570599	1.210225
11	1	0	-2.922459	3.133364	2.136356
12	6	0	-4.741149	5.084387	-0.000428
13	1	0	-4.630463	4.966343	-2.154662
14	1	0	-4.631443	4.965889	2.153840
15	1	0	-5.483314	5.880096	-0.000520
16	8	0	-1.520485	-1.417556	1.137870
17	6	0	-1.930811	-1.799988	-0.000049
18	8	0	-1.520394	-1.417486	-1.137967
19	6	0	-3.034553	-2.828924	-0.000155
20	6	0	-3.549234	-3.309418	-1.212132
21	6	0	-3.549845	-3.308995	1.211730
22	6	0	-4.570865	-4.261955	-1.210871
23	1	0	-3.133327	-2.922119	-2.136738
24	6	0	-4.571470	-4.261529	1.210314
25	1	0	-3.134383	-2.921396	2.136414
26	6	0	-5.084885	-4.740699	-0.000327
27	1	0	-4.966064	-4.630890	-2.154565
28	1	0	-4.967124	-4.630154	2.153938
29	1	0	-5.880702	-5.482749	-0.000400
30	8	0	1.417662	-1.520614	1.138044
31	6	0	1.800070	-1.930884	0.000155
32	8	0	1.417707	-1.520666	-1.137860
33	6	0	2.829212	-3.034626	0.000131
34	6	0	3.309750	-3.549382	-1.211801
35	6	0	3.309383	-3.549768	1.212032
36	6	0	4.262397	-4.570903	-1.210485
37	1	0	2.922380	-3.133594	-2.136436
38	6	0	4.262029	-4.571288	1.210697
39	1	0	2.921735	-3.134250	2.136678
40	6	0	4.741233	-5.084764	0.000099
41	1	0	4.631349	-4.966137	-2.154158
42	1	0	4.630717	-4.966816	2.154352
43	1	0	5.483376	-5.880496	0.000103
44	8	0	1.520399	1.417884	1.138035
45	6	0	1.930661	1.800313	0.000142
46	8	0	1.520524	1.417812	-1.137860
47	6	0	3.034559	2.829257	0.000107
48	6	0	3.549840	3.309220	-1.211829
49	6	0	3.549301	3.309862	1.212007
50	6	0	4.571463	4.261759	-1.210517
51	1	0	3.134356	2.921519	-2.136461
52	6	0	4.570922	4.262400	1.210665
53	1	0	3.133417	2.922619	2.136657
54	6	0	5.084908	4.741048	0.000062
55	1	0	4.967083	4.630293	-2.154191
56	1	0	4.966150	4.631417	2.154317
57	1	0	5.880702	5.483124	0.000059
58	45	0	-0.000139	0.000019	1.246821

59	45	0	0.000086	-0.000010	-1.246591
60	17	0	0.000504	-0.000085	-3.885160

HF=-2822.875789

$[Rh_2(OBz)_4Cl]^-$

Charge=-1, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000028	0.000029	3.514139
2	8	0	-1.668754	1.226604	0.946049
3	6	0	-2.128365	1.564622	-0.187968
4	8	0	-1.667596	1.225408	-1.327798
5	6	0	-3.338820	2.455152	-0.180212
6	6	0	-3.914926	2.878896	-1.385607
7	6	0	-3.896555	2.866414	1.038635
8	6	0	-5.038940	3.706644	-1.372357
9	1	0	-3.469875	2.550987	-2.318741
10	6	0	-5.020513	3.694143	1.048792
11	1	0	-3.436009	2.527886	1.960638
12	6	0	-5.594132	4.116027	-0.155324
13	1	0	-5.481698	4.032451	-2.310007
14	1	0	-5.448716	4.010068	1.996296
15	1	0	-6.469437	4.760748	-0.145501
16	8	0	-1.226571	-1.668706	0.946108
17	6	0	-1.564611	-2.128354	-0.187897
18	8	0	-1.225440	-1.667611	-1.327723
19	6	0	-2.455157	-3.338827	-0.180060
20	6	0	-2.878930	-3.914966	-1.385422
21	6	0	-2.866372	-3.896510	1.038822
22	6	0	-3.706677	-5.038983	-1.372108
23	1	0	-2.551052	-3.469950	-2.318585
24	6	0	-3.694102	-5.020470	1.049042
25	1	0	-2.527819	-3.435937	1.960801
26	6	0	-4.116021	-5.594131	-0.155042
27	1	0	-4.032513	-5.481775	-2.309733
28	1	0	-4.009996	-5.448641	1.996571
29	1	0	-4.760741	-6.469437	-0.145170
30	8	0	1.668751	-1.226594	0.946095
31	6	0	2.128355	-1.564620	-0.187929
32	8	0	1.667567	-1.225427	-1.327752
33	6	0	3.338816	-2.455140	-0.180171
34	6	0	3.914917	-2.878892	-1.385566
35	6	0	3.896565	-2.866385	1.038676
36	6	0	5.038938	-3.706629	-1.372317
37	1	0	3.469854	-2.550996	-2.318700
38	6	0	5.020530	-3.694105	1.048832
39	1	0	3.436025	-2.527850	1.960679
40	6	0	5.594143	-4.115995	-0.155284
41	1	0	5.481692	-4.032441	-2.309968
42	1	0	5.448744	-4.010016	1.996336
43	1	0	6.469454	-4.760709	-0.145462
44	8	0	1.226567	1.668722	0.946116
45	6	0	1.564605	2.128343	-0.187906
46	8	0	1.225416	1.667584	-1.327716
47	6	0	2.455160	3.338809	-0.180094
48	6	0	2.878934	3.914919	-1.385470
49	6	0	2.866384	3.896514	1.038774
50	6	0	3.706691	5.038930	-1.372182
51	1	0	2.551049	3.469887	-2.318623

52	6	0	3.694122	5.020468	1.048968
53	1	0	2.527831	3.435962	1.960764
54	6	0	4.116042	5.594100	-0.155129
55	1	0	4.032528	5.481698	-2.309818
56	1	0	4.010023	5.448656	1.996487
57	1	0	4.760770	6.469400	-0.145277
58	45	0	0.000003	0.000008	1.055903
59	45	0	-0.000017	-0.000012	-1.402999

HF=-2362.6553196

$[Rh_2(OAc)_4]$

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.456440	-1.461190	1.133361
2	6	0	-1.872802	-1.870710	-0.000010
3	8	0	-1.455896	-1.461711	-1.133374
4	8	0	1.452763	-1.458322	1.133372
5	6	0	1.869333	-1.867649	0.000025
6	8	0	1.453315	-1.457788	-1.133332
7	8	0	1.449745	1.454577	1.133368
8	6	0	1.865941	1.864273	0.000032
9	8	0	1.449228	1.455119	-1.133315
10	8	0	-1.461456	1.449430	1.133338
11	6	0	-1.870357	1.866401	-0.000021
12	8	0	-1.461964	1.448903	-1.133367
13	45	0	-0.003619	-0.003711	1.194876
14	45	0	-0.003601	-0.003705	-1.194867
15	6	0	2.963380	2.900403	-0.000026
16	1	0	3.930901	2.386112	-0.002491
17	1	0	2.902008	3.517427	-0.897971
18	1	0	2.904856	3.514640	0.899996
19	6	0	2.965866	-2.904668	0.000037
20	1	0	2.905035	-3.520448	-0.898777
21	1	0	3.933867	-2.391279	-0.000236
22	1	0	2.905322	-3.520145	0.899072
23	6	0	-2.970678	-2.906170	-0.000069
24	1	0	-2.911803	-3.520977	0.899533
25	1	0	-3.937782	-2.391105	-0.001635
26	1	0	-2.909974	-3.522736	-0.898357
27	6	0	-2.904542	2.965556	-0.000002
28	1	0	-3.521096	2.905904	0.898379
29	1	0	-2.388210	3.931984	0.001479
30	1	0	-3.519435	2.907578	-0.899614

HF=-1135.3253968

$[Rh_2(OAc)_3(OBz)]$

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	0.765394	-2.065196	1.133226
2	6	0	0.752797	-2.649125	-0.000169
3	8	0	0.765803	-2.065046	-1.133485
4	8	0	2.835120	-0.021707	1.133372
5	6	0	3.419156	-0.021225	0.000007
6	8	0	2.835124	-0.021175	-1.133361
7	8	0	0.789987	2.050933	1.133482
8	6	0	0.795253	2.635092	0.000191
9	8	0	0.789568	2.051093	-1.133187
10	8	0	-1.278650	0.005335	1.133296
11	6	0	-1.868011	0.009483	0.000005
12	8	0	-1.278654	0.005087	-1.133287
13	6	0	-3.360335	0.019854	0.000007
14	6	0	-4.063502	0.024899	-1.213941
15	6	0	-4.063499	0.024951	1.213956
16	6	0	-5.458215	0.035086	-1.211444
17	1	0	-3.507892	0.021018	-2.145002
18	6	0	-5.458213	0.035137	1.211462
19	1	0	-3.507888	0.021110	2.145016
20	6	0	-6.157210	0.040216	0.000009
21	1	0	-5.999833	0.039128	-2.152731
22	1	0	-5.999829	0.039217	2.152750
23	1	0	-7.243524	0.048264	0.000010
24	45	0	0.777953	-0.007380	1.194494
25	45	0	0.777950	-0.007217	-1.194487
26	6	0	0.841431	4.143521	0.000231
27	1	0	1.889729	4.462361	-0.002143
28	1	0	0.361838	4.536934	-0.897502
29	1	0	0.365705	4.536856	0.900032
30	6	0	4.928002	0.009166	0.000002
31	1	0	5.316577	-0.472500	-0.898753
32	1	0	5.257650	1.054103	-0.000378
33	1	0	5.316591	-0.471910	0.899061
34	6	0	0.689663	-4.156762	-0.000308
35	1	0	1.161224	-4.555975	0.899139
36	1	0	-0.362588	-4.462241	-0.001539
37	1	0	1.163180	-4.555847	-0.898794

HF=-1327.0755005

cis-$[Rh_2(OAc)_2(OBz)_2]$

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.454599	0.483648	1.133234
2	6	0	-1.870907	0.900980	-0.000094
3	8	0	-1.454784	0.483334	-1.133373
4	6	0	-2.926003	1.956139	-0.000154
5	6	0	-3.423592	2.452875	-1.214090
6	6	0	-3.423494	2.453111	1.213725
7	6	0	-4.410512	3.438373	-1.211668
8	1	0	-3.030219	2.060456	-2.145117
9	6	0	-4.410414	3.438610	1.211190
10	1	0	-3.030047	2.060874	2.144797
11	6	0	-4.905113	3.932396	-0.000267
12	1	0	-4.793564	3.821238	-2.152983
13	1	0	-4.793389	3.821660	2.152461
14	1	0	-5.673652	4.700185	-0.000311

15	8	0	-1.455525	-2.423169	1.133296
16	6	0	-1.867300	-2.837512	-0.000065
17	8	0	-1.455122	-2.423474	-1.133391
18	8	0	1.455105	-2.423474	1.133437
19	6	0	1.867286	-2.837525	0.000121
20	8	0	1.455514	-2.423196	-1.133249
21	8	0	1.454798	0.483333	1.133372
22	6	0	1.870919	0.900969	0.000087
23	8	0	1.454610	0.483622	-1.133236
24	6	0	2.926010	1.956131	0.000134
25	6	0	3.423495	2.453096	-1.213751
26	6	0	3.423604	2.452877	1.214064
27	6	0	4.410411	3.438598	-1.211228
28	1	0	3.030044	2.060851	-2.144818
29	6	0	4.410521	3.438379	1.211630
30	1	0	3.030236	2.060464	2.145096
31	6	0	4.905115	3.932394	0.000224
32	1	0	4.793380	3.821643	-2.152504
33	1	0	4.793575	3.821252	2.152941
34	1	0	5.673651	4.700186	0.000258
35	45	0	-0.000061	-0.969515	1.193893
36	45	0	0.000061	-0.969528	-1.193876
37	6	0	2.908796	-3.929539	0.000117
38	1	0	2.399747	-4.899808	-0.002389
39	1	0	3.525730	-3.864120	-0.897546
40	1	0	3.522849	-3.866999	0.899938
41	6	0	-2.908810	-3.929524	-0.000118
42	1	0	-3.524540	-3.865262	-0.898684
43	1	0	-2.399760	-4.899796	-0.000594
44	1	0	-3.524070	-3.865828	0.898804

HF=-1518.8254229

trans-[$Rh_2(OAc)_2(OBz)_2$]

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.003415	2.057689	1.133342
2	6	0	0.011277	2.641873	-0.000004
3	8	0	0.003269	2.057681	-1.133347
4	8	0	-2.055419	0.003451	1.133323
5	6	0	-2.644825	0.004985	0.000002
6	8	0	-2.055418	0.003293	-1.133318
7	6	0	-4.137075	0.008527	0.000002
8	6	0	-4.840263	0.010135	-1.213943
9	6	0	-4.840264	0.010250	1.213947
10	6	0	-6.234998	0.013529	-1.211447
11	1	0	-4.284679	0.008894	-2.145026
12	6	0	-6.234999	0.013644	1.211449
13	1	0	-4.284680	0.009097	2.145029
14	6	0	-6.934010	0.015286	0.000001
15	1	0	-6.776623	0.014897	-2.152737
16	1	0	-6.776624	0.015100	2.152738
17	1	0	-8.020351	0.018025	0.000001
18	8	0	-0.003415	-2.057710	1.133364
19	6	0	-0.011274	-2.641906	0.000025
20	8	0	-0.003268	-2.057724	-1.133325
21	8	0	2.055418	-0.003476	1.133324
22	6	0	2.644825	-0.005048	0.000003
23	8	0	2.055419	-0.003338	-1.133317
24	6	0	4.137075	-0.008513	0.000004

25	6	0	4.840264	-0.010091	-1.213941
26	6	0	4.840263	-0.010193	1.213949
27	6	0	6.234999	-0.013423	-1.211443
28	1	0	4.284680	-0.008882	-2.145023
29	6	0	6.234998	-0.013525	1.211453
30	1	0	4.284679	-0.009063	2.145032
31	6	0	6.934011	-0.015141	0.000005
32	1	0	6.776625	-0.014770	-2.152733
33	1	0	6.776623	-0.014953	2.152742
34	1	0	8.020352	-0.017831	0.000005
35	45	0	-0.000000	-0.000011	1.194002
36	45	0	0.000000	-0.000022	-1.193996
37	6	0	-0.062791	-4.149879	-0.000020
38	1	0	-1.112602	-4.463627	-0.002002
39	1	0	0.414880	-4.545079	-0.897994
40	1	0	0.411687	-4.545098	0.899619
41	6	0	0.062786	4.149847	-0.000041
42	1	0	-0.412361	4.545066	0.899249
43	1	0	1.112597	4.463600	-0.001197
44	1	0	-0.414222	4.545042	-0.898366

HF=-1518.8255919

$[Rh_2(OAc)(OBz)_3]$.

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.004941	1.441576	1.133279
2	6	0	0.006526	2.031163	-0.000021
3	8	0	0.004832	1.441551	-1.133307
4	6	0	0.010465	3.523233	-0.000037
5	6	0	0.012241	4.226324	-1.213921
6	6	0	0.012306	4.226352	1.213831
7	6	0	0.015888	5.621002	-1.211474
8	1	0	0.010769	3.670717	-2.144943
9	6	0	0.015953	5.621029	1.211352
10	1	0	0.010883	3.670765	2.144865
11	6	0	0.017754	6.320026	-0.000069
12	1	0	0.017283	6.162615	-2.152773
13	1	0	0.017400	6.162663	2.152640
14	1	0	0.020612	7.406374	-0.000081
15	8	0	-2.054951	-0.611588	1.133280
16	6	0	-2.644469	-0.609740	-0.000035
17	8	0	-2.054913	-0.611697	-1.133328
18	6	0	-4.136605	-0.608504	-0.000059
19	6	0	-4.839749	-0.608441	-1.213983
20	6	0	-4.839790	-0.608359	1.213840
21	6	0	-6.234460	-0.607998	-1.211526
22	1	0	-4.284157	-0.608108	-2.145043
23	6	0	-6.234501	-0.607916	1.211336
24	1	0	-4.284230	-0.607964	2.144919
25	6	0	-6.933494	-0.607787	-0.000107
26	1	0	-6.776064	-0.607456	-2.152829
27	1	0	-6.776137	-0.607311	2.152620
28	1	0	-8.019841	-0.607117	-0.000126
29	8	0	-0.003431	-2.670861	1.133387
30	6	0	-0.010790	-3.255147	0.000047
31	8	0	-0.003261	-2.670889	-1.133311
32	8	0	2.055305	-0.620201	1.133361
33	6	0	2.644870	-0.621500	0.000051

34	8	0	2.055343	-0.620142	-1.133279
35	6	0	4.136942	-0.627321	0.000077
36	6	0	4.840103	-0.630528	-1.213815
37	6	0	4.840061	-0.630584	1.213993
38	6	0	6.234791	-0.636860	-1.211314
39	1	0	4.284560	-0.627612	-2.144894
40	6	0	6.234749	-0.636916	1.211540
41	1	0	4.284485	-0.627711	2.145052
42	6	0	6.933774	-0.640103	0.000125
43	1	0	6.776421	-0.638986	-2.152599
44	1	0	6.776347	-0.639086	2.152843
45	1	0	8.020112	-0.644803	0.000144
46	45	0	0.000402	-0.614384	1.193529
47	45	0	0.000443	-0.614410	-1.193512
48	6	0	-0.060723	-4.763068	0.000012
49	1	0	-1.110140	-5.078020	-0.002053
50	1	0	0.417521	-5.157680	-0.897862
51	1	0	0.414186	-5.157687	0.899632

HF=-1710.5754439

[$Rh_2(OBz)_4$] (singlet)

Charge=0, Multiplicity=1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.052893	1.764491	-1.133306
2	6	0	-1.354949	2.270894	0.000015
3	8	0	-1.052827	1.764531	1.133339
4	6	0	-2.119331	3.552168	0.000026
5	6	0	-2.479668	4.155910	1.213904
6	6	0	-2.479507	4.156026	-1.213842
7	6	0	-3.194280	5.353581	1.211457
8	1	0	-2.195069	3.678760	2.144947
9	6	0	-3.194117	5.353697	-1.211375
10	1	0	-2.194775	3.678972	-2.144894
11	6	0	-3.552378	5.953893	0.000046
12	1	0	-3.471854	5.818662	2.152752
13	1	0	-3.471568	5.818867	-2.152663
14	1	0	-4.109022	6.886796	0.000052
15	8	0	1.764454	1.052890	-1.133336
16	6	0	2.270854	1.354982	-0.000020
17	8	0	1.764506	1.052831	1.133331
18	6	0	3.552171	2.119305	-0.000034
19	6	0	4.155949	2.479630	1.213830
20	6	0	4.156030	2.479441	-1.213914
21	6	0	5.353652	3.194187	1.211357
22	1	0	3.678800	2.195064	2.144883
23	6	0	5.353733	3.193998	-1.211473
24	1	0	3.678949	2.194721	-2.144956
25	6	0	5.953963	3.552246	-0.000066
26	1	0	5.818759	3.471751	2.152643
27	1	0	5.818903	3.471419	-2.152771
28	1	0	6.886892	4.108847	-0.000079
29	8	0	1.052844	-1.764464	-1.133302
30	6	0	1.354885	-2.270881	0.000014
31	8	0	1.052797	-1.764513	1.133333
32	6	0	2.119314	-3.552123	0.000024
33	6	0	2.479690	-4.155841	1.213903
34	6	0	2.479496	-4.155976	-1.213844
35	6	0	3.194344	-5.353486	1.211455
36	1	0	2.195085	-3.678695	2.144945

37	6	0	3.194150	-5.353621	-1.211377
38	1	0	2.194733	-3.678941	-2.144896
39	6	0	3.552449	-5.953795	0.000044
40	1	0	3.471948	-5.818550	2.152751
41	1	0	3.471605	-5.818789	-2.152665
42	1	0	4.109127	-6.886678	0.000050
43	8	0	-1.764493	-1.052858	-1.133330
44	6	0	-2.270927	-1.354894	-0.000014
45	8	0	-1.764545	-1.052792	1.133340
46	6	0	-3.552176	-2.119334	-0.000030
47	6	0	-4.155923	-2.479713	1.213834
48	6	0	-4.156003	-2.479523	-1.213910
49	6	0	-5.353564	-3.194373	1.211360
50	1	0	-3.678799	-2.195106	2.144888
51	6	0	-5.353645	-3.194182	-1.211470
52	1	0	-3.678946	-2.194761	-2.144951
53	6	0	-5.953845	-3.552482	-0.000063
54	1	0	-5.818648	-3.471978	2.152645
55	1	0	-5.818790	-3.471642	-2.152768
56	1	0	-6.886726	-4.109163	-0.000078
57	45	0	-0.000020	0.000015	-1.193005
58	45	0	-0.000014	0.000011	1.193018

HF=-1902.3252607

[$Rh_2(OBz)_4$] (triplet)

Charge=0, Multiplicity=3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.067372	0.026140	-1.136528
2	6	0	-2.650504	0.033810	-0.000000
3	8	0	-2.067372	0.026159	1.136527
4	6	0	-4.144484	0.053379	-0.000001
5	6	0	-4.847844	0.062833	1.213661
6	6	0	-4.847844	0.062848	-1.213662
7	6	0	-6.242472	0.081611	1.211299
8	1	0	-4.292013	0.055405	2.144510
9	6	0	-6.242472	0.081627	-1.211301
10	1	0	-4.292012	0.055431	-2.144511
11	6	0	-6.941573	0.091092	-0.000001
12	1	0	-6.783933	0.088910	2.152697
13	1	0	-6.783932	0.088940	-2.152699
14	1	0	-8.027849	0.105780	-0.000001
15	8	0	0.026083	2.053355	-1.129483
16	6	0	0.033972	2.650002	-0.000002
17	8	0	0.026101	2.053356	1.129481
18	6	0	0.053507	4.139548	-0.000002
19	6	0	0.062949	4.841850	1.214380
20	6	0	0.062964	4.841849	-1.214384
21	6	0	0.081742	6.236218	1.211682
22	1	0	0.055518	4.286415	2.145527
23	6	0	0.081757	6.236218	-1.211686
24	1	0	0.055543	4.286414	-2.145532
25	6	0	0.091227	6.934772	-0.000002
26	1	0	0.089054	6.777930	2.152813
27	1	0	0.089082	6.777929	-2.152818
28	1	0	0.105933	8.020992	-0.000002
29	8	0	2.067359	-0.026140	-1.136528
30	6	0	2.650490	-0.033822	-0.000000
31	8	0	2.067359	-0.026156	1.136527
32	6	0	4.144471	-0.053386	-0.000001
33	6	0	4.847832	-0.062836	1.213660

34	6	0	4.847830	-0.062855	-1.213663
35	6	0	6.242460	-0.081612	1.211297
36	1	0	4.292002	-0.055408	2.144509
37	6	0	6.242458	-0.081633	-1.211303
38	1	0	4.291998	-0.055441	-2.144511
39	6	0	6.941560	-0.091093	-0.000003
40	1	0	6.783921	-0.088909	2.152695
41	1	0	6.783918	-0.088946	-2.152701
42	1	0	8.027836	-0.105780	-0.000004
43	8	0	-0.026101	-2.053354	-1.129480
44	6	0	-0.034002	-2.649999	0.000002
45	8	0	-0.026118	-2.053352	1.129484
46	6	0	-0.053498	-4.139546	0.000004
47	6	0	-0.062919	-4.841847	1.214387
48	6	0	-0.062936	-4.841849	-1.214378
49	6	0	-0.081680	-6.236216	1.211690
50	1	0	-0.055501	-4.286410	2.145533
51	6	0	-0.081697	-6.236218	-1.211678
52	1	0	-0.055530	-4.286415	-2.145526
53	6	0	-0.091149	-6.934771	0.000007
54	1	0	-0.088979	-6.777926	2.152822
55	1	0	-0.089011	-6.777931	-2.152808
56	1	0	-0.105830	-8.020991	0.000009
57	45	0	-0.000007	0.000001	-1.221671
58	45	0	-0.000007	0.000002	1.221671

HF=-1902.2952939