Supporting Information for

Testing Cuprophilicity with Tetrahedral Ruthenium Hydride Carbonyl Clusters

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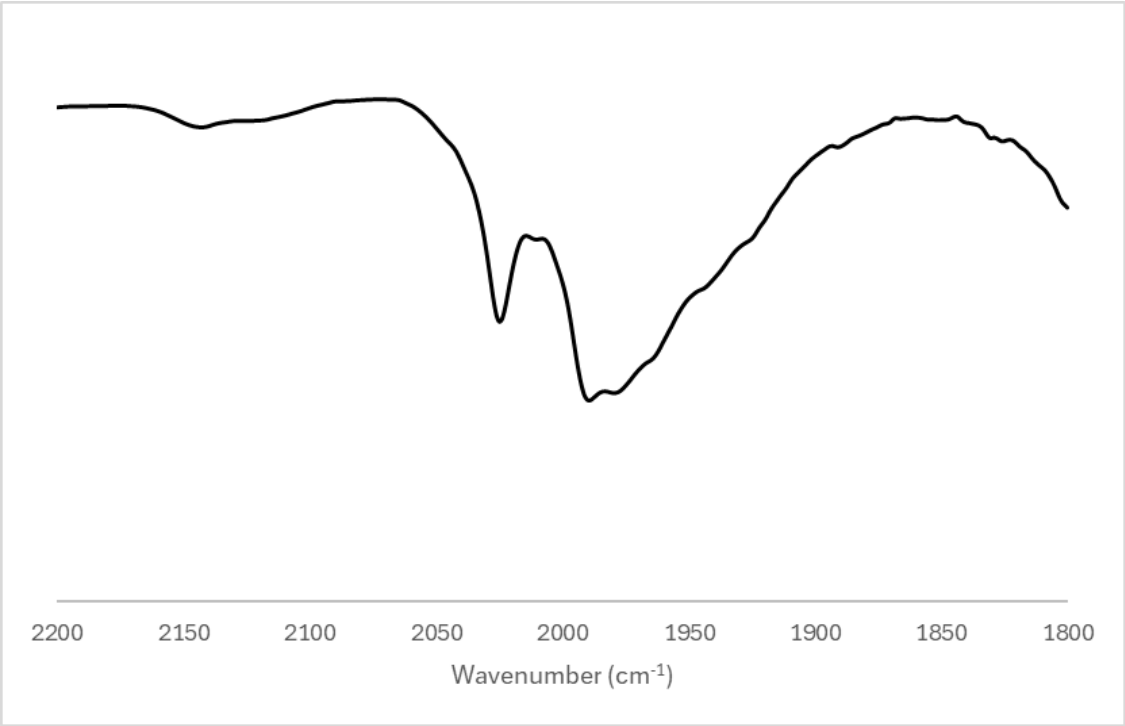

Figure S1. IR spectrum in the ν_{CO} region of $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**) in acetone.

Figure S2. IR spectrum in the ν_{CO} region of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) in CH_2Cl_2.

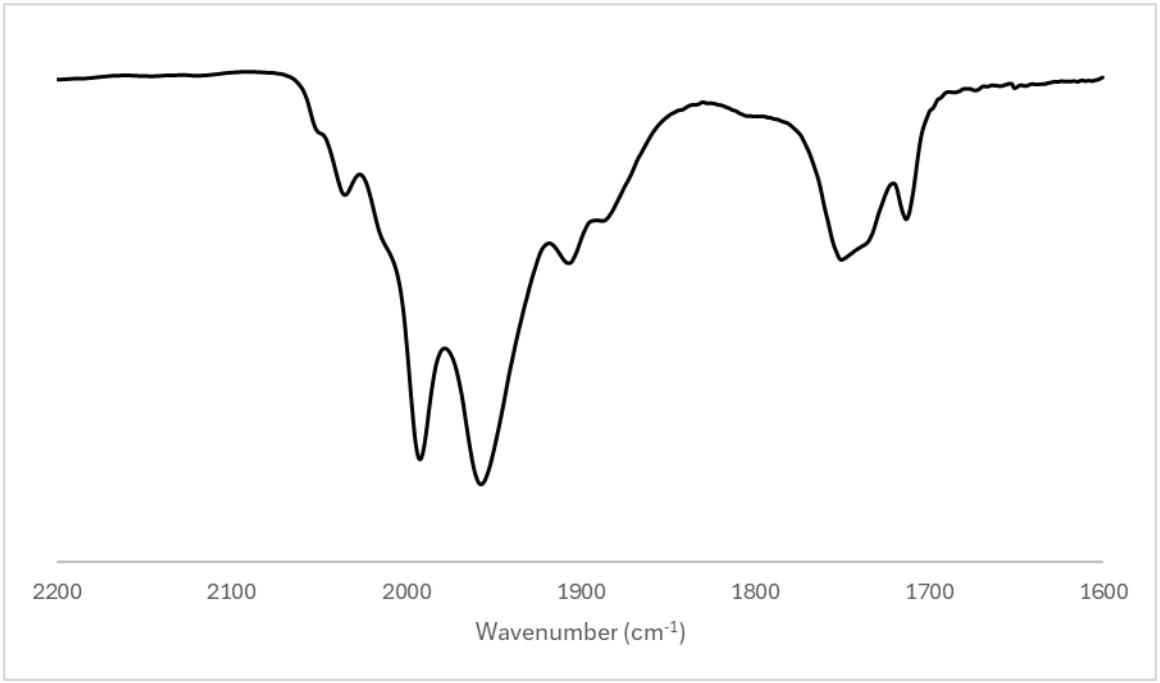

Figure S3. IR spectrum in the ν_{CO} region of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) in CH_2Cl_2.

Figure S4. IR spectrum in the ν_{CO} region of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) in CH_3CN.

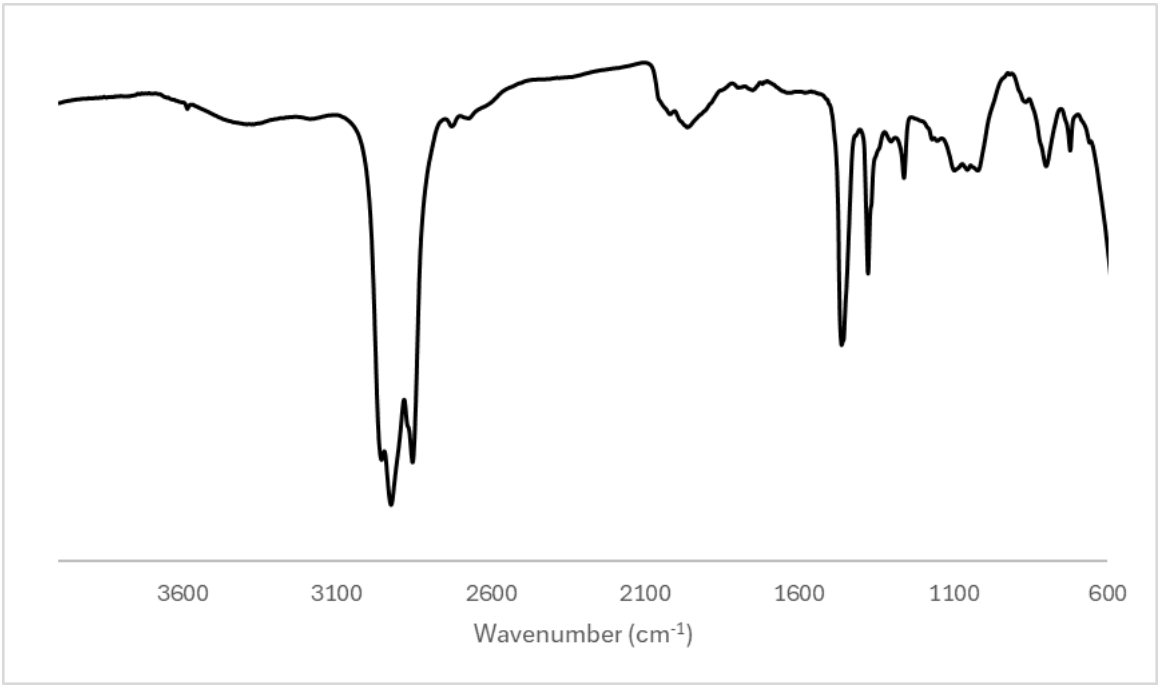

Figure S5. IR spectrum of crystals of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) in nujol mull.

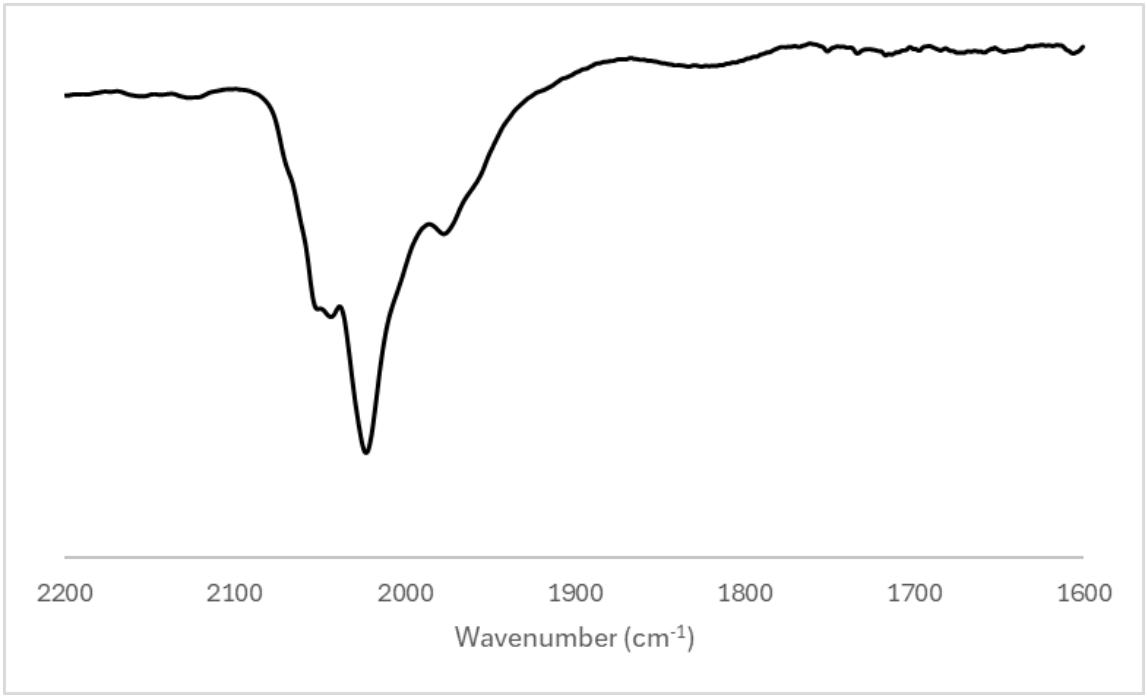

Figure S6. IR spectrum in the ν_{CO} region of $[Ru_5(CO)_{15}(CuMeCN)_2]$ (**5**) in CH_3CN.

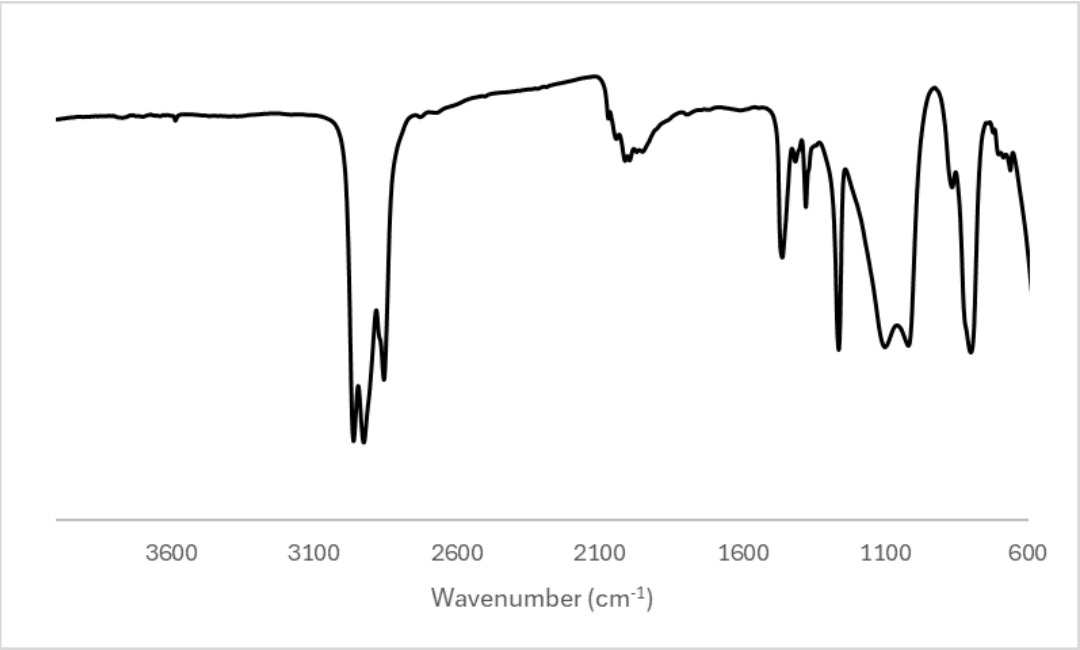

Figure S7. IR spectrum of crystals of $[Ru_5(CO)_{15}(CuMeCN)_2]$ (**5**) in nujol mull.

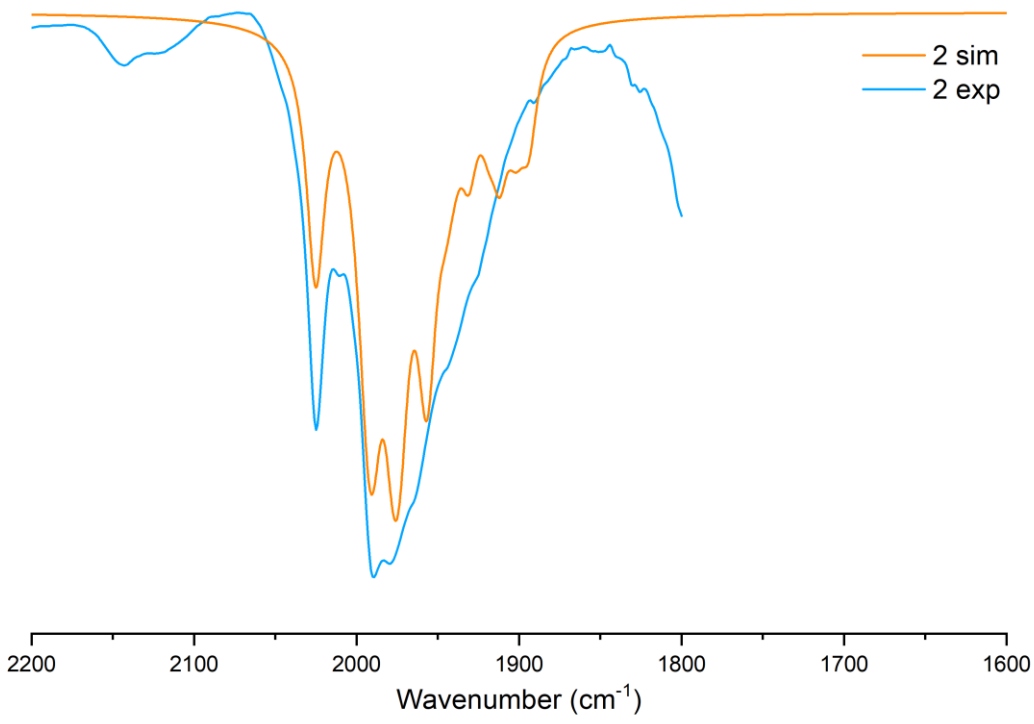

Figure S8. Superimposition of normalized experimental (light blue) and simulated (orange) IR spectra of $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**). Lorentzian broadening functions, FWHM = 12 cm^{-1}.

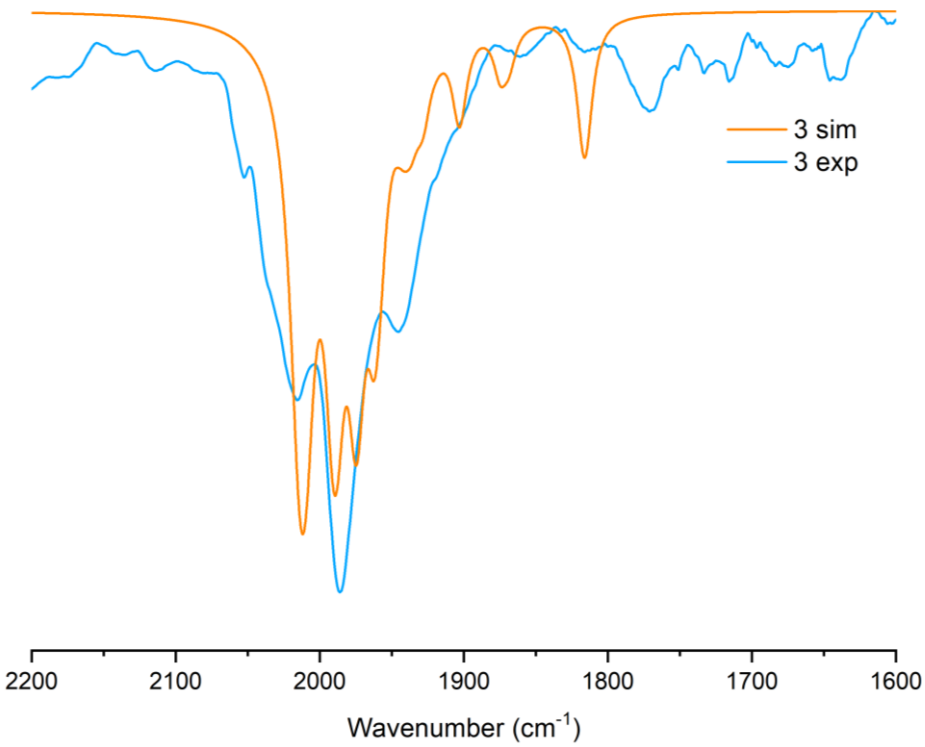

Figure S9. Superimposition of normalized experimental (light blue) and simulated (orange) IR spectra of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**). Lorentzian broadening functions, FWHM = 12 cm^{-1}.

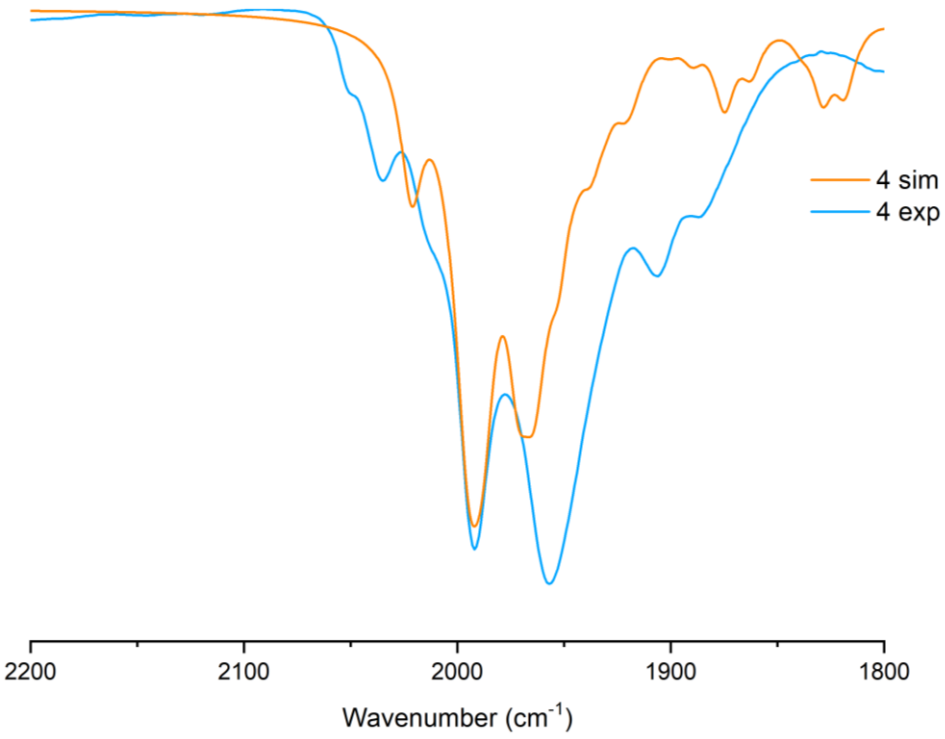

Figure S10. Superimposition of normalized experimental (light blue) and simulated (orange) IR spectra of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**). Lorentzian broadening functions, FWHM = 12 cm^{-1}.

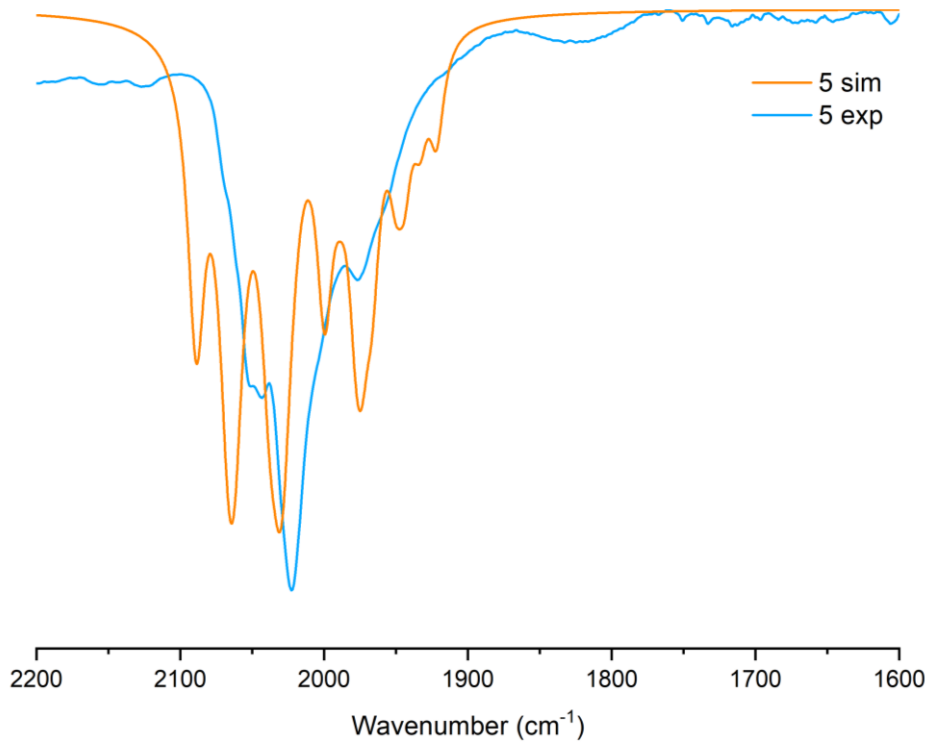

Figure S11. Superimposition of normalized experimental (light blue) and simulated (orange) IR spectra of $[Ru_5(CO)_{15}(CuMeCN)_2]$ (**5**). Lorentzian broadening functions, FWHM = 12 cm^{-1}.

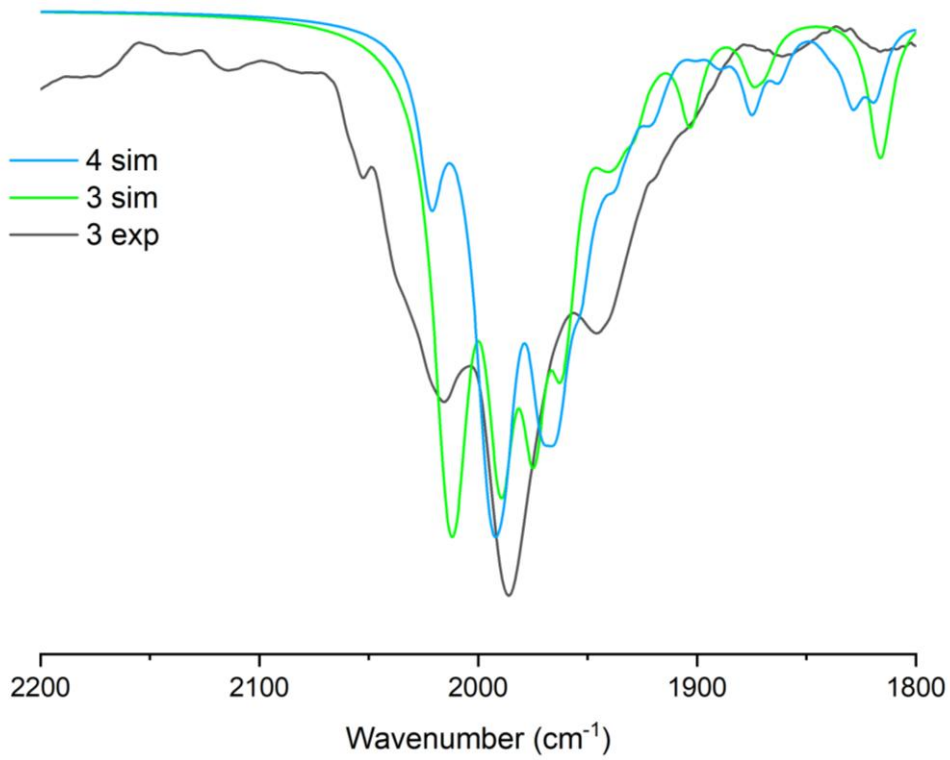

Figure S12. Overlay of normalized experimental IR spectrum (black) and simulated IR spectrum (green) of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) along with the simulated IR spectrum of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**). Lorentzian broadening functions, FWHM = 12 cm^{-1}.

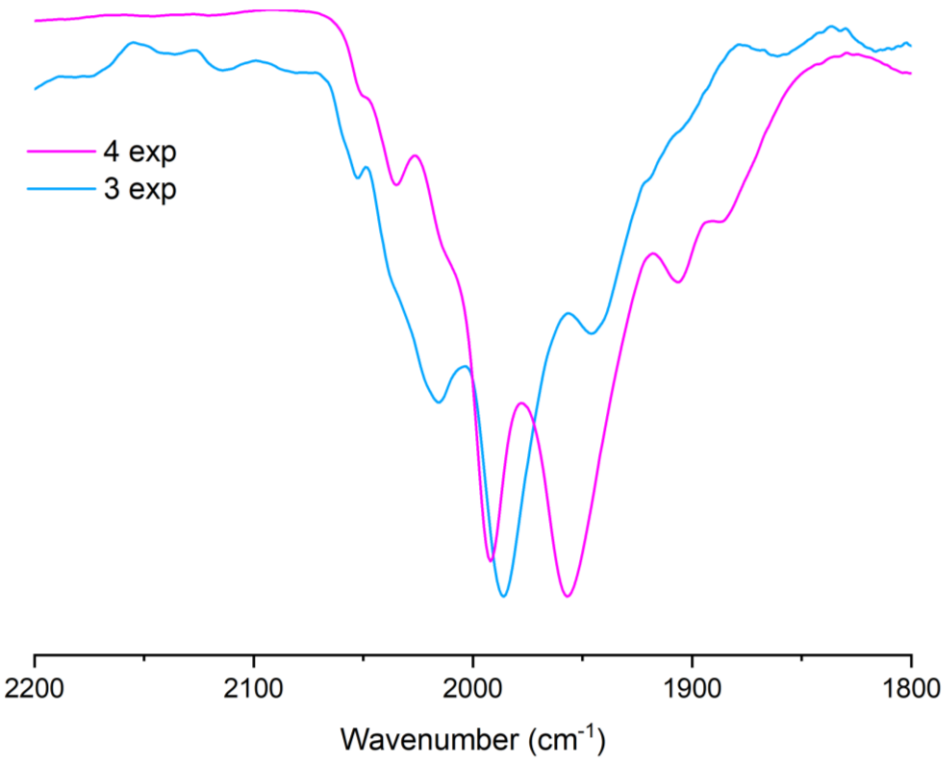

Figure S13. Comparison of normalized experimental IR spectra of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) (light blue) and $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) (purple).

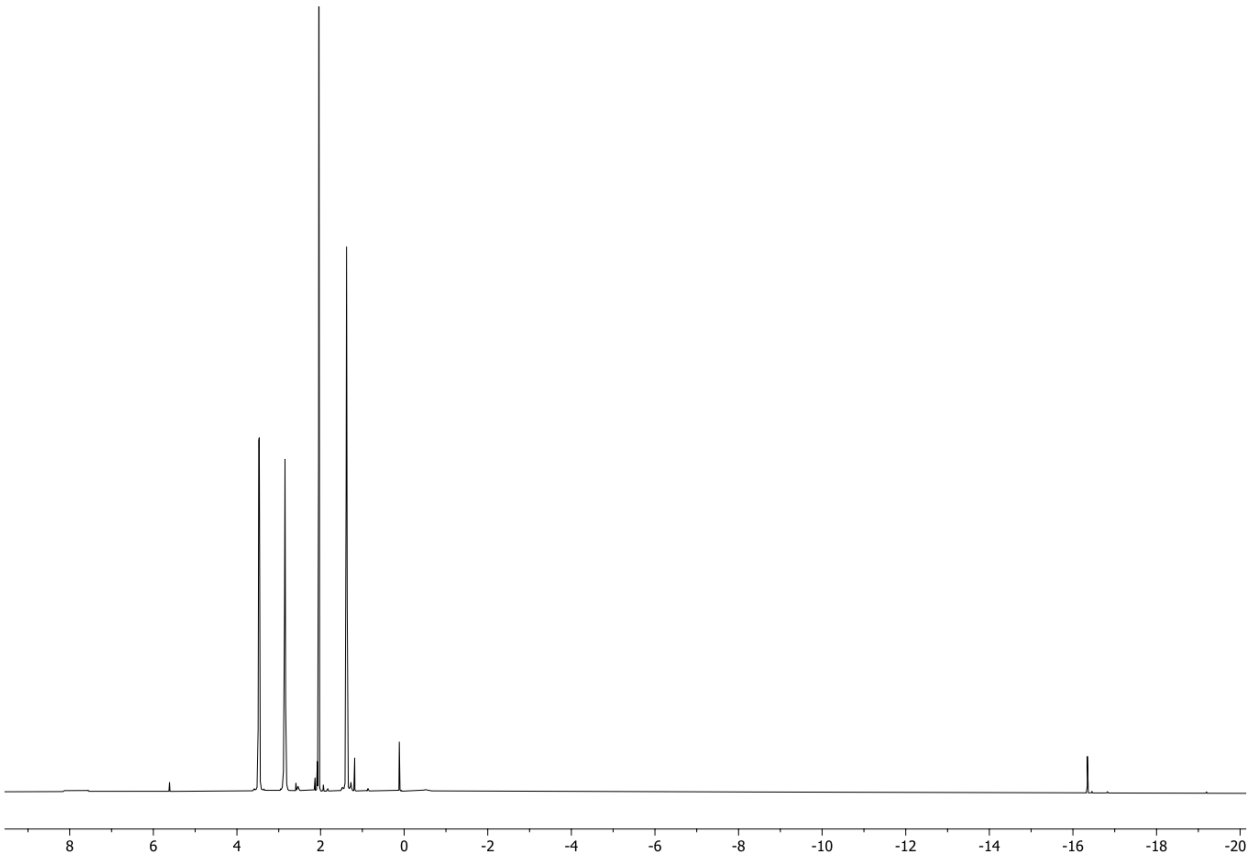

Figure S14. ^{1}H NMR spectrum of crystals of $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**) in acetone-d_6 at 298 K.

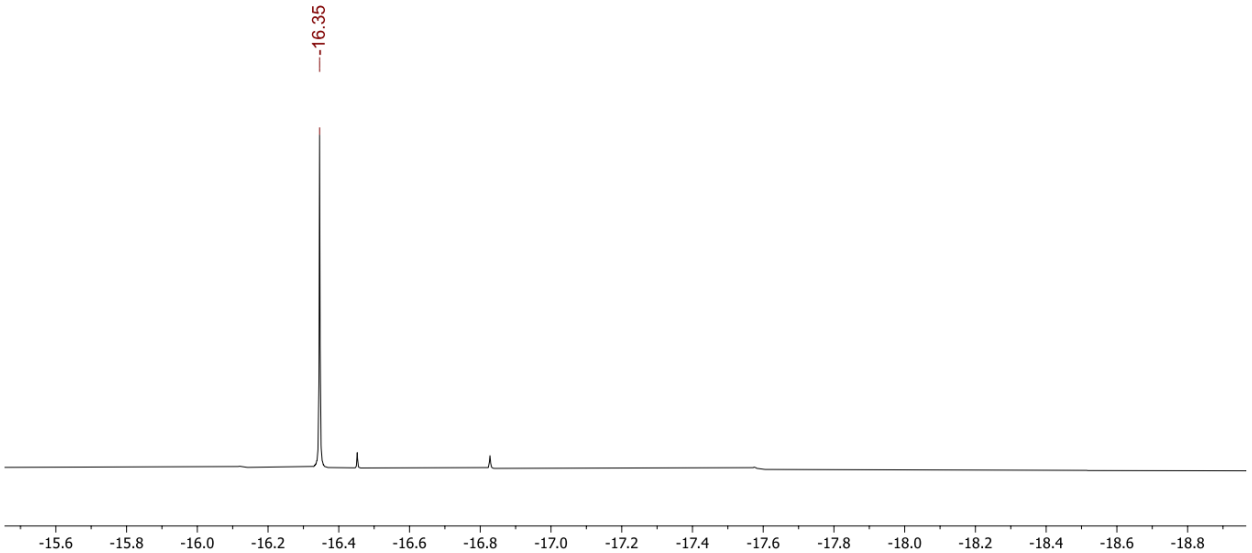

Figure S15. Hydride region of the ^{1}H NMR spectrum of crystals of $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**) in acetone-d_6 at 298 K.

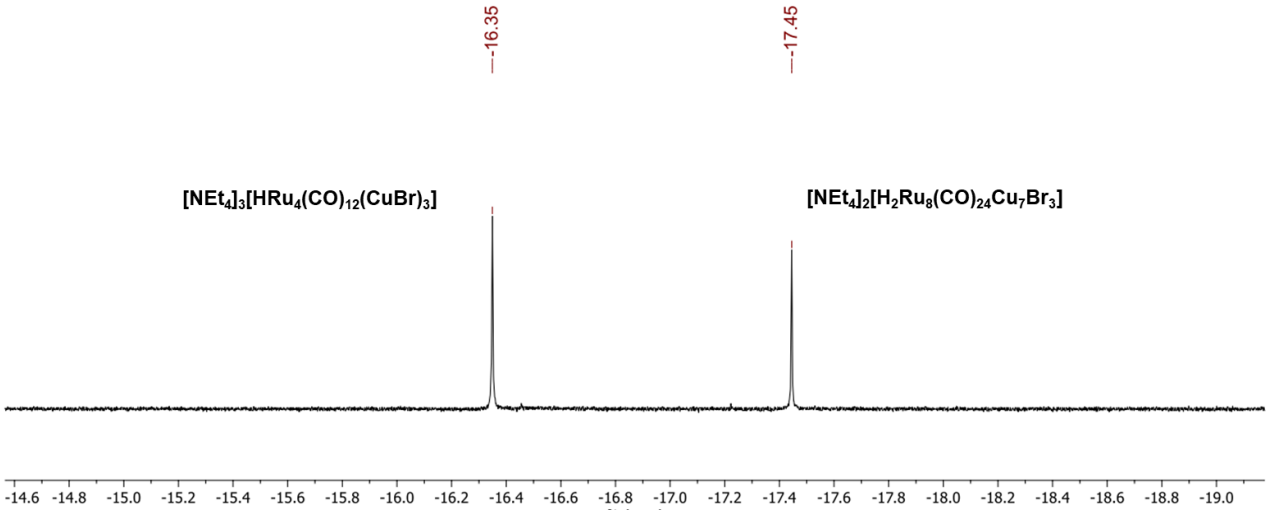

Figure S16. Hydride region of the ^{1}H NMR spectrum of a mixture of $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**) and $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) in acetone-d_6 at 298 K.

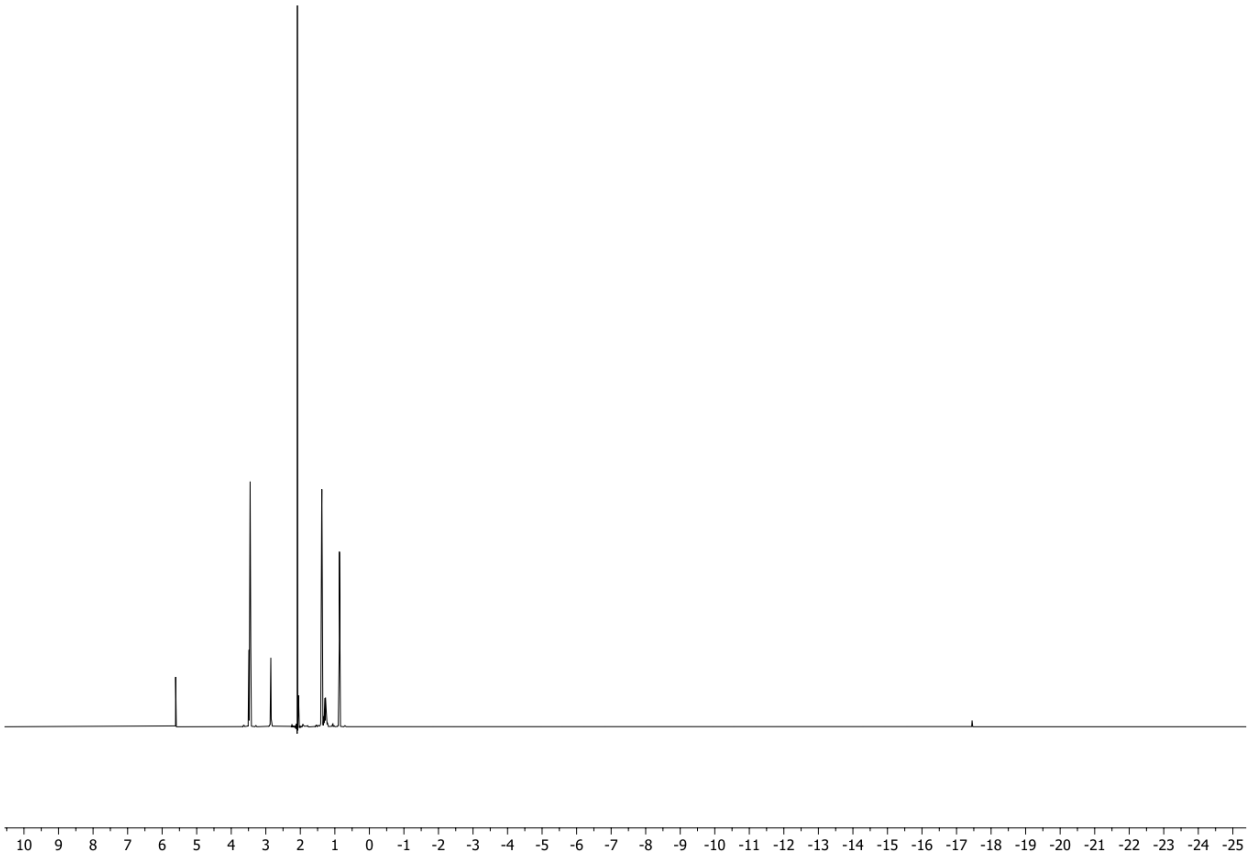

Figure S17. ^{1}H NMR spectrum of crystals of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) in acetone-d_6 at 298 K.

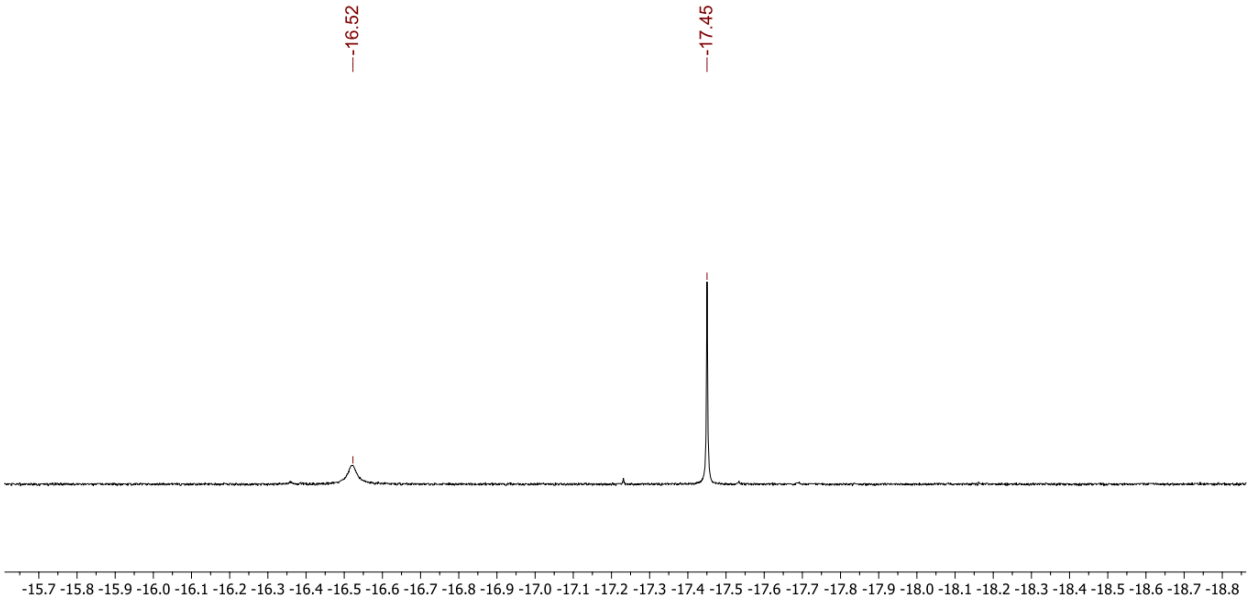

Figure S18. Hydride region of the ^{1}H NMR spectrum of crystals of $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]$ (**3**) in acetone-d_6 at 298 K.

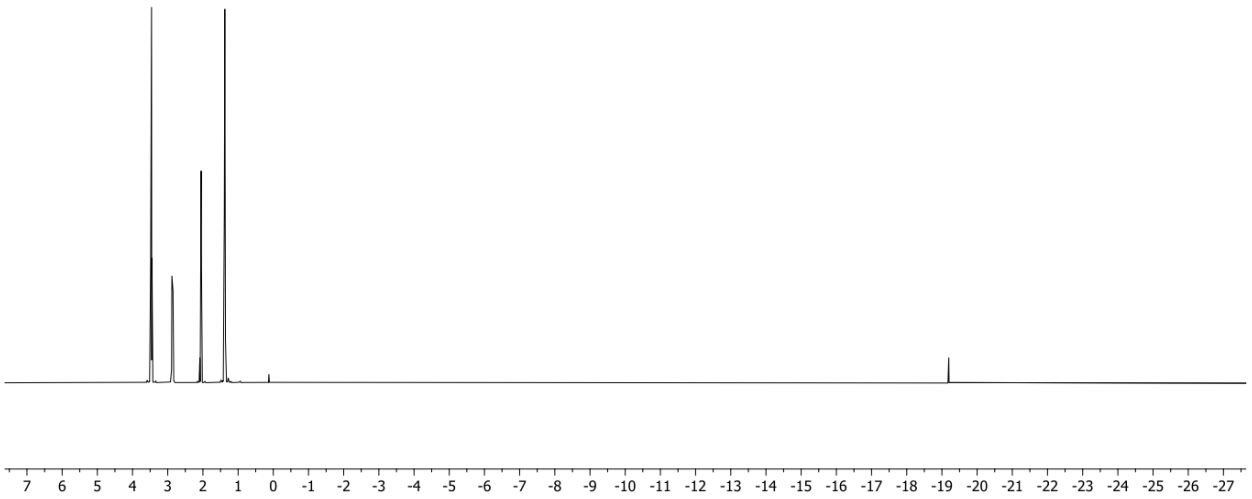

Figure S19. ^{1}H NMR spectrum of crystals of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) in acetone-d_6 at 298 K.

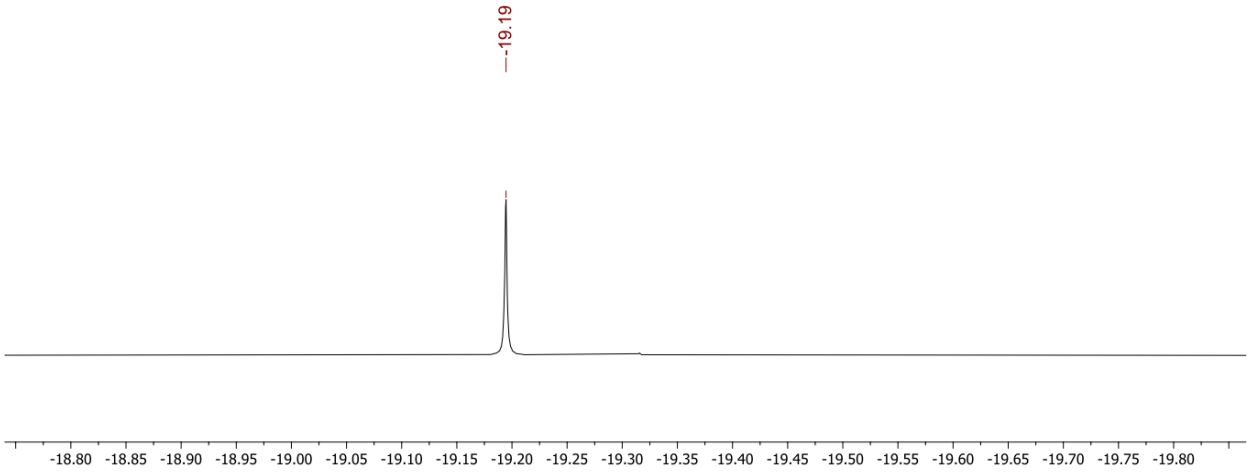

Figure S20. Hydride region of the ^{1}H NMR spectrum of crystals of $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]$ (**4**) in acetone-d_6 at 298 K.

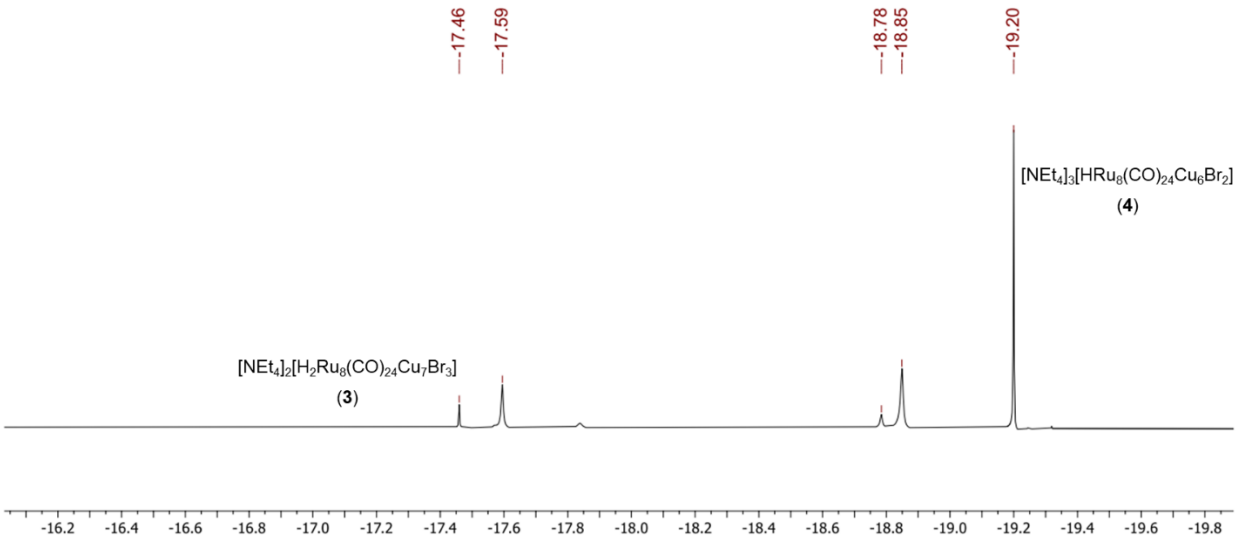

Figure S21. ^{1}H NMR spectrum, in acetone-d_6 at 298 K, of the crude product of the reaction after the addition of 1 equivalent of $[Cu(CH_3CN)_4][BF_4]$ to $[NEt_4]_3[HRu_4(CO)_{12}]$ (**1**).

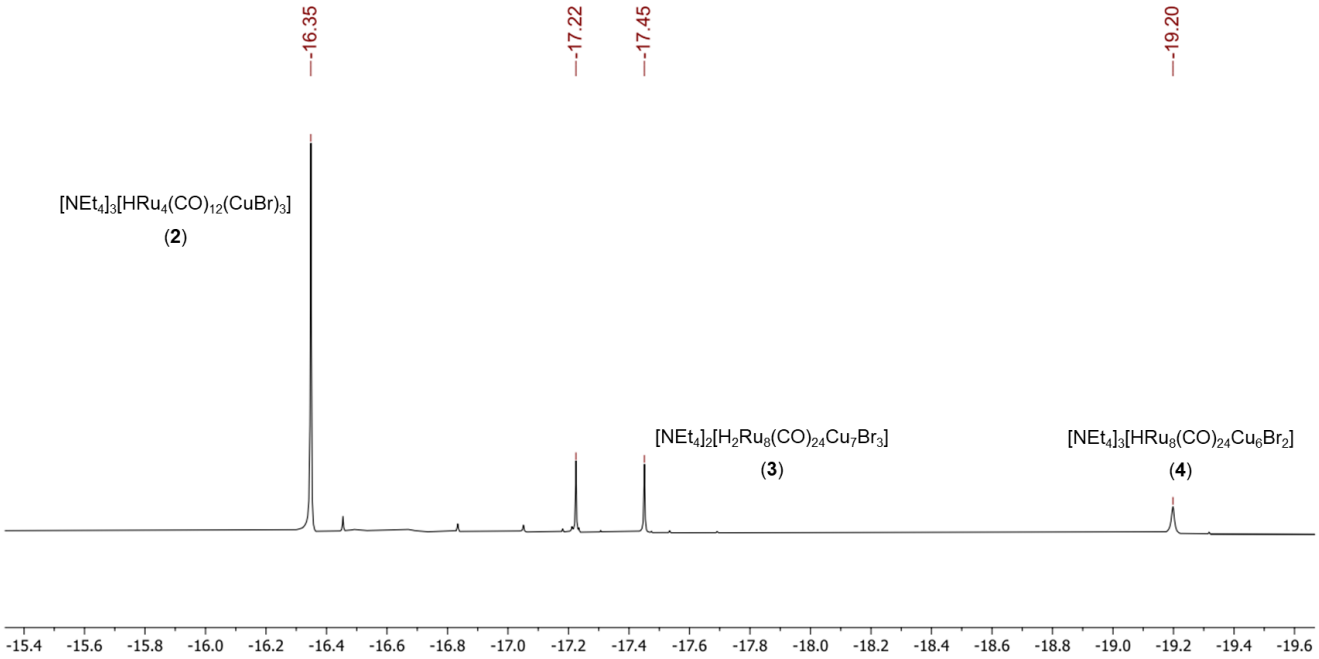

Figure S22. ^{1}H NMR spectrum in acetone-d_6 at 298 K of the mixture extracted in acetone at the end of the reaction of Figure S21.

Table S1. Main bond distances (Å) and angles (°) of $[HRu_4(CO)_{12}(CuBr)_3]^{3-}$ (**2**).

Ru1-Ru2	2.8008(5) *(1.13)*	Ru1-Ru3	2.7873(5) *(1.12)*
Ru1-Ru4	2.7901(5) *(1.12)*	Ru2-Ru3	2.9067(5) *(1.17)*
Ru2-Ru4	2.9537(5) *(1.19)*	Ru3-Ru4	2.9430(5) *(1.19)*
Cu1-Ru2	2.6380(7) *(1.09)*	Cu1-Ru3	2.7808(7) *(1.15)*
Cu1-Ru4	2.6854(7) *(1.11)*	Cu2-Ru2	2.6041(7) *(1.08)*
Cu2-Ru4	2.6211(7) *(1.09)*	Cu3-Ru2	2.6181(7) *(1.08)*
Cu3-Ru3	2.6198(7) *(1.09)*	Cu1-Cu2	2.6380(8) *(1.12)*
Cu1-Cu3	2.5809(8) *(1.10)*	Cu1-Br1	2.3092(7) *(1.00)*
Cu2-Br2	2.3018(9) *(0.99)*	Cu3-Br3	2.2938(7) *(0.99)*
H1-Ru3	1.83(3) *(1.26)*	H1-Ru4	1.83(3) *(1.26)*
H1-Cu1	1.85(3) *(1.32)*	C6-Ru2	1.913(5) *(0.95)*
C6-Cu1	2.558(5) *(1.32)*	C6-Cu2	2.589(5) *(1.33)*
C6-Cu3	2.603(5) *(1.34)*	C9-Ru3	1.918(5) *(0.95)*
C9-Cu3	2.593(5) *(1.33)*	C12-Ru4	1.915(5) *(0.95)*
C12-Cu2	2.657(5) *(1.37)*	Ru2-C6-O6	170.1(4)
Ru3-C9-O9	172.0(4)	Ru4-C12-O12	171.7(5)
α_{CO6}	0.337(6) [*0.373(6)*]	α_{CO9}	0.352(14) [*0.387(14)*]
α_{CO12}	0.388(6) [*0.423(6)*]		

Cotton's FSRs are reported in parentheses. Pauling's atomic radii are employed: Cu 1.173 Å, Ru 1.241 Å, Br 1.142 Å, C 0.771 Å, H 0.230 Å.

α corrected for the different atom radii of Cu (1.173) and Ru (1.241) in parentheses (covalent radii from Pauling).

Table S2. Main bond distances (Å) and angles (°) of $[H_2Ru_8(CO)_{24}Cu_7Br_3]^{2-}$ (**3**).

Ru1-Ru2	2.847(2) *(1.15)*	Ru5-Ru8	2.844(2) *(1.15)*
Ru1-Ru3	2.861(2) *(1.15)*	Ru5-Ru7	2.858(2) *(1.15)*
Ru1-Ru4	2.808(2) *(1.13)*	Ru5-Ru6	2.804(2) *(1.13)*
Ru2-Ru3	2.889(2) *(1.16)*	Ru7-Ru8	2.885(2) *(1.16)*
Ru2-Ru4	2.976(2) *(1.20)*	Ru6-Ru8	2.960(2) *(1.19)*
Ru3-Ru4	2.897(2) *(1.16)*	Ru6-Ru7	2.922(2) *(1.18)*
Cu2-Ru2	2.674(3) *(1.11)*	Cu6-Ru8	2.700(3) *(1.12)*
Cu2-Ru3	2.781(3) *(1.15)*	Cu6-Ru7	2.796(3) *(1.16)*
Cu2-Ru4	2.706(3) *(1.12)*	Cu6-Ru6	2.711(3) *(1.12)*
Cu1-Ru2	2.638(3) *(1.09)*	Cu5-Ru8	2.640(3) *(1.09)*
Cu1-Ru3	2.668(3) *(1.11)*	Cu5-Ru7	2.650(3) *(1.10)*
Cu3-Ru3	2.653(3) *(1.10)*	Cu7-Ru7	2.652(3) *(1.10)*
Cu3-Ru4	2.620(3) *(1.09)*	Cu7-Ru6	2.627(3) *(1.09)*
Cu4-Ru3	2.584(3) *(1.07)*	Cu4-Ru7	2.591(3) *(1.07)*
Cu1-Cu2	2.562(4) *(1.09)*	Cu5-Cu6	2.560(3) *(1.09)*
Cu2-Cu3	2.569(3) *(1.10)*	Cu6-Cu7	2.588(3) *(1.10)*
Cu4-Cu1	2.580(4) *(1.10)*	Cu4-Cu5	2.568(4) *(1.09)*
Cu4-Cu2	2.572(3) *(1.10)*	Cu4-Cu6	2.551(3) *(1.09)*
Cu4-Cu3	2.629(4) *(1.12)*	Cu4-Cu7	2.646(4) *(1.13)*
Cu1-Cu7	2.722(4)	Cu2-Cu6	2.786(3)

	(1.16)		*(1.19)*
Cu3-Cu5	2.721(4) *(1.16)*		
Cu1-Br1	2.353(3) *(1.02)*	Cu7-Br1	2.357(3) *(1.02)*
Cu2-Br2	2.370(3) *(1.02)*	Cu6-Br2	2.381(3) *(1.03)*
Cu3-Br3	2.364(3) *(1.02)*	Cu5-Br3	2.358(3) *(1.02)*
H2-Ru2	1.70(2) *(1.16)*	H1-Ru8	1.70(2) *(1.16)*
H2-Ru4	1.71(2) *(1.16)*	H1-Ru6	1.70(2) *(1.16)*
H2-Cu2	1.60(2) *(1.14)*	H1-Cu6	1.60(2) *(1.16)*
C6-Ru2	1.99(2) *(0.99)*	C24-Ru8	1.96(2) *(0.97)*
C6-Cu1	2.49(2) *(1.28)*	C24-Cu5	2.47(2) *(1.27)*
C10-Ru4	1.91(2) *(0.95)*	C18-Ru6	1.94(2) *(0.96)*
C10-Cu3	2.47(2) *(1.27)*	C18-Cu7	2.54(2) *(1.31)*
C7-Ru3	1.90(2) *(0.94)*	C20-Ru7	1.91(3) *(0.95)*
C7-Cu1	2.53(2) *(1.30)*	C20-Cu5	2.50(3) *(1.29)*
C8-Ru3	1.85(2) *(0.92)*	C21-Ru7	1.91(2) *(0.95)*
C8-Cu3	2.35(2) *(1.21)*	C21-Cu7	2.44(2) *(1.26)*
C8-Cu4	2.35(2) *(1.21)*	C21-Cu4	2.33(2) *(1.20)*
C9-Ru1	2.28(2) *(1.14)*	C19-Ru5	2.25(2) *(1.12)*
C9-Ru3	1.97(2) *(0.98)*	C19-Ru7	1.97(2) *(0.98)*
Ru2-C6-O6	165.2(19)	Ru8-C24-O24	169(2)
Ru4-C10-O10	169(2)	Ru6-C18-O18	171(2)
Ru3-C7-O7	172(2)	Ru7-C20-O20	171(2)

Ru3-C8-O8	167(2)	Ru7-C21-O21	166.1(19)
Ru3-C9-O9	145(2)	Ru5-C19-O19	130.5(18)
α_{CO6}	0.25(2) [*0.28(2)*]	α_{CO24}	0.26(2) [*0.29(2)*]
α_{CO10}	0.29(2) [*0.33(2)*]	α_{CO18}	0.31(2) [*0.34(2)*]
α_{CO7}	0.33(2) [*0.37(2)*]	α_{CO20}	0.31(2) [*0.34(2)*]
α_{CO8}	0.27(2) [*0.31(2)*]	α_{CO21}	0.28(2) [*0.31(2)*]
α_{CO9}	0.16(2)	α_{CO19}	0.14(2)

Cotton's FSRs are reported in parentheses. Pauling's atomic radii are employed: Cu 1.173 Å, Ru 1.241 Å, Br 1.142 Å, C 0.771 Å, H 0.230 Å.

α corrected for the different atom radii of Cu (1.173) and Ru (1.241) in parentheses (covalent radii from Pauling).

Table S3. Main bond distances (Å) and angles (°) of $[HRu_8(CO)_{24}Cu_6Br_2]^{3-}$ (**4**).

Ru1-Ru2	2.9130(10) *(1.17)*	Ru1-Ru3	2.8804(11) *(1.16)*
Ru1-Ru4	2.8341(11) *(1.14)*	Ru2-Ru3	2.9998(11) *(1.21)*
Ru2-Ru4	2.8075(11) *(1.13)*	Ru3-Ru4	2.8519(11) *(1.15)*
Ru5-Ru6	3.0584(11) *(1.23)*	Ru5-Ru7	2.8441(11) *(1.15)*
Ru5-Ru8	2.7983(11) *(1.13)*	Ru6-Ru7	2.8228(11) *(1.14)*
Ru6-Ru8	2.9352(11) *(1.18)*	Ru7-Ru8	2.8146(11) *(1.13)*
Cu1-Ru1	2.6896(14) *(1.11)*	Cu1-Ru3	2.6652(14) *(1.10)*
Cu2-Ru1	2.8642(14) *(1.19)*	Cu2-Ru2	2.7221(14) *(1.13)*
Cu2-Ru3	2.7383(14) *(1.13)*	Cu2-Ru5	2.6337(14) *(1.09)*
Cu3-Ru1	2.6627(14) *(1.10)*	Cu3-Ru2	2.5947(14) *(1.07)*
Cu4-Ru1	2.6461(14) *(1.10)*	Cu4-Ru5	2.7710(14) *(1.15)*
Cu4-Ru6	2.6058(14)	Cu5-Ru5	2.6506(14)

	(1.08)		*(1.10)*
Cu5-Ru6	2.6403(14) *(1.09)*	Cu5-Ru8	2.6889(14) *(1.11)*
Cu6-Ru5	2.6077(13) *(1.08)*	Cu6-Ru6	2.7099(14) *(1.12)*
Cu6-Ru7	2.6457(14) *(1.10)*	Cu1-Cu2	2.5432(16) *(1.10)*
Cu1-Cu4	2.4669(16) *(1.07)*	Cu1-Cu6	2.6596(17) *(1.13)*
Cu2-Cu3	2.5712(17) *(1.10)*	Cu2-Cu4	2.4669(16) *(1.05)*
Cu3-Cu4	2.5590(16) *(1.09)*	Cu3-Cu5	2.7095(17) *(1.15)*
Cu4-Cu5	2.5762(16) *(1.10)*	Cu4-Cu6	2.6492(17) *(1.13)*
Cu1-Br1	2.3915(15) *(1.03)*	Cu6-Br1	2.3864(15) *(1.03)*
Cu3-Br2	2.3459(15) *(1.01)*	Cu5-Br2	2.3816(15) *(1.03)*
H1-Ru2	1.83(10) *(1.24)*	H1-Ru3	1.95(10) *(1.33)*
H1-Cu2	1.79(10) *(1.28)*	C1-Ru1	1.894(11) *(0.94)*
C1-Cu3	2.461(10) *(1.27)*	C1-Cu4	2.241(10) *(1.15)*
C2-Ru1	1.892(9) *(0.94)*	C2-Cu1	2.546(10) *(1.31)*
C4-Ru2	1.911(11) *(0.95)*	C4-Cu3	2.501(10) *(1.29)*
C7-Ru3	1.906(11) *(0.95)*	C7-Cu1	2.301(10) *(1.18)*
C13-Ru5	1.882(10) *(0.94)*	C13-Cu2	2.145(10) *(1.10)*
C16-Ru6	1.879(11) *(0.93)*	C16-Cu4	2.359(10) *(1.21)*
C16-Cu6	2.595(10) *(1.33)*	C17-Ru6	1.907(10) *(0.95)*
C17-Cu5	2.619(10) *(1.35)*	C19-Ru7	1.899(11) *(0.94)*
C19-Cu6	2.379(10)	C22-Ru8	1.906(10)

	(1.22)		*(0.95)*
C22-Cu5	2.535(10) *(1.30)*	C3-Ru1	1.935(10) *(0.96)*
C3-Ru4	2.340(10) *(1.16)*	C15-Ru5	1.959(9) *(0.97)*
C15-Ru8	2.180(10) *(1.08)*	Ru1-C1-O1	163.0(9)
Ru1-C2-O2	173.8(9)	Ru2-C4-O4	169.6(9)
Ru3-C7-O7	164.0(9)	Ru5-C13-O13	157.7(8)
Ru6-C16-O16	168.6(9)	Ru6-C17-O17	171.5(9)
Ru7-C19-O19	167.1(10)	Ru8-C22-O22	173.1(9)
Ru1-C3-O3	149.5(8)	Ru5-C15-O15	141.1(8)
α_{CO1}	0.183(12) [*0.219(12)*]	α_{CO2}	0.346(12) [*0.382(12)*]
α_{CO4}	0.309(13) [*0.344(13)*]	α_{CO7}	0.207(12) [*0.243(12)*]
α_{CO13}	0.141(11) [*0.176(11)*]	α_{CO16}	0.255(13) [*0.292(13)*]
α_{CO17}	0.373(12) [*0.409(12)*]	α_{CO19}	0.253(13) [*0.289(13)*]
α_{CO22}	0.330(12) [*0.366(12)*]		
α_{CO3}	0.209(11)	α_{CO15}	0.113(10)

Cotton's FSRs are reported in parentheses. Pauling's atomic radii are employed: Cu 1.173 Å, Ru 1.241 Å, Br 1.142 Å, C 0.771 Å, H 0.230 Å.

α corrected for the different atom radii of Cu (1.173) and Ru (1.241) in parentheses (covalent radii from Pauling).

Table S4. Main bond distances (Å) and angles (°) of $[Ru_5(CO)_{15}(CuMeCN)_2]$ (**5**).

Ru1-Ru2	2.8526(12) *(1.15)*	Ru1-Ru3	2.9839(12) *(1.20)*
Ru1-Ru4	2.6894(12) *(1.08)*	Ru2-Ru3	2.7792(12) *(1.12)*
Ru2-Ru4	2.9112(13) *(1.17)*	Ru2-Ru5	2.8226(13) *(1.14)*
Ru3-Ru4	2.9056(12) *(1.17)*	Ru3-Ru5	2.9325(12) *(1.18)*
Ru4-Ru5	2.6944(12) *(1.09)*	Cu1-Ru1	2.7336(16) *(1.13)*
Cu1-Ru3	2.5655(16)	Cu1-Ru4	2.7180(15)

	(1.06)		*(1.13)*
Cu2-Ru3	2.5860(17) *(1.07)*	Cu2-Ru4	2.6729(16) *(1.11)*
Cu2-Ru5	2.7358(16) *(1.13)*	Cu1-Cu2	2.6726(18) *(1.11)*
Cu1-N1	1.920(9) *(0.99)*	Cu2-N2	1.925(10) *(0.99)*
C7-Ru3	1.886(12) *(0.94)*	C7-Cu1	2.497(11) *(1.28)*
C9-Ru3	1.894(13) *(0.94)*	C9-Cu2	2.404(13) *(1.24)*
C11-Ru4	1.901(12) *(0.94)*	C11-Cu2	2.610(13) *(1.34)*
C8-Ru2	2.512(12) *(1.29)*	C8-Ru3	1.903(13) *(0.95)*
C10-Ru1	2.393(11) *(1.19)*	C10-Ru4	1.929(12) *(0.96)*
Ru3-C7-O7	171.9(10)	Ru3-C9-O9	170.5(11)
Ru4-C11-O11	174.2(10)	Ru3-C8-O8	159.4(10)
Ru4-C10-O10	156.2(10)	α_{CO7}	0.324(14) [*0.360(14)*]
α_{CO9}	0.269(16) [*0.305(16)*]	α_{CO11}	0.373(16) [*0.409(16)*]
α_{CO8}	0.320(15)	α_{CO10}	0.241(13)

Cotton's FSRs are reported in parentheses. Pauling's atomic radii are employed: Cu 1.173 Å, Ru 1.241 Å, Br 1.142 Å, C 0.771 Å, H 0.230 Å.

α corrected for the different atom radii of Cu (1.173) and Ru (1.241) in parentheses (covalent radii from Pauling).

Table S5. Crystal data and experimental details for $[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$ (**2**), $[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]\cdot 3CH_3COCH_3$ (**3**$\cdot 3CH_3COCH_3$), $[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]\cdot CH_2Cl_2$ (**4**$\cdot CH_2Cl_2$), and $[Ru_5(CO)_{15}(CuMeCN)_2]\cdot CH_2Cl_2$ (**5**$\cdot CH_2Cl_2$).

	$[NEt_4]_3[HRu_4(CO)_{12}(CuBr)_3]$	**$[NEt_4]_2[H_2Ru_8(CO)_{24}Cu_7Br_3]\cdot 3CH_3COCH_3$**
Formula	$C_{36}H_{61}Br_3Cu_3N_3O_{12}Ru_4$	$C_{49}H_{60}Br_3Cu_7N_2O_{27}Ru_8$
Fw	1562.50	2602.06
T, K	100(2)	100(2)
λ, Å	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space Group	$P2_1/n$	$P2_1/c$
a, Å	12.6129(5)	14.292(3)
b, Å	27.7074(10)	23.458(5)
c, Å	14.6211(6)	22.443(5)
α, °	90	90
β, °	96.0210(10)	93.240(9)
γ, °	90	90
Cell Volume, $Å^3$	5081.5(3)	7512(3)
Z	4	4
D_c, g cm^{-3}	2.042	2.301
μ, mm^{-1}	4.802	5.159
F(000)	3048	4976
Crystal size, mm	0.20×0.16×0.14	0.22×0.16×0.13
θ limits, °	1.582-26.000	1.648-25.200
Index ranges	$-15 \le h \le 15$ $-34 \le k \le 34$ $-18 \le l \le 18$	$-17 \le h \le 17$ $-28 \le k \le 28$ $-26 \le l \le 26$
Reflections collected	72054	80943
Independent reflections	9987 [R_{int} = 0.0445]	13546 [R_{int} = 0.0868]
Completeness to θ max	100.0%	100.0%
Data / restraints / parameters	9987 / 4 / 569	13546 / 605 / 852
Goodness on fit on F^2	1.213	1.078
R_1 ($I > 2\sigma(I)$)	0.0369	0.0929
wR_2 (all data)	0.0752	0.2460
Largest diff. peak and hole, e $Å^{-3}$	1.278 / -0.620	3.188 / -2.388

	$[NEt_4]_3[HRu_8(CO)_{24}Cu_6Br_2]\cdot CH_2Cl_2$	$[Ru_5(CO)_{15}(CuMeCN)_2]\cdot CH_2Cl_2$
Formula	$C_{49}H_{63}Br_2Cl_2Cu_6N_3O_{24}Ru_8$	$C_{20}H_8Cl_2Cu_2N_2O_{15}Ru_5$
Fw	2498.54	1219.61
T, K	100(2)	100(2)
λ, Å	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$
a, Å	12.5448(6)	9.0648(10)
b, Å	13.5388(6)	11.3026(13)
c, Å	22.7631(10)	17.3140(19)
α, °	87.1610(10)	107.816(4)
β, °	85.5450(10)	93.116(4)
γ, °	67.5230(10)	109.764(4)
Cell Volume, $Å^3$	3560.8(3)	1564.7(3)
Z	2	2
D_c, g cm^{-3}	2.330	2.589
μ, mm^{-1}	4.662	3.921
F(000)	2400	1148
Crystal size, mm	0.12×0.09×0.07	0.13×0.10×0.06
θ limits, °	1.628-26.407	1.992-25.099
Index ranges	$-15 \le h \le 15$ $-16 \le k \le 16$ $-28 \le l \le 28$	$-10 \le h \le 10$ $-13 \le k \le 13$ $-20 \le l \le 20$
Reflections collected	34169	11164
Independent reflections	14580 [R_{int} = 0.0674]	5534 [R_{int} = 0.0510]
Completeness to θ max	100.0%	99.3%
Data / restraints / parameters	14580 / 48 / 862	5534 / 0 / 417
Goodness on fit on F^2	1.081	1.061
R_1 ($I > 2\sigma(I)$)	0.0640	0.0588
wR_2 (all data)	0.1265	0.1534
Largest diff. peak and hole, e $Å^{-3}$	1.888 / -1.585	1.946 / -1.326