Electronic Supplementary Information for Dalton Transactions

ESI pages for

Kinetic study of the reaction of $[Rh_6(CO)_{16}]$ with NO_2^-: Insertion of the nitrogen atom into a Rh_6 cluster core

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Fig. S1 Typical absorbance changes at 450 nm during step 1 at 25 °C under N_2. Data fitted using a single exponential function.

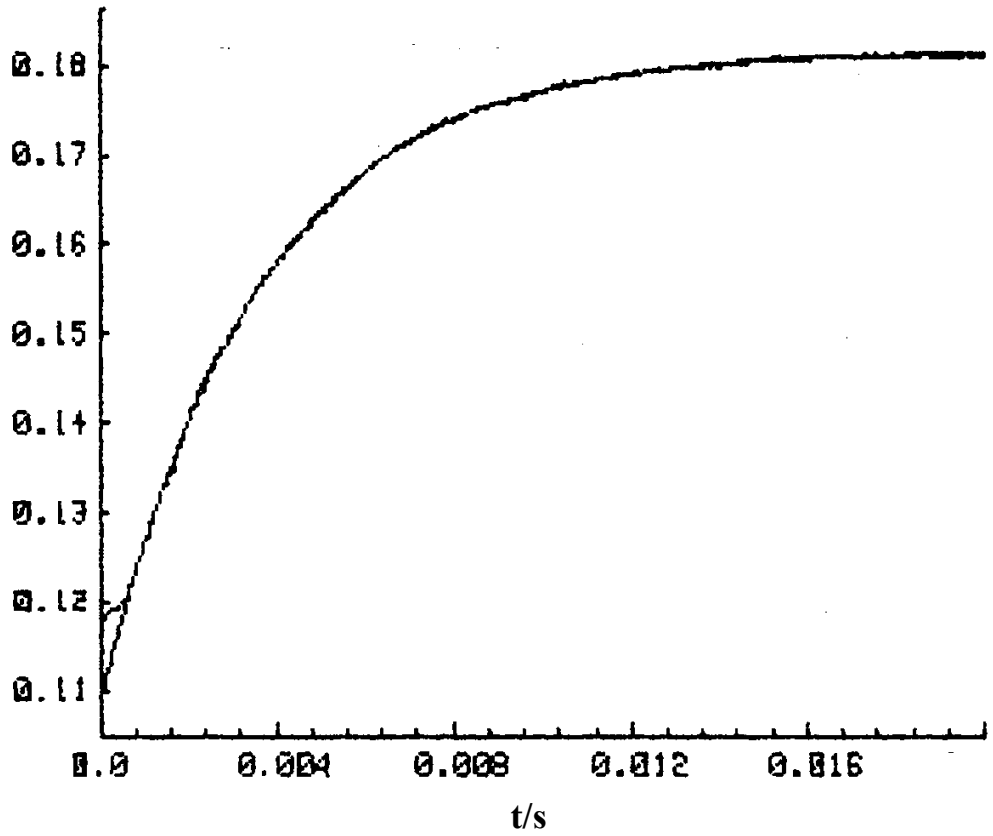

Fig. S2 Typical plot of absorbance (425 nm) vs. time (t/s) for step 2 at 10 °C under CO. Data fitted using a single exponential function and the "residuals" are also shown (with a much expanded scale).

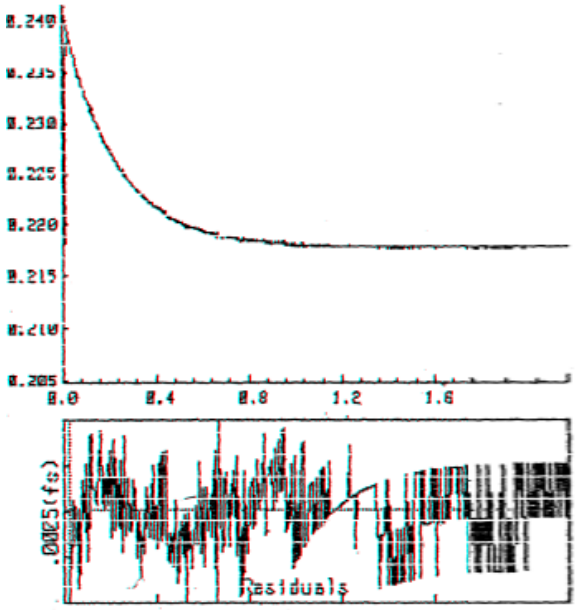

Fig. S3 Spectrum of the "2013 cm^{-1} species" established by subtracting the spectra of $[Rh_6(CO)_{14}(\kappa^2\text{-}O\underline{C}O\underline{N}O)]^-$ and $Rh_6N(CO)_{15}]^-$ from that of the mixture when the concentration of the "2013 cm^{-1} species" is at a maximum.

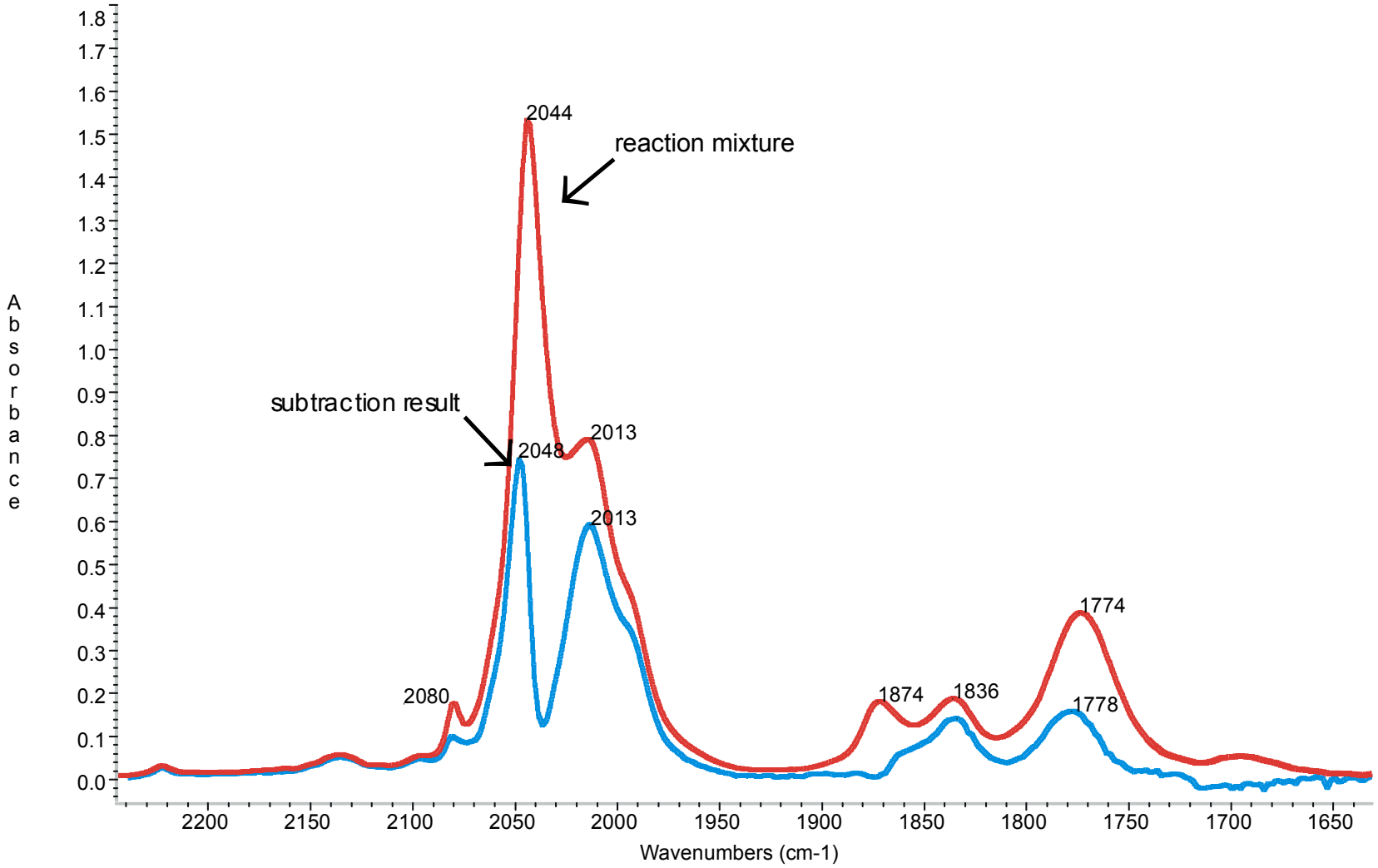

Table S1 Crystal Data and Structure Refinement for PPN[$Rh_6N(CO)_{15}$] (Using *SHELXTL/PC*; Bruker Analytical X-ray : Madison, WI, 1997).

Identification code	k99228
Empirical formula	C51 H30 N O16 P2 Rh6
Formula weight	1592.16
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.0540(18) Å α= 109.80(3)°.
	b = 15.826(3) Å β= 91.07(3)°.
	c = 19.596(4) Å γ = 97.02(3)°.
Volume	2616.7(9) $Å^3$
Z	2
Density (calculated)	2.021 Mg/m^3
Absorption coefficient	1.980 mm^{-1}
F(000)	1542
Crystal size	0.25 x 0.20 x 0.20 mm^3
Theta range for data collection	2.59 to 27.51°.
Index ranges	0<=h<=11, -20<=k<=20, -25<=l<=25
Independent reflections	11788 [R(int) = 0.064]
Completeness to theta = 27.51°	97.9 %
Absorption correction	None
Max. and min. transmission	0.6929 and 0.6374
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	11788 / 0 / 686
Goodness-of-fit on F2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0815
R indices (all data)	R1 = 0.0496, wR2 = 0.0866
Extinction coefficient	0.00098(9)

Largest diff. peak and hole	0.948 and -1.210 e.Å^{-3}