Binding of CO, and NH_3, at a five-coordinate Ru(II) centre in the solid state and in solution

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SUPPLEMENTARY MATERIAL

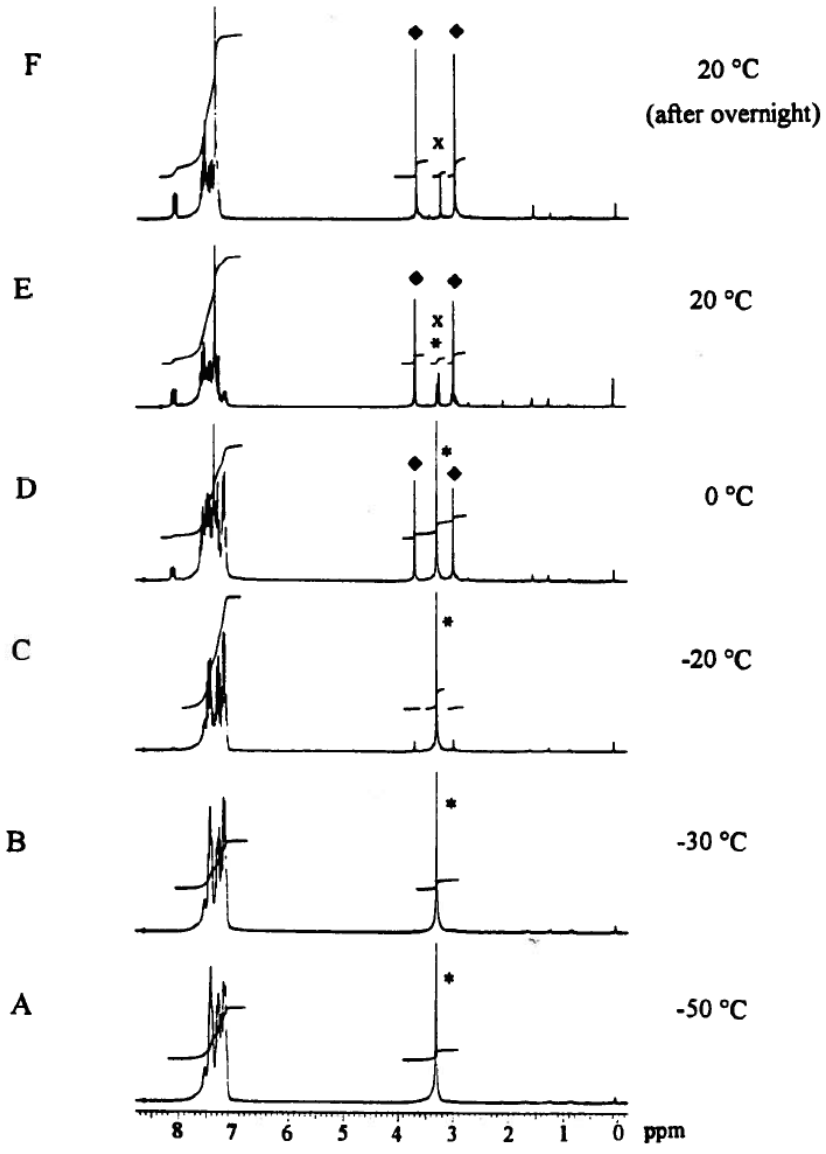

Fig. S1. Variable temperature ^{1}H NMR spectra ($CDCl_3$) of **1a** under 1 atm CO; * = NMe_2 of **2a**, ♦ = NMe of *cis*,*cis*-**3**, **x** = NMe_2 of *tran,cis*-**3**.

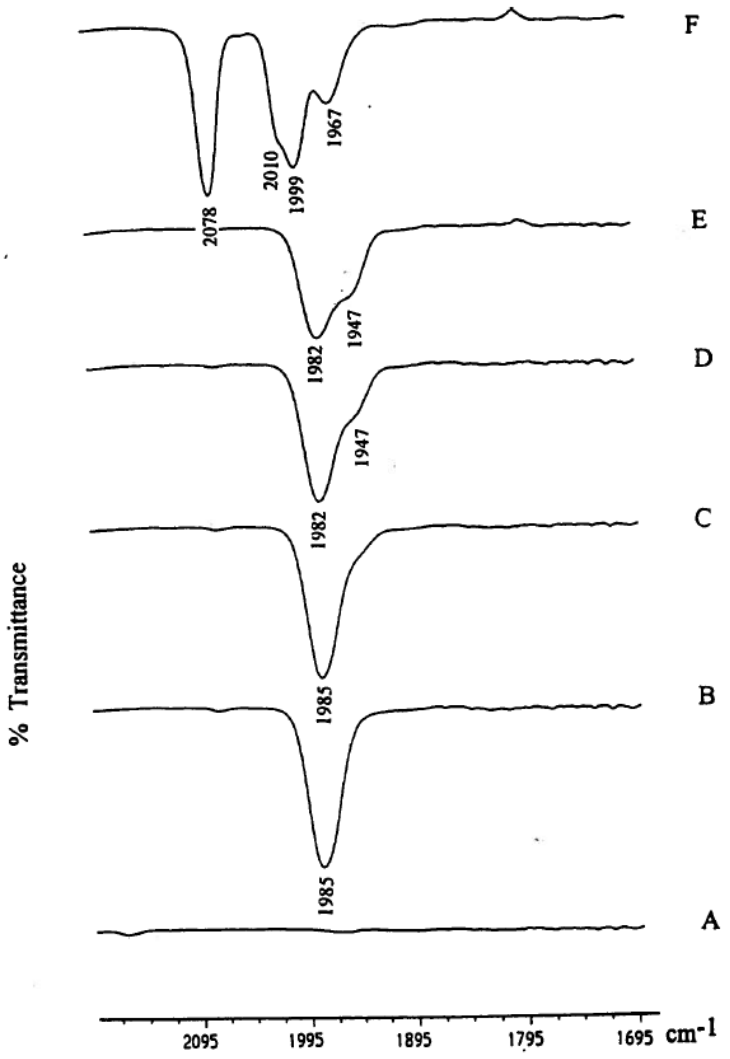

Fig. S2. IR spectra ($CHCl_3$, 0.1 mm KBr cell) of **1a** under Ar (A), and **1a** under 1 atm CO at different temperatures: ~ –50 °C (B), between ~ C50 and 20 °C (C–E), and 50 °C (F).

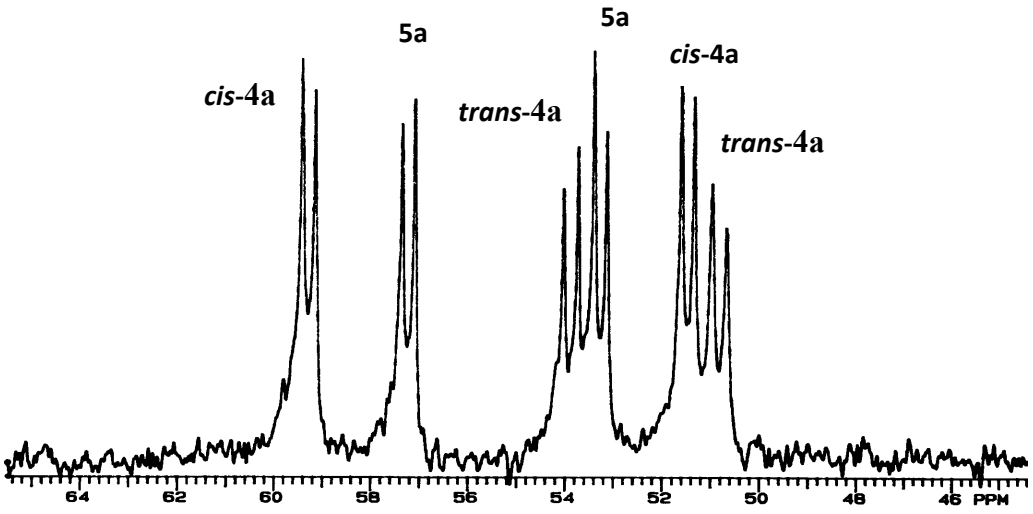

Fig. S3. $^{31}P\{^{1}H\}$ NMR spectrum of *trans*-$RuCl_2(P–N)(PPh_3)(NH_3)$ (*trans*-**4a**), 5 min after dissolution in $CDCl_3$ at 20 °C; see Experimental section for assignments.

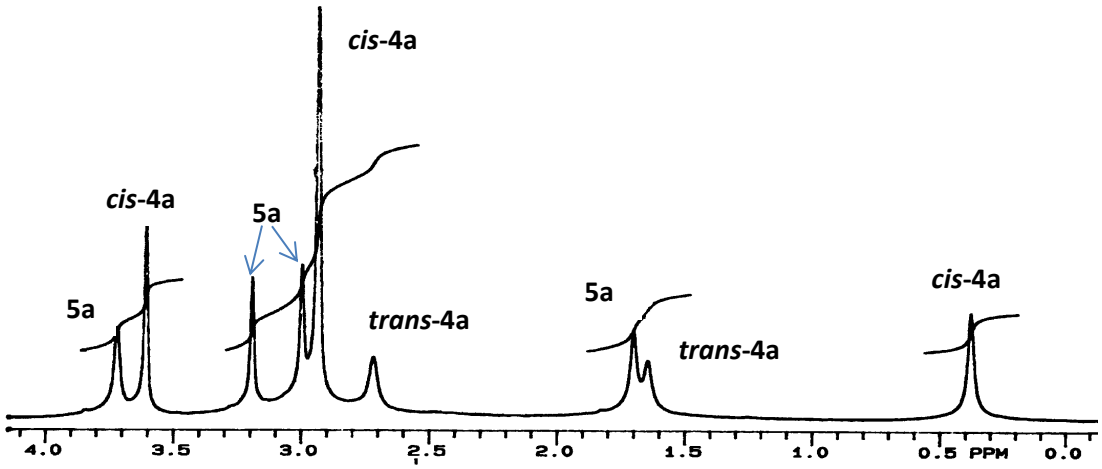

Fig. S4. ^{1}H NMR spectrum (in the δ 4.0 to 0.0 region) of *trans*-$RuCl_2(P–N)(PPh_3)(NH_3)$ (*trans*-**4a**), 5 min after dissolution in $CDCl_3$ at 20 °C; see Experimental section for assignments.

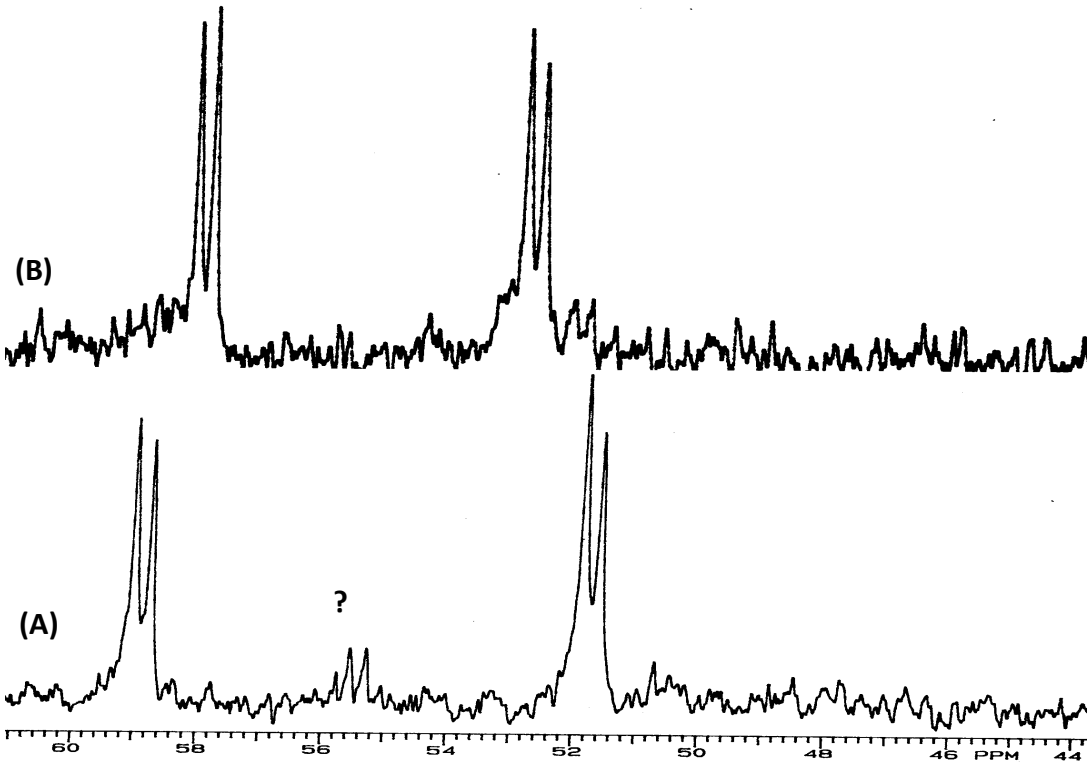

Fig. S5. $^{31}P\{^{1}H\}$ NMR spectra (d_6-acetone at 20 °C) of: (A) $[RuCl(P–N)(PPh_3)(NH_3)_2][PF_6]$ **(6)** − the septet of PF_6^- is at δ-143.4; and (B) **5a**, $[RuCl(P–N)(PPh_3)(NH_3)_2\cdots Cl]$, or $RuCl_2(P–N)(PPh_3)(NH_3)_2$ with monodentate P–N (see text).

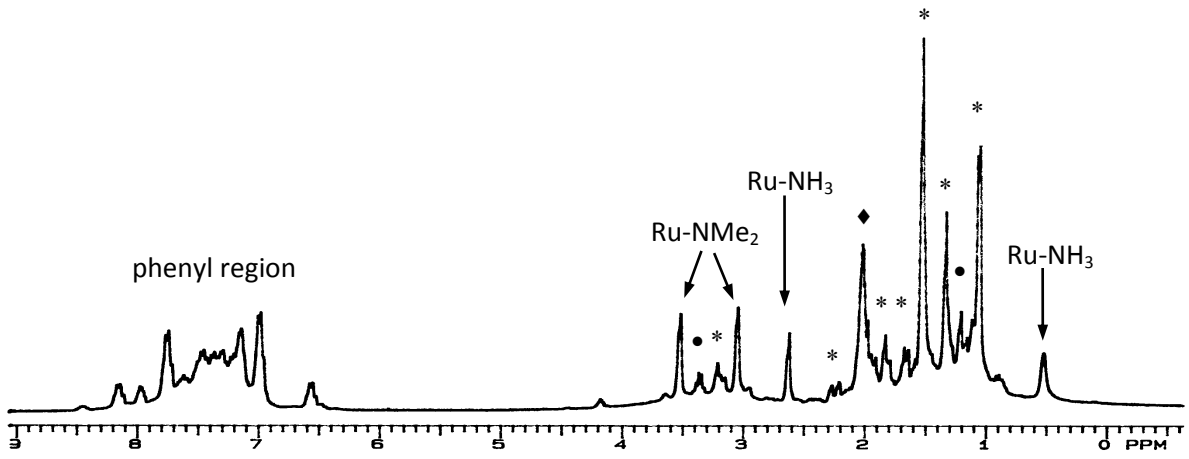

Fig. S6. ^{1}H NMR spectrum of $[RuCl(P\text{-}N)(PPh_3)(NH_3)_2]PF_6$ **(6)** in d_6-acetone at 20 °C;
♦ = acetone (δ2.0); • = Et_2O (δ3.4, 1.2) from isolation of **6**; * = unidentified.

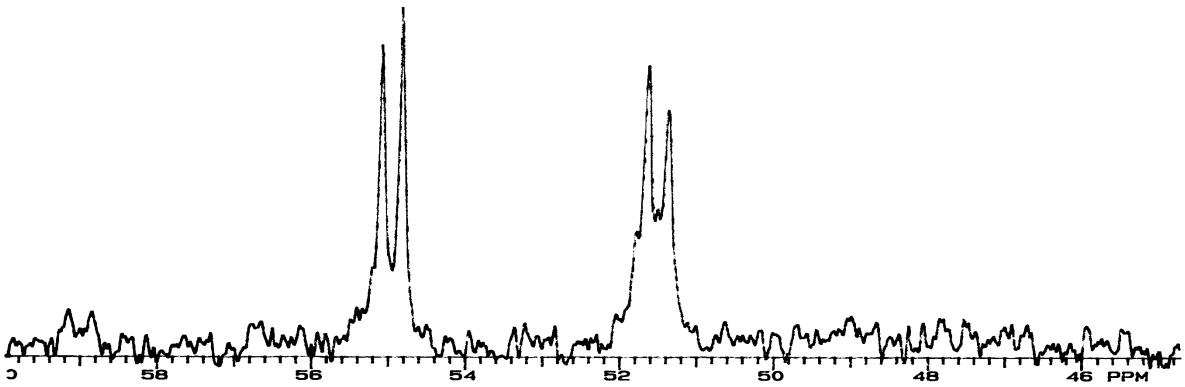

Fig. S7. $^{31}P\{^{1}H\}$ NMR spectrum for *in situ* formation (d_6-acetone, 20 °C) of $[Ru(P{-}N)(PPh_3)(NH_3)_3](PF_6)_2$ (**8**) from reaction of **1a** and 2 equiv. NH_4PF_6 with 1 atm NH_3 in d_6-actone at 20 °C – the septet of PF_6^- is at δ-143.4.