Supporting Information

Hydrogen-bond networks in polymorphs and solvates in metallorganic complexes containing ruthenium and aminoamide ligands

Alessia Bacchi, Giulia Cantoni, Domenico Crocco, Matteo Granelli,† Paolo Pagano, Paolo Pelagatti*

Dipartimento di Chimica, Università degli Studi di Parma, Viale delle Scienze 17/A, 43124 Parma, Italy

† Department of Chemistry, University of Genève, Quai Ernest A. 30, 1205 Genève, Switzerland

*Paolo Pelagatti, Department of Chemistry, University of Parma, Parco Area Scienze 17/A, 43124 Parma, Italy. Email paolo.pelagatti@unipr.it. Tel. +39 0521 905426. Fax +39 0521 905557

Index

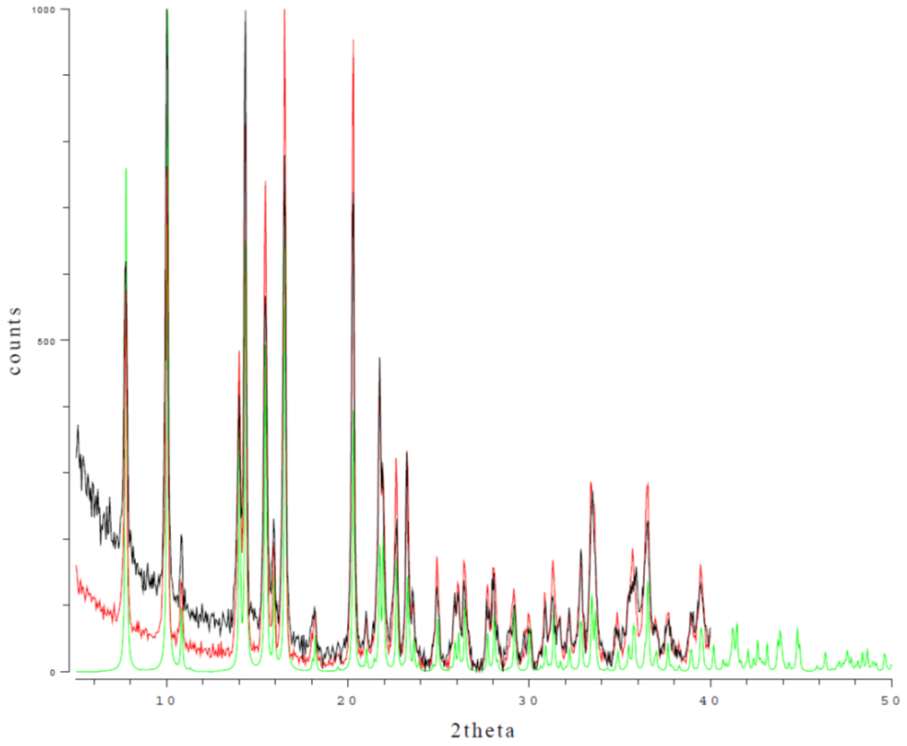

Figure S1 Comparison between the XRPD traces of **1α** synthesized in methanol (red trace), water (black trace) and calculated from X-ray structure (green trace).

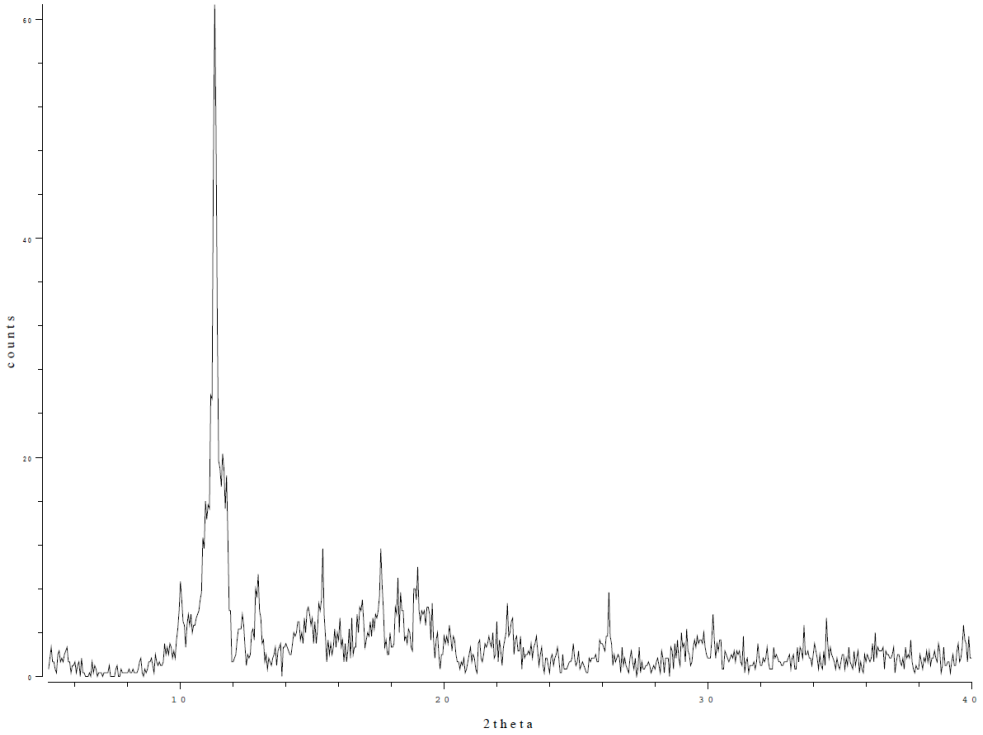

Figure S2 XRPD trace of complex **2**

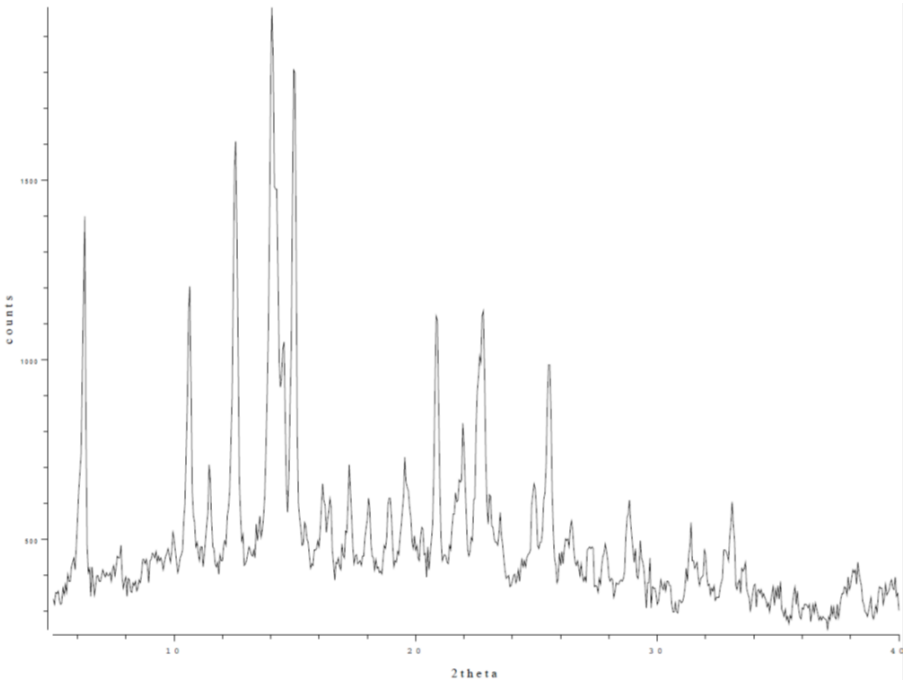

Figure S3 XRPD trace of the yellow microcrystalline solid obtained after exposure of **1α** to vapors of anhydrous ammonia.

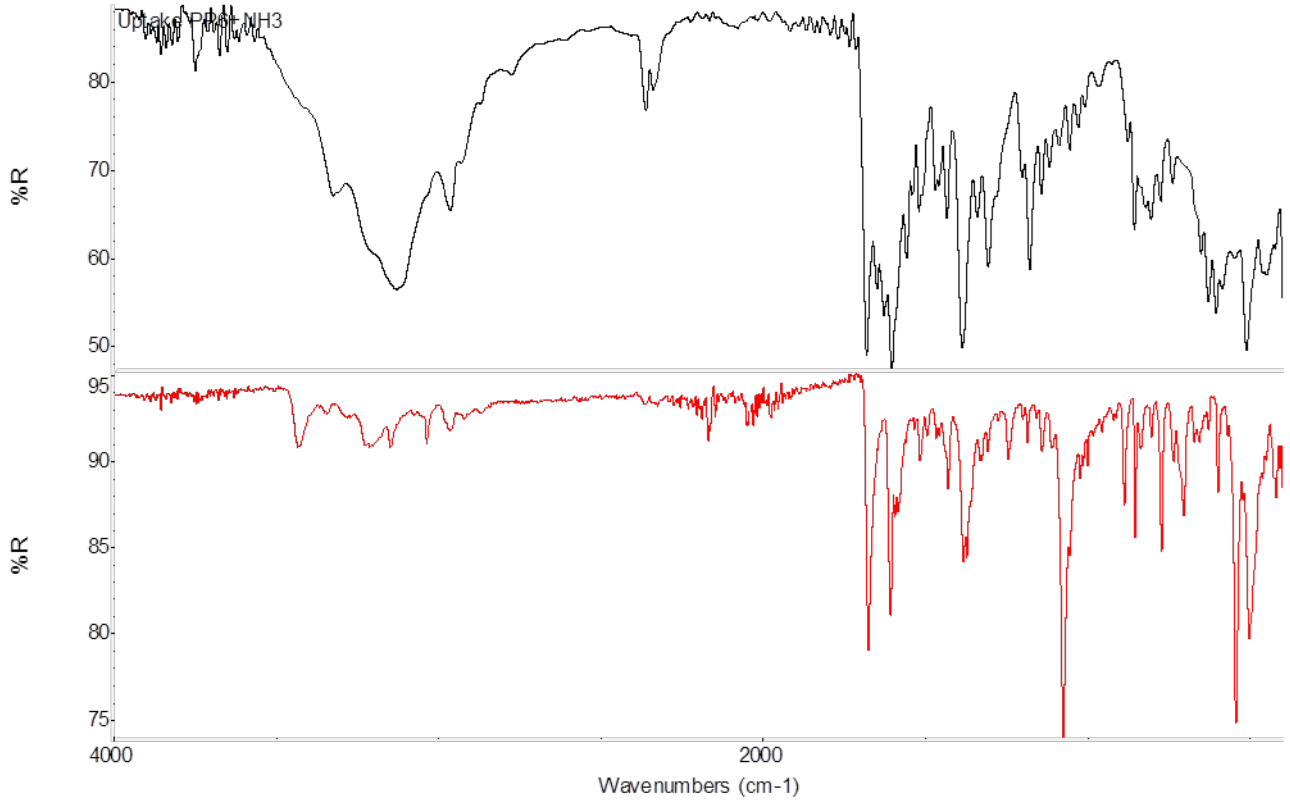

Figure S4 Comparison between the FTIR (ATR) spectra after (black) and before (red) ammonia uptake by complex **1α**.

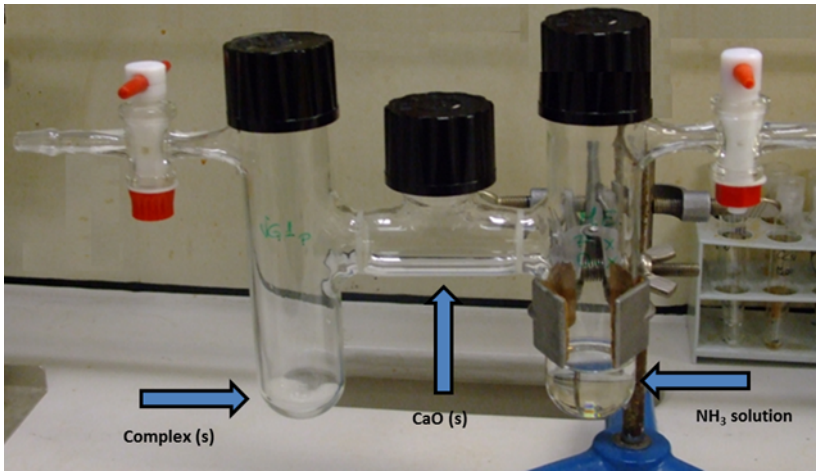

Figure S4 Apparatus used for the ammonia uptake.

Solution ^{1}H-NMR data

^{1}H NMR spectra were recorded on an AV-300 or an AV-400 MHz Bruker spectrophotometers at 25 °C, the chemical shift values are referred to TMS. *J* values are given in Hz.

[(p-cymene)RuCl$_2$(κN-4AB)] (1) δ_H (400MHz; CDCl3/one drop of DMSO-d6): 7.54 (2H, d, Aniline, $^{3}J_{HH}$ 7.2), 6.54 (2H, d, Aniline, $^{3}J_{HH}$ 7.2), 5.74 (1H, br, NH), 5.53 (2H, d, p-cymene, $^{3}J_{HH}$ 5.4), 5.46 (2H, d, p-cymene, $^{3}J_{HH}$ 5.4), 4.33 (1H, br, NH), 2.90 (1H, m, C*H*(CH$_3$)$_2$, $^{3}J_{HH}$ 6.6), 2.53 (2H, br, NH), 2.13 (3H, s, CH$_3$), 1.17 (6H, d, CH(C*H*$_3$)$_3$, $^{3}J_{HH}$ 6.6).

[(p-cymene)RuCl$_2$(κN-4ABN)] (2·2H$_2$O) δ_H (300MHz; CD$_2$Cl$_2$): 7.95 (3H, br, NH+Aniline), 7.70 (2H, d, Ph, $^{3}J_{HH}$ 7.6), 7.43 (3H, t, Aniline+Ph), 7.21 (1H, t, Ph, $^{3}J_{HH}$ 7.6), 5.08 (2H, d, p-cymene, $^{3}J_{HH}$ 6), 4.94 (2H, d, p-cymene, $^{3}J_{HH}$ 6), 4.84 (2H, br, NH$_2$), 2.89 (1H, m, C*H*(CH$_3$)$_2$), 2.16 (3H, s, CH$_3$), 1.28 (6H, d, CH(C*H*$_3$)$_2$).

The ^{1}H-NMR spectrum of complex **2** was identical to that of complex **2·2H$_2$O**.