

Electronic Supplementary Data

Copper (II) chlorofluorophosphate: a new layered square-net for intercalating amines

S1. Infrared Spectra in the range 4000 -550 cm^{-1} for the three new compounds described in the main manuscript

Figure S1a IR spectrum of compound 1 $[\text{NH}_4]\text{Cu}_4\text{Cl}(\text{PO}_3\text{F})_4$:

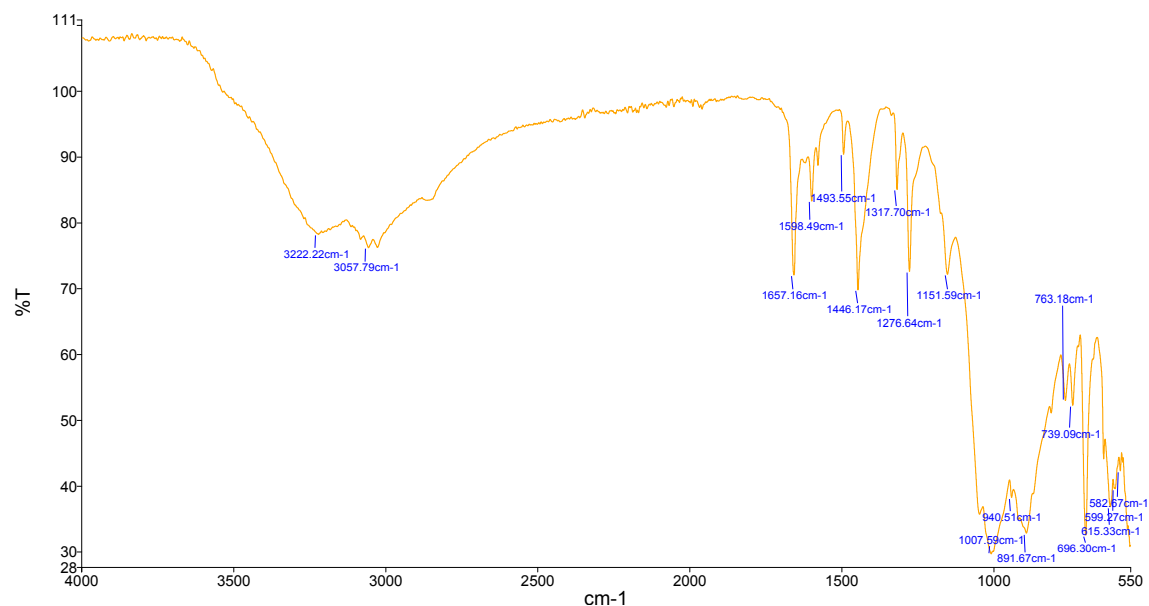


Figure S1b IR spectrum of Compound 2. $[\text{H-piperazine}]\text{Cu}_4\text{Cl}(\text{PO}_3\text{F})_4$:

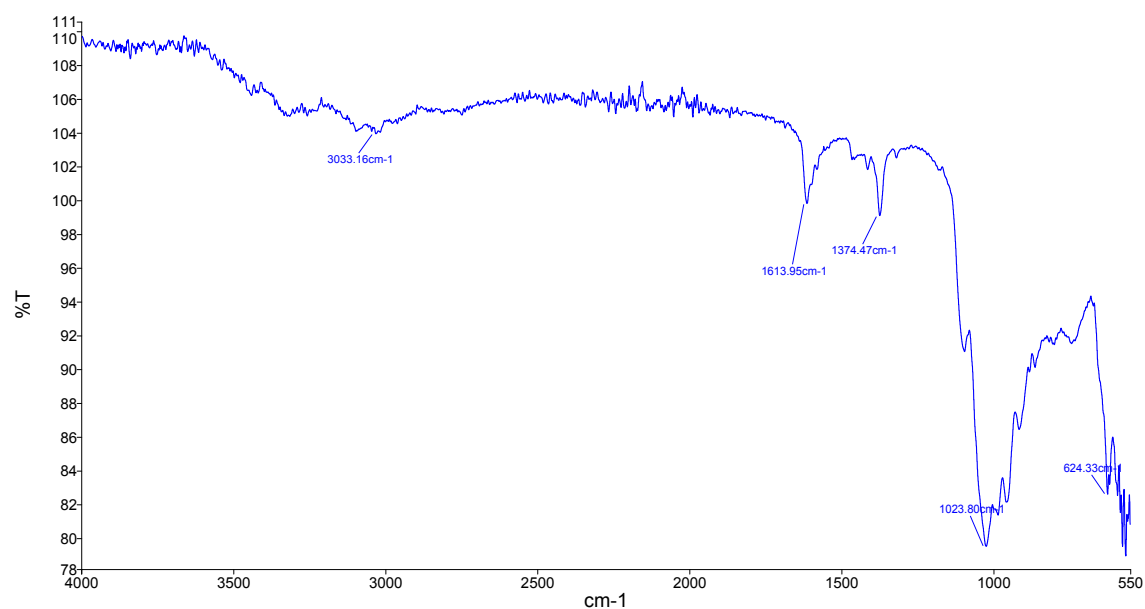
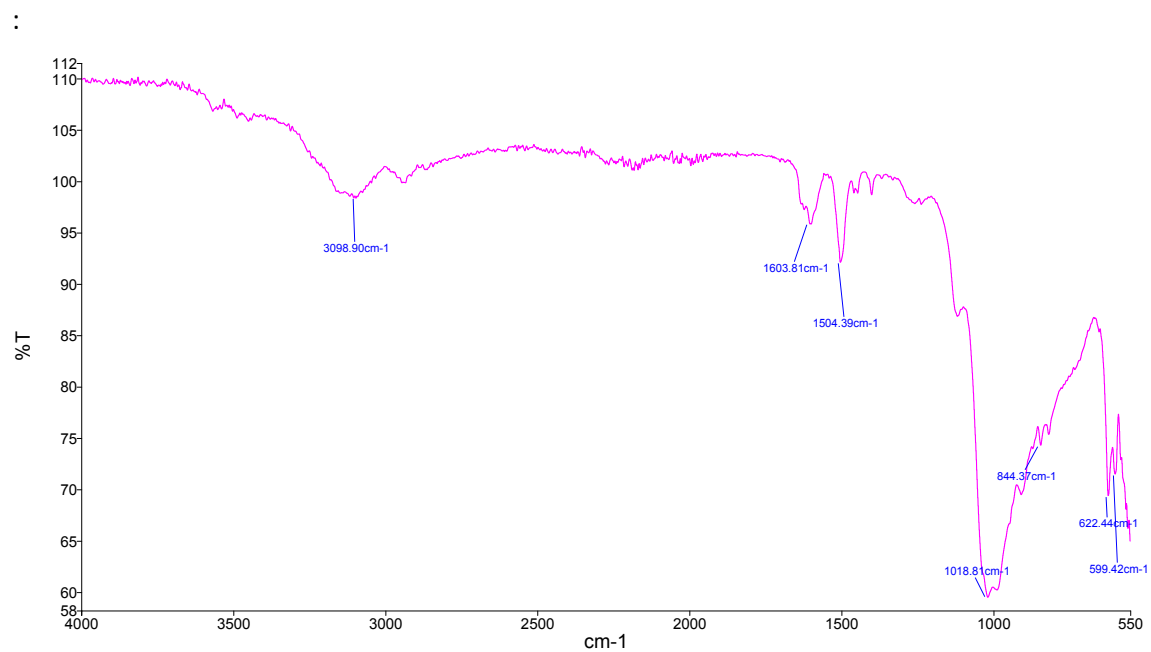


Figure S1c IR spectrum of Compound 3 [H-trans-1,4-diaminocyclohexane] Cu₄Cl(PO₃F)₄



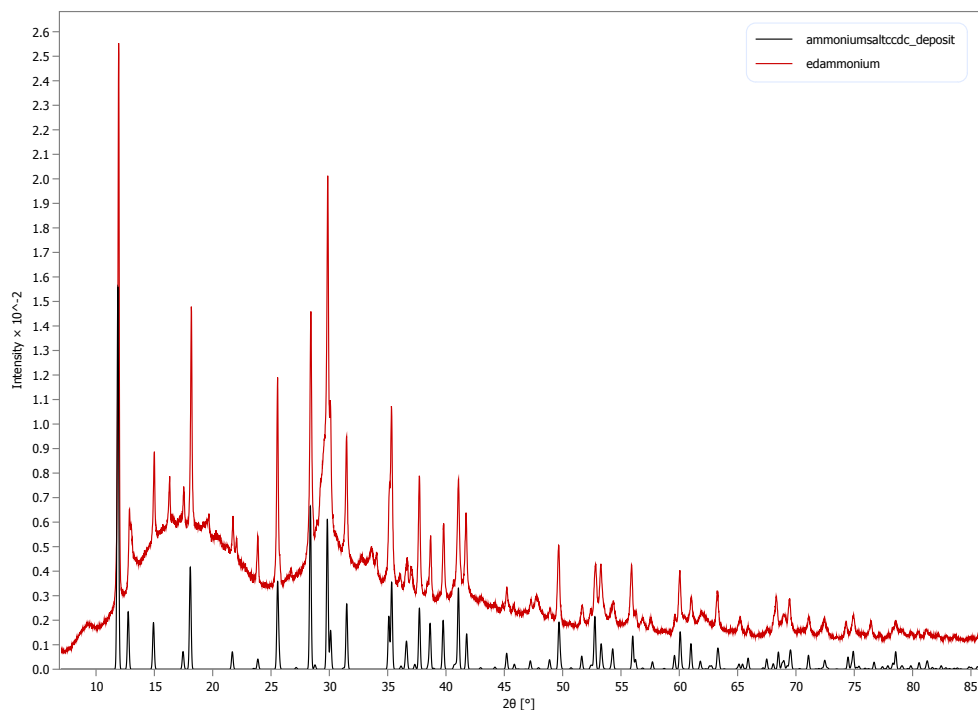


Figure S2a Comparison of calculated and experimental powder diffraction patterns from Compound 1 $[\text{NH}_4]\text{Cu}_4\text{Cl}(\text{PO}_3\text{F})_4$: between 5 and 85 degrees with CuK α radiation. Experimental data were collected from a 10 mg sample mounted on a plastic sample holder producing the observed background

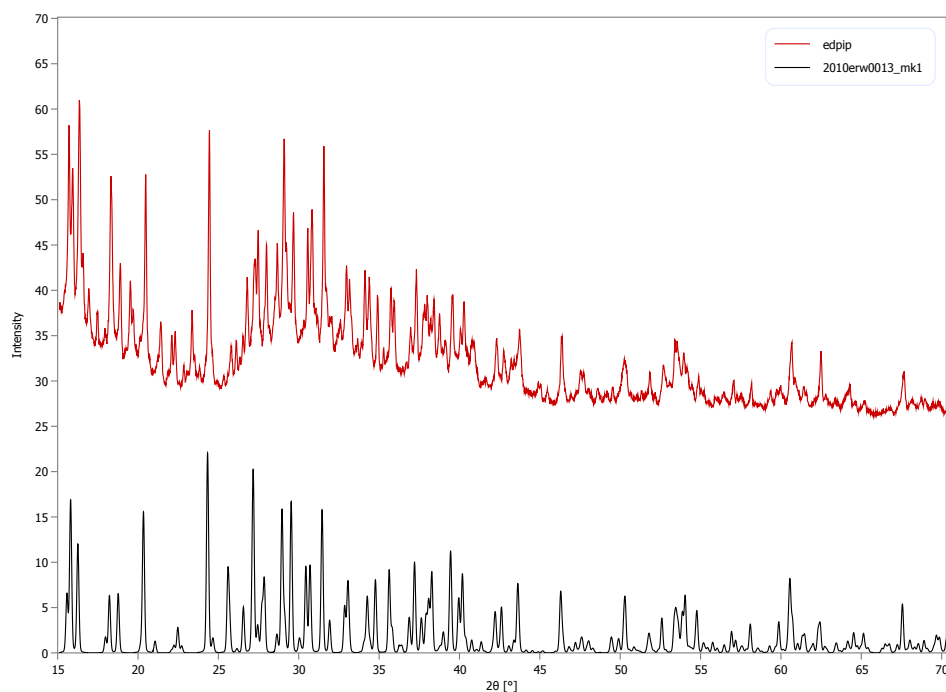


Figure S2b. Comparison of calculated and experimental powder diffraction patterns from Compound 2 $[\text{H-piperazine}]\text{Cu}_4\text{Cl}(\text{PO}_3\text{F})_4$: between 15 and 70 degrees with CuK α radiation. Experimental data were collected from a 10 mg sample mounted on a plastic sample holder producing the observed background

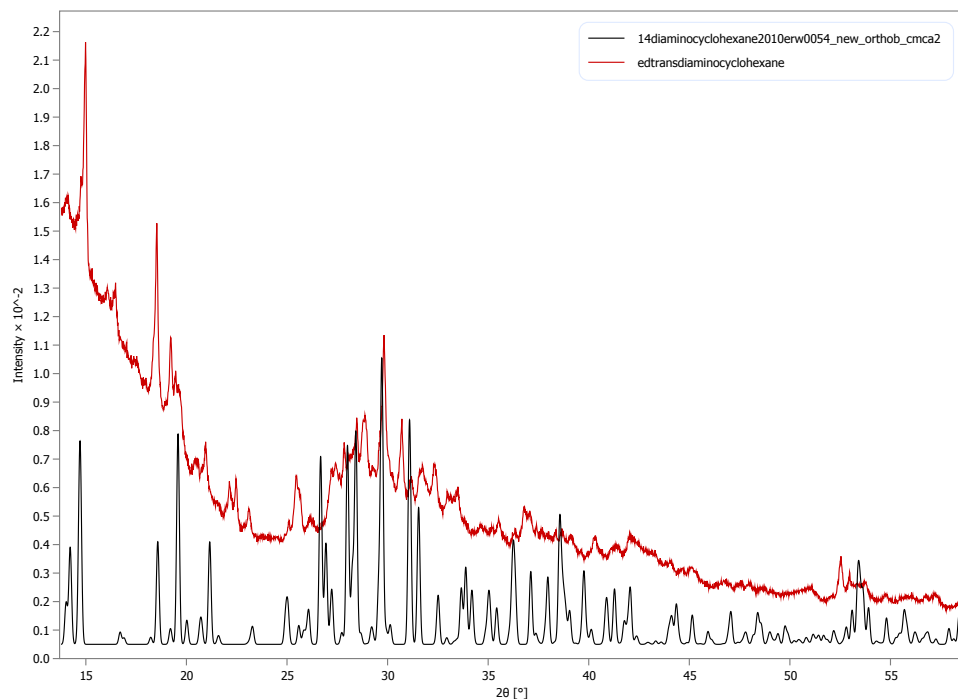


Figure S2c Comparison of calculated and experimental powder diffraction patterns from Compound 3, [H-trans-1,4-diaminocyclohexane] $\text{Cu}_4\text{Cl}(\text{PO}_3\text{F})_4$ between 12 and 60 degrees with CuK α radiation. Experimental data were collected from a 10 mg sample mounted on a plastic sample holder producing the observed background