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Supporting Information

Structures and trends of one-dimensional halide-bridged polymers of five-coordinate cadmium(II) and mercury(II) with benzopyridine and –pyrazine type N-donor ligands

C. Slabbert and M. Rademeyer*

Department of Chemistry, University of Pretoria, cnr Lynnwood Road & Roper Street, Hatfield, Pretoria 0002, South Africa

Simulated and experimental powder X-ray diffraction patterns

In Figures S1 to S13 below, the experimental powder X-ray diffraction patterns of the bulk samples are compared with powder patterns simulated from the single crystal structures. In this comparison, the experimental powder patterns are shown in red, while the calculated patterns are given in black. It was found that compound **6** decomposed upon preparative grinding of the powder X-ray diffraction sample. For the rest of the compounds the single crystal structure was determined to be representative of the bulk sample.

Fig. S1: Experimental and simulated powder diffraction pattern for compound **1: [Cd(μ-Cl)$_2$acr]$_\infty$**

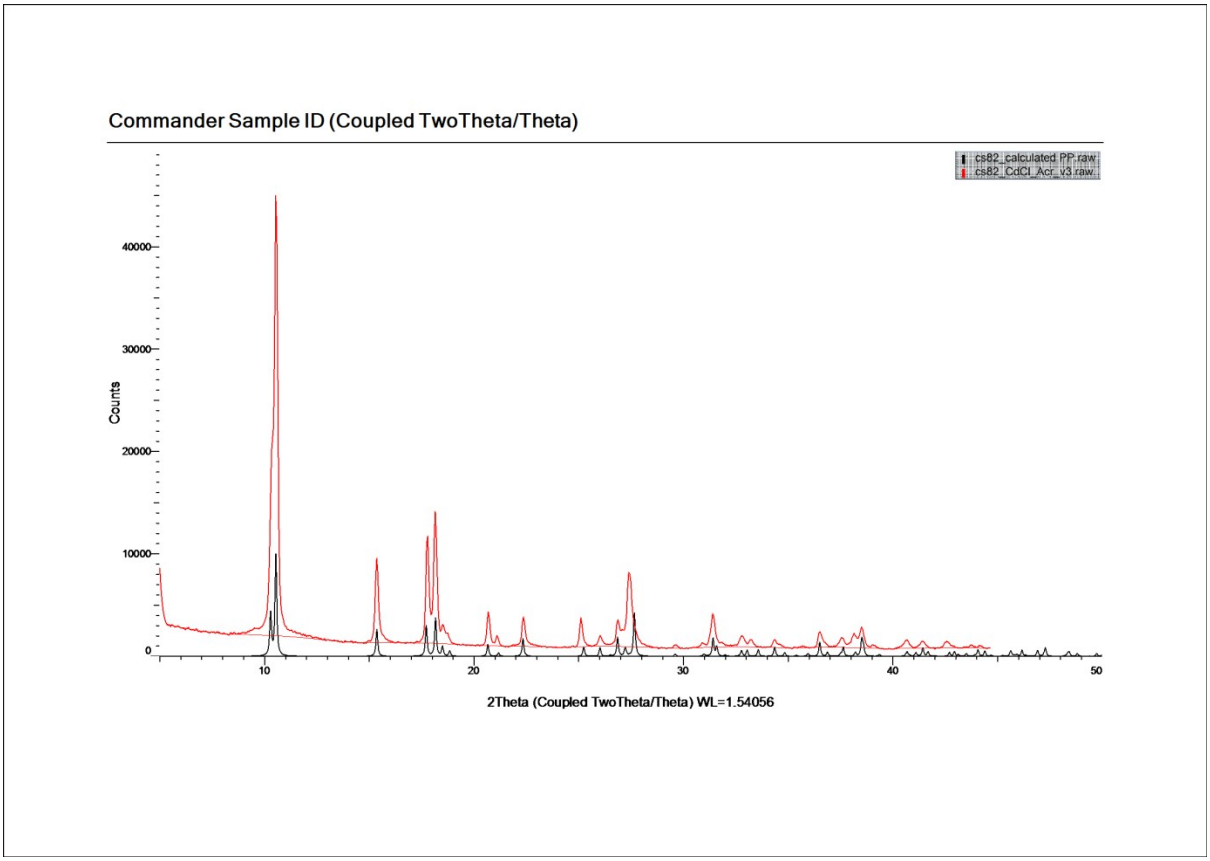

Fig. S2: Experimental and simulated powder diffraction pattern for compound **2: [Cd(μ-Br)$_2$acr]$_\infty$**

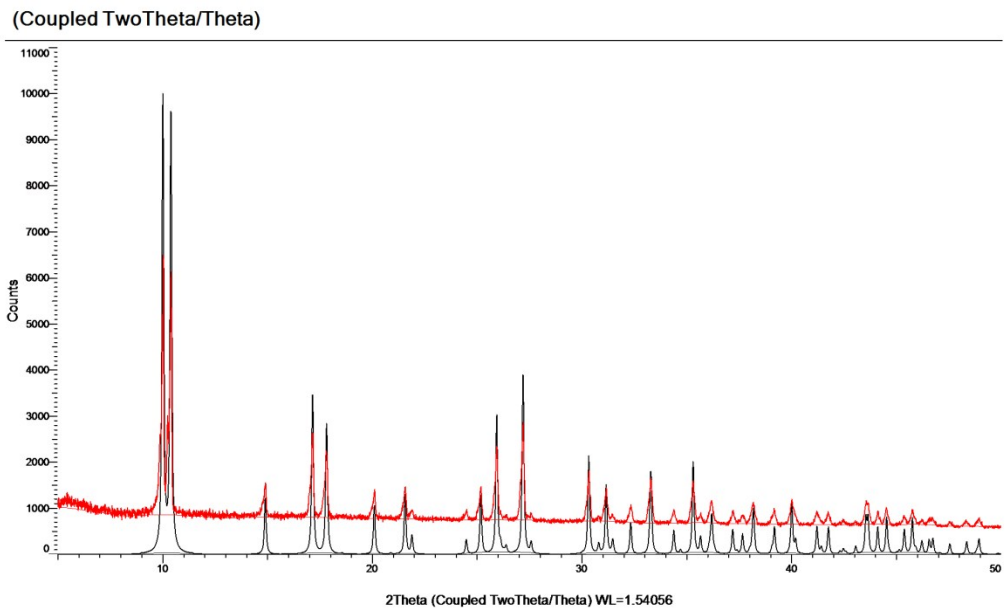

Fig. S3: Experimental and simulated powder diffraction pattern for compound **3: [Cd(μ-I)$_2$acr]$_\infty$**

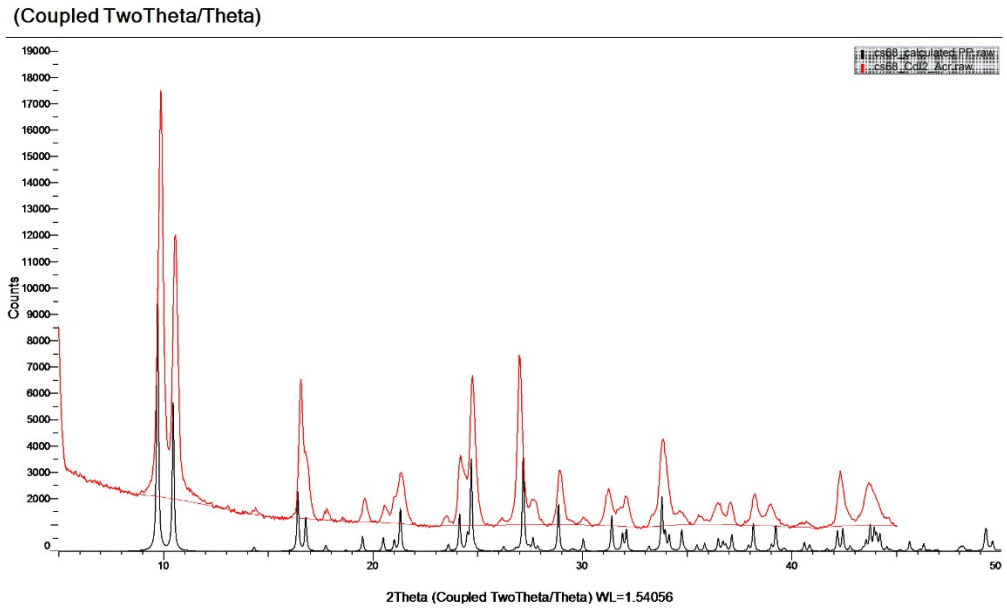

Fig. S4: Experimental and simulated powder diffraction pattern for compound **4: [Hg(μ-Cl)$_2$acr]$_\infty$**

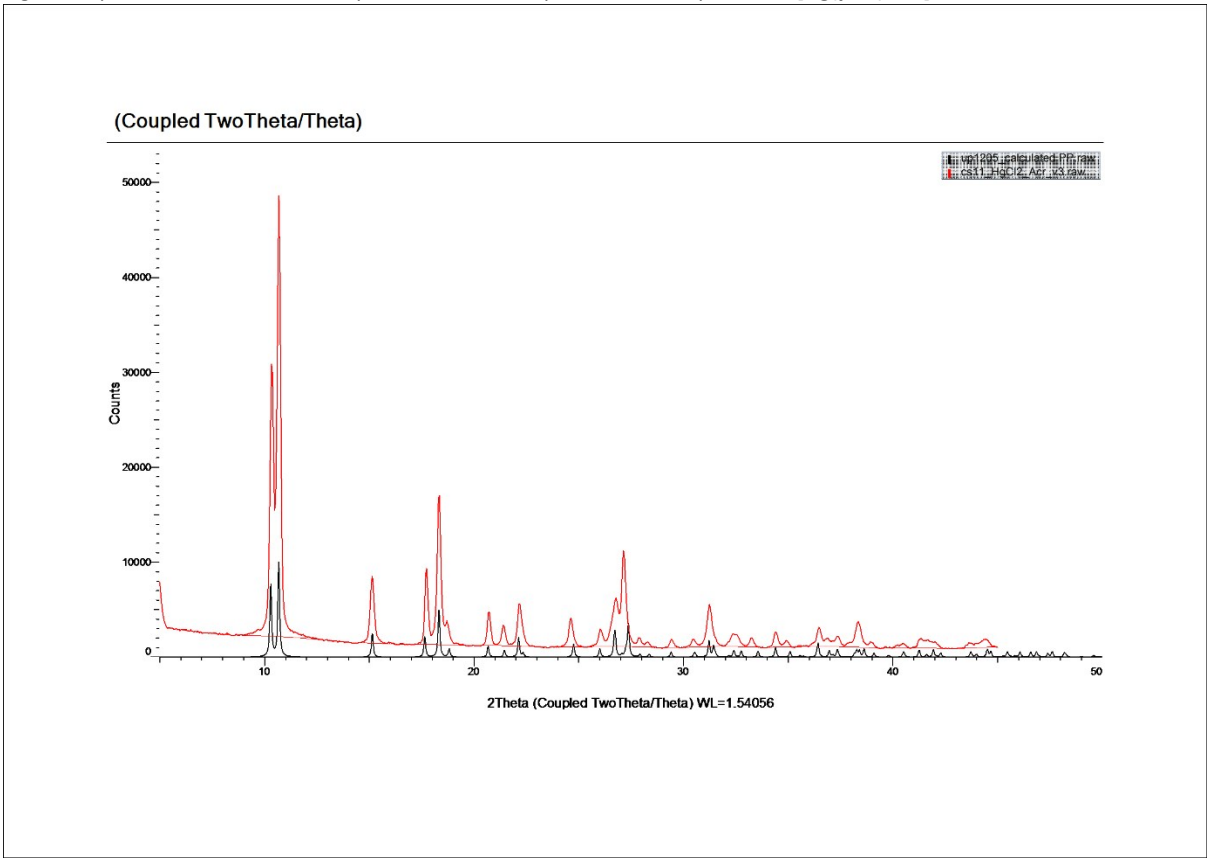

Fig. S5: Experimental and simulated powder diffraction pattern for compound **5: [Hg(μ-Br)$_2$acr]$_\infty$**

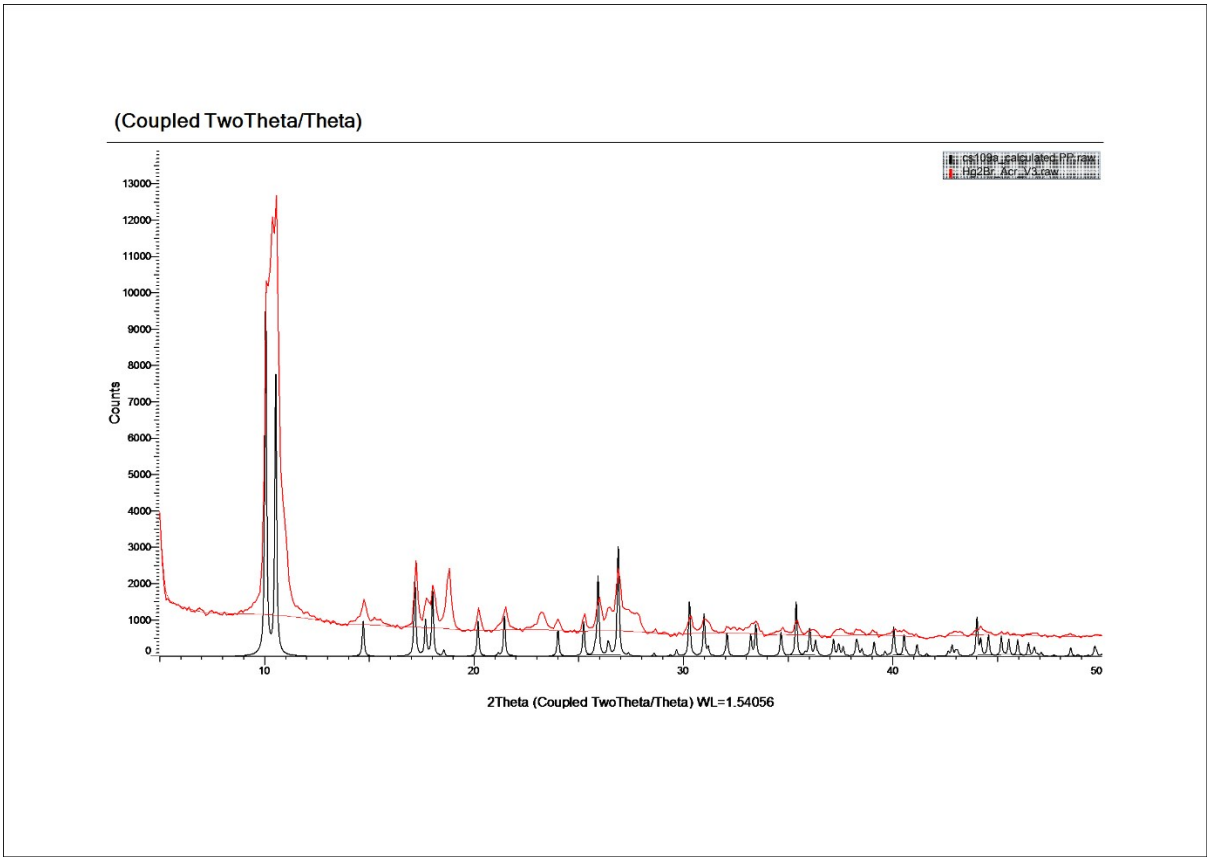

Fig. S6: Experimental and simulated powder diffraction pattern for compound **6: [Hg(μ-I)$_2$(I)acr]**

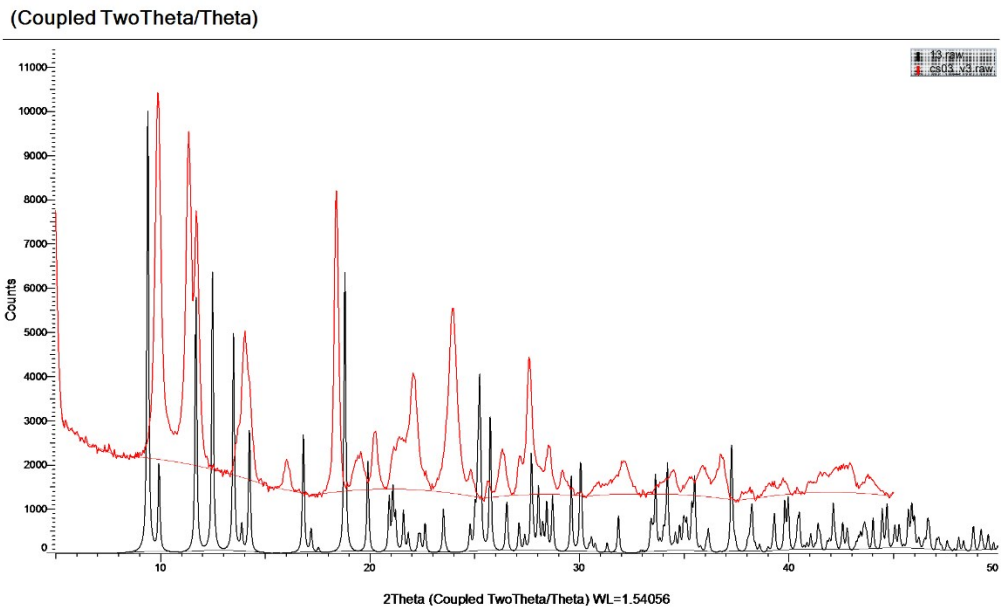

Fig. S7: Experimental and simulated powder diffraction pattern for compound **7: [Cd(μ-Cl)$_2$phe]$_\infty$**

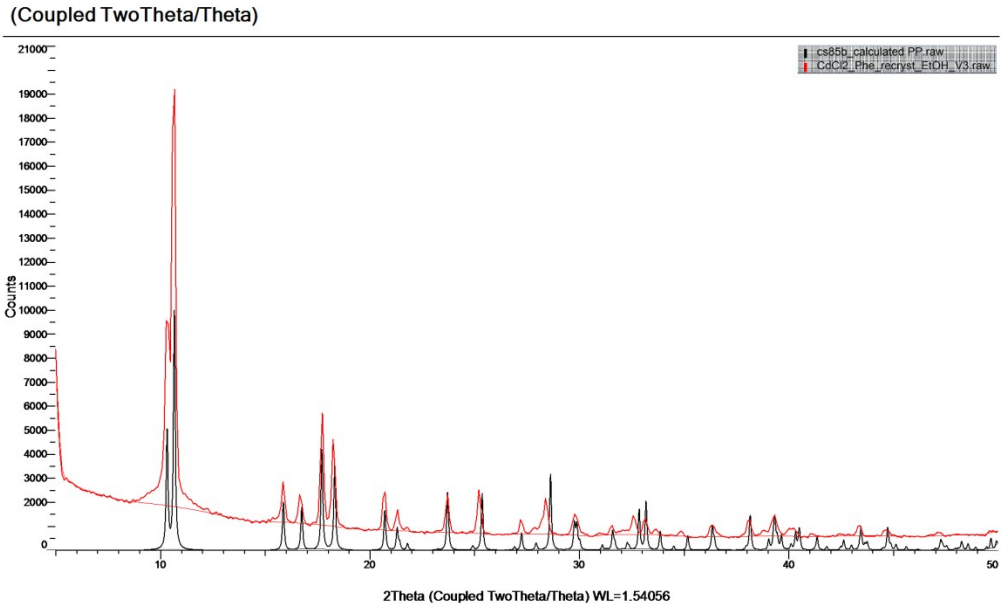

Fig. S8: Experimental and simulated powder diffraction pattern for compound **8: [Hg(μ-Cl)$_2$phe]$_\infty$**

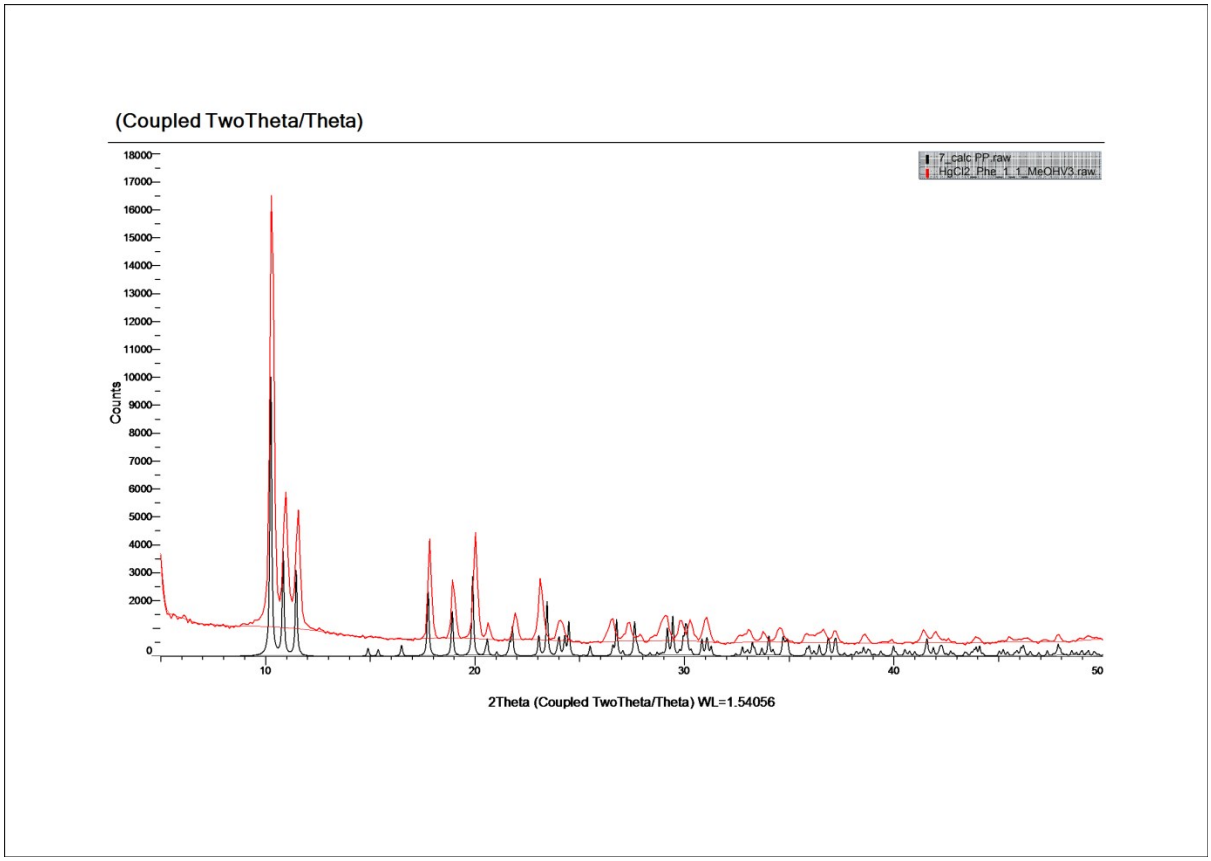

Fig. S9: Experimental and simulated powder diffraction pattern for compound **9: [Hg(μ-Br)$_2$phe]$_\infty$**

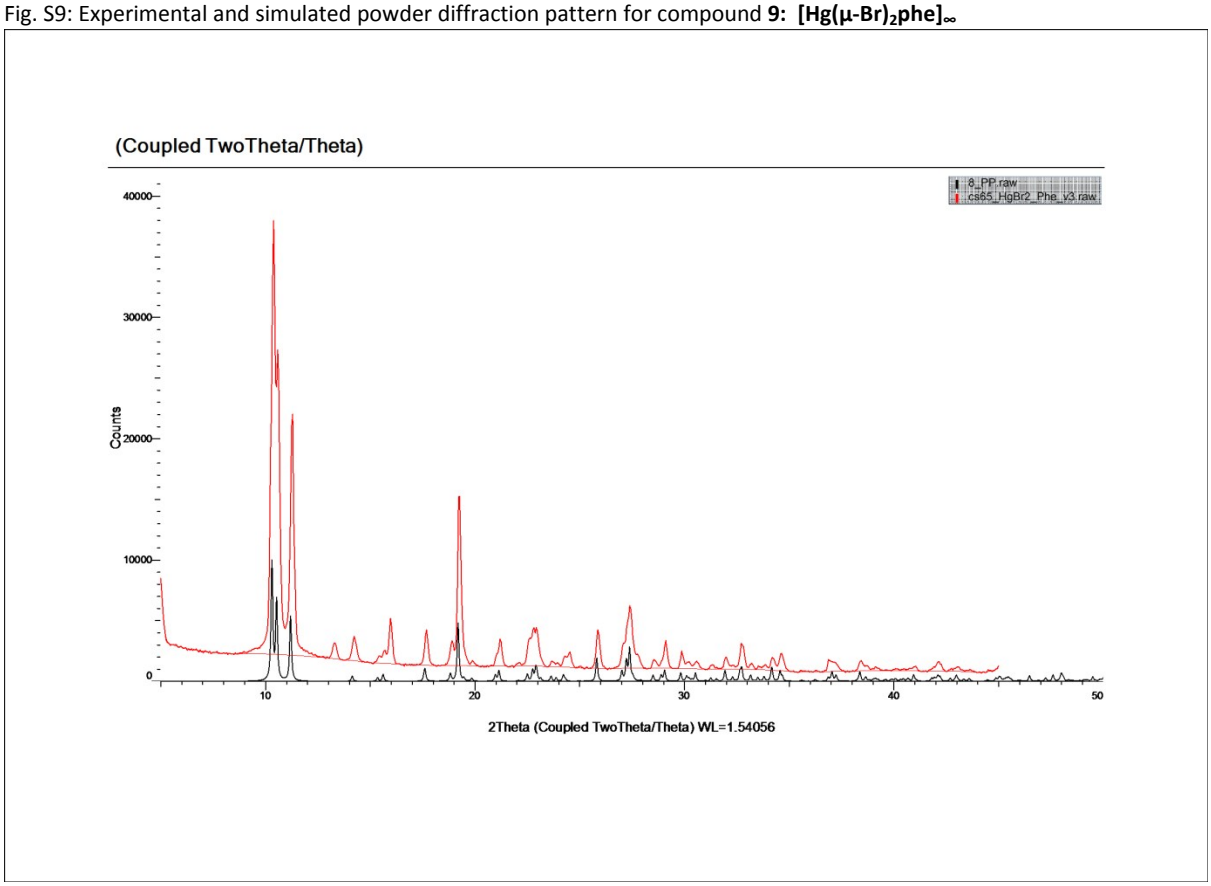

Fig. S10: Experimental and simulated powder diffraction pattern for compound **10: $[Hg_2(\mu\text{-}Br)_2(\mu\text{-}phe)]_\infty$**

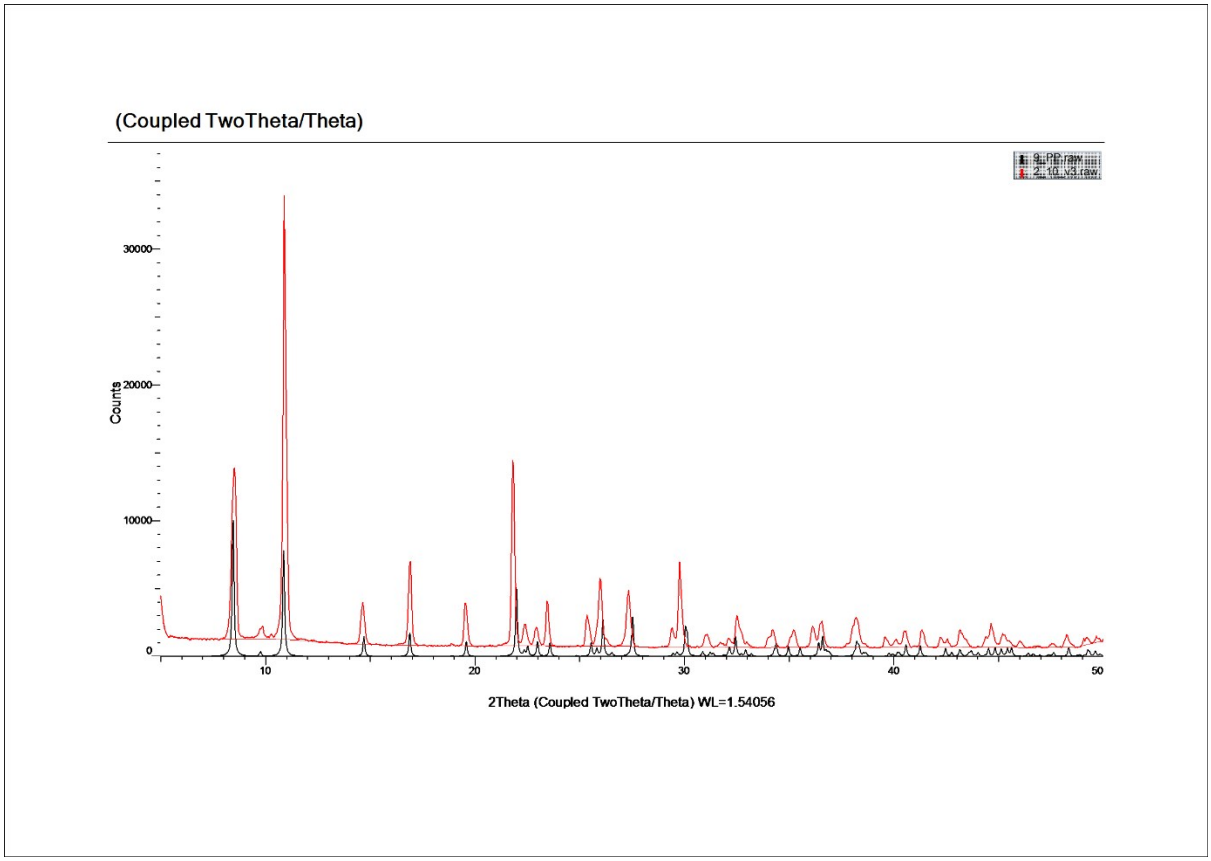

Fig. S11: Experimental and simulated powder diffraction pattern for compound **11: $[Hg(\mu\text{-}Cl)_2quin]_\infty$**

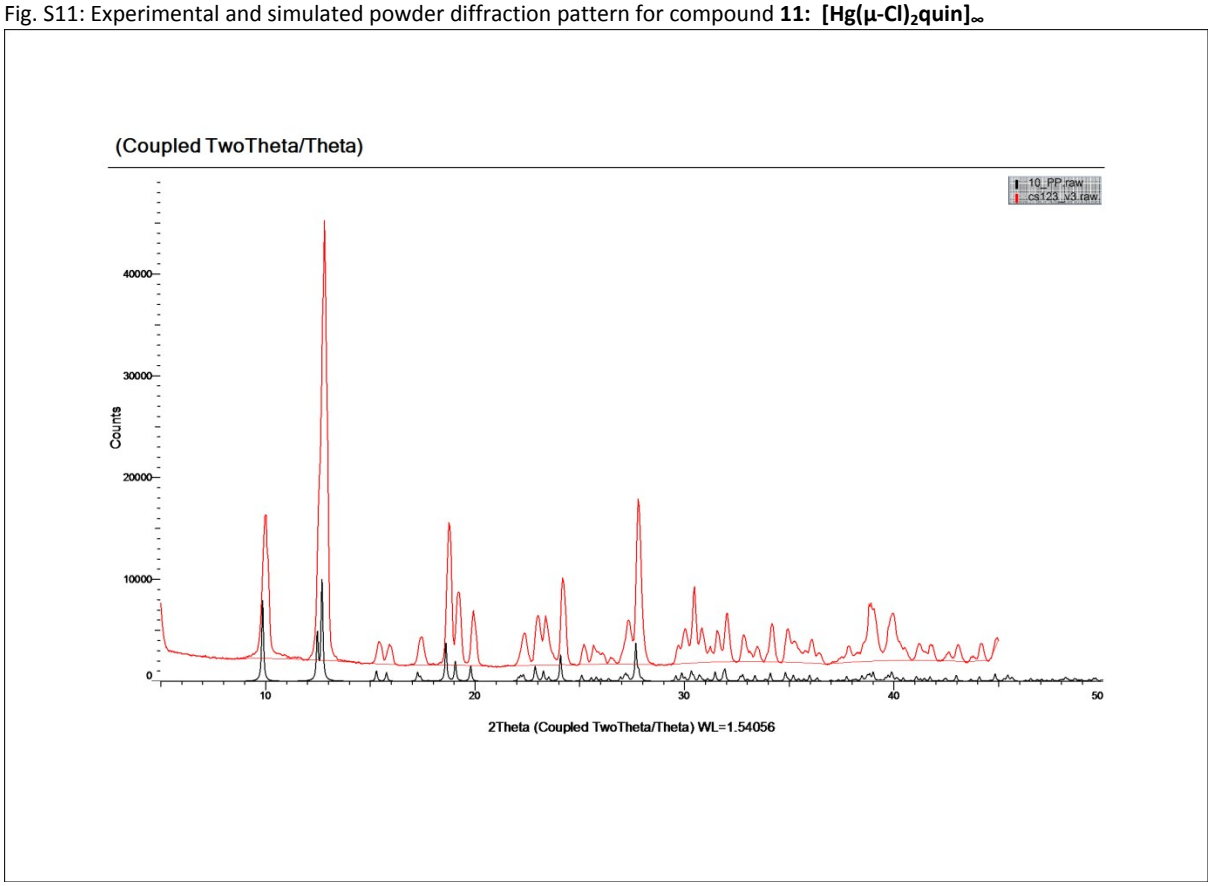

Fig. S12: Experimental and simulated powder diffraction pattern for compound **12: [Hg(μ-Br)$_2$quin]$_\infty$**

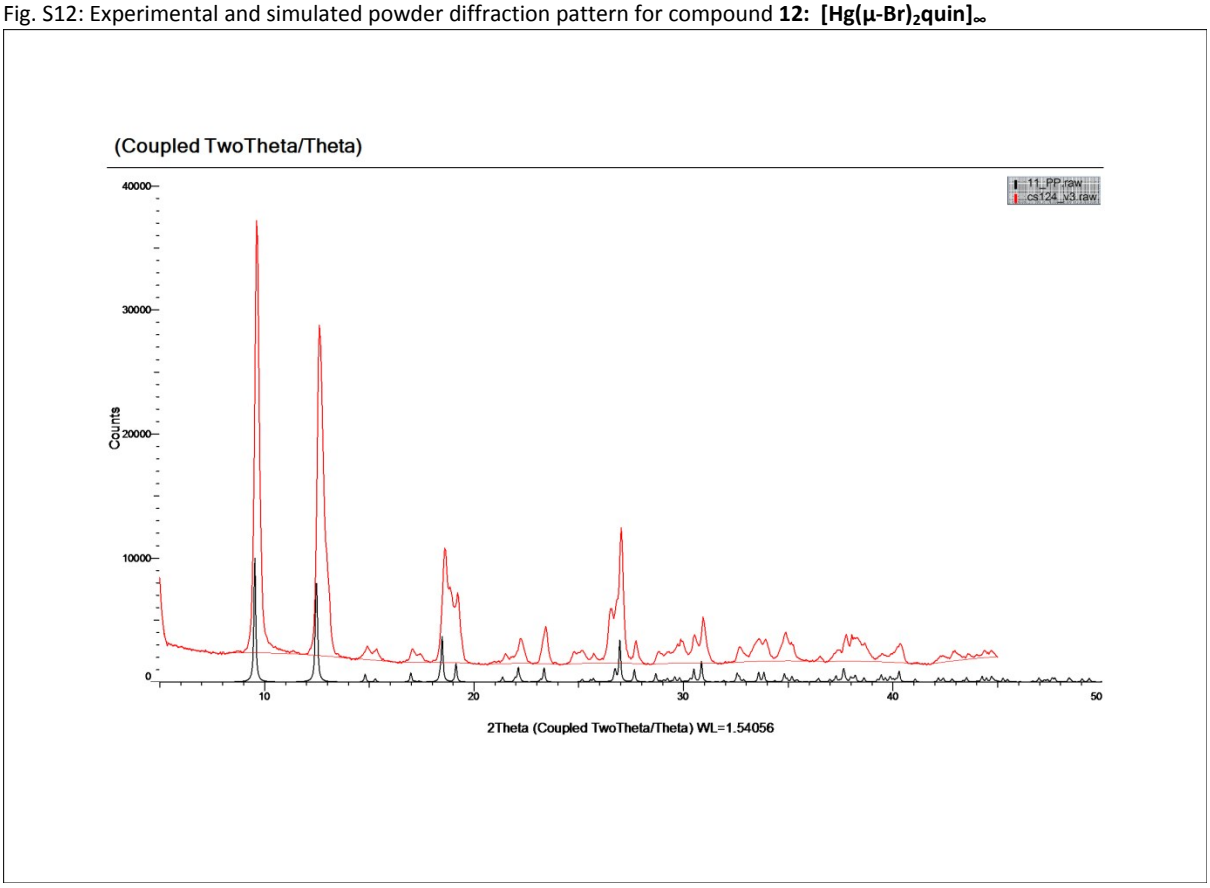

Fig. S13: Experimental and simulated powder diffraction pattern for compound **13: [Hg(μ-I)$_2$(I)quin]**