

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

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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**: $[\text{Cd}(\mu\text{-Cl})_2\text{acr}]_\infty$

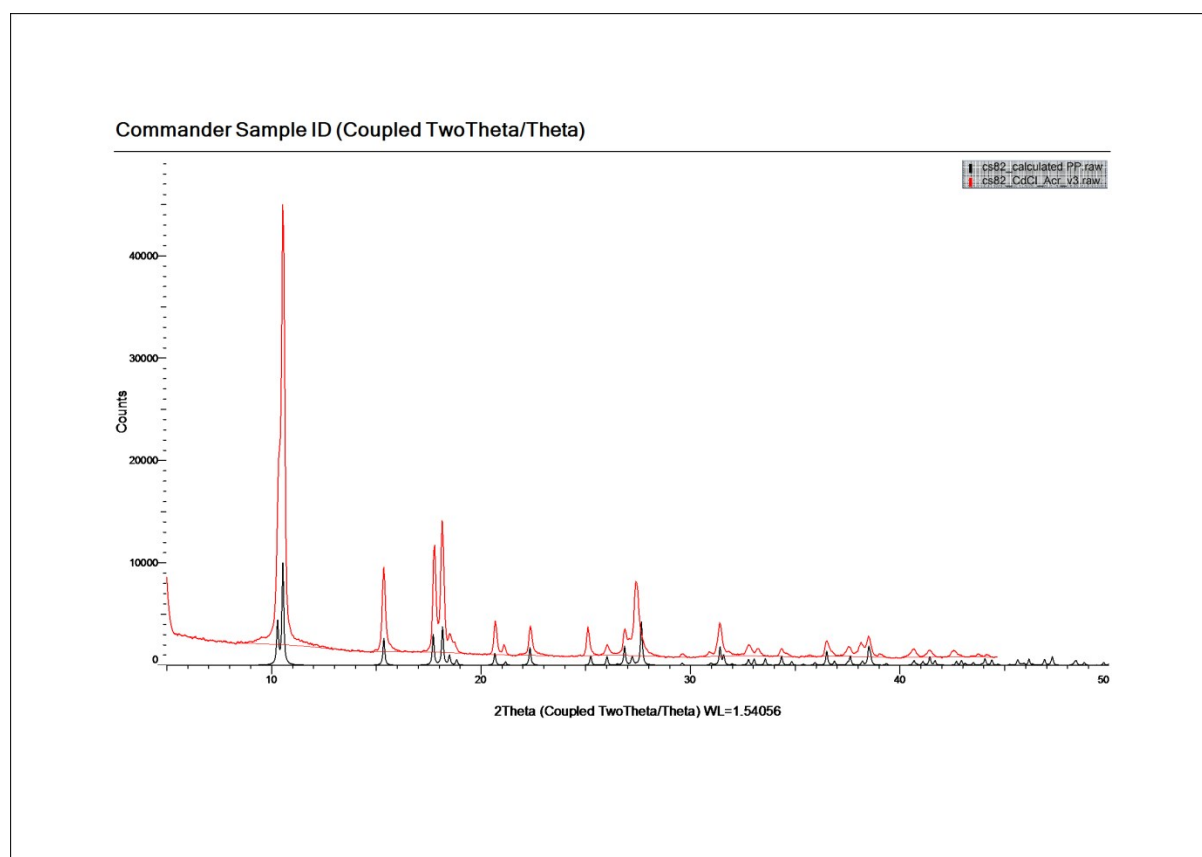


Fig. S2: Experimental and simulated powder diffraction pattern for compound **2**: $[\text{Cd}(\mu\text{-Br})_2\text{acr}]_\infty$

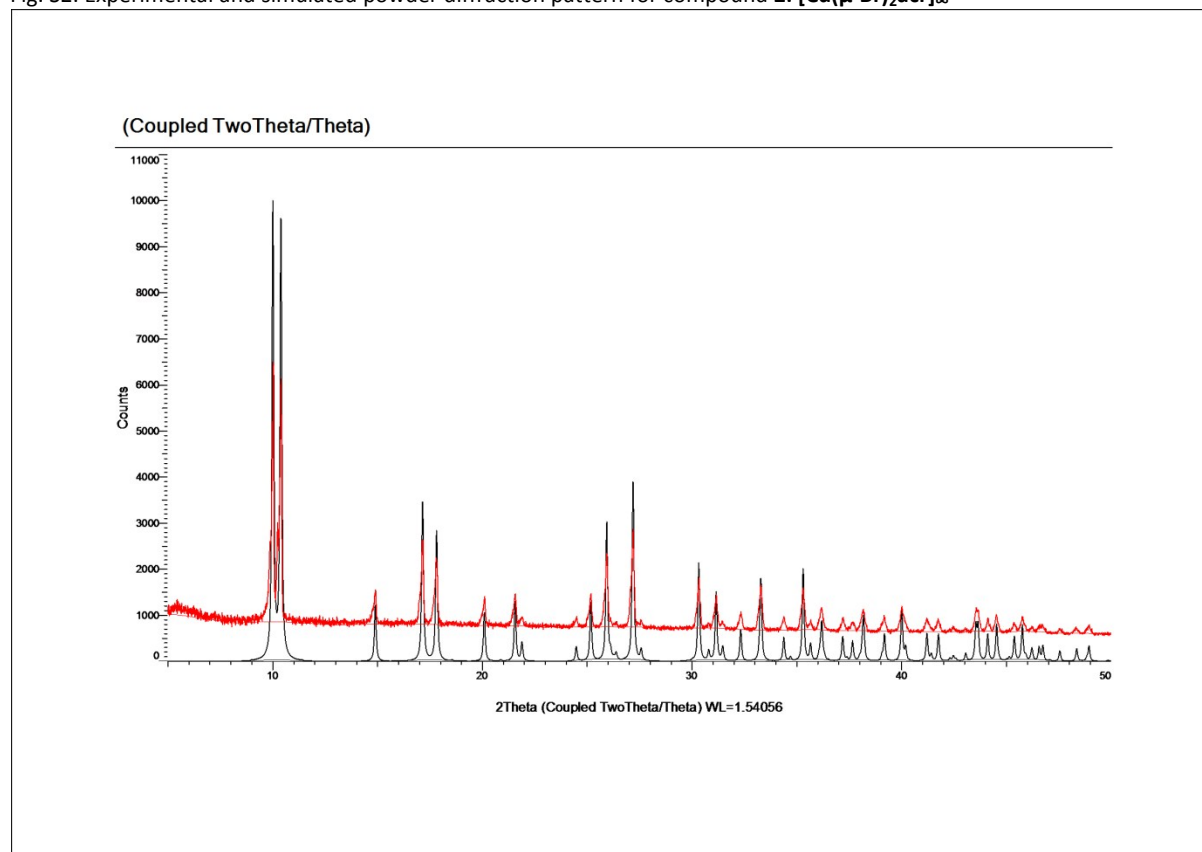


Fig. S3: Experimental and simulated powder diffraction pattern for compound **3**: $[\text{Cd}(\mu\text{-I})_2\text{acr}]_\infty$

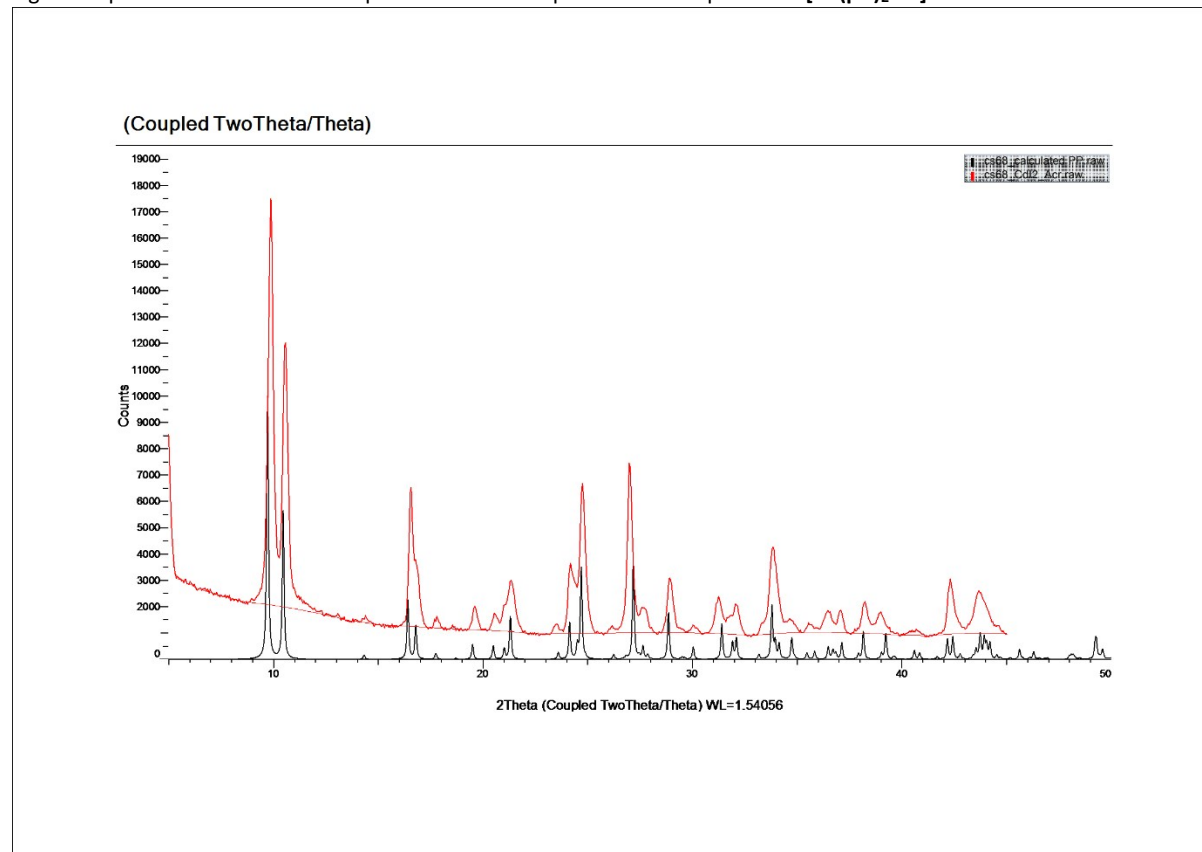


Fig. S4: Experimental and simulated powder diffraction pattern for compound **4**: $[\text{Hg}(\mu\text{-Cl})_2\text{acr}]_\infty$

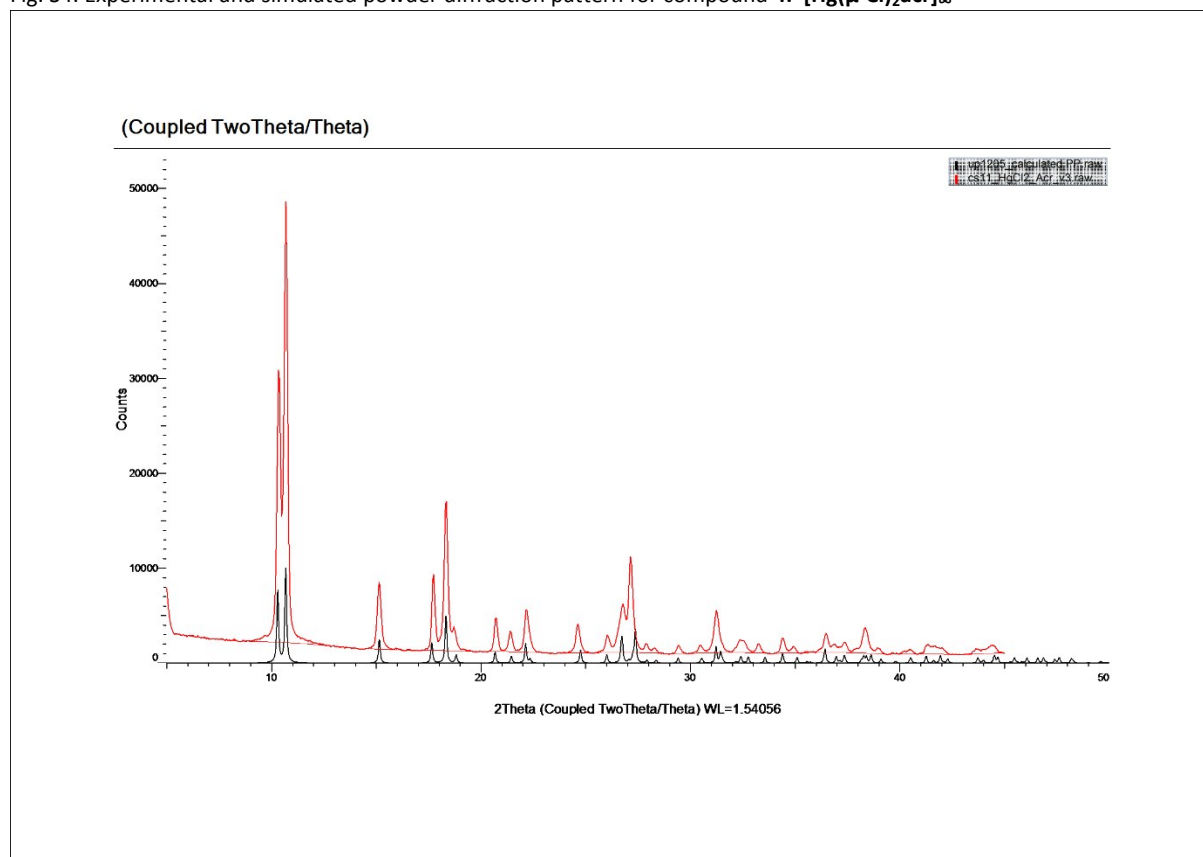
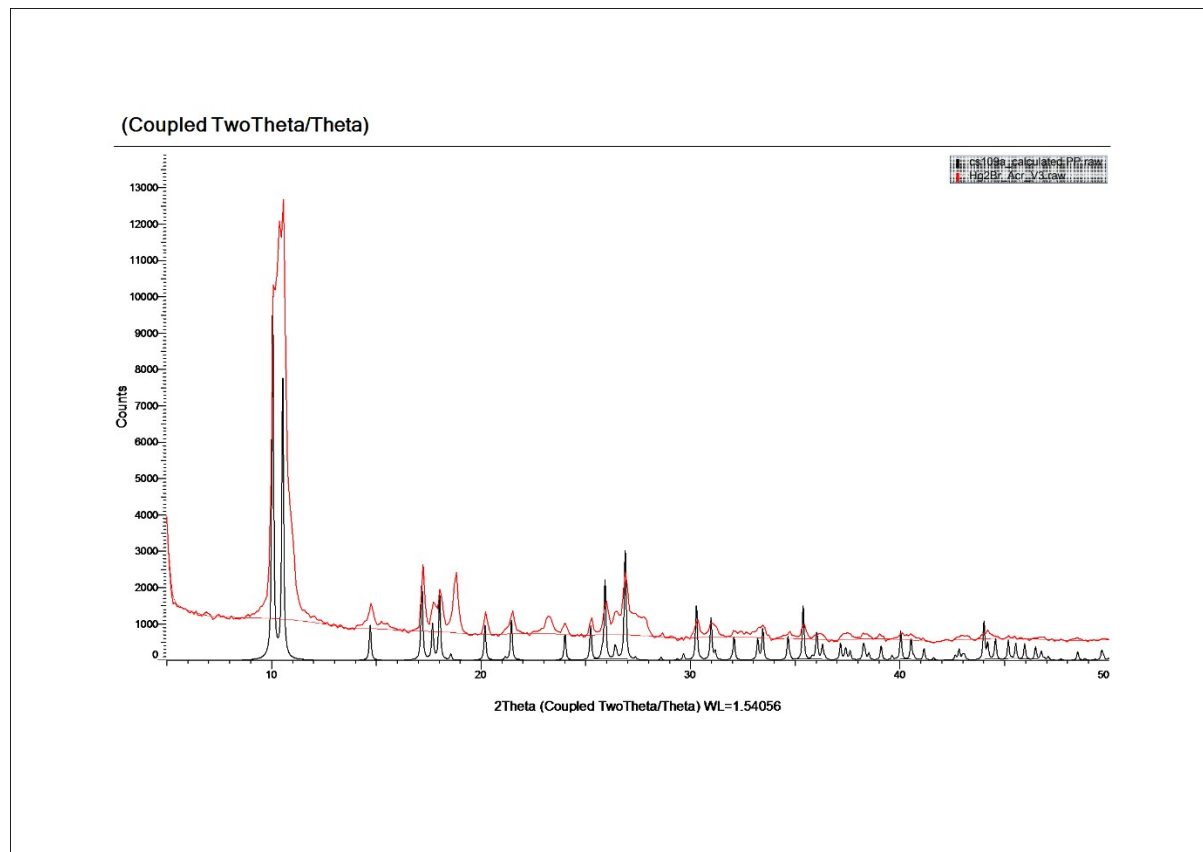


Fig. S5: Experimental and simulated powder diffraction pattern for compound **5**: $[\text{Hg}(\mu\text{-Br})_2\text{acr}]_\infty$



(Coupled TwoTheta/Theta)

Counts

21000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
0

10 20 30 40 50

2Theta (Coupled TwoTheta/Theta) WL=1.54056

cs85b_calculated PP.raw
CdCl2·Ph6 recryst EtOH V3.raw

The figure is an X-ray diffraction (XRD) pattern. The y-axis is labeled 'Counts' and ranges from 0 to 21,000. The x-axis is labeled '2Theta (Coupled TwoTheta/Theta) WL=1.54056' and ranges from 10 to 50. There are two data series: a black line representing 'cs85b_calculated PP.raw' and a red line representing 'CdCl2·Ph6 recryst EtOH V3.raw'. The red line shows a very sharp, intense peak at approximately 11.5 degrees 2Theta, reaching a count of about 19,000. The black line shows a much smaller peak at the same position, reaching about 5,000 counts. Both lines show several smaller peaks at higher 2Theta values, with the red line generally having higher intensity than the black line in this region.

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

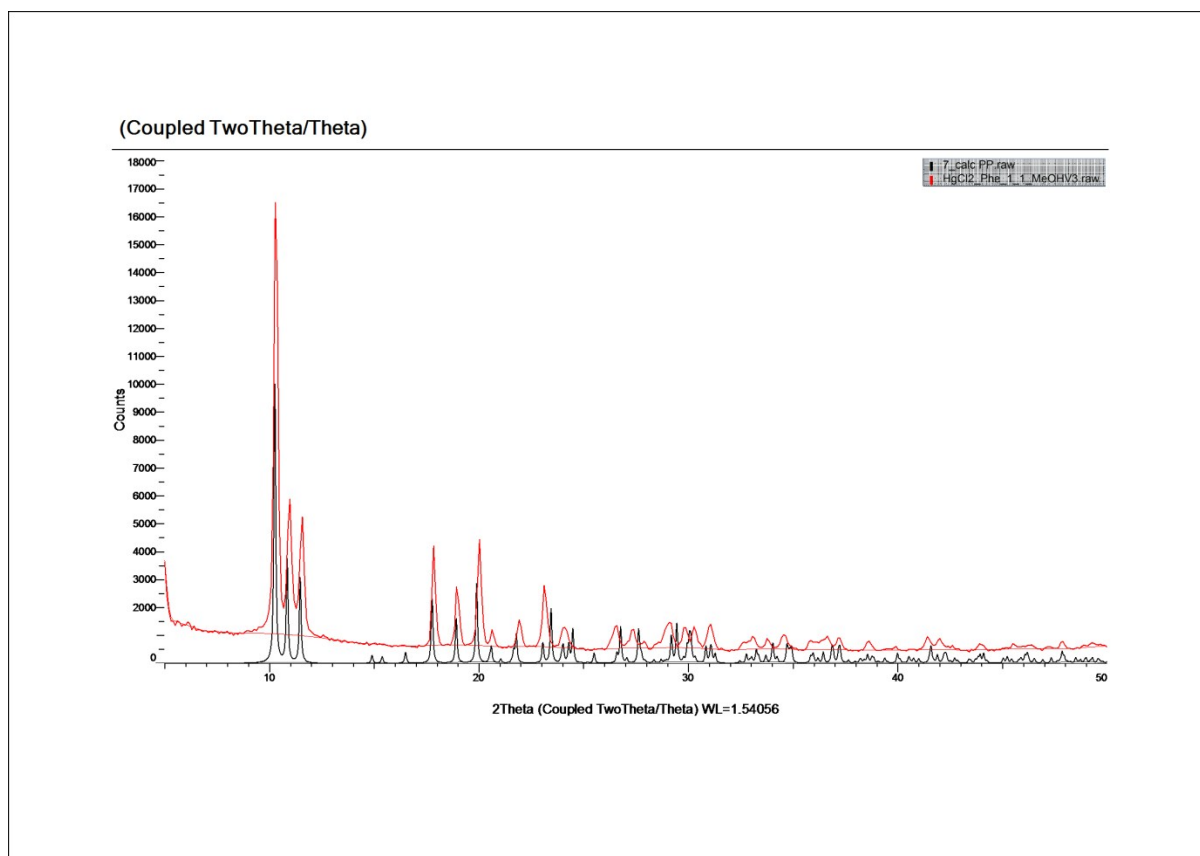


Fig. S9: Experimental and simulated powder diffraction pattern for compound **9**: $[\text{Hg}(\mu\text{-Br})_2\text{phe}]_\infty$

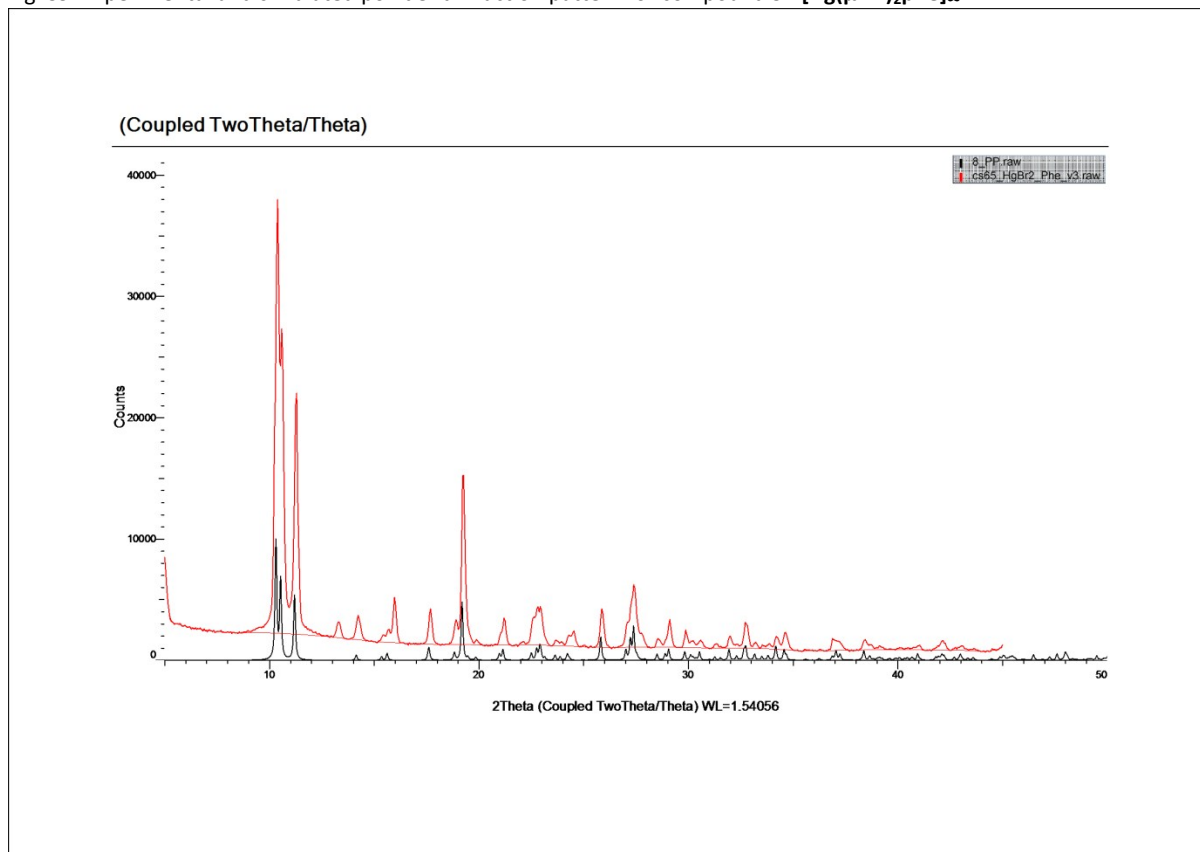


Fig. S10: Experimental and simulated powder diffraction pattern for compound **10**: $[\text{Hg}_2(\mu\text{-Br})_2(\mu\text{-phe})]_\infty$

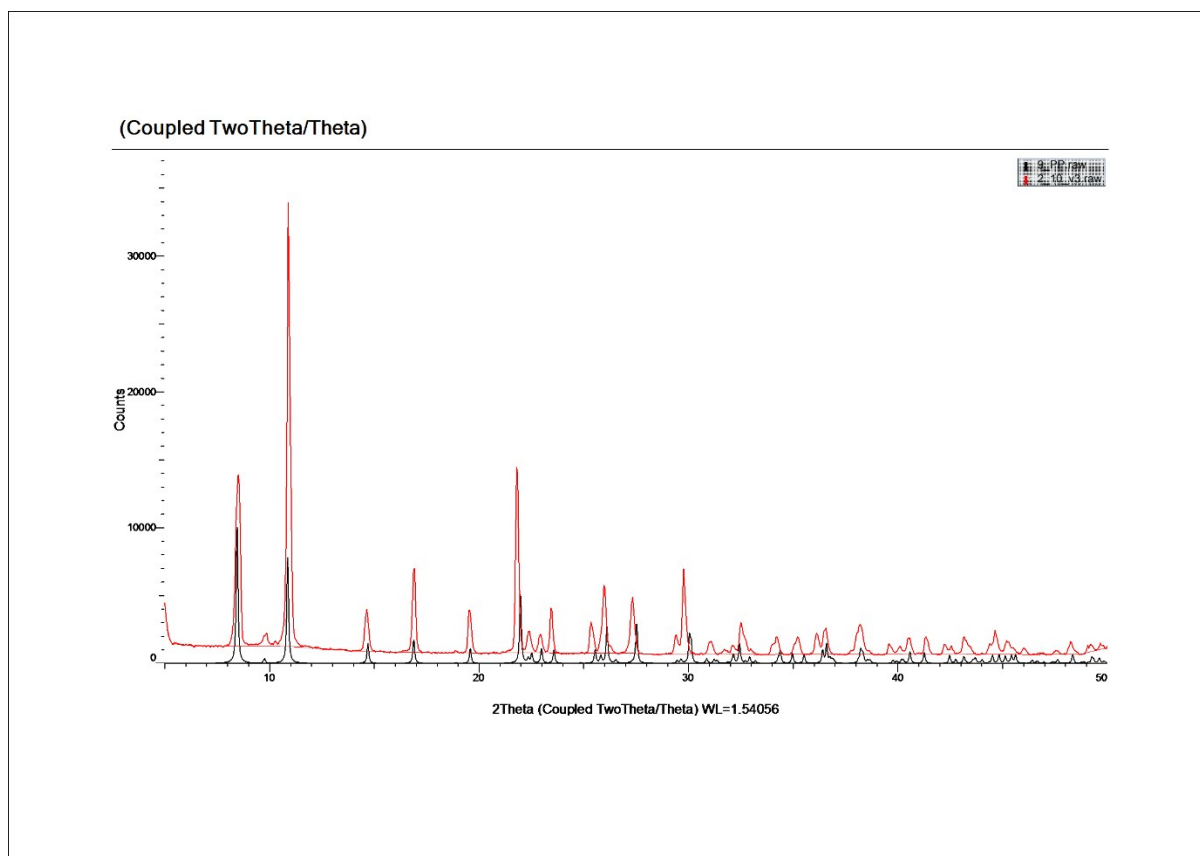


Fig. S11: Experimental and simulated powder diffraction pattern for compound **11**: $[\text{Hg}(\mu\text{-Cl})_2\text{quin}]_\infty$

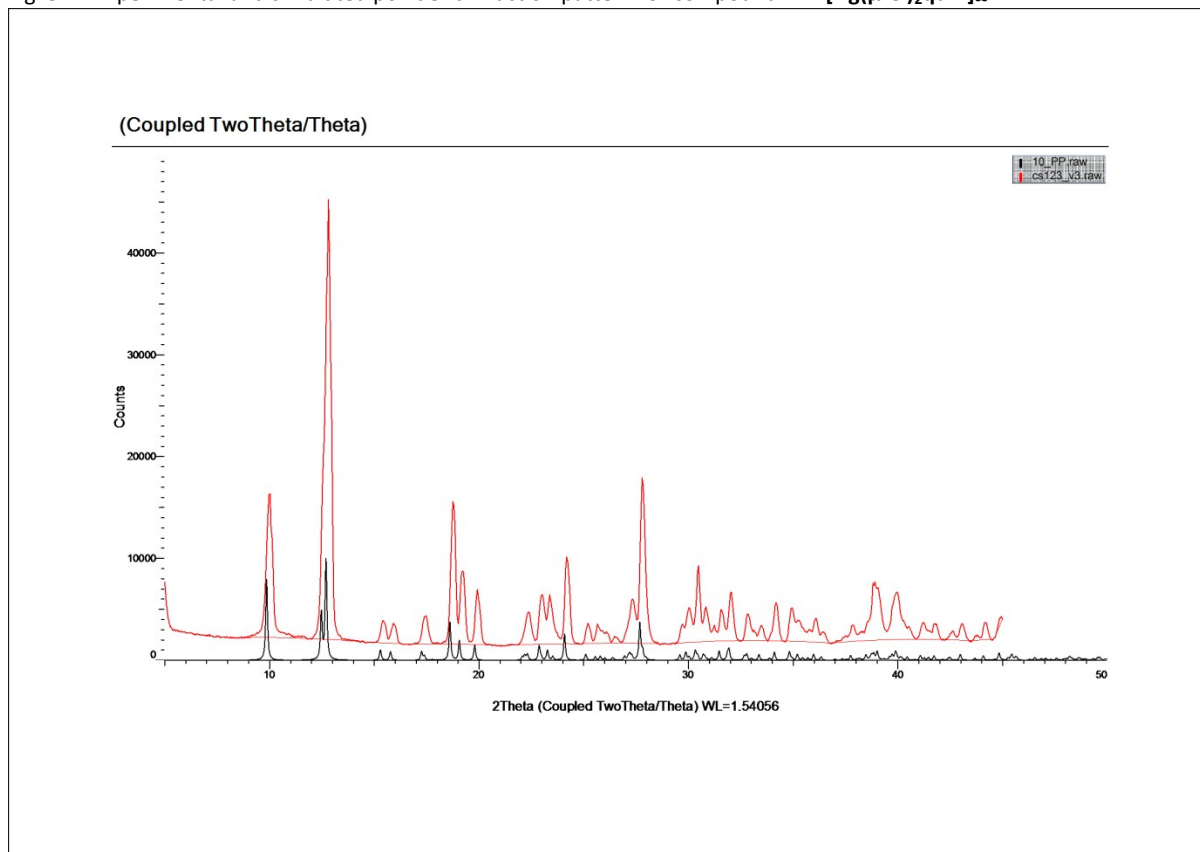


Fig. S12: Experimental and simulated powder diffraction pattern for compound **12**: $[\text{Hg}(\mu\text{-Br})_2\text{quin}]_\infty$

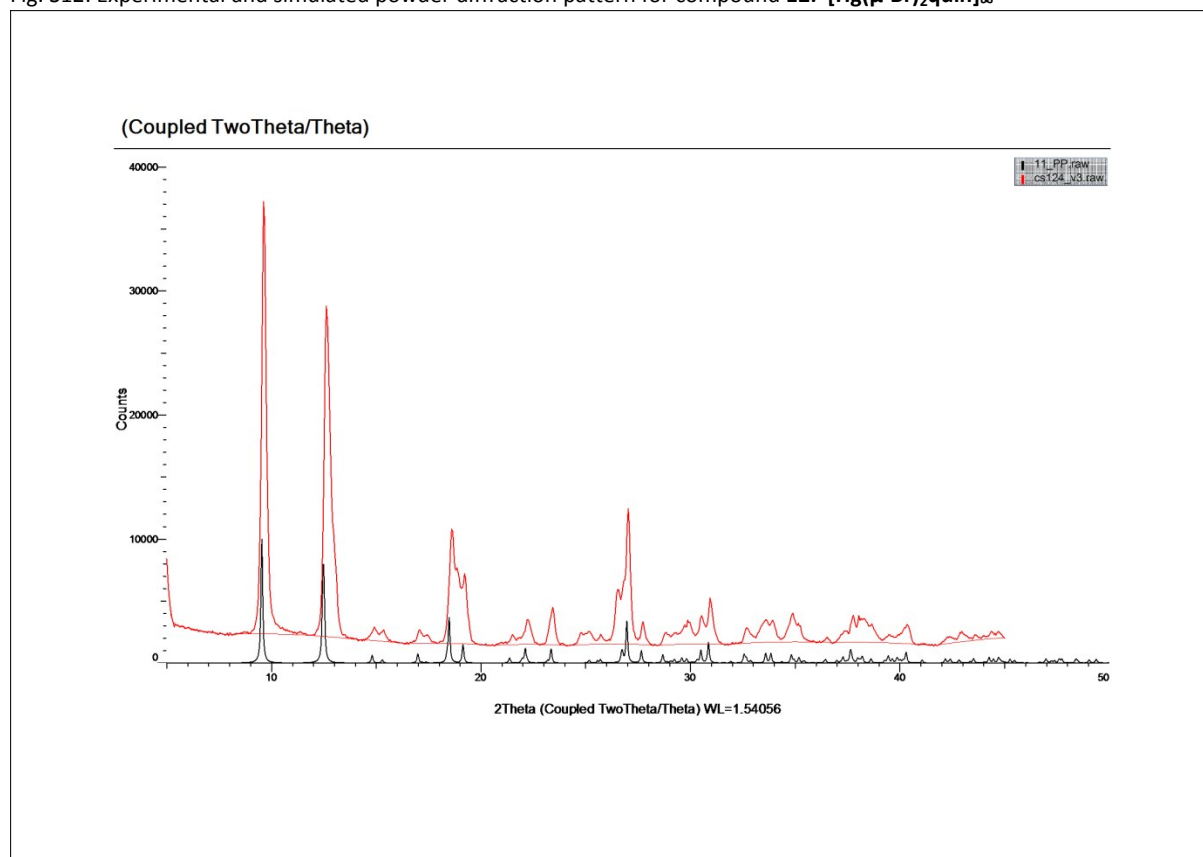


Fig. S13: Experimental and simulated powder diffraction pattern for compound **13**: $[\text{Hg}(\mu\text{-I})_2(\text{I})\text{quin}]$

