Structure prediction as a tool for solution of the crystal structures of metallo-organic complexes using powder X-ray diffraction data
Andrew D. Bond and William Jones

Supplementary Information
Overlay of predicted (black) and observed (red) structures

Zn(PT)\textsubscript{2} 1
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\( \text{Cu(PT)}_2 \)
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Ni(PT)$_2$ 3
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Zn(MPT)₂ 4
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Cu(MPT)$_2$ 5
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Ni(MPT)$_2$ 6 (equivalent to Cu(MPT)$_2$ 5)
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Zn(MTT)₂ 7
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Supplementary Information
Overlay of predicted (black) and observed (red) structures
PXRD profiles simulated from them (predicted (top) and observed (bottom))

Cu(MTT)₂
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Supplementary Information
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Ni(MTT)$_2$ 9