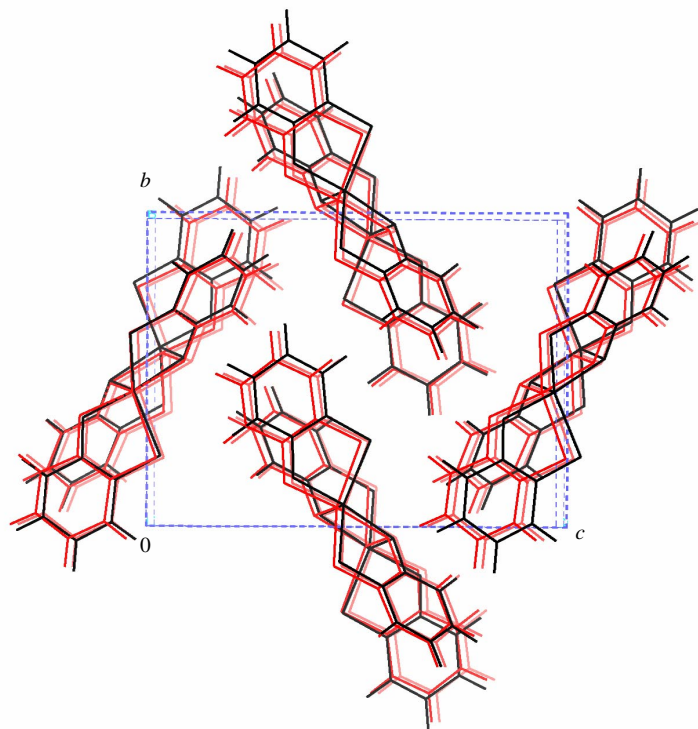


**Structure prediction as a tool for solution of the crystal structures of
metallo-organic complexes using powder X-ray diffraction data**
Andrew D. Bond and William Jones

Supplementary Information

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

Zn(PT)₂ 1

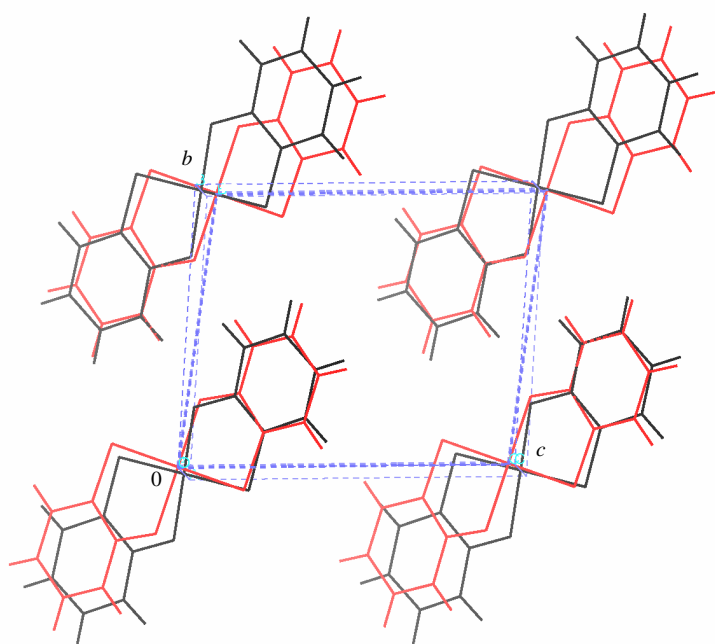


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$\text{Cu}(\text{PT})_2 \cdot 2$

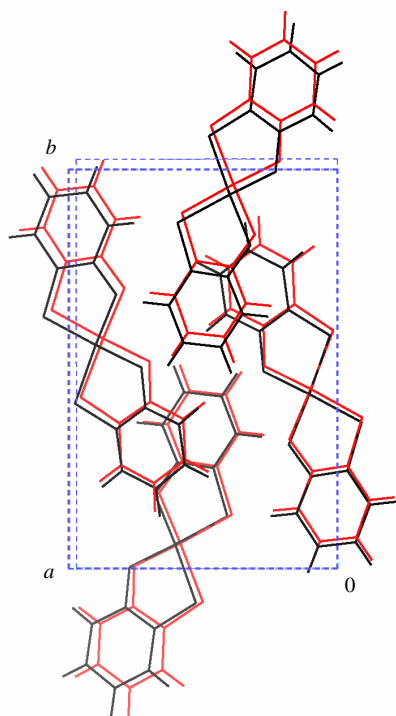


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$\text{Ni}(\text{PT})_2 \cdot 3$

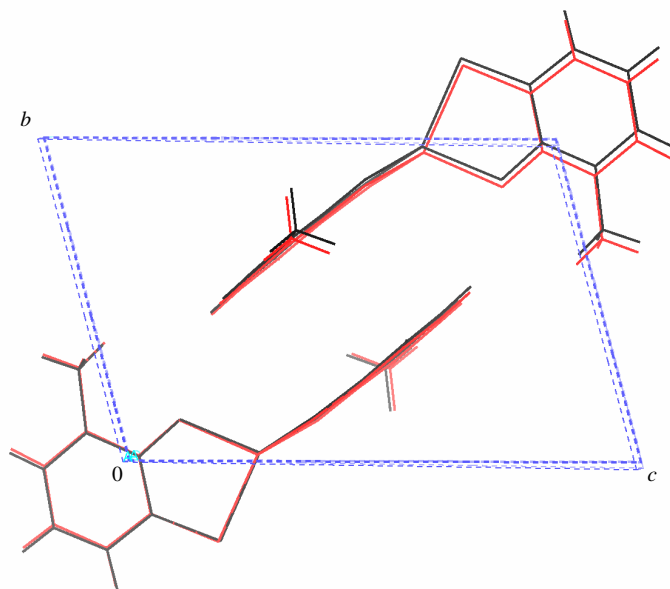


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$\text{Zn}(\text{MPT})_2 \cdot 4$

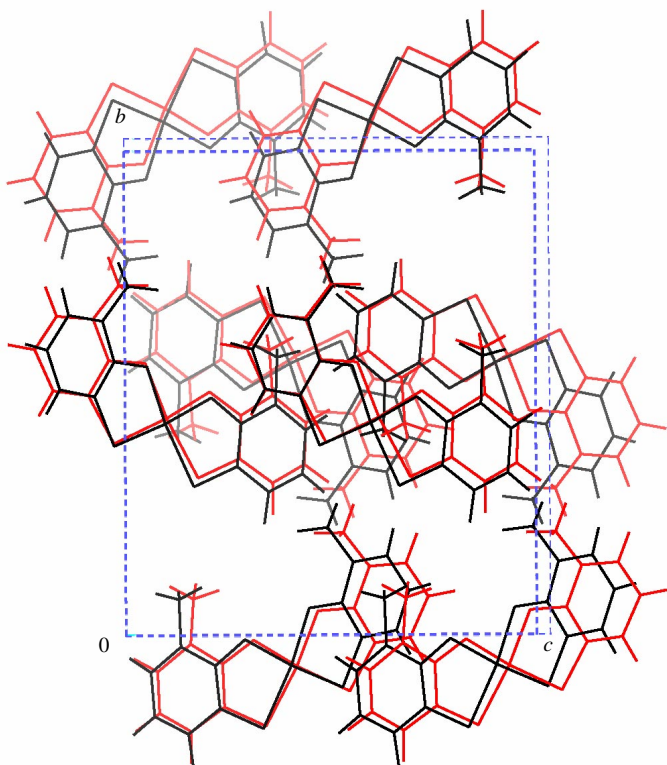


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$\text{Cu}(\text{MPT})_2 \cdot 5$

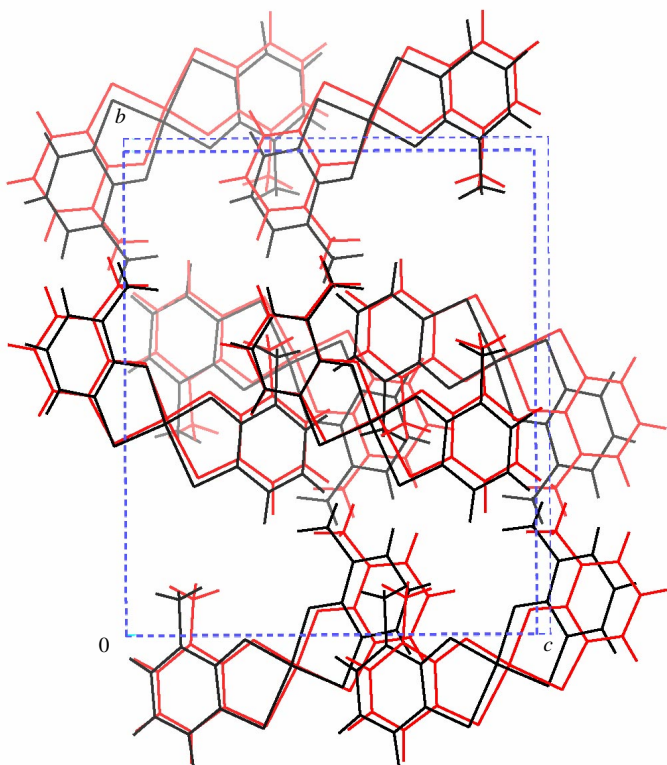


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Ni(MPT)₂ 6 (equivalent to Cu(MPT)₂ 5)

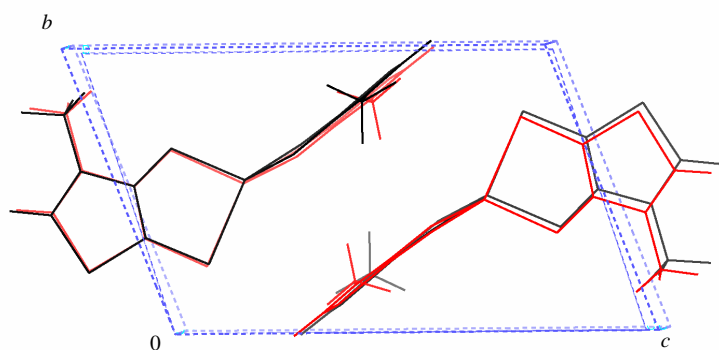


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$\text{Zn}(\text{MTT})_2 \cdot 7$

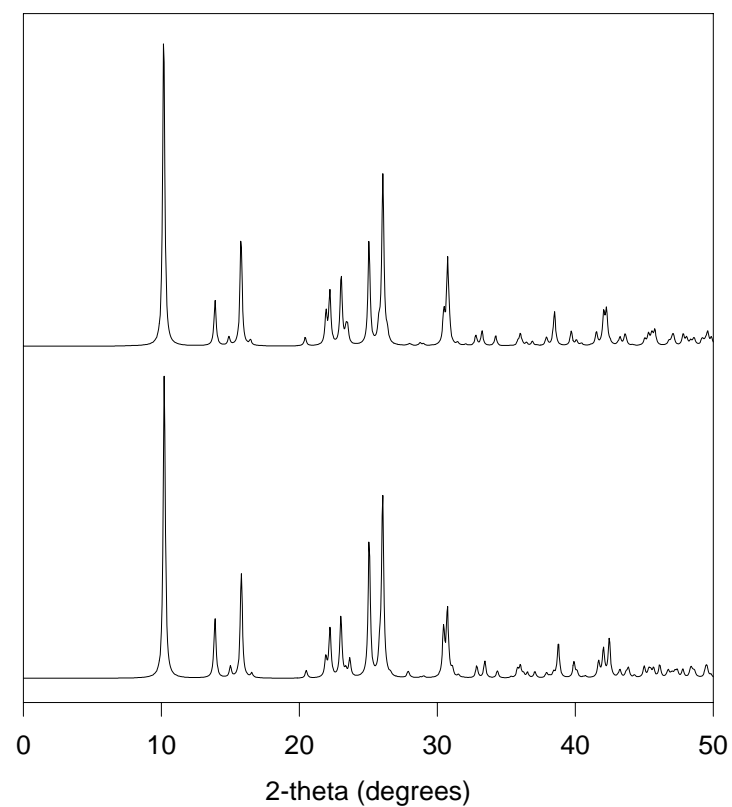
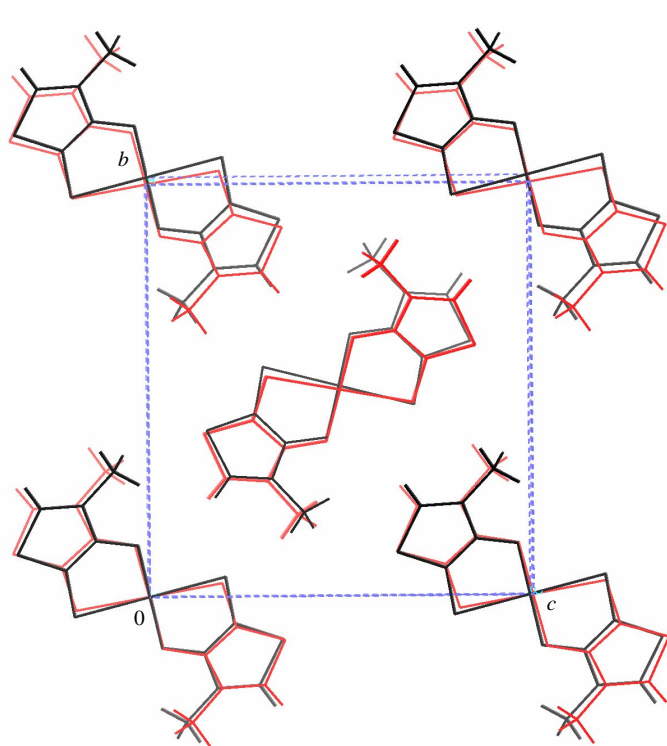


Structure prediction as a tool for solution of the c metallo-organic complexes using powder X-ray d Andrew D. Bond and William Jones

Supplementary Information

Overlay of predicted (black) and observed (red) structure
PXRD profiles simulated from them (predicted (top) and

$\text{Cu}(\text{MTT})_2 \cdot 8$



**Structure prediction as a tool for solution of the crystal structures of
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Supplementary Information

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

$\text{Ni}(\text{MTT})_2 \cdot 9$

