

Supporting information for the article

**Porphyrin-Fullerene, C₆₀ Cocrystallates:
Influence of C₆₀ on the Porphyrin Ring Conformation**

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SFigure 1. ORTEP of $\text{Co}(\text{TPP})(\text{Ph})_4 \cdot \text{C}_{60}$ cocrystallate. The asymmetric unit of the porphyrin and the C_{60} are labelled for clarity. Thermal ellipsoids are shown at 40% probability level.

SFigure 2. Shows capped stick model for $\text{CoTPP}(\text{Ph})_4 \cdot \text{C}_{60}$ cocrystallate (a) short contacts between C_{60} and porphyrin along the one dimensional chains. Symmetry related short contact atoms are labelled for clarity. Intermolecular contacts are shown in dotted red lines. (b) Relative orientation of paracylene 6:6 junction of C_{60} to the porphyrin ring. C, grey; N, blue; Co, orange; C_{60} is shown in grey colour. The phenyl rings and hydrogens are not shown.

SFigure 3. van der Waals packing diagram (100% vdw) showing the one-dimensional array of $\text{Co}(\text{TPP})(\text{Ph})_4 \cdot \text{C}_{60}$ cocrystallate.

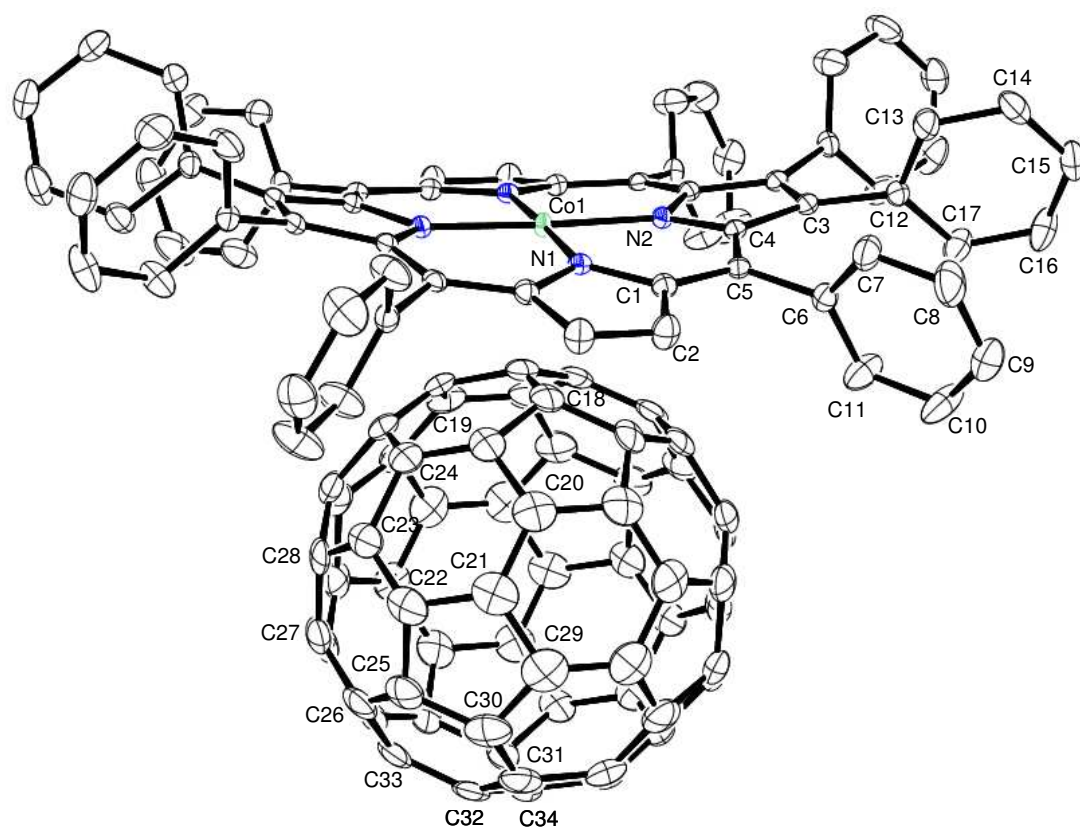
SFigure 4. (a) Capped stick model for $\text{CuTPP}(\text{Ph})_4 \cdot \text{C}_{60}$ showing the intermolecular contacts along the array. Short contacts atom are labelled for clarity. (b) Shows the orientation of 6:6 junction of paracylene unit in C_{60} relative to the porphyrin ring. Porphyrin: N, blue; Cu, orange; C, grey. C_{60} : purple colour.

SFigure 5. Capped stick model showing the interconnected one-dimensional array of $\text{Cu}(\text{TPP})(\text{Ph})_4 \cdot \text{C}_{60}$ cocrystallate oriented parallel to unit cell 'bc' plane. Intermolecular contacts are shown in dotted red lines. Color scheme: C_{60} , purple and $\text{CuTPP}(\text{Ph})_4$, grey.

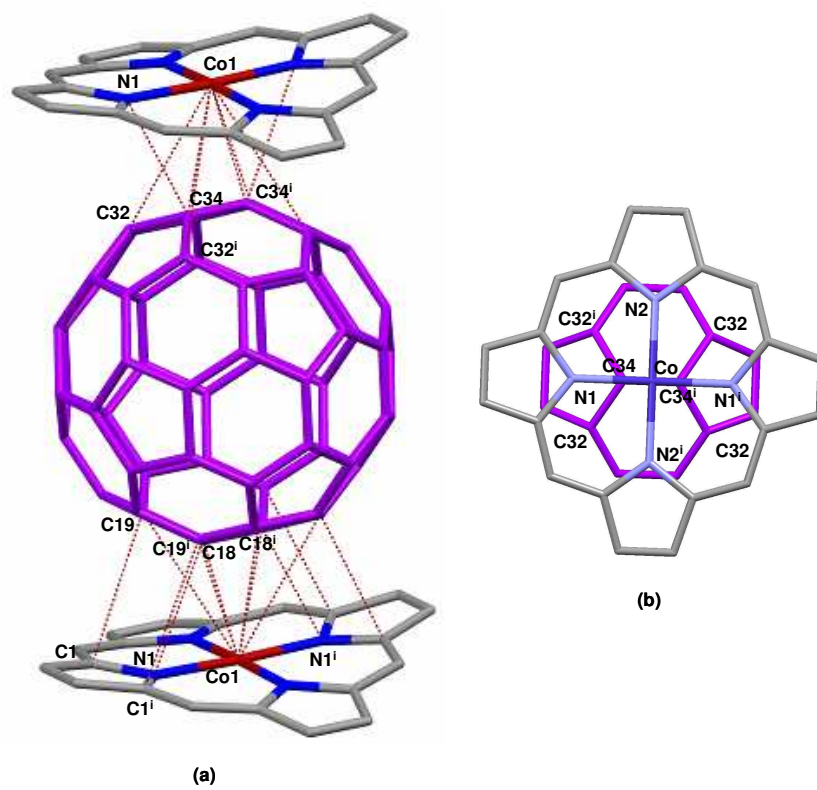
SFigure 6. ORTEP diagram of $\text{CuTPP}(\text{Ph})_4(\text{CH}_3)_4 \cdot \text{C}_{60}$ complex. Hydrogens are not shown for clarity. Thermal ellipsoids at 40% probability level.

SFigure 7. (a) ORTEP of $\text{CoTPP}(\text{Ph})_4$ complex (thermal ellipsoids at 40% probability). Hydrogens are not shown for clarity. (b) Side view of the complex 24 atom core. The peripheral phenyl groups are omitted for simplicity. (c) Mean plane displacement of the core atoms in Å (esd's, 0.002).

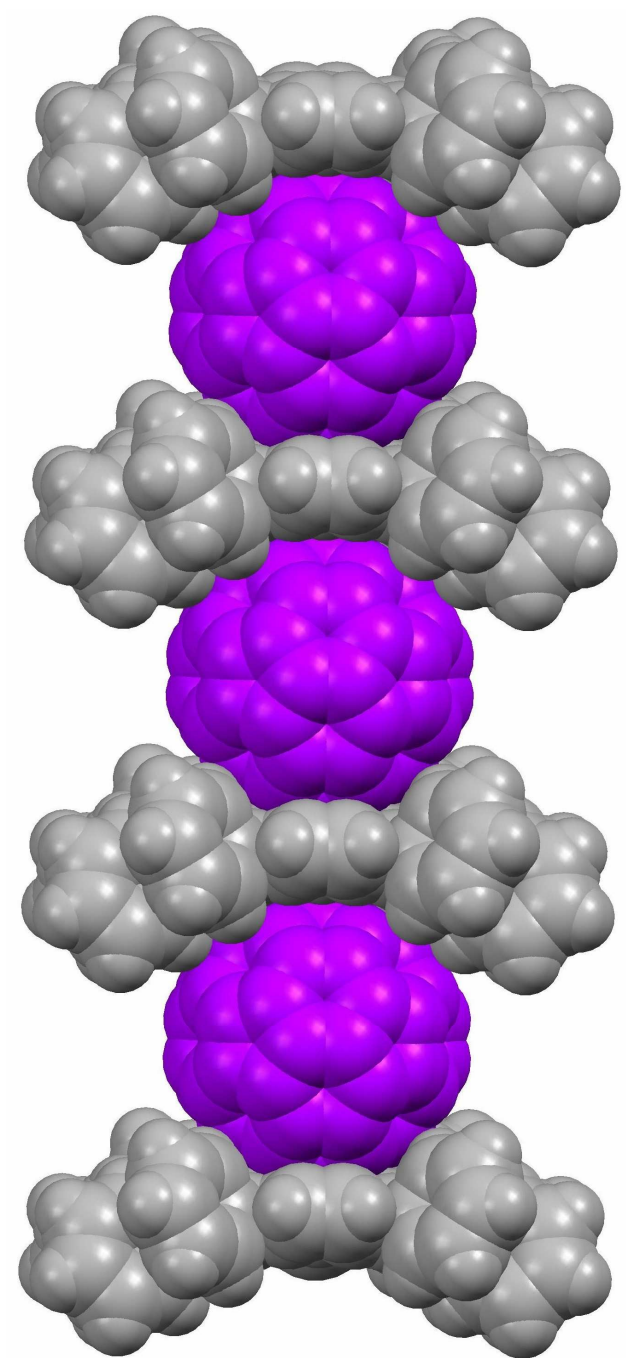
SFigure 8. (a) ORTEP of $\text{CuTPP}(\text{Ph})_4$ complex (thermal ellipsoids at 40% probability level). (b) Side view of the complex 24 atom core. Phenyl groups are not shown. (c) Mean plane displacement of the core atoms in Å (esd's, 0.002).



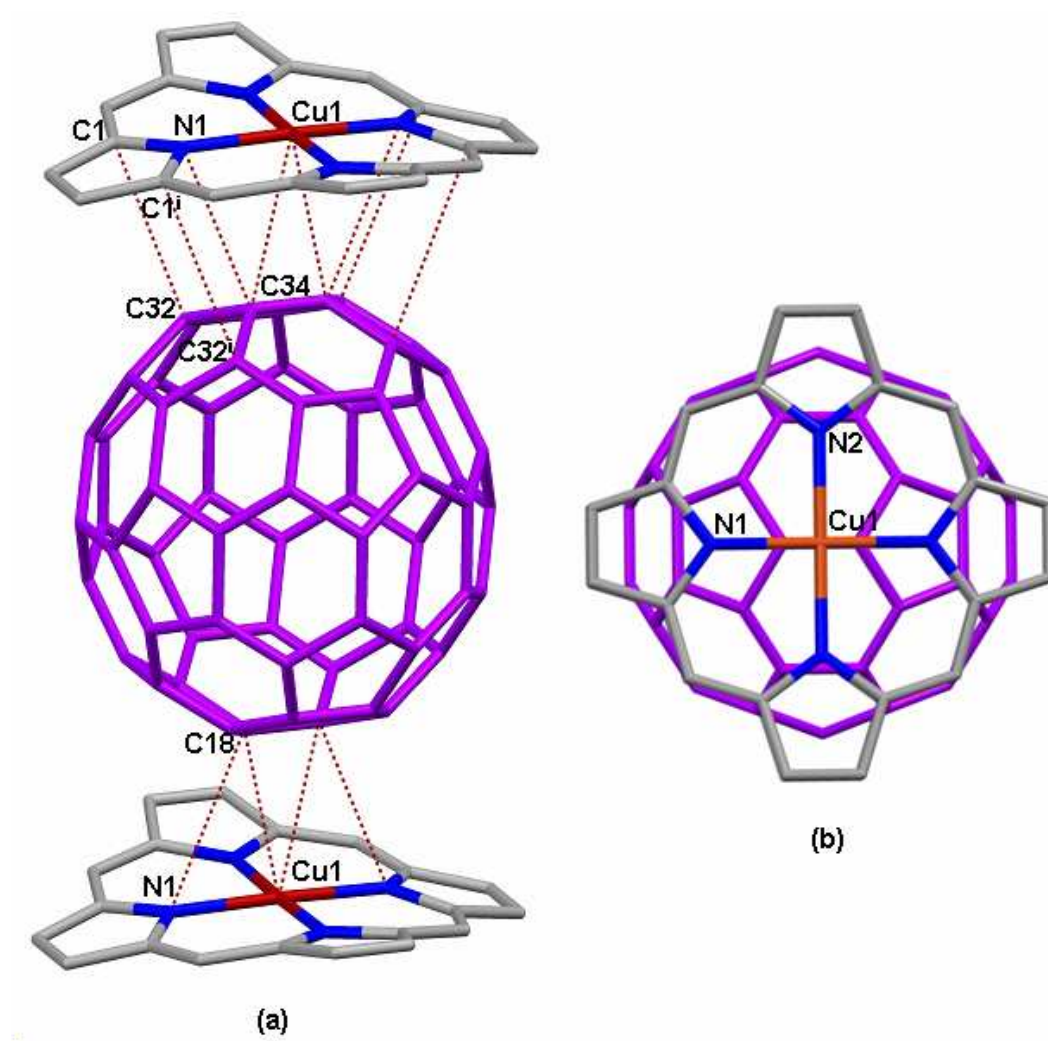
SFigure 1



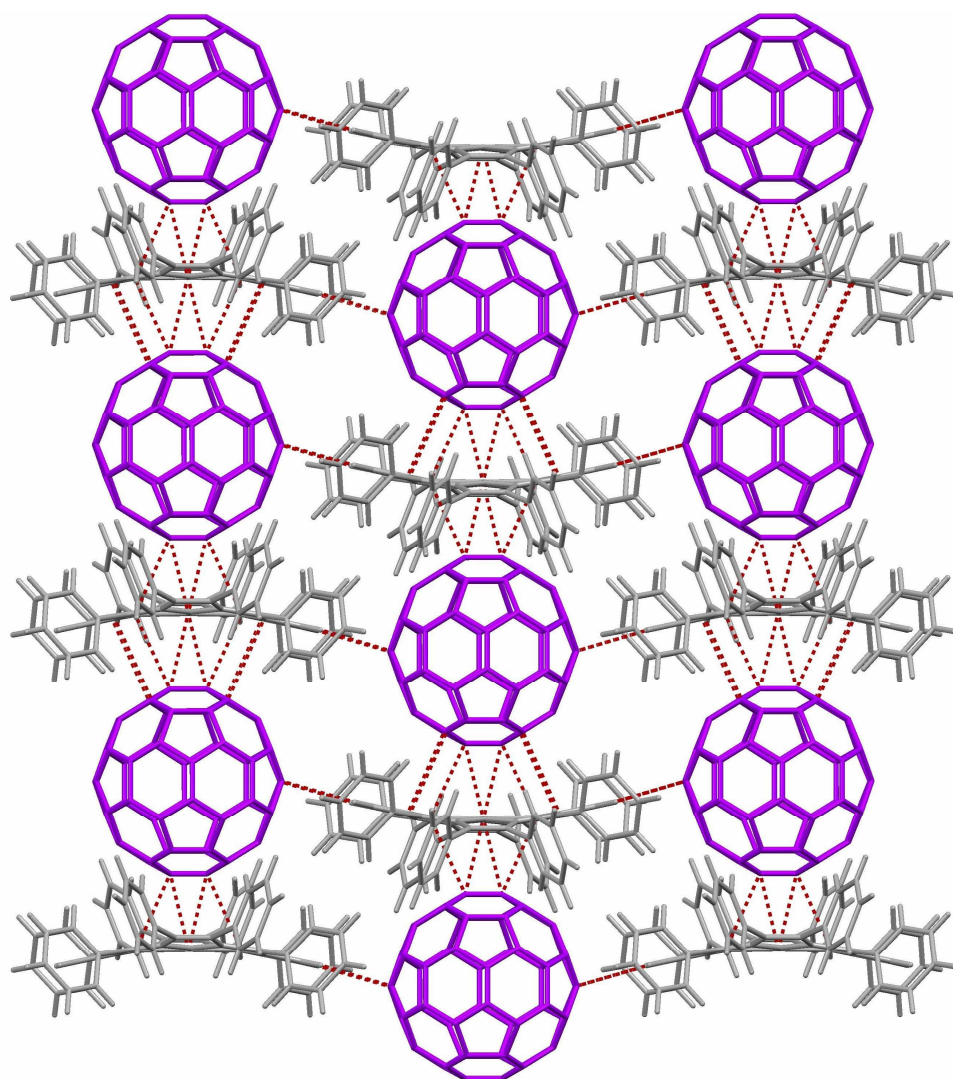
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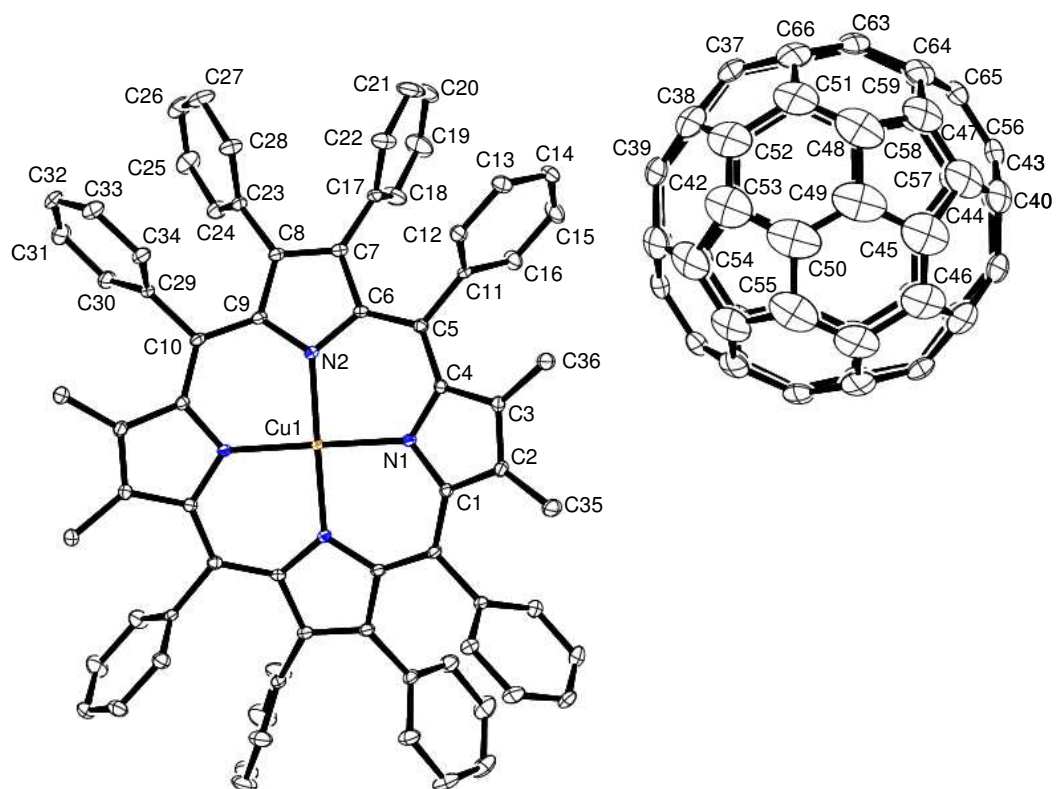
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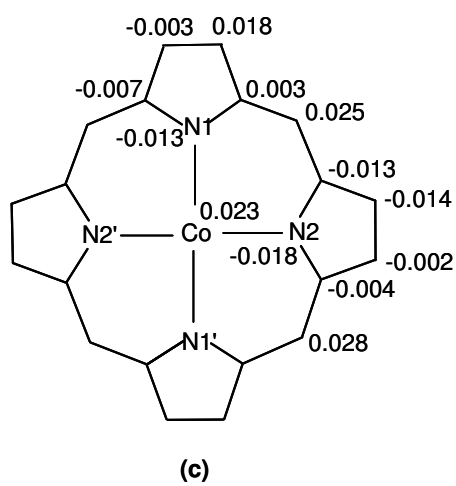
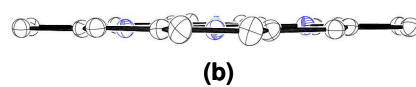
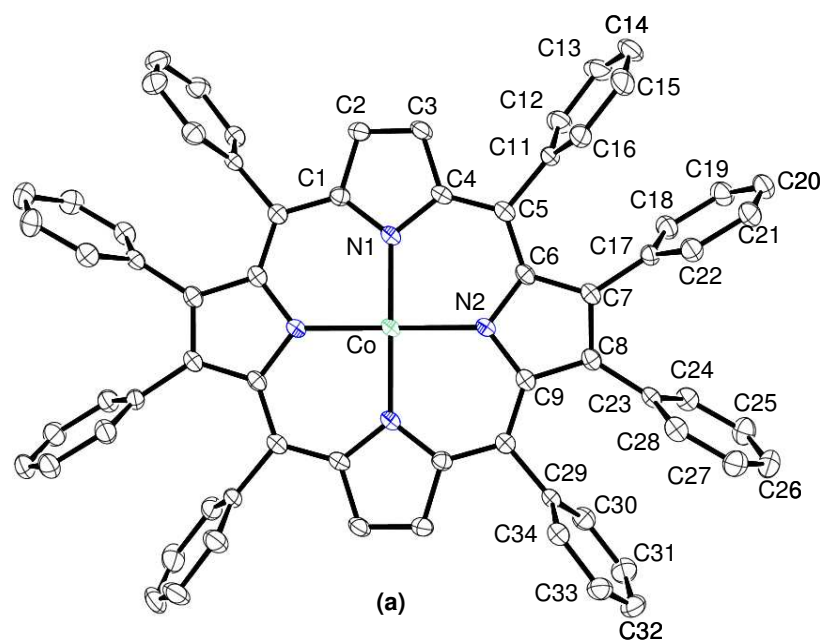
SFigure 4



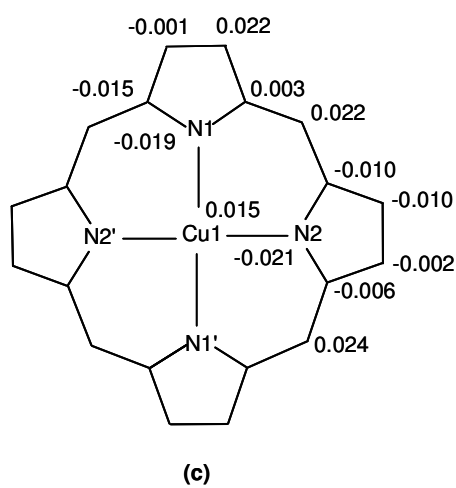
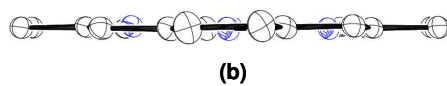
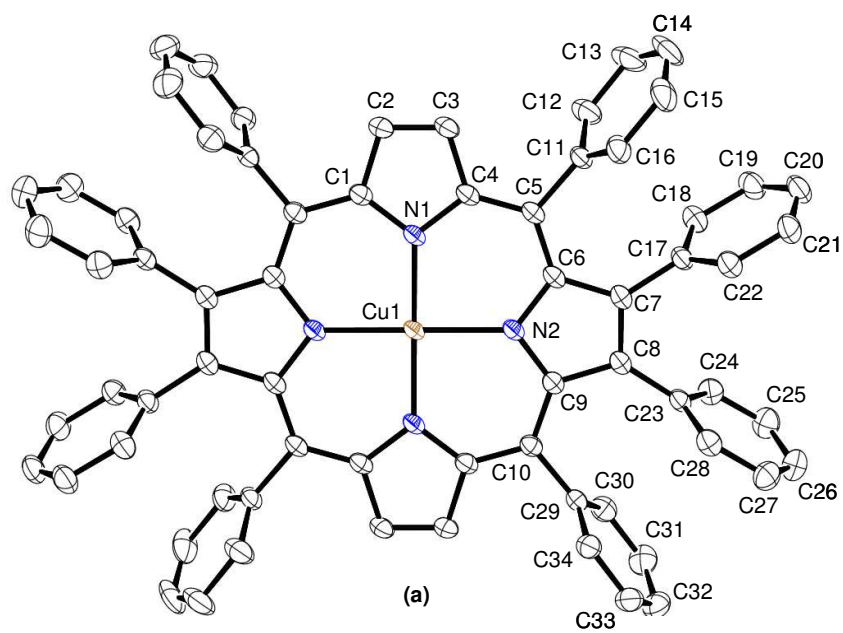
SFigure 5



SFigure 6



SFigure 7



SFigure 8