A triple-triangle cluster derived from a simple tridentate ligand

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Experimental Procedures

The multidentate ligand H_2L (2,6-bis(1,5-diphenyl-1H-pyrazole-3-yl)pyridine) was synthesized the previously reported synthetic method.[1]

Elemental analyses for carbon, hydrogen, and nitrogen were performed with a PerkinElmer CHN analyzer (Model 2400). The IR spectra (KBr pellets, 4000-400 cm^{-1}) were recorded by using a Shimadzu Model IR Affinity-1 spectrometer. The magnetic data were obtained with a Quantum Design MPMS 5XL super conducting quantum interface device (SQUID) susceptometer. The magnetic susceptibility measurements were performed in the 1.8 - 300 K temperature range under a 0.05 T dc applied magnetic field. Diamagnetic corrections were applied using Pascal's constants. Variable-temperature Mössbauer experiments were carried out using a ^{57}Co/Rh source in a constant acceleration transmission spectrometer (Topologic Systems) equipped with an Iwatani HE05/CW404 Cryostat. The spectra were recorded at 20 K. The spectrometer was calibrated using standard α-Fe foil.

Data collections for single crystal X-ray diffraction for **1** were performed on a Bruker SMART APEX II, with a CCD area detector with graphite monochromated Mo-Kα (λ = 0.71073 Å) radiation. The structure was solved by direct methods and refined by full-matrix least-squares methods based on F^2 using the SHELXL software. Non-hydrogen atoms were refined anisotropically. All hydrogen atoms were positioned geometrically and refined with isotropic displacement parameters according to the riding model. All geometrical calculations were performed using the SHELXL software. Data sets for **1** were treated with the SQUEEZE program from the PLATON suite to remove highly disordered solvent molecules from the calculations.
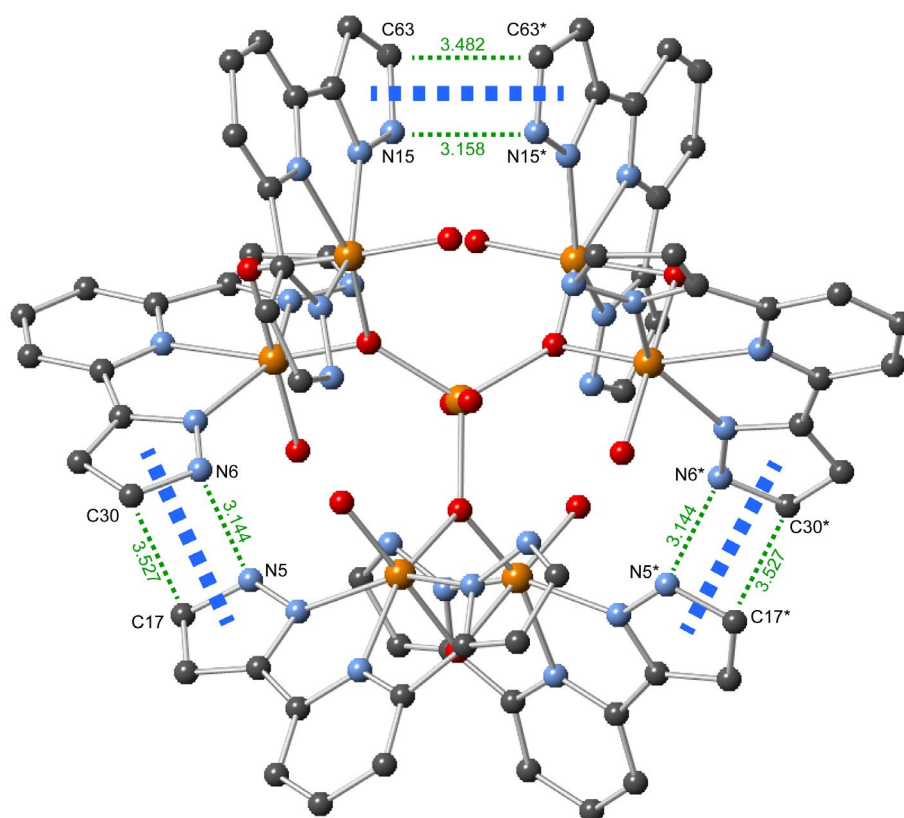
Figure S1 π–π stacking interactions of **1**. Phenyl rings were omitted for clarity. Blue dotted lines represent π–π stacking interactions.

References

1   Y. Zhou, W. Chem and D. Wang, *Dalton Trans.*, 2008, 1444.