Pentasubstituted Ferrocene and Dirhodium Tetracarboxylate as Building Blocks for Discrete Fullerene-like and Extended Supramolecular Structures

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Supplementary material

Contents :

SR-XRD analysis on compound 3 (measured in glass capillary 0.8mm)

Ratio Ligand/linkers = 1 / 2.5. Final expected composition if the spheroid is formed with 12 ligand + 30 linkers : $C_{1416}H_{2364}Fe_{12}N_{120}O_{252}P_{12}Rh_{60}$, MM = 32318.92g/mol

The SR-XRD pattern corrected for empty capillary (Fig. S1) shows six broad reflections which could be indexed using the Dicvol04 program[1] in a cubic body centred (*I*) system, with cell parameter *a*=44.40(2)Å and cell volume *V*=87548(70)Å^3

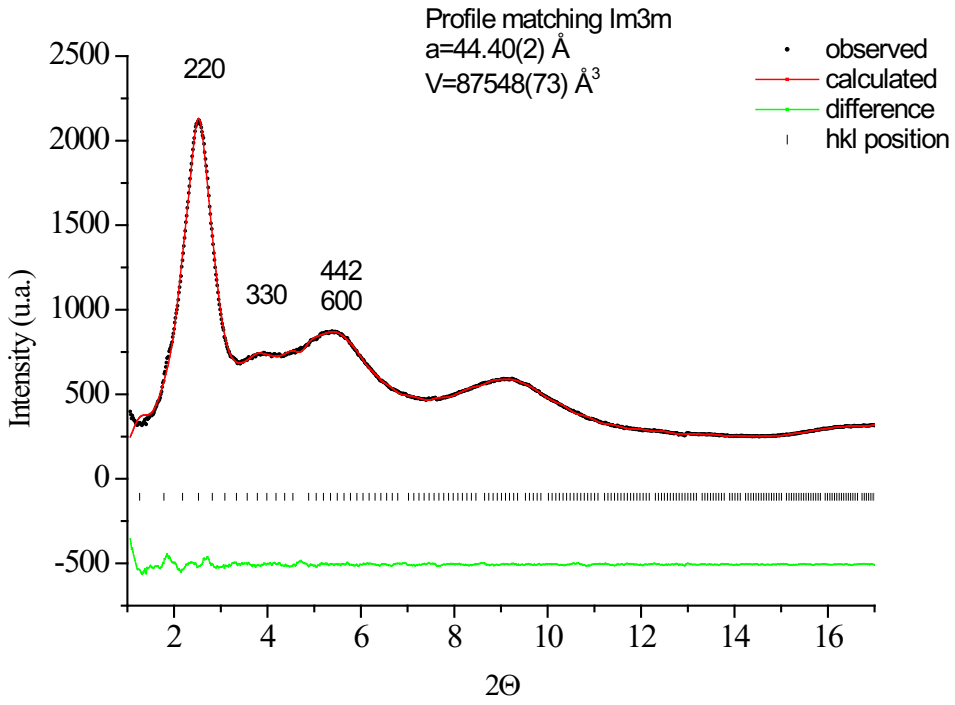

Fig. S1. X-Ray powder diffraction results for **(3)**. Profile matching fitting results in space group Im-3m using the Fullprof program[2]. Experimental pattern (dot black), calculated (red), difference (green) and hkl position (ticks).

[1] *Dicvol04 :* A. Boultif, D. Louer, J. Appl. Cryst. (2004) 37, 724-731

[2] *Fullprof* : J. Rodriguez-Carvajal, Physica B (1993) 192, 55.

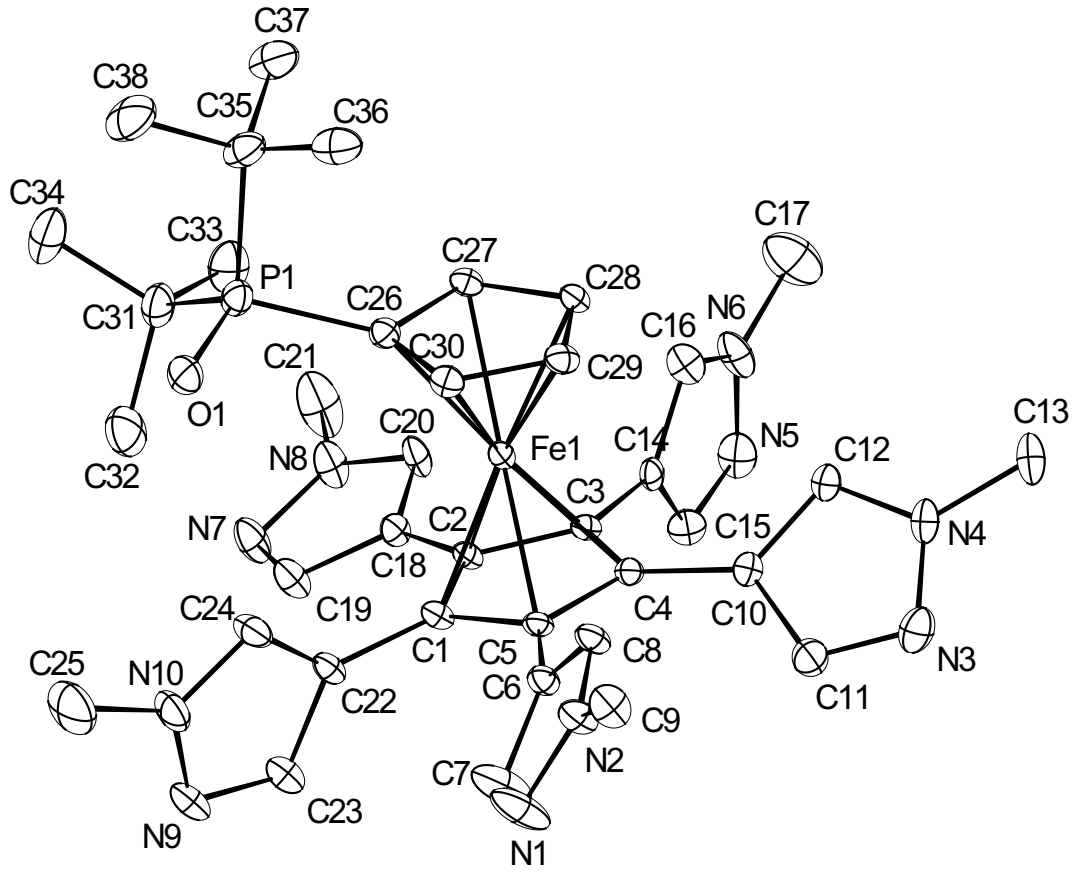

Fig. S2 Molecular X-Ray single crystal structure of ligand **1** (ORTEP representation, 30% probability) with numbering scheme. Hydrogen atoms and chloroform solvent molecule are omitted for clarity.

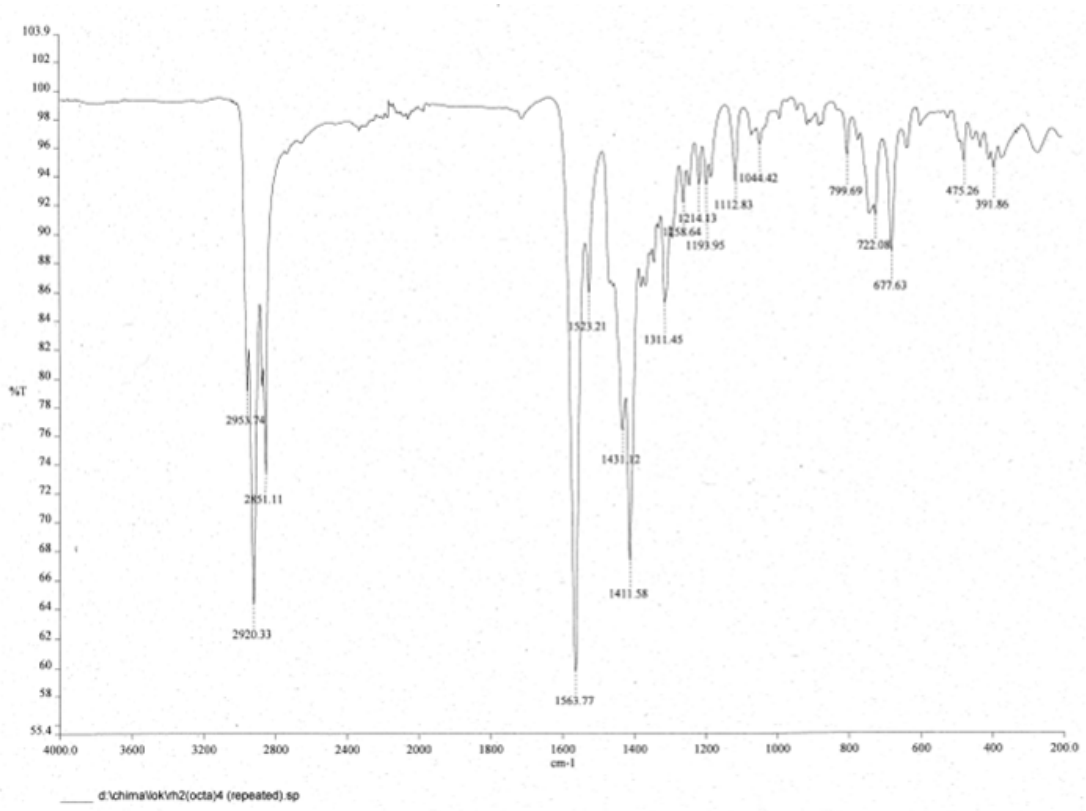

Fig. S3. IR spectrum of dirhodium tetracarboxylate **2**

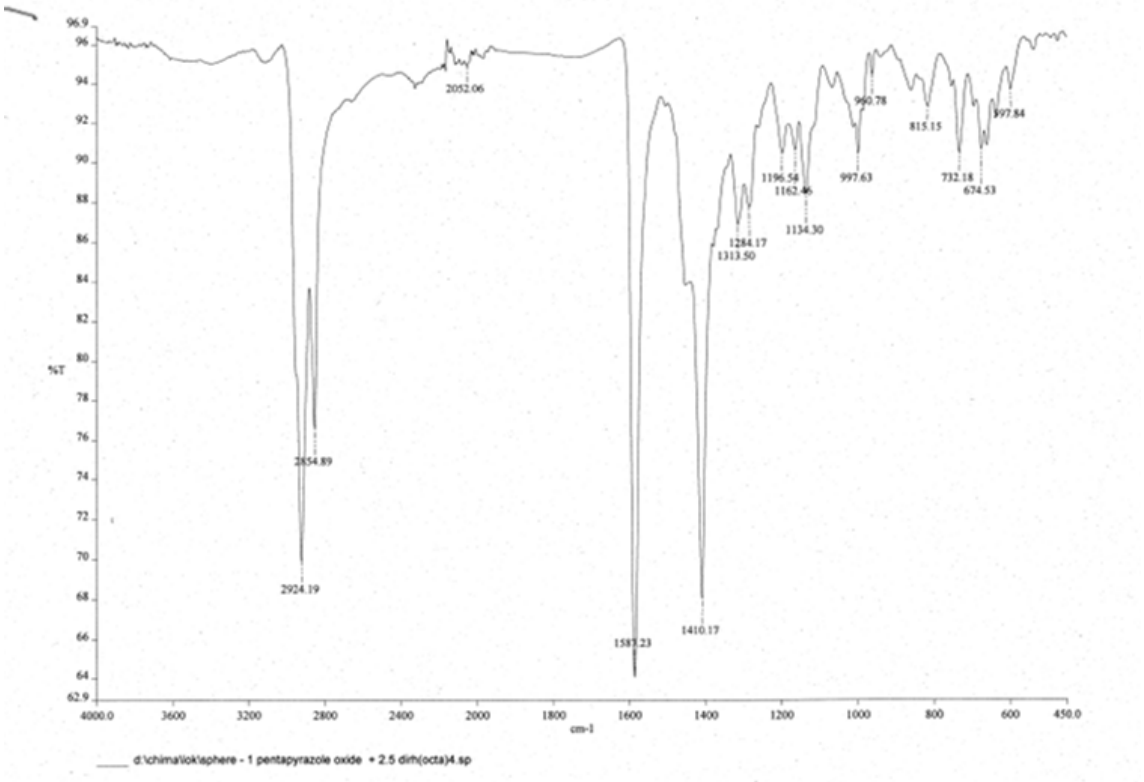

Fig. S4. IR spectrum of precipitate **3**

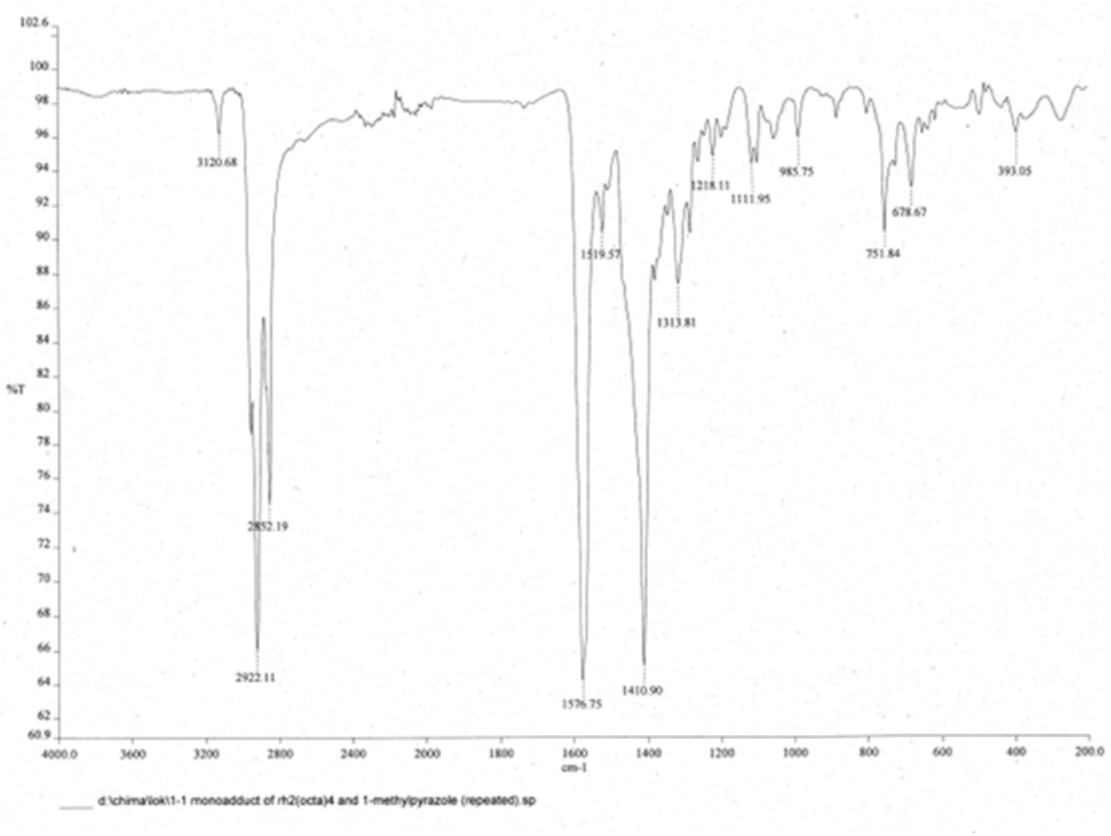

Fig. S5. IR spectrum of *mono*-adduct **4**

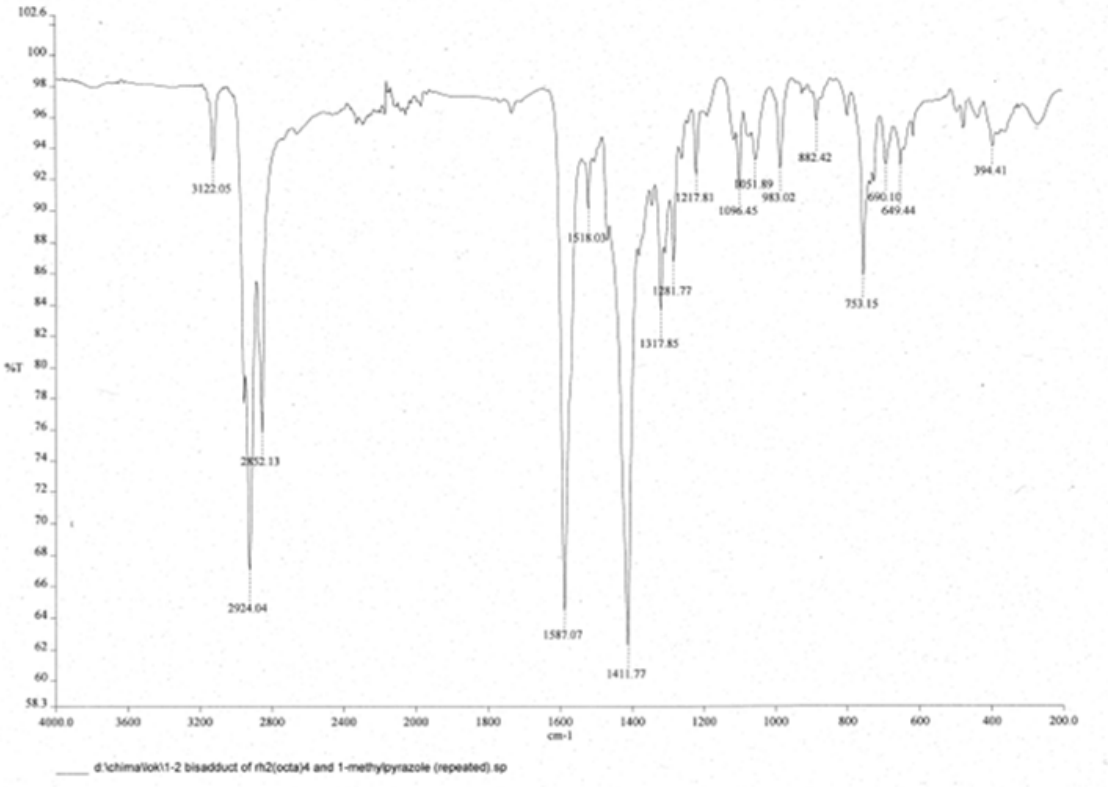

Fig. S6. IR spectrum of *bis*-adduct **5**

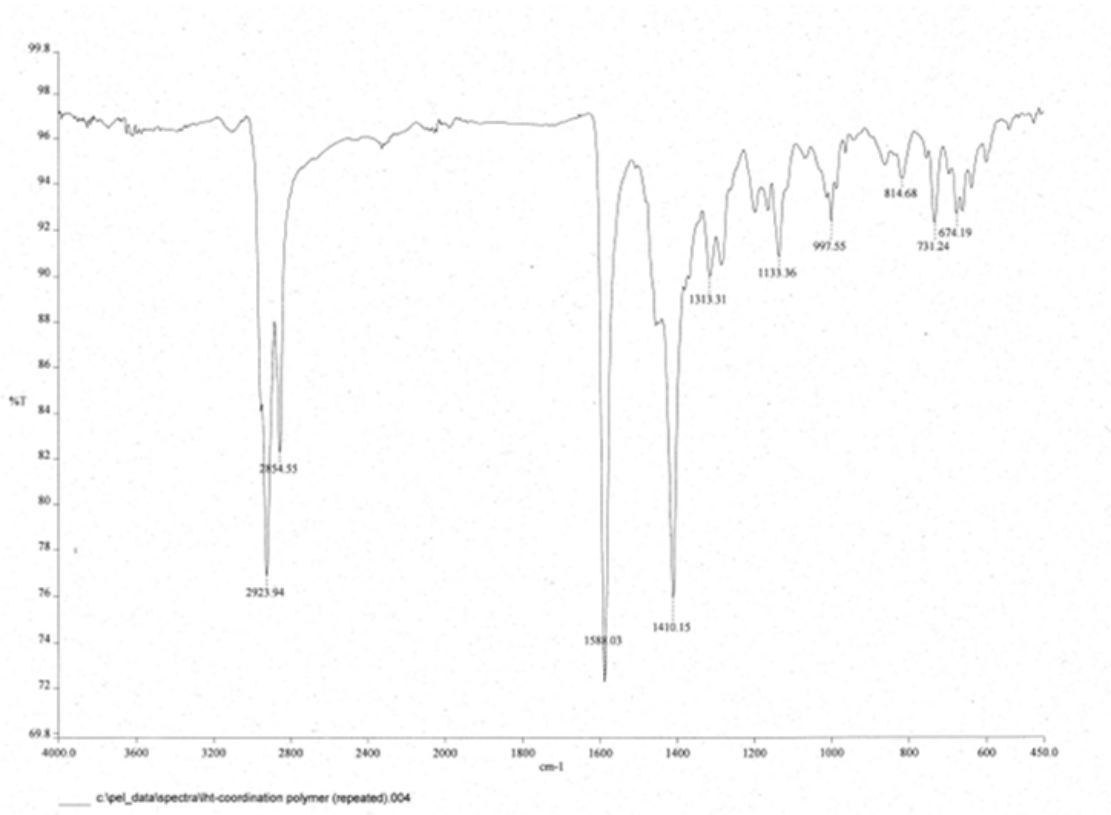

Fig S.7. IR spectrum of crystal **6**