



STRUCTURAL
CHEMISTRY

Volume 78 (2022)

Supporting information for article:

Coordination chemistry of polynitriles. Part 9. Decacyanoferrrocene revisited. Crystal and molecular structure of *cis*- $[\{C_5(CN)_5\}_2(MeCN)_4Fe]$

Karlheinz Sünkel and Tobias Blockhaus

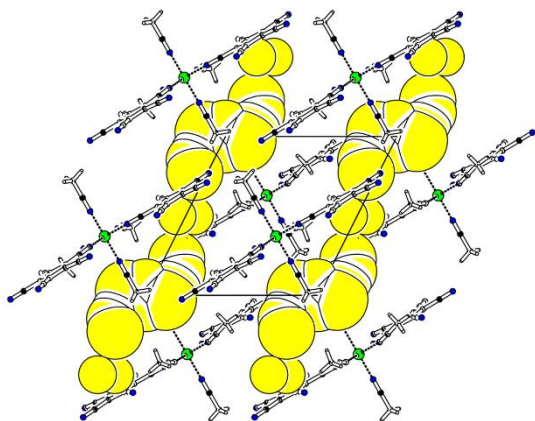


Figure S1 Platon cavity plot.

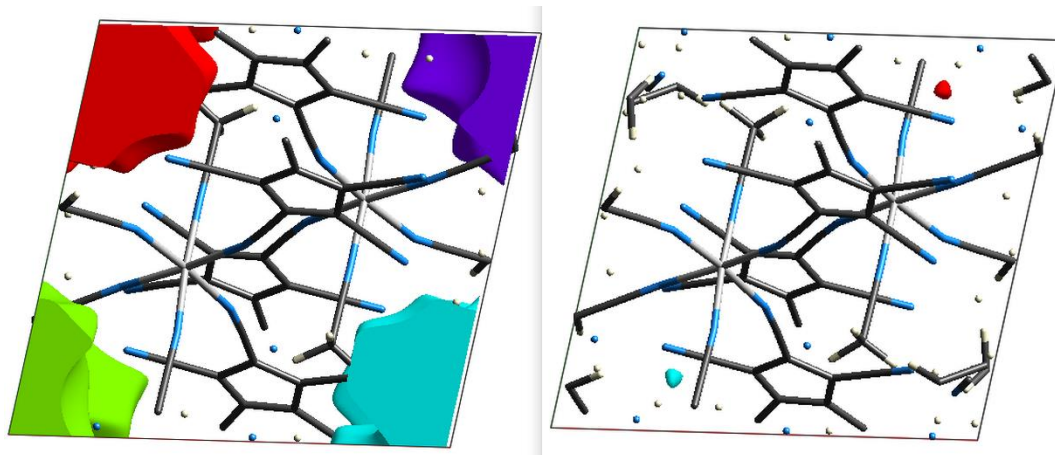


Figure S2 Void plots (0.0003 au Isosurface) for the structure solution without the lattice MeCN (left) and including the 2 MeCN lattice solvents (right). The surface area range from 65.8 (light blue) to 51.3 (violet) \AA^2 in the left and both (light blue and red) 1.6 \AA^2 .

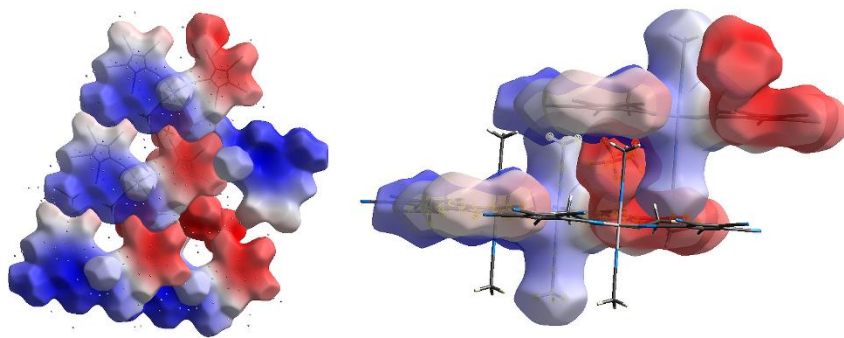


Figure S3 Top and side view of several "cloned" Hirshfeld surfaces displaying the electrostatic potentials and their complementarity in neighbouring molecules.

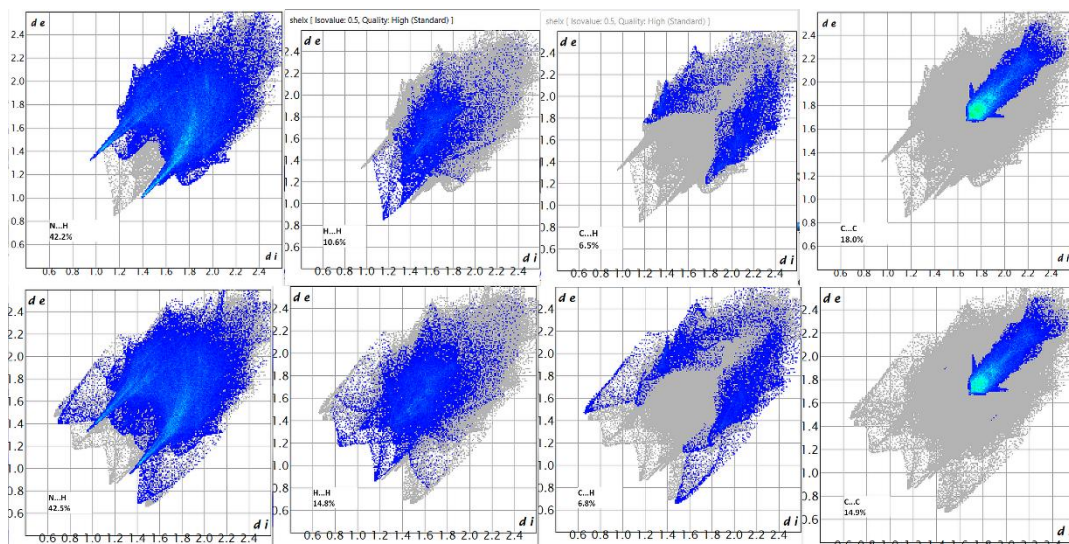


Figure S4 Individual Fingerprint plots corresponding to Figures 8a (top row) and 8b (bottom row).

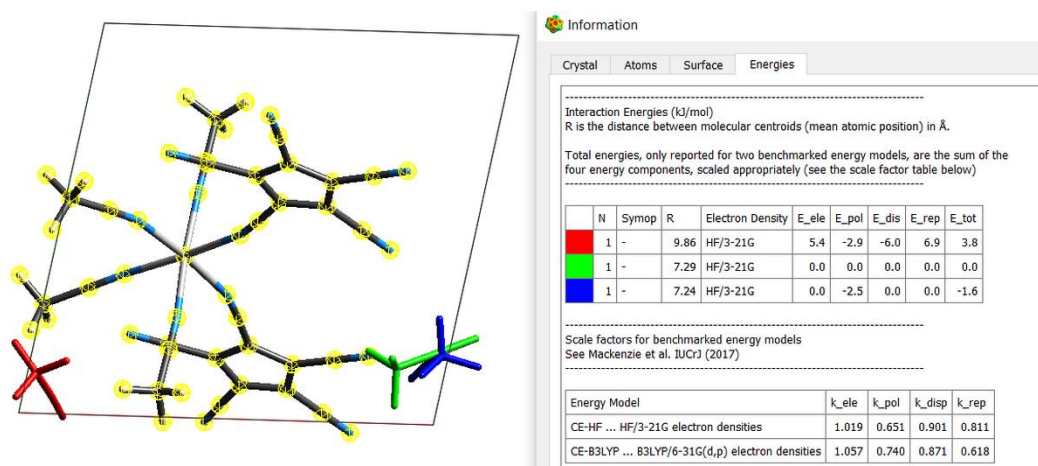


Figure S5 Interaction energies (HF/3-21G) between a single Fe complex and the two lattice MeCN molecules

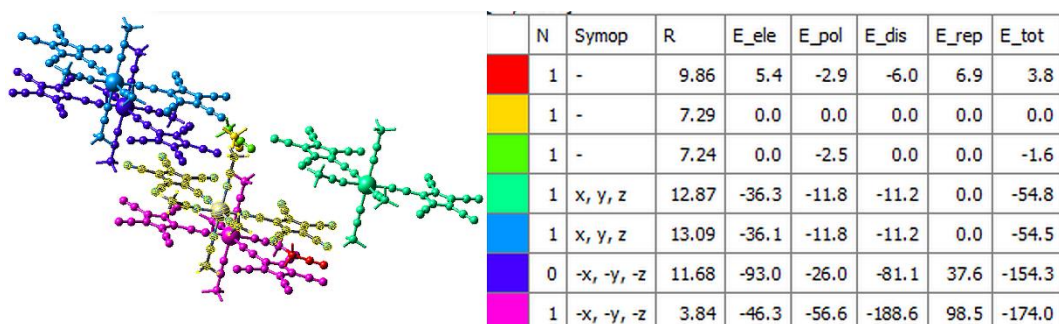


Figure S6 Interaction energies (HF/3-21G) between the asymmetric unit and four close neighbours.