Molecular, Supramolecular Structures Combined with Hirshfeld and DFT Studies of Centrosymmetric M(II)-azido {M=Ni(II), Fe(II) or Zn(II)} Complexes of 4-Benzoylpyridine

Morsy A. M. Abu-Youssef [1,*], Vratislav Langer [2], Assem Barakat [3], Matti Haukka [4] and Saied M. Soliman [1,*]

[1] Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia,
Alexandria 21321, Egypt.
[2] Department of Chemical and Biological Engineering, Chalmers University of Technology,
SE-41296 Gothenburg, Sweden; vratislav@hotmail.com or langer@chalmers.se
[3] Department of Chemistry, College of Science, King Saud University, P. O. Box 2455, Riyadh 11451,
Saudi Arabia; ambarakat@ksu.edu.sa
[4] Department of Chemistry, University of Jyväskylä, P.O. Box 35, FI-40014 Jyväskylä, Finland; matti.o.haukka@jyu.fi
* Correspondence: morsy5@alexu.edu.eg (M.A.M.A.-Y.);
saeed.soliman@alexu.edu.eg (S.M.S.);
Tel.: +20-1010003021 (M.A.M.A.-Y.); +20-1111361059 (S.M.S.).

X-ray structure determination

Crystallographic measurements were made on a Siemens Smart CCD diffractometer with graphite monochromated Mo Kα radiation at 173 K. CCD data were integrated with the SAINT package [S1] and a multiscan absorption correction was applied (3) using SADABS [S2]. Structures were solved by direct methods (**1**, **2**, SHELXS) [S3] or by intrinsic phasing (**3**, SHELXT [S4]) and refined against all F^2 data by full-matrix least-squares (SHELXL [S5] including anisotropic displacement parameters for all non-H atoms. The N3-moiety in **3** was disordered over two positions with occupancy ratio on 0.50/0.50. The hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95 Å and $U_{iso} = 1.2 \cdot U_{eq}$(parent atom).

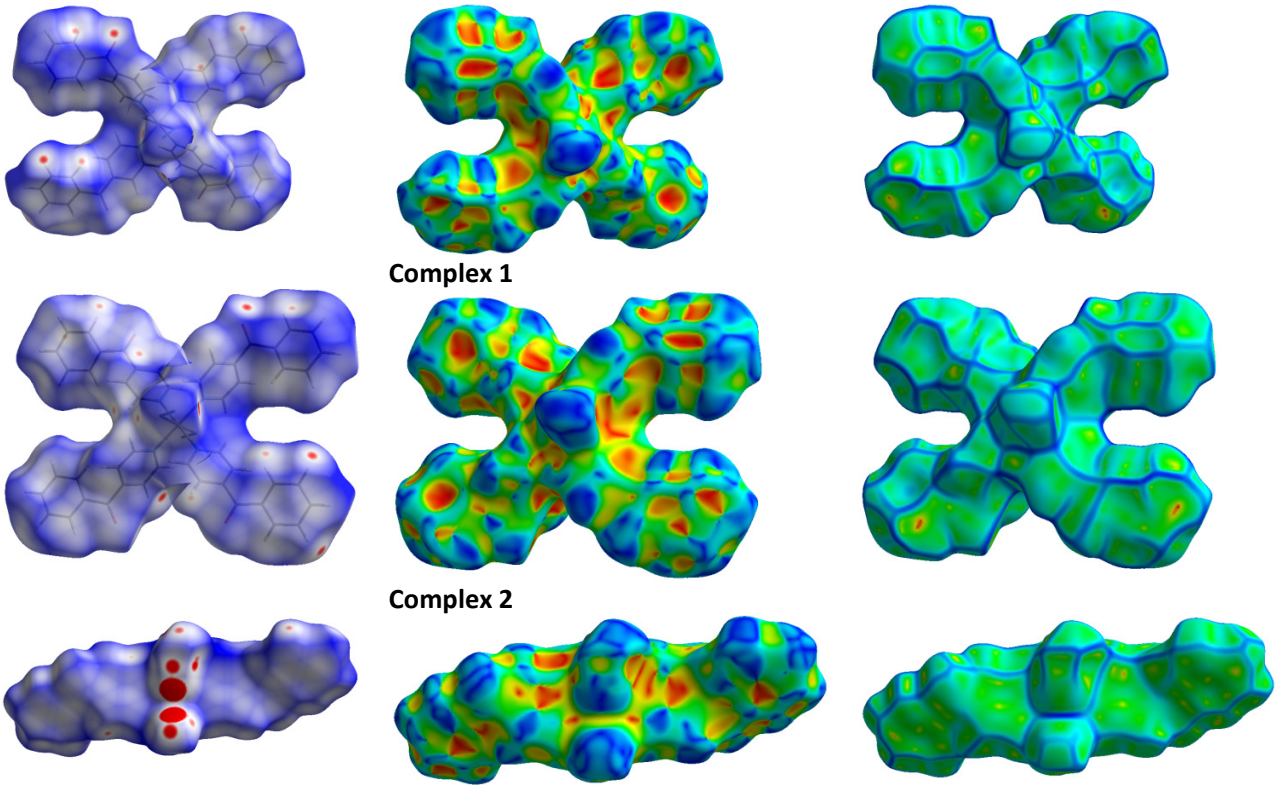
[S1] SAINT; Siemens analytical X-ray Instruments Inc.: Madison, WI, **1995**.

[S2] Sheldrick, G. M. SADABS; University of Göttingen: Göttingen, Germany, **1996**.

[S3] Sheldrick, G. M. A short history of SHELX. *Acta Crystallogr. A64*, **2008**, 112-122.

[S4] Sheldrick; G. M. *SHELXT* - Integrated space-group and crystal-structure determination. *Acta Cryst.* **2015**, *A71*, 3-8.

[S5] Sheldrick, G. M. Crystal structure refinement with *SHELXL*. *Acta Cryst.* **2015**, *C71*, 3-8.



Complex 1

Complex 2

Complex 3

Figure. S1 Hirshfeld surfaces of the studied complexes