

Supporting Information

Synthesis, Supramolecular Structural Investigations of Co(II) and Cu(II) Azido Complexes with Pyridine-Type Ligands

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Physicochemical characterizations

All chemical were purchased from Sigma-Aldrich Company. CHN analyses were performed using Perkin Elmer 2400 Elemental Analyzer. The Cu and Co contents were determined using Shimadzu atomic absorption spectrophotometer (AA-7000 series, Shimadzu, Ltd, Japan).

X-ray single crystal diffraction measurement

The crystal structures of the two azides were determined by using a Bruker APEX II diffractometer equipped with graphite monochromated MoK α radiation source. All details regarding the crystallographic measurements are included in **Table 1**. SADABS was used for absorption corrections [S1] and all calculations were performed using SHELXTL program package [S2]. The positions of the heavy atoms were detected by the direct methods of SHELXS. The hydrogen atoms bonded to carbon atoms are refined according to the riding model implemented in SHELX. The hydrogen atoms in the crystal structures bonded to oxygen atoms (water and the hydrogen atoms in the hydroxyl group of **HAId** were refined with DFIX restraints and with fixed thermal parameter at a value of 1.5 times the displacement parameters of the respective oxygen atoms. The CIF deposition numbers are CCDC – 2158205 and CCDC – 2158206 for the Co- and the Cu complex, respectively and can be obtained from the CCDC at <https://www.ccdc.cam.ac.uk/structures>.

Computational details

With the aid of Gaussian 09 software package [S3], natural charge calculations [S4] were performed using WB97XD method [S5] at the X-ray structure coordinates and employing the TZVP basis sets. Atoms in molecules (AIM) [S6] topology analyses were performed using Multiwfn program [S7].

References

- S1. Sheldrick, G.M. SADABS, Program for Empirical Absorption Correction of Area Detector Data; ScienceOpen, Burlington, USA, 1996.
- S2. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Crystallogr. C Struct. Chem.* 2015, 71, 3–8.
- S3. M. J. Turner, J. J. McKinnon, S. K. Wolff, D. J. Grimwood, P. R. Spackman, D. Jayatilaka, M. A. Spackman, *Crystal Explorer17* (2017) University of Western Australia. <http://hirshfeldsurface.net>
- S4. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; et al. GAUSSIAN 09; Revision A02; Gaussian Inc.: Wallingford, CT, USA, 2009.
- S5. Glendening, E.D.; Reed, A.E. ; Carpenter, J.E.; Weinhold, F. NBO Version 3.1, CI, University of Wisconsin, Madison, 1998.
- S6. Chai J. D.; Head-Gordon M. *Phys. Chem. Chem. Phys.* 2008, 10,6615-6620.
- S7. Bader, R. F. W. *Atoms in Molecules: A Quantum Theory*, Oxford University Press, Oxford, U.K., 1990.

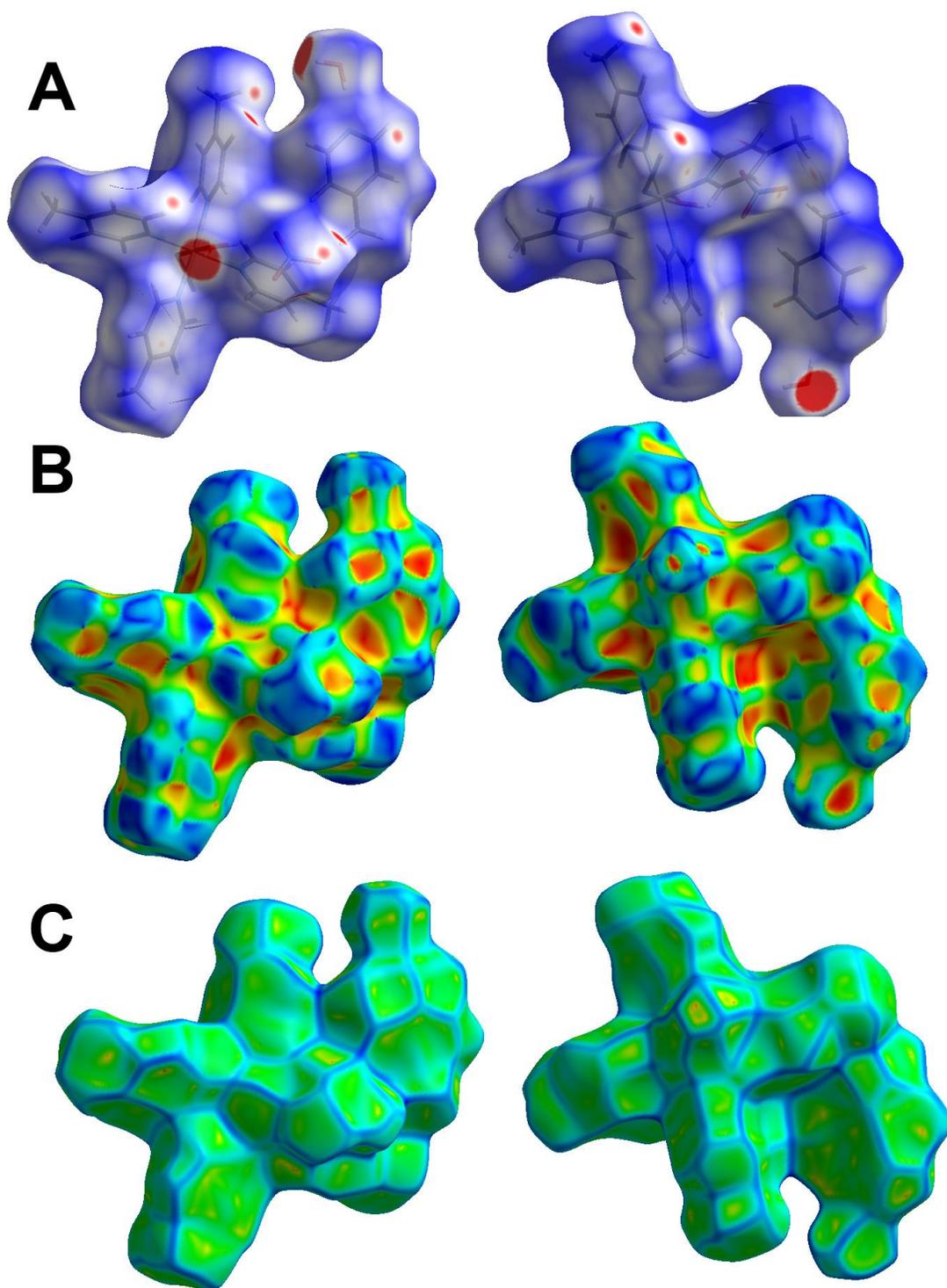


Figure S1. Hirshfeld surfaces of 1.

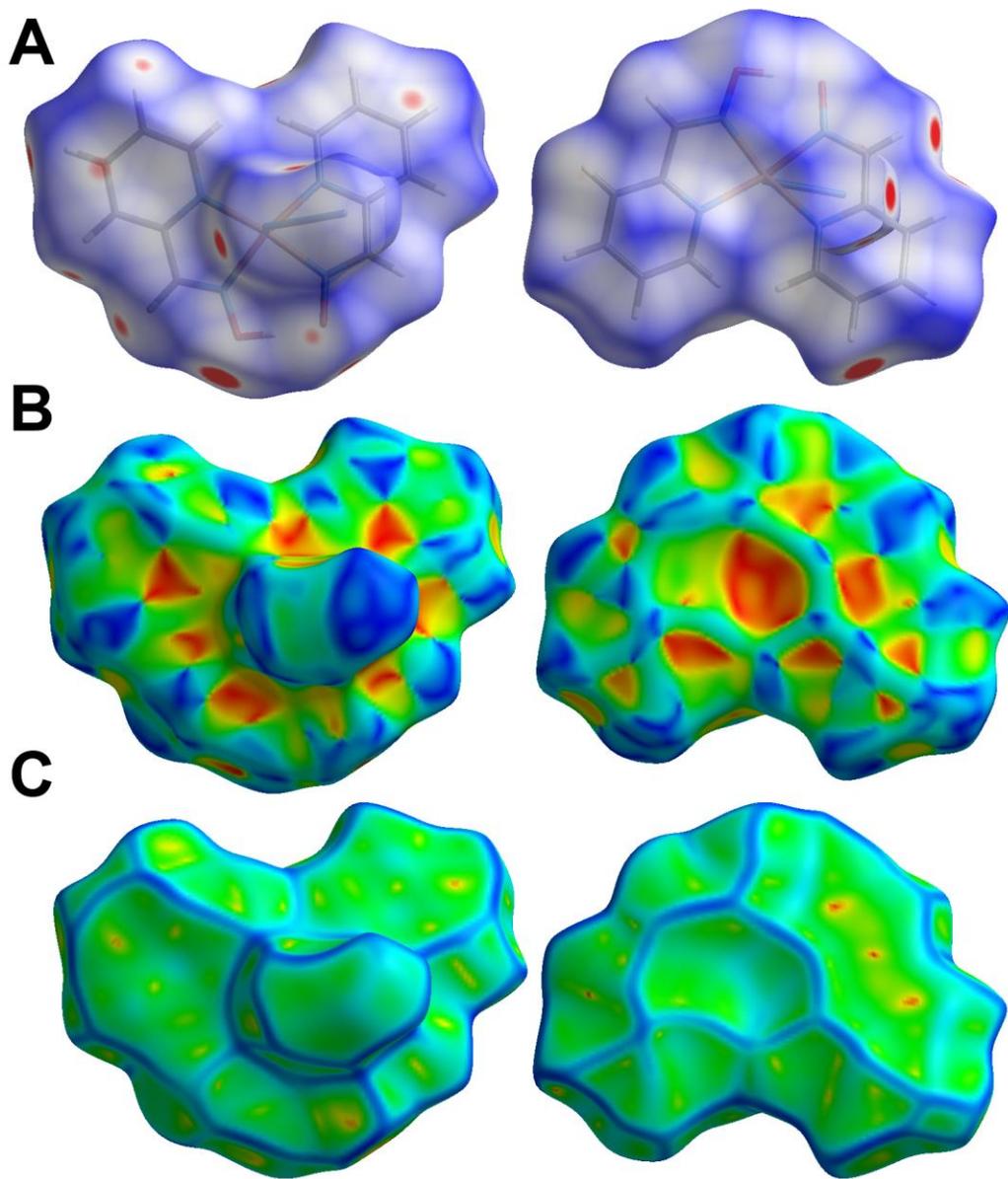


Figure S2. Hirshfeld surfaces of 2.