STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 77 (2021)

Supporting information for article:

Crystal structure and enantiomeric layer disorder of a copper(I) nitrate π-coordination compound

Dorota A. Kowalska, Vasyl Kinzhybalo, Yuriy I. Slyvka and Marek Wołcyrz

Supporting information

Table S1 The comparison between fits from SHELX structure refinement and JANA2006 taking into account enantiomeric layer disorder in [Cu(*m-dmphast*)NO_3].

This is a table headnote (style: IUCr table headnote)

	SHELX	JANA2006
Data/restrains/constrains/parameters	3247/0/0/201	13521/0/345/200
Goodness-of-fit on F^2	1.065	1.64*
R [F_0^2>2σ(F_0^2)]	R_1 = 0.0493, wR_1 = 0.1162	R_1 = 0.0376, wR_1 = 0.0665
R (all)	R_2 = 0.0609, wR_2 = 0.1247	R_2 = 0.0504, wR_2 = 0.0687
Largest diff. peak and hole (e Å^{-3})	2.69 and -0.62	0.40 and -0.62

* The formulae for goodness-of-fit calculation are different in SHELX and JANA2006 programs.

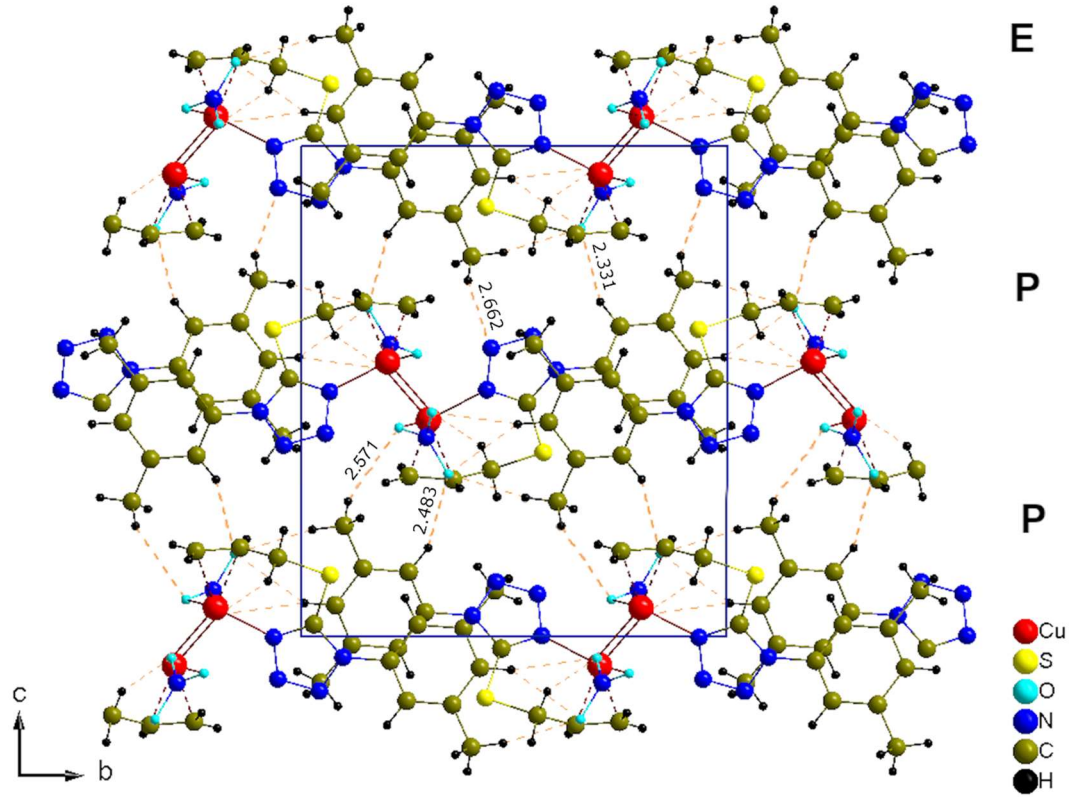

Figure S1 View at the three layers of the [Cu(*m-dmphast*)NO_3] disordered structure perpendicular to the *a*-direction. The C-H···O and C-H···N bonds between adjacent (**E**, **P** and **P**, **P**) layers are marked with orange thick dashed lines.

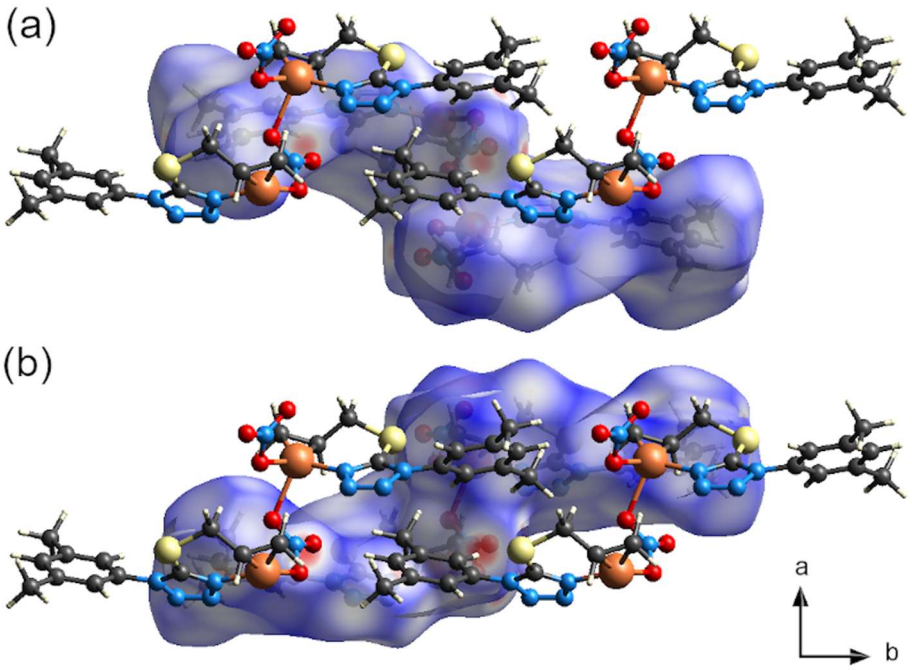

Figure S2 The Hirshfeld surface of layer **P** (a) and **E** (b) segment between two layers of **P** type. A view down the *c* crystallographic direction.

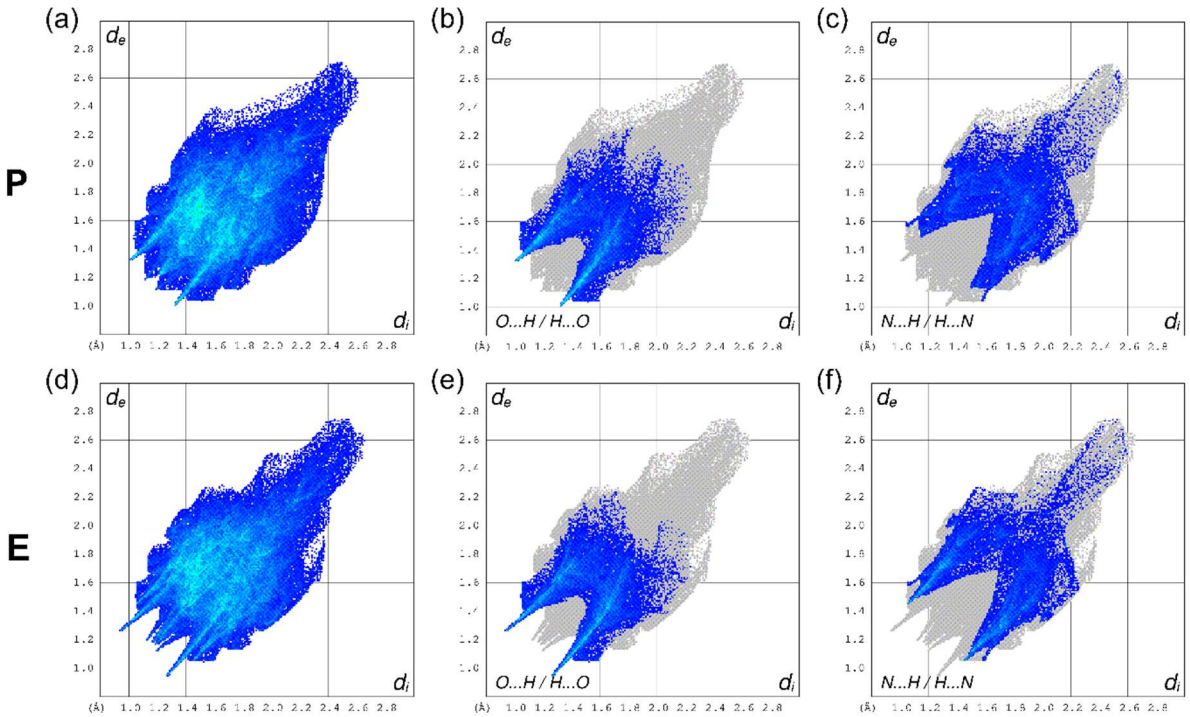

Figure S3 The 2D fingerprint plot of molecules in **P** (a)-(c) and **E** (d)-(f) layers situated between two layers of **P** type; d_e – the distance from the point to the nearest nucleus external to the surface, d_i – the distance to the nearest nucleus internal to the surface.

Figure S4 Graphical representation of the [Cu(*m-dmphast*)NO_3] crystal final 1-*D* NNI model (J = -2). One thousand layers of **P** (→ , blue colour) and **E** (←, red colour) types are presented. Each arrow represents a single layer. The layers (arrows) should form one column; for simplicity, they are placed in the following lines.