Hydro/ Solvothermal Synthesis and Crystal Structure of Novel Ni(II) Coordination Polymer Containing Pamoic Acid and Ethylenediamine Mixed Ligands : $\{[Ni(\mu\text{-}pam)(en)_2]\cdot H_2O\}_n$

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Supplementary Materials

APPENDIX A. SUPPLEMENTARY DATA

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 1482735. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk).

THE STRUCTURE SOLVED METHODS

The structure was solved by direct methods using SHELXS-97 (1) and refined by full-matrix least-squares methods on F^2 using SHELXL-2013 (2). All non-hydrogen atoms were refined with anisotropic parameters. The water H atom was located in a difference map refined freely. The other H atoms were located from different maps and then treated as riding atoms with C-H distances of 0.93-0.97 Å, N-H distances of 0.97 Å and O-H distance of 0.82 Å. The following procedures were implemented in our analysis: data collection: Bruker APEX2 (3); program used for molecular graphics were as follow: MERCURY programs (4); software used to prepare material for publication: WinGX (5).

REFERENCES

1. Sheldrick GM. Acta Cryst. 2008; A64: 112-122. doi.org/10.1107/S0108767307043930.
2. Sheldrick GM. Acta Cryst. 2015; C71: 3-8. DOI:10.1107/S2053273314026370
3. APEX2, Bruker AXS Inc. Madison Wisconsin USA, 2013.
4. Mercury, version 3.3; CCDC, available online via ccdc.cam.ac.uk/products/mercury.
5. Farrugia LJ. J. Apply. Cryst. 1999; *32*: 837-838.

Table S1: Crystal data and structure refinement parameters of **1**

Empirical formula	$C_{27}H_{32}N_4O_7Ni$
Formula weight	583.27
Crystal system	Orthorhombic
Space group	Fddd
a (Å)	16.920 (3)
b (Å)	24.186 (5)
c (Å)	25.770 (5)
V (Å^3)	10546 (4)
Z	16
D_c (g cm^{-3})	1.469
μ (mm^{-1})	0.79
θ range (°)	2.9-28.2
Measured refls.	46515
Independent refls.	3284
R_{int}	0.051
S	1.05
R1/wR2	0.042/0.120
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^{-3})	0.86/-0.96

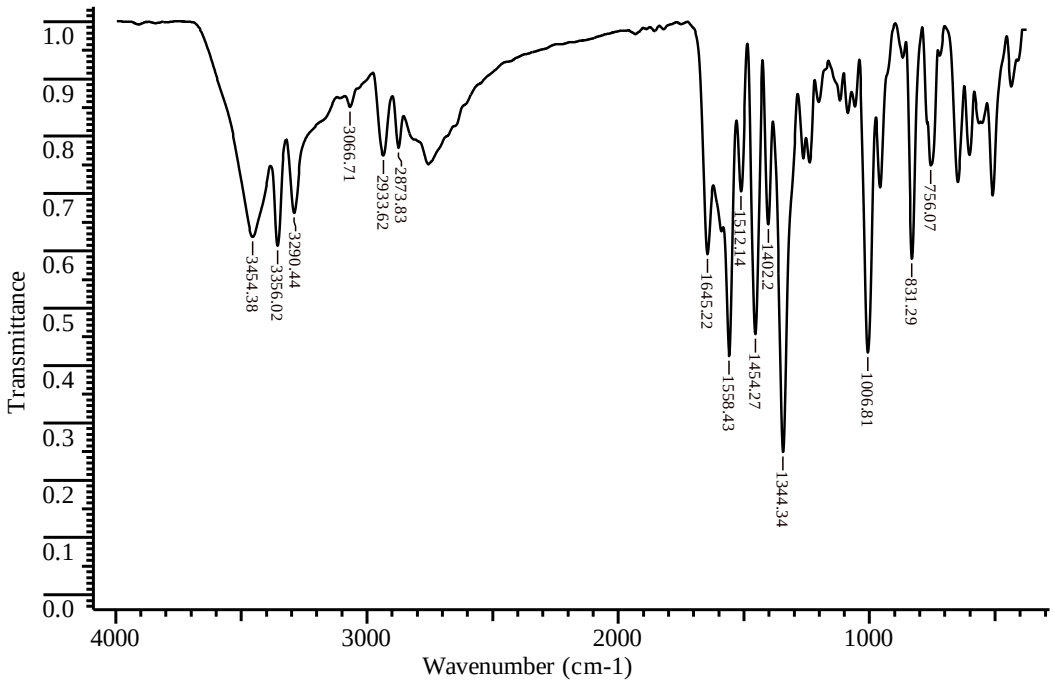

Figure S1: The FT-IR spectra of **1.**