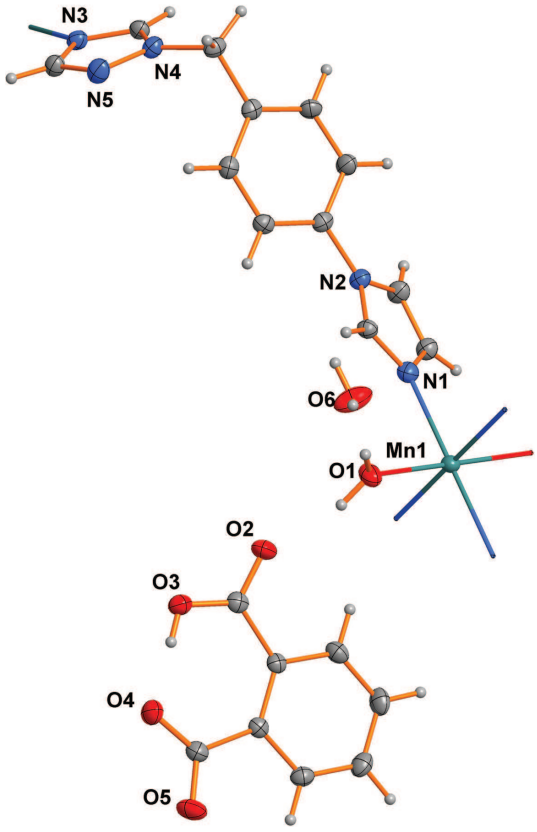
Wen Li, Xia Zhu*, Xue-heng Zhu and Shi-jing-min Li

Crystal structure of poly[diaqua-bis(μ$_2$-1-(4-(1*H*-imidazol-1-yl)benzyl)-1*H*-1,2,4-triazole-κ^2*N*:*N*′)manganese(II)]bis(2-carboxybenzoate) dihydrate, $MnC_{40}H_{40}N_{10}O_{12}$



https://doi.org/10.1515/ncrs-2018-0223
Received July 1, 2018; accepted October 4, 2018; available online October 17, 2018

Abstract

$MnC_{40}H_{40}N_{10}O_{12}$, monoclinic, $P2_1/c$ (no. 14), $a = 8.252(6)$ Å, $b = 18.144(10)$ Å, $c = 13.580(8)$ Å, $\beta = 97.61(3)°$, $V = 2015(2)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0390$, $wR_{ref}(F^2) = 0.1027$, $T = 120$ K.

CCDC no.: 1871360

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Block, clear light colourless
Size:	0.1 × 0.1 × 0.05 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.5 mm^{-1}
Diffractometer, scan mode:	Bruker D8 VENTURE, φ and ω-scans
θ_{max}, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	43860, 4601, 0.127
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3338
$N(param)_{refined}$:	286
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

Source of materials

A mixture of $Mn(CH_3COO)_2{\cdot}4H_2O$ (0.5 mmol), phthalic acid (0.5 mmol), 1-(imidazo-1-ly)-4-(1,2,4-triazol-1-ylmethyl) benzene (itmb) (0.50 mmol) and distilled water (25 mL) was heated in a 50 mL stainless steel reactor with a Teflon liner 373 K for 8 h, followed by slow cooling to room temperature until colourless crystals of the title compound formed.

Experimental details

All H atoms were positioned geometrically (O—H = 0.85 Å and C—H = 0.95 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$, $U_{iso}(H) = 1.5U_{eq}(O)$.

Discussion

The design and construction of metal-organic frameworks (MOFs) with well-regulated network structures has been provoked significant interest on these functional materials [4–7]. The organic ligands, which have their differences in the size, the flexibility, the coordination ability, the number of the carboxylate groups, the positions of the carboxylate groups and so on, are important in the design of frameworks [8–10]. In addition, containing triazol ligands [11, 12] are known to be connectors of coordination networks.

In this paper, we select phthalic acid to react with Mn(II) ions and 1-(imidazo-1-ly)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb) to obtain a new coordination polymer. The asymmetric

***Corresponding author: Xia Zhu,** Science College, Civil Aviation University of China, Tianjin 300300, P.R. China, e-mail: xzhu@cauc.edu.cn
Wen Li, Xue-heng Zhu and Shi-jing-min Li: Science College, Civil Aviation University of China, Tianjin 300300, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
Mn1	0.000000	0.000000	0.000000	0.01591(12)
O1	0.23902(17)	−0.04362(8)	−0.01765(10)	0.0248(3)
H1A	0.292834	−0.033306	−0.065320	0.037*
H1B	0.291054	−0.080096	0.012660	0.037*
N1	0.1114(2)	0.10800(8)	0.05850(12)	0.0191(4)
N2	0.25537(19)	0.20944(9)	0.09256(12)	0.0177(3)
N3	0.97252(19)	0.45931(8)	0.34069(12)	0.0176(3)
N4	0.85932(19)	0.43703(9)	0.18888(12)	0.0185(4)
N5	0.9985(2)	0.39503(9)	0.20147(13)	0.0233(4)
C1	0.2493(2)	0.14254(10)	0.04809(14)	0.0184(4)
H1	0.332922	0.122997	0.013928	0.022*
C2	0.0264(3)	0.15509(11)	0.11314(15)	0.0213(4)
H2	−0.077380	0.144876	0.133049	0.026*
C3	0.1122(2)	0.21753(11)	0.13402(15)	0.0220(4)
H3	0.080629	0.258856	0.170010	0.026*
C4	0.3805(2)	0.26439(10)	0.09358(14)	0.0181(4)
C5	0.3342(3)	0.33788(11)	0.08898(15)	0.0229(4)
H5	0.222062	0.351144	0.084179	0.027*
C6	0.4538(2)	0.39179(11)	0.09149(15)	0.0220(4)
H6	0.422667	0.442223	0.089353	0.026*
C7	0.6187(2)	0.37351(10)	0.09707(14)	0.0184(4)
C8	0.6631(2)	0.29933(11)	0.10118(14)	0.0197(4)
H8	0.775011	0.286047	0.104560	0.024*
C9	0.5448(2)	0.24454(11)	0.10039(14)	0.0191(4)
H9	0.575815	0.194092	0.104456	0.023*
C10	0.7458(2)	0.43358(11)	0.09610(14)	0.0210(4)
H10A	0.808793	0.424815	0.040042	0.025*
H10B	0.689738	0.481682	0.084908	0.025*
C11	1.0616(2)	0.41036(11)	0.29349(15)	0.0211(4)
H11	1.160796	0.389151	0.324371	0.025*
C12	0.8459(2)	0.47431(10)	0.27148(14)	0.0178(4)
H12	0.758967	0.506960	0.280203	0.021*
O2	0.42794(19)	−0.13192(8)	0.11365(11)	0.0302(4)
O3	0.62177(17)	−0.21294(7)	0.15563(11)	0.0250(3)
H3A	0.631676	−0.257783	0.161452	0.037*
O4	0.65484(17)	−0.34316(8)	0.17316(12)	0.0288(4)
O5	0.50637(18)	−0.44257(7)	0.17755(12)	0.0301(4)
C13	0.4709(2)	−0.19626(11)	0.13597(14)	0.0199(4)
C14	0.3374(2)	−0.25385(10)	0.13877(14)	0.0172(4)
C15	0.1781(2)	−0.22569(11)	0.12284(15)	0.0230(4)
H15	0.163904	−0.174289	0.111500	0.028*
C16	0.0402(3)	−0.26926(12)	0.12282(16)	0.0271(5)
H16	−0.065799	−0.248003	0.111371	0.033*
C17	0.0591(3)	−0.34423(12)	0.13972(15)	0.0255(5)
H17	−0.033715	−0.375071	0.140663	0.031*
C18	0.2154(3)	−0.37356(11)	0.15524(14)	0.0215(4)
H18	0.227297	−0.425051	0.166664	0.026*
C19	0.3569(2)	−0.33077(10)	0.15487(13)	0.0171(4)
C20	0.5152(2)	−0.37512(10)	0.16967(14)	0.0196(4)
O6	0.4085(2)	0.00414(9)	−0.15526(12)	0.0383(4)
H6A	0.442268	−0.015374	−0.205635	0.058*
H6B	0.464438	0.043396	−0.145045	0.058*

unit of the title structure consists of one half Mn^{2+} ion, one 1-(imidazo-1-ly)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb), two water molecules and one phthalate monoanion. Each Mn(II) atom is coordinated by two triazolyl nitrogen atoms and two imidazolyl nitrogen atoms from four different itmb ligands and two oxygen atoms from two water molecule to furnish a $[MnN_4O_2]$ six-coordinate distorted octahedral geometry (*cf.* the figure). The Mn—O bond lengths are 2.1678(19) Å, and the Mn—N distances are 2.2634(18) and 2.269(2) Å, both of which are in the normal range. The bond angles around the Mn(II) are in the ranges of 87.84(6)–180°. Moreover, the coordinated water molecules and the solvated water molecules, the solvated water molecules and carboxyl O atoms, the coordination water molecules and carboxyl O atoms show hydrogen bonding interactions with d(O—H$\cdots$O) = 2.625(2)–2.7460 Å. Through hydrogen bonds coordination polymers and water molecules are interlinked to form the 3D network.

Acknowledgements: We acknowledge support for the publication fee by Innovation and entrepreneurship fund for Undergraduates (201710059045).

References

1. Bruker. APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, WI, USA (2012).
2. Sheldrick, G. M.: SHELXT-integrated space-group and crystal-structure determination. Acta Crystallogr. **A71** (2015) 3–8.
3. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Crystallogr. **42** (2009) 339–341.
4. Mahmudov, K. T.; Kopylovich, M. N.; da Silva, M. F. C. G.; Pombeiro, A. J. L.: Non-covalent interactions in the synthesis of coordination compounds: Recent advances. Coord. Chem. Rev. **345** (2017) 54–72.
5. Wang, X. F.; Du, K. J.; Wang, H. Q.; Zhang, X. L.; Nie, C. M.: A novel asymmetric chair-like hydroxyl-bridged tetra-copper compound: Synthesis, supramolecular structure and magnetic property. J. Mol. Struc. **1138** (2017) 155–160.
6. Li, S. H.; Li, X. L.: A cadmium complex based on 5-methylisophthalic acid and 1,6-bis(imidazol-1-yl)hexane: synthesis, crystal structure, and photoluminescence properties. Synth. React. Inorg. Met. Org. Chem. **43** (2013) 710–713.
7. Vahovska, L.; Potocnak, I.; Vitushkina, S.; Walko, M.: Low-dimensional compounds containing cyanido groups. Part XXX. Recrystallization of Co(II) complexes with pseudohalogenide ligands leading to CO_2 uptake and formation of dicyanoguanidine anion in newly created Co(III) complexes. Polyhedron. **117** (2016) 359–366.
8. Zhu, X.; Sun, P. P.; Ding, J. G.; Li, B. L.; Li, H. Y.: Tuning cobalt coordination architectures by bis(1,2,4-triazol-1-ylmethyl)benzene position isomers and 5-nitroisophthalate. Cryst. Growth Des. **12** (2012) 3992–C3997.
9. Li, S. H.; Han, M. L.; Liu, G. Z.; Ma, L. F.; Wang, L. Y.: Guestin-duced single-crystal-to-single-crystal transformations of a new 4-connected 3D cadmium(II) metal-organic framework. RSC Adv. **5** (2015) 17588–17591.

10. Zhao, Y.; Li, S. H.: Synthesis and crystal structure of a new three-dimensional complex constructed from thiophene-2,5-dicarboxylic aid. Synth. React. Inorg. Met. Org. Chem. **45** (2015) 921–925.
11. Qian, X.; Sun, P. P.; Ding, J. G.; Li, B. L.; Li, H. Y.: Syntheses, structures and properties of Mn(II), Zn(II) and Ag(I) coordination polymers with 2-(1,2,4-triazol-1-yl)acetate. J. Mol. Struc. **1031** (2013) 175–179.
12. Zhu, W. F.; Zhu, X.: Crystal structure of poly[bis-μ_3-[(2-(1,2,4-triazol-1-yl)acetato-κ^3O:O':N)]-cobalt(II), $[Co(C_4H_4N_3O_2)_2]_n$, $C_8H_8CoN_6O_4$. Z. Kristallogr. NCS **229** (2014) 289–290.