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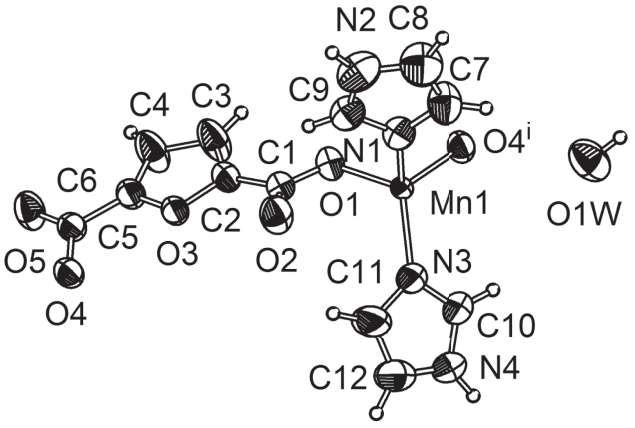
Crystal structure of the catena-poly[bis(1H-imidazole-κ*N*)-(μ$_2$-furan-2,5-dicarboxylato-κ^2*O*^{1}:*O*^{4})manganese(II)]monohydrate, $C_{12}H_{12}MnN_4O_6$



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Abstract

$C_{12}H_{12}MnN_4O_6$, monoclinic, $P2_1/c$ (no. 14), $a = 8.1583(16)$ Å, $b = 16.525(3)$ Å, $c = 13.134(3)$ Å, $\beta = 117.96(3)°$, $V = 1564.0(7)$ Å^3, $4 = 2$, $R_{gt}(F) = 0.0503$, $wR_{ref}(F^2) = 0.1579$, $T = 293$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a typically synthetic protocol, furan-2,5-dicarboxyl acid (0.0156 g, 0.10 mmol), $MnCl_2{\cdot}4H_2O$ (0.0198 g, 0.10 mmol), $C_3N_2H_4$ (0.020, 0.30 mmol) and NaOH (0.004, 0.10 mmol) were dissolved in water (5 ml, 278 mmol) under stirring. The mixture with a molar ratio of 1 (furan-2,5-dicarboxyl acid) : 1 ($MnCl_2{\cdot}4H_2O$) : 3 ($C_3N_2H_4$) : 1 NaOH : 2780 H_2O was stored at room temperature for 4 days. The pink product was collected as a single phase.

Experimental details

Water H atoms were located in a difference Fourier map and refined with O—H = 0.82 Å and $U_{iso}(H) = 1.2U_{eq}(O)$). The carbon H-atoms and nitrogen H-atoms were placed in calculated positions (C—H = 0.93 Å and N—H = 0.86 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Table 1: Data collection and handling.

Crystal:	Pink, block, size 0.23×0.38×0.44 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.79 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS RAPID, ω
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	15160, 3586
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3121
$N(param)_{refined}$:	215
Programs:	SHELX [5], Diamond [6]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(3)	4*e*	−0.2028	0.6543	0.8450	0.090
H(4)	4*e*	−0.3596	0.5354	0.8842	0.092
H(2)	4*e*	0.7509	0.7018	1.1071	0.091
H(7)	4*e*	0.6152	0.8385	0.8396	0.084
H(8)	4*e*	0.8422	0.8241	1.0422	0.101
H(9)	4*e*	0.4823	0.6448	0.9561	0.067
H(4A)	4*e*	0.1218	0.6417	0.3284	0.087
H(10)	4*e*	0.1592	0.7452	0.4600	0.072
H(11)	4*e*	0.2676	0.5410	0.6217	0.137
H(12)	4*e*	0.1949	0.5134	0.4231	0.161
H(1A)	4*e*	0.765(6)	0.944(2)	0.711(5)	0.101
H(1B)	4*e*	0.606(2)	0.898(3)	0.653(4)	0.101

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	4*e*	0.25204(5)	0.72008(2)	0.71535(3)	0.0290(3)	0.0215(3)	0.0257(3)	0.0014(1)	0.0129(2)	−0.0002(1)
O(1)	4*e*	0.0730(4)	0.6807(2)	0.7681(2)	0.062(2)	0.041(1)	0.058(2)	−0.005(1)	0.031(1)	0.002(1)
O(2)	4*e*	0.2236(4)	0.5645(2)	0.7968(3)	0.069(2)	0.054(2)	0.091(2)	0.002(1)	0.054(2)	0.003(2)
O(3)	4*e*	−0.0446(3)	0.4862(1)	0.8267(2)	0.051(1)	0.035(1)	0.052(1)	−0.003(1)	0.032(1)	−0.002(1)
O(4)	4*e*	−0.1371(3)	0.3300(1)	0.8232(2)	0.053(1)	0.037(1)	0.055(1)	−0.001(1)	0.029(1)	−0.003(1)
O(5)	4*e*	−0.3382(4)	0.3597(2)	0.8871(3)	0.067(2)	0.047(2)	0.096(2)	−0.005(1)	0.055(2)	0.002(2)
C(1)	4*e*	0.0955(5)	0.6058(2)	0.7940(3)	0.053(2)	0.039(2)	0.045(2)	−0.004(1)	0.026(2)	−0.001(1)
C(2)	4*e*	−0.0441(5)	0.5691(2)	0.8209(3)	0.056(2)	0.034(2)	0.054(2)	−0.001(1)	0.030(2)	−0.001(1)
C(3)	4*e*	−0.1751(7)	0.5999(2)	0.8437(6)	0.086(3)	0.036(2)	0.139(5)	0.001(2)	0.082(4)	−0.003(2)
C(4)	4*e*	−0.2631(7)	0.5331(2)	0.8654(5)	0.089(3)	0.039(2)	0.141(5)	−0.001(2)	0.086(4)	−0.006(2)
C(5)	4*e*	−0.1809(5)	0.4663(2)	0.8537(3)	0.053(2)	0.039(2)	0.058(2)	−0.003(1)	0.035(2)	−0.003(2)
C(6)	4*e*	−0.2221(5)	0.3795(2)	0.8566(3)	0.045(2)	0.038(2)	0.048(2)	−0.002(1)	0.026(2)	−0.003(1)
N(1)	4*e*	0.4903(4)	0.7363(2)	0.8589(3)	0.045(2)	0.052(2)	0.048(2)	0.004(1)	0.019(1)	0.003(1)
N(2)	4*e*	0.6935(6)	0.7215(3)	1.0386(4)	0.056(2)	0.105(4)	0.050(2)	0.011(2)	0.011(2)	0.008(2)
C(7)	4*e*	0.6164(6)	0.7977(3)	0.8887(4)	0.055(2)	0.073(3)	0.068(3)	−0.011(2)	0.016(2)	0.010(2)
C(8)	4*e*	0.7423(8)	0.7901(4)	0.9999(5)	0.059(3)	0.097(4)	0.069(3)	−0.016(3)	0.008(2)	−0.001(3)
C(9)	4*e*	0.5429(6)	0.6913(3)	0.9520(3)	0.051(2)	0.062(2)	0.050(2)	0.007(2)	0.020(2)	0.005(2)
N(3)	4*e*	0.2277(5)	0.6595(2)	0.5785(3)	0.062(2)	0.046(2)	0.044(2)	0.004(1)	0.027(1)	0.002(1)
N(4)	4*e*	0.1557(7)	0.6341(2)	0.4003(3)	0.108(3)	0.068(2)	0.044(2)	−0.007(2)	0.038(2)	−0.005(2)
C(10)	4*e*	0.1775(7)	0.6902(3)	0.4766(4)	0.083(3)	0.053(2)	0.053(2)	0.000(2)	0.039(2)	0.004(2)
C(11)	4*e*	0.237(1)	0.5797(3)	0.5641(5)	0.237(9)	0.044(2)	0.067(3)	0.017(4)	0.075(5)	0.001(2)
C(12)	4*e*	0.196(2)	0.5639(4)	0.4547(5)	0.28(1)	0.060(3)	0.077(4)	0.000(5)	0.098(6)	−0.009(3)
O(1W)	4*e*	0.7188(5)	0.8969(2)	0.6978(4)	0.076(2)	0.069(2)	0.112(3)	−0.019(2)	0.047(2)	−0.016(2)

Discussion

In the past decades, the MOF materials (metal-organic framework materials) have being attracted extensive attentions due to the applications for gas absorption and catalyst reactions [1, 2]. So far, thousands of MOFs have been synthesized, which reveals the diversities of the compositions and structures. MOF is generally constructed by the means of metal ions/metal clusters as the nodes and bidentate/multi-dentate organic molecule as the linkers [3, 4].

The asymmetric unit of the title structure consists of one Mn(II) cation, one furan-2,5-dicarboxylate anion, two imidazoles and one water molecule (see the Figure). Each manganese is tetrahedrally coordinated by two carboxylate oxygens (d_{Mn1-O} of 1.997(14) Å and 1.997(3) Å) from different furan-2,5-dicarboxylate, and two imidazoles (d_{Mn1-N} of 1.984(3) Å and 1.992(3) Å).

In the title coordination polymer, an infinite chain is formed along [010] by linking the $Mn(C_3N_2H_4)_2$ entities with two bridging monodentate carboxylate groups of two crystallographically dependent furan-2,5-dicarboxylate dianions. The dihedral angle between the imidazole planes is 49.6(3)°. O_w—H···O and N_i—H···O (w = water and i = imidazole) hydrogen bonds help to establish the packing.

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References

1. Murray, L. J.; Dinca, M.; Long, J. R.: Hydrogen storage in metal-organic frameworks. Chem. Soc. Rev. **38** (2009) 1294–1314.
2. Corma, A.; Garcia, H.; Xamena, F. X. L. I.: Engineering metal organic frameworks for heterogeneous catalysis. Chem. Rev. **110** (2010) 4606–4655.
3. Tranchemontagne, D. J.; Mendoza-Cortés, J. L.; O'Keeffe, M.; Yaghi, O. M.: Secondary building units, nets and bonding in the chemistry of metal-organic frameworks. Chem. Soc. Rev. **38** (2009) 1257–1283.
4. Li, M.; Li, D.; O'Keeffe, M.; Yaghi, O. M.: Topological analysis of metal-organic frameworks with polytopic linkers and/or multiple building units and the minimal transitivity principle. Chem. Rev. **114** (2014) 1343–1370.
5. Brandenburg, K.: DIAMOND. Visual crystal structure information system. Version 3.2i. Crystal Impact, Bonn, Germany 2012.
6. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.