Crystal structure of 2-(2-methyl-5-(6-(1-methyl-5-(pyrazin-2-yl)-1*H*-1,2,4-triazol-3-yl)pyridin-2-yl)-2*H*-1,2,4-triazol-3-yl)pyrazine manganese(II) dibromide, $C_{19}H_{15}Br_2MnN_{11}$

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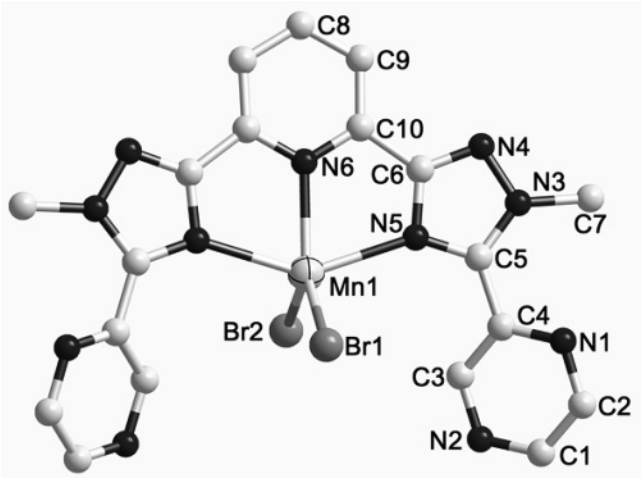

Abstract

$C_{19}H_{15}Br_2MnN_{11}$, monoclinic, $P2_1/m$ (no. 11), a = 8.442(2) Å, b = 15.478(3) Å, c = 9.266(2) Å, β = 111.54(3)°, V = 1126.3 Å^3, Z = 2, $R_{gt}(F)$ = 0.0568, $wR_{ref}(F^2)$ = 0.1554, T = 293 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.25×0.28×0.34 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	41.67 cm^{-1}
Diffractometer, scan mode:	Bruker P4, ω
$2\theta_{max}$:	50.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5701, 2167
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1719
$N(param)_{refined}$:	157
Programs:	SHELX [11]

Source of material

A mixture of 2-(2-methyl-5-(6-(1-methyl-5-(pyrazin-2-yl)-1*H*-1,2,4-triazol-3-yl)pyridin-2-yl)-2*H*-1,2,4-triazol-3-yl)pyrazine (0.05 mmol) and $MnBr_2$ (0.1 mmol) in 10 mL mixed solvent (CH_3CN/H_2O, *v*/*v*, 7:3) was placed in a 25 mL Teflon-lined stainless steel vessel, and the vessel was sealed and heated to 160 °C for 72 h. After the mixture had been cooled to room temperature over 24 h. Yellow crystals of the title complex were obtained with a yield of 74% (based on Mn).

Discussion

The construction of metal-organic frameworks (MOFs) has become an exciting and expanding approach to novel materials. The interest is stimulated not only by the MOFs' structural diversities but also by their extensive potential applications in such areas as separation, molecular recognition, ion exchange, gas sorption and storage, nonlinear optics, magnetics and catalysis [1–3]. A successful strategy in building such networks is to employ appropriate bridging ligands that can bind metal ions in different modes and provide a possible way to achieve more robust polymeric structures [4–8]. In constructing MOFs, flexible ligands are usually selected because they may act as bridging to extend the architecture to 1D chains, 2D layers and 3D networks [9, 10]. In our work, we selected 2-(2-methyl-5-(6-(1-methyl-5-(pyrazin-2-yl)-1*H*-1,2,4-triazol-3-yl)pyridin-2-yl)-2*H*-1,2,4-triazol-3-yl)-pyrazine ligand as the linker on the basis of the following considerations: (i) excellent characteristics in thermal/chemical stability and photoluminescence properties, and (ii) the heterocyclic ligand can rotate around the central C–C bond and adopt different conformations; no matter which conformation it adopts, the ligand will provide potential tridentate binding site and terminal pyrazine nitrogen atom. The asymmetric unit contains one half of a Mn(II) ion, two half Br ligands, and one half of a 2-(2-methyl-5-(6-(1-methyl-5-(pyrazin-2-yl)-1*H*-1,2,4-triazol-3-yl)pyridin-2-yl)-2*H*-1,2,4-triazol-3-yl)pyrazine ligand. The Mn(II) ion is coordinated by the central tridentate binding site of 2-(2-methyl-5-(6-(1-methyl-5-(pyrazin-2-yl)-1*H*-1,2,4-triazol-3-yl)pyridin-2-yl)-2*H*-1,2,4-triazol-3-yl)pyrazine ligand, and two bromido ligands, resulting in a $\{N_3Br_2\}$coordination environment. The Mn–N bond lengths are 2.235(6) and 2.339(4) Å, whereas the Mn–Br bond lengths are 2.4569(16) and 2.4688(15) Å, respectively. The bond angles around the Mn(II) ion vary from 72.70(10) to 145.3(2)°. Each mononuclear complex is potentially connected to adjacent complexes by weak C–H···π, C–H···N, and C–H···Br interactions.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*f*	0.0160	–0.0750	0.3003	0.064
H(2)	4*f*	0.0892	–0.1507	0.5259	0.060
H(3)	4*f*	0.3705	0.0927	0.4993	0.056
H(7A)	4*f*	0.5142	–0.1463	0.8767	0.077
H(7B)	4*f*	0.7066	–0.1412	0.9853	0.077
H(7C)	4*f*	0.6557	–0.1443	0.8048	0.077
H(8)	2*e*	1.1178	¼	1.2956	0.063
H(9)	4*f*	0.9932	0.1205	1.1876	0.056

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	2*e*	0.4862(1)	¼	0.7393(1)	0.0338(6)	0.0345(6)	0.0304(6)	0	–0.0002(5)	0
Br(1)	2*e*	0.1880(1)	¼	0.7239(1)	0.0396(5)	0.0534(6)	0.0725(7)	0	0.0052(4)	0
Br(2)	2*e*	0.5332(2)	¼	0.4929(1)	0.0915(8)	0.0577(7)	0.0593(6)	0	0.0341(6)	0
N(1)	4*f*	0.2777(6)	–0.0763(3)	0.6523(6)	0.052(3)	0.037(3)	0.048(3)	–0.002(2)	0.014(2)	–0.003(2)
N(2)	4*f*	0.1845(6)	0.0167(3)	0.3742(6)	0.049(3)	0.050(3)	0.043(3)	–0.001(2)	–0.001(2)	–0.001(2)
N(3)	4*f*	0.6145(6)	–0.0282(3)	0.8816(5)	0.045(3)	0.034(2)	0.036(2)	0.005(2)	0.010(2)	0.002(2)
N(4)	4*f*	0.7394(6)	0.0179(3)	0.9869(5)	0.040(3)	0.040(3)	0.034(2)	0.005(2)	0.004(2)	0.002(2)
N(5)	4*f*	0.5551(5)	0.1058(3)	0.8099(5)	0.032(2)	0.032(2)	0.034(2)	0.003(2)	0.004(2)	0.002(2)
N(6)	2*e*	0.7197(8)	¼	0.9554(7)	0.035(3)	0.030(3)	0.035(3)	0	0.000(3)	0
C(1)	4*f*	0.1053(8)	–0.0549(4)	0.3869(7)	0.045(3)	0.056(4)	0.046(3)	0.002(3)	0.001(3)	–0.014(3)
C(2)	4*f*	0.1499(8)	–0.1009(4)	0.5234(7)	0.051(4)	0.042(3)	0.055(4)	–0.009(3)	0.017(3)	–0.010(3)
C(3)	4*f*	0.3117(7)	0.0423(4)	0.5025(7)	0.041(3)	0.041(3)	0.049(3)	0.002(3)	0.005(3)	0.003(3)
C(4)	4*f*	0.3588(6)	–0.0037(3)	0.6402(6)	0.037(3)	0.033(3)	0.035(3)	0.004(2)	0.009(2)	–0.005(2)
C(5)	4*f*	0.5045(6)	0.0246(3)	0.7754(6)	0.037(3)	0.033(3)	0.035(3)	0.002(2)	0.011(2)	0.002(2)
C(6)	4*f*	0.6986(7)	0.0980(3)	0.9399(6)	0.034(3)	0.036(3)	0.033(3)	0.003(2)	0.003(2)	0.000(2)
C(7)	4*f*	0.6236(8)	–0.1233(4)	0.8876(7)	0.062(4)	0.031(3)	0.050(4)	0.013(3)	0.008(3)	0.004(3)
C(8)	2*e*	1.017(1)	¼	1.209(1)	0.033(4)	0.059(6)	0.043(5)	0	–0.010(4)	0
C(9)	4*f*	0.9431(7)	0.1729(4)	1.1458(6)	0.037(3)	0.048(4)	0.041(3)	0.004(3)	–0.003(2)	0.009(3)
C(10)	4*f*	0.7925(6)	0.1752(4)	1.0187(6)	0.036(3)	0.040(3)	0.035(3)	0.000(2)	0.006(2)	0.000(2)

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