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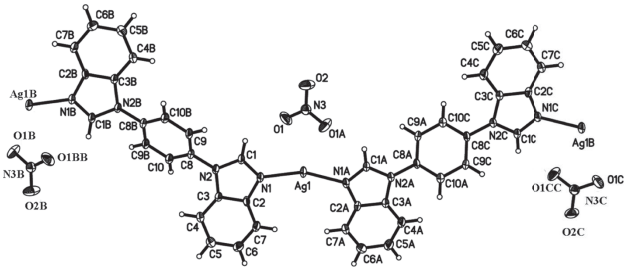
The crystal structure of catena-poly[(μ_2-1,1′-benzene-1,4-diylbis(1*H*-benzimidazole-κ^2N:*N*′) silver(I)] nitrate, $C_{20}H_{14}N_5AgO_3$



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Abstract

$C_{20}H_{14}N_5O_3Ag$, monoclinic, $C2/c$ (no. 15), $a = 17.501$ Å, $b = 9.896$ Å, $c = 12.768$ Å, $\beta = 124.84°$, $V = 1814.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0484$, $wR_{ref}(F^2) = 0.1042$, $T = 293$ 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.

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.170×0.180×0.200 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.45 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ and ω scans
$2\theta_{max}$:	54.97°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9363, 2065
$N(param)_{refined}$:	133
Programs:	Bruker programs [8], SHELXTL [9, 10]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(10)	8*f*	0.8118	0.0432	0.5979	0.046
H(9)	8*f*	0.6181	0.3326	0.4795	0.046
H(1)	8*f*	0.6255	0.2466	0.6664	0.046
H(7)	8*f*	0.5481	−0.2027	0.7004	0.051
H(5)	8*f*	0.6599	−0.3473	0.5226	0.062
H(4)	8*f*	0.7033	−0.1317	0.5029	0.053
H(6)	8*f*	0.5871	−0.3826	0.6243	0.061

Source of material

The title complex was synthesized from a mixture of $AgNO_3$ (0.169 g, 1 mmol), 1,4-bis(benzoimidazo-1-yl)benzene and deionized (0.310 g, 1 mmol) water (8 mL), which was sealed under reaction kettle and heated to 120 °C for 3 days, followed by cooling to roomtemperature at 25 °C/h. The solid products were recovered by filtration and washed with distilled water. Colourless block-shaped, crystals which were suitable for X-ray diffraction analysis were obtained. The product was stable in air and common organic solvents. The yield of the compound was about 62% based on silver.

Experimental details

H atoms were placed in geometrically idealized positions with Csp^2—H = 0.93 Å.

Discussion

In recent dacades, the rational design and synthesis of cationic metal-organic frameworks (CMOFs) have attracted sigificant interests due to their intriguing structures and potential application in many fields, such as nonlinear optics, magnetism, catalyst, adsorption, ion exchange, luminescence and drug deliver [1–5]. The common strategy to synthesize the CMOFs is to select a pyridine/imidazole and other N-donor ligands to react with a metal salt. Use some positive methods to control the anion from metal salt or solvent

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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}
Ag(1)	4*e*	0.5	0.10666(5)	0.75	0.0579(3)	0.0474(3)	0.0656(4)	0.0	0.0545(3)	0.0
N(2)	8*f*	0.6636(2)	0.1012(3)	0.5934(3)	0.043(2)	0.036(2)	0.046(2)	0.001(2)	0.037(2)	0.004(2)
C(10)	8*f*	0.7869(3)	0.1260(4)	0.5583(4)	0.041(2)	0.040(2)	0.049(2)	0.000(2)	0.034(2)	0.002(2)
N(1)	8*f*	0.5883(2)	0.0644(3)	0.6855(3)	0.049(2)	0.039(2)	0.046(2)	−0.001(2)	0.040(2)	0.001(2)
C(8)	8*f*	0.7072(3)	0.1755(4)	0.5449(4)	0.037(2)	0.038(2)	0.040(2)	−0.004(2)	0.032(2)	0.000(2)
C(9)	8*f*	0.6709(3)	0.2993(4)	0.4875(4)	0.041(2)	0.041(2)	0.054(3)	0.003(2)	0.039(2)	0.002(2)
C(2)	8*f*	0.6037(3)	−0.0603(4)	0.6490(4)	0.036(2)	0.039(2)	0.036(2)	0.002(2)	0.029(2)	−0.000(2)
C(1)	8*f*	0.6254(3)	0.1545(4)	0.6517(4)	0.047(3)	0.038(2)	0.053(3)	0.002(2)	0.042(2)	0.002(2)
C(7)	8*f*	0.5792(3)	−0.1887(4)	0.6616(4)	0.052(3)	0.043(2)	0.054(3)	−0.001(2)	0.043(2)	0.005(2)
C(3)	8*f*	0.6512(3)	−0.0401(4)	0.5913(4)	0.036(2)	0.034(2)	0.042(2)	−0.000(2)	0.030(2)	0.001(2)
C(5)	8*f*	0.6470(3)	−0.2735(5)	0.5551(5)	0.061(3)	0.044(3)	0.070(3)	0.001(2)	0.049(3)	−0.008(2)
C(4)	8*f*	0.6729(3)	−0.1456(4)	0.5424(4)	0.054(3)	0.043(2)	0.057(3)	−0.001(2)	0.045(3)	−0.005(2)
C(6)	8*f*	0.6019(3)	−0.2950(4)	0.6154(5)	0.061(3)	0.036(2)	0.071(3)	−0.002(2)	0.046(3)	0.004(2)
N(3)	4*e*	0.5	0.4276(5)	0.75	0.045(3)	0.042(3)	0.041(3)	0.0	0.026(3)	0.0
O(1)	8*f*	0.5645(3)	0.3653(4)	0.7572(4)	0.071(3)	0.070(2)	0.097(3)	0.011(2)	0.057(2)	−0.021(2)
O(2)	4*e*	0.5	0.5514(5)	0.75	0.054(3)	0.035(3)	0.136(5)	0.0	0.047(4)	0.0

and other kinds atoms like O/ F/ Cl do not coordinate with metals and then the whole structure may be constructed as a new CMOFs. As a result, we choose 1,4-bis(benzoimidazo-1-yl)benzene and Ag to constructed a new CMOFs. Fortunately, controlling serial reaction factors, we succeed to construct the title compound. The asymmetric unit contains one half of a Ag(I)ion, one half of a 1,4-bis(benzoimidazo-1-yl)benzene molecule and one half of a nitrate anion. Ag(I) is typically two-coordinated by two N atoms from two organic ligands. The bond length of Ag-N is 2.138(3) Å and the angle of N1A-Ag-N1 is 157.7(2)°, which is similar to those in reported Ag(I) complexes [6, 7].

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