Crystal structure of poly[(μ₂-5-bromoisophthalato-κ⁴O,O':O'',O''')-(μ₂-1,4-bis(2-methylimidazol-1-ylmethyl)benzene-N:N')cadmium(II)], C_{24}H_{21}BrCdN_{4}O_{4}

Abstract

C_{24}H_{21}BrCdN_{4}O_{4}, orthorhombic, Pnna (no. 52), a = 7.4860(5) Å, b = 17.7424(13) Å, c = 17.2241(12) Å, V = 2,287.7(3) Å³, Z = 4, R_{gt}(F) = 0.0363, wR_{ref}(F^2) = 0.0866, T = 296(2) K.

CCDC no.: 2360971

The molecular structure is shown in the Figure 1. Table 1 contains crystallographic data and Table 2 contains the list of

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Colorless block</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.20 x 0.15 x 0.10 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>Mo Kα radiation (0.71073 Å)</td>
</tr>
<tr>
<td>μ:</td>
<td>2.74 mm⁻¹</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>Bruker APEX-II, φ and ω</td>
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<tr>
<td>θ_{max}, completeness:</td>
<td>27.5°, &gt;99 %</td>
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<tr>
<td>N(hklo)measured-N(hklo)unique, R_measured:</td>
<td>11,540, 2,646, 0.063</td>
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<tr>
<td>Criterion for I_{obs}, N(hklo)_gt:</td>
<td>I_{obs} &gt; 2σ(I_{obs}), 1.865</td>
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<tr>
<td>N[param]refined:</td>
<td>157</td>
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<td>Programs:</td>
<td>Bruker</td>
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</table>

1 Source of materials

A mixture of cadmium nitrate hexahydrate (30.8 mg, 0.1 mmol), 5-bromoisophthalic acid(5-Brip) (24.0 mg, 0.1 mmol), 1,4-bis(2-methylimidazol-1-ylmethyl)benzene (bmimb) (15.0 mg, 0.05 mmol), and KOH (11.0 mg, 0.2 mmol) was added to 10 mL H₂O, stirred to form a clear
solution. The mixture was heated in an oven at 413 K for 72 h. Many colorless crystals were filtered, washed with distilled water, and dried in air. Yield: 24.5% (based on 5-bromoxyisophthalic acid).

2 Experimental details

The structure was solved by Direct Methods with the SHELXS-2018 program. All H-atoms from C atoms were positioned with idealized geometry and refined isotropic using a riding model with C–H = 0.93–0.97 Å. Their $U_{iso}$ values were set to 1.2$U_{eq}$ or 1.5$U_{eq}$ of the parent atoms.

3 Comment

The flexible bis(imidazole) bidentate ligands can adopt the coordinated nitrogen atom(s) for the fabrication of highly connected CPs. And the aromatic multicarboxylate ligands play an important role in tuning the coordination framework structures, which satisfy the geometric requirement of metal centers leading to fascinating structural architectures through different coordination modes. To date, there is only one complex about the study of cadmium MOFs based on 1,4-bis(2-methylimidazol-1-ylmethyl)benzene with 5-substituted isophthalate. Single-crystal X-ray structural analysis displays that the asymmetric unit consists of half a Cd(II) ion, half a 5-Brip$^2$ anion and half a bmimb co-ligand. Each Cd(II) atom is coordinated with four oxygen atoms from two 5-Brip$^2$ ligands, two nitrogen atom from two different bmimb ligands, which forms a distorted octahedral CdO$_4$N$_2$ coordination geometry. The molecular structure is presented in the Figure. The Cd–O and Cd–N lengths are 2.297(3)–2.424(3) Å and 2.287(3) Å, respectively. In the title compound, the 5-Brip$^2$ ligand serves as a μ$_2$-bridge linking two adjacent Cd$^{2+}$ ions to give rise to a one-dimensional chain, while such one-dimensional chains are further bridged by bmimb ligands into a three-dimensional three-fold interpenetrated network structure, which is different to the reported [Cd$_2$(Tcph)$_2$(4,4-bmimb)$_0.5$(H$_2$O)$_4$]$_n$ and [Cd(bmimb)$_2$(nec)$_1$.5H$_2$O]$_{10}$.$^5$.$^1$

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References


