Ning Ling, Xia Wang, Ya-Wen Zhang, Tian-Tian Zhao, Yuan Ruan and Jing Yang*

Crystal structure of dimethanol-bis(1-((2-methyl-1H-benzo[d]imidazol-1-yl)methyl)-1H-benzo[d][1,2,3]triazole-κN)-bis(thiocyanato-κN) cadmium(II) \( \text{C}_{34}\text{H}_{34}\text{CdN}_{12}\text{O}_{2}\text{S}_{2} \)

Abstract

\( \text{C}_{34}\text{H}_{34}\text{CdN}_{12}\text{O}_{2}\text{S}_{2}, \text{triclinic, } P\bar{1}, \ a = 9.6872(6) \AA, \)
\( b = 10.6523(7) \AA, \ c = 10.8422(9) \AA, \ a = 113.022(7)^\circ, \)
\( \beta = 96.919(6)^\circ, \ \gamma = 104.526(6)^\circ, \ Z = 1, \ V = 948.20(13) \AA^3, \)
\( R_{gt}(F) = 0.0564, \ wR_{ref}(F^2) = 0.1511, \ T = 293(2) \text{ K}. \)

CCDC no.: 1905432

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All starting materials are commercially available, and are used without further purification. 1-[(2-methyl-1H-benzoimidazol-1-yl)methyl]-1H-benzotriazole (L) was prepared according to the literature method [3]. The ligand L (0.02 mmol, 0.0053 g) in methanol (6 mL) was added dropwise to a methanol solution (6 mL) of \( \text{Cd(NO}_{3}\text{)}_{2} \) (0.02 mmol, 0.0047 g). Then an aqueous solution (2 mL) of KSCN (0.02 mmol, 0.0019 g) was added dropwise. The resulting solution was allowed to stand at room temperature. After 2 weeks colorless crystals were obtained.

Experimental details

H atoms were generated geometrically with C—H = 0.93 Å and \( U_{eq}(C) \) for aromatic H atoms, with C—H = 0.97 Å and \( U_{eq}(C) \) for methylene H atoms, and with C—H = 0.96 Å and \( U_{eq}(C) \) for methyl H atoms.

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Plate, colorless</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.33 × 0.21 × 0.09 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>Cu Ka radiation (1.54184 Å)</td>
</tr>
<tr>
<td>µ:</td>
<td>0.5 mm⁻¹</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>Xcalibur, ω-scans</td>
</tr>
<tr>
<td>θmax, completeness:</td>
<td>67.1°, &gt;99%</td>
</tr>
<tr>
<td>N(hkl)measured, N(hkl)unique, Rint:</td>
<td>6842, 3378, 0.043</td>
</tr>
<tr>
<td>Criterion for Iobs, N(hkl)gt:</td>
<td>Iobs &gt; 2σ(Iobs), 3129</td>
</tr>
<tr>
<td>N(param)refined:</td>
<td>137</td>
</tr>
<tr>
<td>Programs:</td>
<td>CrysAlisPRO [1], SHELX [2]</td>
</tr>
</tbody>
</table>

Comment

N-Heterocyclic organic compounds such as benzimidazole and benzotriazole are extensively used as ligands and crystal engineering [4–6]. The incorporation of benzotriazole and benzimidazole is an interesting strategy for the design of novel drug candidate molecules [7]. In addition, Cd ion is easy to coordinate to N/O-containing ligands and Cd(II)-containing coordination polymers have attracted
considerable recent interest owing to its various coordination modes and special physical properties [8].

The title compound contains a mononuclear complex. As is shown in the figure, the Cd(II) atom is six-coordinated by two N atoms from two crystallographically dependent ligands L, two O atoms from two methanol molecules and two crystallographically dependent thiocyanato ligands in a distorted octahedral geometry (with the Cd1–N1 bond length of 2.399(4) Å, the Cd1–N6 bond length of 2.249(4) Å, and the Cd1–O1 bond lengths of 2.386(4) Å). The bond angles around Cd(II) ion range from 87.01(16) to 180°. Adjacent molecules are linked through O—H⋯N hydrogen bonds (with the bond length of 1.98(3) Å) involving N5 and the coordinated methanol molecules. In addition, the benzotriazole rings in adjacent molecules are parallel, with a centroid-centroid distance of 3.707 Å. Thus π–π interactions are not to be ruled out [9]. Bond lengths and angles are in accord with related structures [5].

Acknowledgements: This work was financially supported by the Science and Technology Department of Henan Province (no. 182102310315) and the Foundation for Henan Provincial Institute of Henan University of Chinese Medicine (2014KYWWF-QN11).

References