Crystal structure of *catena*-(acetato-*O*,*O*′)(bromo)-[μ-1,1′-(1,4-butanediyl)bis(benzimidazole)-*N*:*N*′]cadmium(II), $CdBr(C_2H_3O_2)(C_{18}H_{18}N_2)$

Jian-Hua Qin*,[I] and Xiang-Dong Han[II]

[I] Luoyang Normal University, College of Chemistry and Chemical Engineering, Luoyang 471022, Henan, P. R. China
[II] Luoyang City Environmental Monitoring Station, Luoyang 471000, Henan, P. R. China

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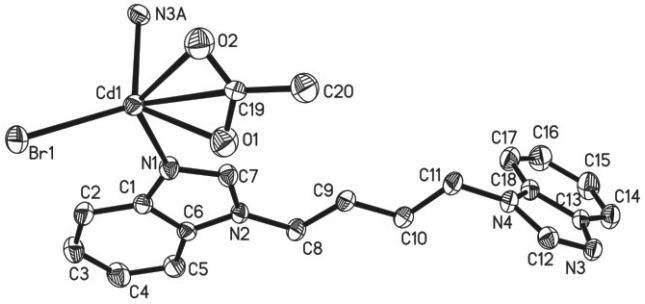

Abstract

$C_{20}H_{21}BrCdN_4O_2$, monoclinic, $P12_1/c1$ (no. 14), a = 10.253(3) Å, b = 14.323(4) Å, c = 17.137(4) Å, β = 124.29(1)°, V = 2079.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.032, $wR_{ref}(F^2)$ = 0.079, T = 296 K.

Source of material

A mixture of 1,1′-(1,4-butanediyl)bis(benzimidazole) (0.1 mmol), $CdBr_2 \cdot 4H_2O$ (0.1 mmol) and acetic acid (0.1 mmol) in distilled water (15 mL) was placed in a Teflon-lined stainless steel vessel, heated to 120 °C for 3 days, and then cooled to room temperature over 24 h. Colorless block-shaped crystals of the title complex were obtained.

Discussion

In recent years, there has been great interest in the construction of metal-organic frameworks (MOFs) due to their interesting magnetic, electronic, nonlinear optical properties and intriguing structural motifs varying from extended coordination polymers to discrete molecular entities such as cages or metallomacrocycles [1-6]. Among the distinct factors involved in the syntheses of complexes, ligand design is often a useful way of manipulating the overall resulting frameworks. In particular, the uses of flexible ligands have attracted remarkable attention because their conformations are expected to produce many intriguing architectures. Bis(imidazole) ligands are excellent candidates for the construction of extended architectures and supramolecular architectures [7-10]. 1,1′-(1,4-butanediyl)bis(benzimidazole) (bbim), bearing a longer methylene (-CH_2-)$_4$ skeleton, is a good candidate for N-donor linkers. To further understand the coordination chemistry of nonrigid long-chain linear spacers, we here report on a new complex with the flexible ligand bbim.

In the title crystal structure, the asymmetric unit consists of one Cd^{2+} ion, one 1,1′-(1,4-butanediyl)bis(benzimidazole) (bbim) ligand, one Br^- anion and one acetate anion. The Cd^{2+} ion is five-coordinated in a distorted square-pyramidal arrangement (CdN_2O_2Br) defined by two oxygen atoms from one acetate anion, two nitrogen atoms from two bbim ligands and one Br^- anion. The Cd^{2+} ion deviates from the mean plane of the basal atoms towards the Br^- anion by 0.95 Å. Each *trans*-bbim ligand links two Cd^{2+} ions by its aromatic nitrogen atoms acting as a bridging bidentate ligand. Thus, the neighboring Cd^{2+} ions are bridged into a chain, with the bridged Cd···Cd distance of 12.902(3) Å. These chains are further interconnected by C–H···O hydrogen bonds and weak C–H···π interactions to generate a three-dimensional supramolecular structure .

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.13 × 0.14 × 0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	29.95 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11907, 3843
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2960
$N(param)_{refined}$:	254
Programs:	SHELXS-97, SHELXL-97, SHELXTL [11]

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

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.7877	0.2551	0.2396	0.052
H(3)	4*e*	0.5770	0.1856	0.2313	0.064
H(4)	4*e*	0.3454	0.2668	0.1760	0.068
H(5)	4*e*	0.3154	0.4198	0.1253	0.059
H(7)	4*e*	0.7467	0.5700	0.1365	0.046
H(8A)	4*e*	0.4098	0.6051	0.1315	0.051
H(8B)	4*e*	0.3455	0.5714	0.0288	0.051
H(9A)	4*e*	0.5318	0.6647	0.0285	0.052
H(9B)	4*e*	0.5958	0.6984	0.1311	0.052
H(10A)	4*e*	0.2918	0.7416	–0.0301	0.053
H(10B)	4*e*	0.3495	0.7721	0.0727	0.053
H(11A)	4*e*	0.5460	0.8652	0.0846	0.060
H(11B)	4*e*	0.5040	0.8296	–0.0135	0.060
H(12)	4*e*	0.2985	0.9174	–0.1566	0.052
H(14)	4*e*	0.0207	1.1422	–0.0981	0.064
H(15)	4*e*	0.0654	1.1531	0.0497	0.079
H(16)	4*e*	0.2490	1.0583	0.1718	0.080
H(17)	4*e*	0.3883	0.9477	0.1504	0.072
H(20A)	4*e*	1.1245	0.6872	0.0903	0.086
H(20B)	4*e*	0.9402	0.6773	0.0281	0.086
H(20C)	4*e*	1.0414	0.6245	–0.0004	0.086

* Correspondence author (e-mail: jh_q128105@126.com)

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}
Cd(1)	4*e*	1.02754(3)	0.42454(2)	0.21134(2)	0.0321(2)	0.0372(2)	0.0368(2)	0.0022(1)	0.0173(1)	–0.0014(1)
Br(1)	4*e*	1.07223(5)	0.24973(3)	0.21288(4)	0.0516(3)	0.0409(3)	0.0675(3)	0.0100(2)	0.0296(2)	–0.0036(2)
O(1)	4*e*	0.9257(4)	0.5207(2)	0.0837(2)	0.062(2)	0.063(2)	0.066(2)	–0.002(2)	0.038(2)	0.013(2)
O(2)	4*e*	1.1776(4)	0.5392(2)	0.1787(2)	0.069(2)	0.066(2)	0.061(2)	0.000(2)	0.037(2)	0.007(2)
N(1)	4*e*	0.7809(4)	0.4383(2)	0.1818(2)	0.035(2)	0.036(2)	0.052(2)	0.005(1)	0.027(2)	0.004(2)
N(2)	4*e*	0.5563(3)	0.5159(2)	0.1268(2)	0.033(2)	0.030(2)	0.043(2)	0.006(1)	0.020(2)	0.001(1)
N(3)	4*e*	0.1739(4)	1.0146(2)	–0.1427(2)	0.044(2)	0.035(2)	0.037(2)	0.007(2)	0.021(2)	0.005(2)
N(4)	4*e*	0.3485(4)	0.9226(2)	–0.0247(2)	0.042(2)	0.037(2)	0.043(2)	0.006(2)	0.018(2)	0.010(2)
C(1)	4*e*	0.6764(4)	0.3797(3)	0.1855(3)	0.033(2)	0.035(2)	0.037(2)	0.001(2)	0.020(2)	–0.002(2)
C(2)	4*e*	0.6943(5)	0.2877(3)	0.2165(3)	0.041(2)	0.040(2)	0.048(3)	0.008(2)	0.025(2)	0.006(2)
C(3)	4*e*	0.5687(5)	0.2471(3)	0.2117(3)	0.061(3)	0.039(2)	0.066(3)	0.002(2)	0.039(3)	0.008(2)
C(4)	4*e*	0.4277(5)	0.2965(3)	0.1779(4)	0.052(3)	0.050(3)	0.076(4)	–0.008(2)	0.040(3)	0.000(2)
C(5)	4*e*	0.4085(5)	0.3872(3)	0.1475(3)	0.036(2)	0.046(2)	0.064(3)	0.001(2)	0.028(2)	–0.001(2)
C(6)	4*e*	0.5346(4)	0.4275(2)	0.1517(3)	0.035(2)	0.034(2)	0.034(2)	–0.000(2)	0.018(2)	–0.004(2)
C(7)	4*e*	0.7038(4)	0.5180(3)	0.1466(3)	0.037(2)	0.033(2)	0.049(3)	0.003(2)	0.026(2)	0.002(2)
C(8)	4*e*	0.4394(4)	0.5916(3)	0.0880(3)	0.035(2)	0.039(2)	0.051(3)	0.011(2)	0.022(2)	0.003(2)
C(9)	4*e*	0.5016(5)	0.6787(3)	0.0717(3)	0.035(2)	0.039(2)	0.045(3)	0.008(2)	0.015(2)	0.003(2)
C(10)	4*e*	0.3838(5)	0.7589(3)	0.0314(3)	0.036(2)	0.040(2)	0.046(3)	0.007(2)	0.017(2)	0.004(2)
C(11)	4*e*	0.4599(5)	0.8453(3)	0.0222(3)	0.038(2)	0.044(2)	0.054(3)	0.009(2)	0.016(2)	0.013(2)
C(12)	4*e*	0.2772(5)	0.9462(3)	–0.1163(3)	0.045(2)	0.038(2)	0.046(3)	0.002(2)	0.026(2)	0.001(2)
C(13)	4*e*	0.1777(5)	1.0368(3)	–0.0629(3)	0.046(2)	0.032(2)	0.036(2)	–0.001(2)	0.020(2)	0.004(2)
C(14)	4*e*	0.0935(6)	1.1033(3)	–0.0492(3)	0.068(3)	0.042(2)	0.048(3)	0.012(2)	0.032(3)	0.006(2)
C(15)	4*e*	0.1211(7)	1.1097(3)	0.0389(4)	0.096(4)	0.051(3)	0.062(4)	0.012(3)	0.052(3)	–0.001(3)
C(16)	4*e*	0.2319(7)	1.0518(3)	0.1128(4)	0.096(4)	0.061(3)	0.043(3)	0.002(3)	0.038(3)	–0.002(2)
C(17)	4*e*	0.3157(6)	0.9862(3)	0.1010(3)	0.073(3)	0.050(3)	0.042(3)	0.005(2)	0.024(3)	0.008(2)
C(18)	4*e*	0.2879(5)	0.9795(3)	0.0122(3)	0.048(2)	0.034(2)	0.039(3)	0.001(2)	0.022(2)	0.003(2)
C(19)	4*e*	1.0512(4)	0.5604(2)	0.1113(3)	0.027(2)	0.031(2)	0.030(2)	–0.002(2)	0.020(2)	–0.005(2)
C(20)	4*e*	1.0381(5)	0.6454(3)	0.0517(3)	0.059(3)	0.055(3)	0.060(3)	–0.003(2)	0.034(3)	0.005(2)

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