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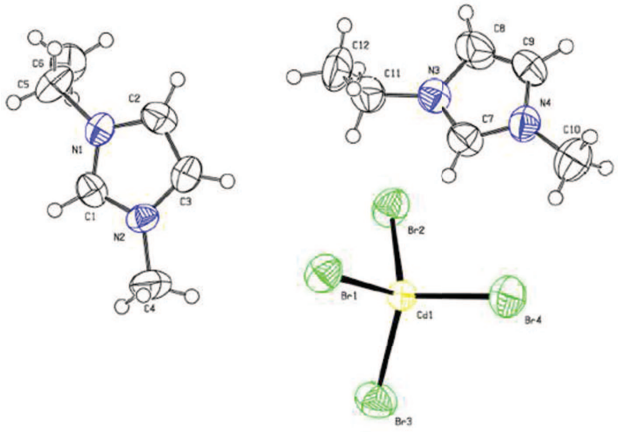
Crystal structure of bis(1-ethyl-3-methylimidazolium) tetrabromidocadmate(II), $[C_6H_{11}N_2]_2[CdBr_4]$



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Abstract

$(C_6H_{11}N_2)_2[CdBr_4]$, monoclinic, $P2_1/c$, $a = 13.8943(17)$ Å, $b = 10.2820(13)$ Å, $c = 14.7986(18)$ Å, $\beta = 94.241(3)°$, $V = 2108.4(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0477$, $wR_{ref}(F^2) = 0.1332$, $T = 273$ 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.

Source of material

All the reagents and solvents were commercially available and used as purchased. A mixture of $CdCl_2{\cdot}2.5\ H_2O$ (0.129 g, 0.56 mmol) and excessive amount of 1-ethyl-3-methylimidazolium bromide (0.5 g, 2.6 mmol) was placed in a Teflon-lined stainless vessel and heated to 433 K for 72 h. After cooling to room temperature, the colorless crystals were obtained (yield, 76% based on cadmium). Elemental analysis-found: C, 21.99%; H, 3.38%; N, 8.57%; calc. for $C_{12}H_{22}Br_4\ N_4Cd$: C, 22.02%; H, 3.39%; N, 8.56%.

Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.20×0.28×0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	86.15 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	50.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10279, 3719
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2332
$N(param)_{refined}$:	194
Programs:	SHELX [10]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.5545	0.6828	0.7910	0.060
H(2)	4e	0.3394	0.6765	0.9491	0.070
H(3)	4e	0.2899	0.5555	0.8084	0.067
H(4A)	4e	0.3994	0.6124	0.6348	0.120
H(4B)	4e	0.3882	0.4714	0.6728	0.120
H(4C)	4e	0.4913	0.5302	0.6649	0.120
H(5A)	4e	0.4960	0.8371	0.9907	0.078
H(5B)	4e	0.5857	0.8067	0.9357	0.078
H(6A)	4e	0.5145	0.6416	1.0679	0.100
H(6B)	4e	0.6146	0.7125	1.0766	0.100
H(6C)	4e	0.5966	0.5984	1.0072	0.100
H(7)	4e	0.0380	0.2369	0.8482	0.068
H(8)	4e	0.0417	0.2331	1.1133	0.092
H(9)	4e	−0.1008	0.1248	1.0555	0.087
H(10A)	4e	−0.1931	0.1654	0.8733	0.132
H(10B)	4e	−0.1457	0.0270	0.8759	0.132
H(10C)	4e	−0.1165	0.1298	0.8047	0.132
H(11A)	4e	0.2010	0.3118	1.0399	0.082
H(11B)	4e	0.2009	0.3041	0.9340	0.082
H(12A)	4e	0.0973	0.4874	0.9285	0.123
H(12B)	4e	0.2036	0.5153	0.9666	0.123
H(12C)	4e	0.1216	0.5007	1.0332	0.123

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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}
Cd(1)	4*e*	0.23815(4)	0.02440(6)	0.76994(4)	0.0447(4)	0.0460(4)	0.0441(4)	−0.0031(3)	0.0043(3)	−0.0014(3)
Br(1)	4*e*	0.24952(7)	0.27167(9)	0.73408(7)	0.0767(7)	0.0542(6)	0.0674(7)	−0.0007(5)	−0.0013(5)	0.0029(5)
Br(2)	4*e*	0.29923(8)	−0.0051(1)	0.93678(7)	0.0726(7)	0.0681(6)	0.0593(6)	−0.0079(5)	−0.0107(5)	0.0051(5)
Br(3)	4*e*	0.34387(8)	−0.0996(1)	0.66475(7)	0.0841(8)	0.0698(7)	0.0779(8)	0.0114(6)	0.0252(6)	−0.0058(6)
Br(4)	4*e*	0.06126(8)	−0.0379(1)	0.74107(8)	0.0652(8)	0.121(1)	0.0850(8)	−0.0236(7)	0.0023(6)	−0.0171(7)
N(1)	4*e*	0.4682(5)	0.7040(6)	0.8930(5)	0.043(4)	0.042(4)	0.050(5)	−0.002(3)	−0.005(3)	−0.001(3)
N(2)	4*e*	0.4249(5)	0.6018(6)	0.7691(4)	0.056(5)	0.037(4)	0.041(4)	0.002(3)	0.003(4)	−0.003(3)
N(3)	4*e*	0.0730(5)	0.2572(7)	0.9799(5)	0.049(5)	0.057(4)	0.056(5)	0.004(4)	0.003(4)	0.001(4)
N(4)	4*e*	−0.0587(5)	0.1645(7)	0.9290(5)	0.047(5)	0.051(4)	0.070(6)	−0.002(4)	0.004(4)	−0.006(4)
C(1)	4*e*	0.4947(6)	0.6660(8)	0.8129(6)	0.046(5)	0.055(5)	0.050(6)	0.000(4)	0.007(4)	0.010(5)
C(2)	4*e*	0.3766(7)	0.6626(9)	0.9003(6)	0.061(7)	0.069(6)	0.047(6)	0.002(5)	0.011(5)	0.003(5)
C(3)	4*e*	0.3489(7)	0.5962(8)	0.8223(6)	0.048(6)	0.056(5)	0.061(6)	−0.007(5)	−0.008(5)	−0.003(5)
C(4)	4*e*	0.4260(8)	0.550(1)	0.6776(6)	0.111(9)	0.083(7)	0.048(6)	−0.015(7)	0.018(6)	−0.018(5)
C(5)	4*e*	0.5312(7)	0.7680(9)	0.9630(6)	0.076(7)	0.056(6)	0.061(6)	−0.005(5)	−0.019(5)	−0.012(5)
C(6)	4*e*	0.5676(7)	0.6712(9)	1.0354(6)	0.069(7)	0.074(7)	0.054(6)	−0.009(5)	−0.008(5)	0.012(5)
C(7)	4*e*	0.0213(7)	0.2227(9)	0.9071(6)	0.049(6)	0.076(7)	0.045(6)	0.004(5)	−0.001(5)	0.006(5)
C(8)	4*e*	0.0228(8)	0.219(1)	1.0525(7)	0.082(8)	0.101(9)	0.048(6)	−0.010(7)	0.008(6)	0.016(6)
C(9)	4*e*	−0.0548(8)	0.162(1)	1.0210(7)	0.078(8)	0.084(7)	0.057(7)	−0.019(6)	0.024(6)	0.006(6)
C(10)	4*e*	−0.1349(7)	0.118(1)	0.8654(7)	0.064(7)	0.115(9)	0.083(8)	−0.022(7)	−0.015(6)	−0.014(7)
C(11)	4*e*	0.1635(7)	0.331(1)	0.9836(7)	0.054(6)	0.087(8)	0.063(7)	−0.008(5)	0.006(5)	−0.005(6)
C(12)	4*e*	0.1449(8)	0.471(1)	0.9774(8)	0.065(7)	0.092(8)	0.088(8)	−0.034(6)	−0.008(6)	−0.008(7)

Discussion

Room temperature ionic liquids have attracted attention due to their interesting and useful physicochemical properties such as high thermal and chemical stability, negligible vapor pressures and extended electrochemical windows. Particularly, ionic liquids composed of or containing transition metal ions are of great interest regarding their potential catalytic applications [1–5]. So far, some solid-state studies have examined the influence of the cation and anion structures and interionic interactions on the behavior of metal containing ion liquids, such as [EMIM] $[AlCl_4]$ [6, 7], [EMIM]$[AuCl_4]$ [8], $[EMIM]_2$ $[MCl_4]$ [9] $M = Ni^{2+}$, Co^{2+} (EMIM = 1-ethyl-3-methylimidazolium). The structure of title compound contains two crystallographically independent $[EMIM]^+$ cations and one $[CdBr_4]^{2-}$ anion. $[CdBr_4]^{2-}$ is approximately tetrahedral with Cd-Br bond lengths in the range of 0.25452(1)–0.26044(1) nm. No obvious strong hydrogen bonds exist, except for some weak C–H$\cdots$Br interactions between imidazolium-bound H atoms and Br atoms. These interactions, although relatively weak, seem to direct the orientation between ions and might govern the overall assembly.

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