Xiao-jing Liu, E. Liu, Ze-shen Jin, Zhuang-yu Li, Fang-fang Jian* and Tong-ling Liang

Crystal structure of dichlorido-bis(1-hexyl-1*H*-benzotriazole-*k*¹*N*)zinc(II), C₂₄H₃₄N₆Cl₂Zn

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.30 × 0.29 × 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.11 mm ⁻¹
Diffractometer, scan mode:	Enraf-Nonius CAD-4, ω
$\theta_{\max}$, completeness:	28.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	17,642, 6715, 0.026
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4725
$N(\text{param})_{\text{refined}}$:	357
Programs:	CAD-4 [1,2], Olex2 [3]

Source of material

1-Hexyl-1*H* benzotriazole (2.03 g, 0.01 mol) and zinc chloride (0.6815 g, 0.005 mol) were added into 30 ml ethanol and refluxed for 2 h, and then evaporated to obtain a white solid. Then, it was recrystallized from acetonitrile to obtain colorless transparent crystal.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Ionic liquids have shown good application prospects in organic synthesis [4], organic catalysis [5], solar cell preparation [6], electrochemistry [7], analytical chemistry [8], preparation of functional materials [9] and so on. More and more attention has been paid to the application of *n*-dialkylbenzimidazolium ionic liquids in catalytic systems. As we know, the reports about ionic liquids of benzimidazole salt are rare. As a result, we focused on the benzimidazole salts and synthesized a new benzimidazole ionic liquid.

The molecular structure of the title compound is shown in the figure. Bond lengths and angles are within normal ranges [10]. The angle between two benzimidazole ligands is 101.05(9)°.

<https://doi.org/10.1515/ncrs-2020-0535>

Received October 13, 2020; accepted November 26, 2020;
published online December 21, 2020

Abstract

C₂₄H₃₄N₆Cl₂Zn, monoclinic, $P2_1/c$ (no. 14), $a = 9.513(3)$ Å, $b = 9.546(3)$ Å, $c = 30.956(10)$ Å, $\beta = 101.228(9)^\circ$, $V = 2757.3(15)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0452$, $wR_{\text{ref}}(F^2) = 0.1299$, $T = 293$ K.

CCDC no.: 2046616

The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Fang-fang Jian**, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang, Henan 471003, P. R. China; and Heke University Renewable Energy Co. LTD, Luoyang 471000, P. R. China, E-mail: Fangfjian@126.com

Xiao-jing Liu, E. Liu, Ze-shen Jin and Zhuang-yu Li, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang, Henan 471003, P. R. China

Tong-ling Liang, Institute of Chemistry, Chinese Academy of Sciences, Zhongguancun, Beijing 100190, P. R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Zn1	0.18393 (3)	−0.79303 (3)	−0.124785 (10)	0.04692 (12)
Cl1	0.24479 (9)	−0.86321 (8)	−0.18697 (2)	0.0629 (2)
Cl2	0.28309 (7)	−0.90830 (8)	−0.06427 (2)	0.0596 (2)
N1	0.2951 (3)	−0.3880 (3)	−0.09031 (9)	0.0657 (7)
N2	0.2874 (3)	−0.5250 (3)	−0.08325 (8)	0.0636 (6)
N3	0.2281 (3)	−0.5840 (2)	−0.12055 (7)	0.0528 (5)
N4	−0.2532 (3)	−0.7642 (3)	−0.16008 (9)	0.0716 (7)
N5	−0.1187 (3)	−0.7555 (3)	−0.16595 (8)	0.0668 (7)
N6	−0.0339 (2)	−0.7918 (3)	−0.12902 (8)	0.0542 (6)
C1 ^a	−0.322 (2)	−0.0895 (15)	−0.1882 (5)	0.166 (8)
H1a ^a	−0.360 (12)	−0.045 (5)	−0.2158 (5)	0.249 (11)*
H1b ^a	−0.398 (9)	−0.0995 (17)	−0.172 (3)	0.249 (11)*
H1c ^a	−0.247 (3)	−0.033 (4)	−0.172 (3)	0.249 (11)*
C25 ^a	−0.2634 (17)	−0.2343 (13)	−0.1964 (6)	0.152 (7)
H25a ^a	−0.2462 (17)	−0.2436 (13)	−0.2262 (6)	0.182 (9)*
H25b ^a	−0.1767 (17)	−0.2565 (13)	−0.1754 (6)	0.182 (9)*
C3	−0.3914 (7)	−0.3225 (7)	−0.1891 (2)	0.138 (2)
H3aa ^a	−0.4106 (7)	−0.3107 (7)	−0.1597 (2)	0.165 (2)*
H3ab ^a	−0.4774 (7)	−0.3022 (7)	−0.2107 (2)	0.165 (2)*
H3bc ^b	−0.515 (15)	−0.324 (13)	−0.208 (4)	0.207 (3)*
H3bd ^b	−0.399 (14)	−0.388 (14)	−0.155 (5)	0.207 (3)*
C4	−0.3315 (6)	−0.4672 (6)	−0.19573 (17)	0.1329 (19)
H4a	−0.3138 (6)	−0.4744 (6)	−0.22547 (17)	0.160 (2)*
H4b	−0.2407 (6)	−0.4793 (6)	−0.17547 (17)	0.160 (2)*
C26	−0.4320 (4)	−0.5801 (6)	−0.18827 (16)	0.1165 (15)
H26a	−0.4485 (4)	−0.5737 (6)	−0.15838 (16)	0.1398 (18)*
H26b	−0.5232 (4)	−0.5670 (6)	−0.20821 (16)	0.1398 (18)*
C6	−0.3731 (4)	−0.7267 (5)	−0.19563 (13)	0.1008 (13)
H6a	−0.3411 (4)	−0.7283 (5)	−0.22353 (13)	0.1210 (15)*
H6b	−0.4489 (4)	−0.7955 (5)	−0.19704 (13)	0.1210 (15)*
C7 ^c	0.9799 (12)	−0.3779 (14)	−0.0588 (4)	0.210 (4)
H7a ^c	0.981 (5)	−0.372 (11)	−0.0897 (4)	0.315 (7)*
H7b ^c	0.990 (6)	−0.286 (5)	−0.046 (3)	0.315 (7)*
H7c ^c	1.0577 (14)	−0.436 (6)	−0.044 (3)	0.315 (7)*
C8 ^c	0.8362 (11)	−0.4423 (12)	−0.0524 (5)	0.204 (4)
H8a ^c	0.7936 (11)	−0.5016 (12)	−0.0770 (5)	0.245 (5)*
H8b ^c	0.8461 (11)	−0.4944 (12)	−0.0251 (5)	0.245 (5)*
C9 ^d	0.7524 (9)	−0.3060 (13)	−0.0512 (5)	0.164 (3)
H9a ^d	0.7931 (9)	−0.2483 (13)	−0.0260 (5)	0.197 (4)*
H9b ^d	0.7457 (9)	−0.2522 (13)	−0.0781 (5)	0.197 (4)*
C10	0.6058 (6)	−0.3695 (7)	−0.0466 (2)	0.1427 (19)
H10a ^d	0.5772 (6)	−0.4428 (7)	−0.0682 (2)	0.171 (2)*
H10b ^d	0.6104 (6)	−0.4082 (7)	−0.0174 (2)	0.171 (2)*
H10c ^e	0.5701 (6)	−0.4270 (7)	−0.0252 (2)	0.171 (2)*
H10d ^e	0.5858 (6)	−0.4220 (7)	−0.0739 (2)	0.171 (2)*
C11	0.5039 (5)	−0.2498 (5)	−0.05448 (16)	0.1127 (16)
H11a	0.5331 (5)	−0.1793 (5)	−0.03196 (16)	0.1353 (19)*
H11b	0.5075 (5)	−0.2078 (5)	−0.08278 (16)	0.1353 (19)*
C12	0.3537 (5)	−0.2936 (4)	−0.05397 (13)	0.0834 (11)
H12a	0.2936 (5)	−0.2108 (4)	−0.05572 (13)	0.1001 (13)*
H12b	0.3512 (5)	−0.3400 (4)	−0.02626 (13)	0.1001 (13)*
C13	0.2416 (3)	−0.3563 (3)	−0.13316 (10)	0.0597 (7)
C14	0.2240 (4)	−0.2302 (3)	−0.15645 (13)	0.0777 (10)
H14	0.2529 (4)	−0.1445 (3)	−0.14333 (13)	0.0933 (12)*
C15	0.1616 (5)	−0.2417 (4)	−0.19967 (14)	0.0872 (11)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H15	0.1492 (5)	−0.1608 (4)	−0.21675 (14)	0.1047 (14)*
C16	0.1155 (5)	−0.3687 (4)	−0.21967 (12)	0.0856 (11)
H16	0.0721 (5)	−0.3694 (4)	−0.24931 (12)	0.1027 (13)*
C17	0.1321 (4)	−0.4925 (4)	−0.19691 (11)	0.0692 (8)
H17	0.1018 (4)	−0.5775 (4)	−0.21020 (11)	0.0831 (10)*
C18	0.1978 (3)	−0.4832 (3)	−0.15237 (9)	0.0548 (7)
C19	−0.1161 (3)	−0.8232 (3)	−0.09854 (9)	0.0547 (7)
C20	−0.0794 (3)	−0.8669 (4)	−0.05470 (10)	0.0653 (8)
H20	0.0155 (3)	−0.8789 (4)	−0.04070 (10)	0.0784 (10)*
C21	−0.1903 (4)	−0.8911 (4)	−0.03345 (12)	0.0797 (10)
H21	−0.1700 (4)	−0.9196 (4)	−0.00417 (12)	0.0956 (12)*
C22	−0.3332 (4)	−0.8742 (4)	−0.05441 (13)	0.0832 (11)
H22	−0.4048 (4)	−0.8933 (4)	−0.03866 (13)	0.0999 (13)*
C23	−0.3713 (3)	−0.8313 (4)	−0.09642 (13)	0.0782 (10)
H23	−0.4667 (3)	−0.8192 (4)	−0.11002 (13)	0.0938 (12)*
C24	−0.2582 (3)	−0.8061 (4)	−0.11849 (10)	0.0625 (8)
C2a ^b	−0.187 (2)	−0.154 (2)	−0.1770 (6)	0.206 (8)
H2aa ^b	−0.183 (6)	−0.159 (16)	−0.1457 (6)	0.309 (13)*
H2ab ^b	−0.117 (2)	−0.216 (11)	−0.185 (4)	0.309 (13)*
H2ac ^b	−0.169 (7)	−0.060 (6)	−0.185 (4)	0.309 (13)*
C1a ^b	−0.320 (3)	−0.195 (2)	−0.1983 (9)	0.200 (9)
H1aa ^b	−0.316 (3)	−0.197 (2)	−0.2293 (9)	0.240 (10)*
H1ab ^b	−0.384 (3)	−0.118 (2)	−0.1947 (9)	0.240 (10)*
C8a ^f	0.883 (4)	−0.316 (3)	−0.0513 (11)	0.152 (7)
H8aa ^f	0.964 (4)	−0.286 (3)	−0.0290 (11)	0.182 (8)*
H8ab ^f	0.851 (4)	−0.239 (3)	−0.0716 (11)	0.182 (8)*
C7a ^f	0.915 (4)	−0.463 (3)	−0.0766 (10)	0.150 (7)
H7aa ^f	0.835 (11)	−0.483 (13)	−0.100 (5)	0.226 (11)*
H7ab ^f	1.000 (14)	−0.453 (9)	−0.089 (7)	0.226 (11)*
H7ac ^f	0.93 (2)	−0.539 (6)	−0.0559 (19)	0.226 (11)*
C9a ^e	0.767 (4)	−0.377 (5)	−0.0325 (13)	0.145 (5)
H9aa ^e	0.785 (4)	−0.345 (5)	−0.0021 (13)	0.173 (6)*
H9ab ^e	0.787 (4)	−0.477 (5)	−0.0310 (13)	0.173 (6)*

^aOccupancy: 0.483 (17), ^bOccupancy: 0.517 (17), ^cOccupancy: 0.761 (13), ^dOccupancy: 0.786 (18), ^eOccupancy: 0.214 (18), ^fOccupancy: 0.239 (13)

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

Research funding: Henan University of Science and Technology Distinguished Professor Open Fund (Grant No. 135100001).

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

References

1. *Enraf-Nonius: CAD-4 Software. Version 5.0*; Enraf-Nonius: Delft, The Netherlands, 1985.
2. Harms K., Wocadlo S. *XCAD4*; University of Marburg: Germany, 1995.

3. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, 42, 339–341.
4. Ochędzan-Siodłak W., Bihun A., Olszowy A., Rajfur M., Jesionowski T., Siwińska-Stefańska K. Ethylene polymerization using vanadium catalyst supported on silica modified by pyridinium ionic liquid. *Polym. Int.* 2016, 65, 1089–1097.
5. Mazloumi M., Shirini F. Introduction of a new catalyst containing an ionic liquid bridge on nanoporous Na^+ - montmorillonite for the synthesis of hexahydroquinolines and 1,8-dioxo-decahydroacridines via Hantzsch condensation. *J. Mol. Struct.* 2020, 1217, 128326.
6. Gupta A., Jain A., Tripathi S. K. Structural and electrochemical studies of bromide derived ionic liquid-based gel polymer electrolyte for energy storage application. *J. Energy Storage* 2020, 32, 101723.
7. Wang G. J., Fang S. H., Luo D., Yang L., Hirano S. I. Functionalized 1,3-dialkylimidazolium bis(fluorosulfonyl)imide as neat ionic liquid electrolytes for lithium-ion batteries. *Electrochem. Commun.* 2016, 72, 148–152.
8. Yavir K., Jedrkiewicz L., Marcinkowska R., Namiesnik J., Kloskowski A. Analytical applications and physicochemical properties of ionic liquid-based hybrid materials: a review. *Anal. Chim. Acta* 2019, 1054, 1–16.
9. Wang Y. N., Hou Q. D., Ju M. T., Li W. Z. New developments in material preparation using a combination of ionic liquids and microwave irradiation. *Nanomaterials* 2019, 9, 1–16.
10. Wang X., Ling N., Li Y., Zhang S. Crystal structure of dichlorido bis [1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole- κ^1N]cadmium(II), $C_{30}H_{26}CdCl_2N_{10}$. *Z. Kristallogr. NCS* 2018, 233, 215–216.