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Crystallographic report

catena-Aqua(2,2′-bipyrimidine)lithium(I) perchlorate

Ming-Liang Tong[1,2]*, Sheng Hu[1], Xiao-Lan Yu[1] and Xiao-Ming Chen[1]

[1]School of Chemistry and Chemical Engineering, Sun Yat-Sen University, 510275 Guangzhou, People's Republic of China
[2]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, People's Republic of China

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A lithium(I) coordination polymer has been formed from $LiClO_4$ and the 2,2′-bipyrimidine (bpym) ligand in which each square pyramidal lithium(I) atom is coordinated in the basal plane by four nitrogen donor atoms derived from two bpym ligands and one water molecule at the apical position. These are connected into a layer structure via hydrogen-bonding interactions involving the perchlorate anions. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; lithium; 2,2′-bipyrimidine; layer structure

COMMENT

A two-dimensional coordination polymer is found in the crystal structure of $[Li(bpym)(H_2O)]ClO_4$ (bpym = 2, 2′-bipyrimidine). Each lithium(I) atom is coordinated in a distorted square-pyramidal geometry by four nitrogen donors from two bpym ligands, which occupy the basal positions, and one water molecule at the apical position. Each water molecule hydrogen bonds to two oxygen atoms of two perchlorate anions (O1w $\cdots$ O2^{i} = 2.920(4) and O1w $\cdots$ O3 = 2.918(4) Å; symmetry code, i: x, $\frac{1}{2}-y$, $\frac{1}{2}+z$) to form a two-dimensional hydrogen-bonded layer structure (Fig. 1). The structure represents a rare example of a lithium(I) complex with oligopyridine-like ligands.[1,2]

EXPERIMENTAL

The complex was synthesized by the self-assembly of lithium perchlorate and 2, 2′-bipyrimidine in 1:1 molar stoichiometry in methanol/water (v/v 1:1). Colorless crystals separated from

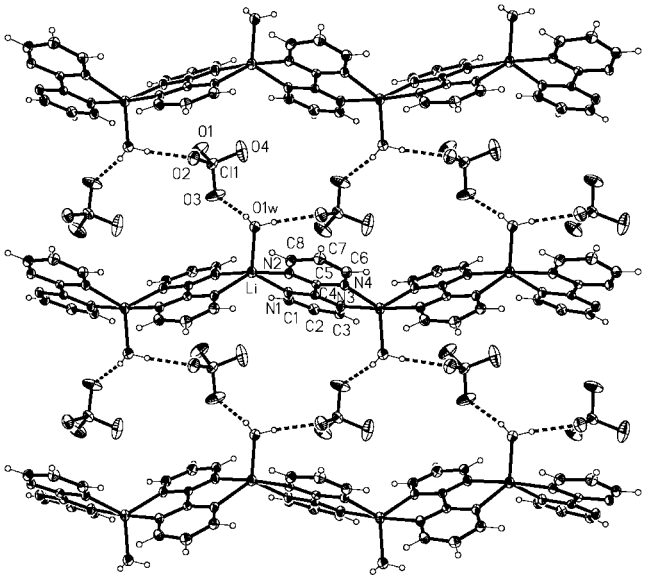

Figure 1. ORTEP plot (50% probability level) showing the supramolecular association operating in polymeric aqua(2,2′-bipyrimidine)lithium(I). Selected bond distances and angles: Li–O1w 1.961(6), Li–N1 2.099(6), Li–N2 2.200(6), Li–N3^{i} 2.156(6), Li–N4^{i} 2.160(6) Å; O1w–Li–N1 109.8(3), O1w–Li–N2 90.5(2), O1w–Li–N3^{i} 93.7(3), O1w–Li–N4^{i} 122.3(3), N1–Li–N2 77.6(2), N1–Li–N3^{i} 102.5(3), N1–Li–N4^{i} 127.8(3), N2–Li–N3^{i} 175.4(3), N2–Li–N4^{i} 99.4(2), N3^{i}–Li–N4^{i}76.9(2)°. Symmetry code, i: x, $\frac{3}{2}-y$, $-\frac{1}{2}+z$.

*Correspondence to: Ming-Liang Tong, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, 510275 Guangzhou, People's Republic of China.
E-mail: cestml@zsu.edu.cn
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solution when the mixture was set aside. Anal. Found: C, 33.93; H, 2.72; N, 19.67. Calc. for $C_8H_8LiClN_4O_5$: C, 34.01; H, 2.85; N, 19.83%. A $0.36 \times 0.40 \times 0.48$ mm^3 specimen was used for data collection on a Bruker CCD diffractometer using Mo Kα radiation. $C_8H_8ClLiN_4O_5$, $M = 282.6$, monoclinic, space group $P2_1/c$, $a = 12.558(4)$, $b = 8.958(3)$, $c = 11.048(3)$ Å, $\beta = 110.085(7)°$, $V = 1167.2(6)$ Å^3, $Z = 4$, $D_x = 1.608$ g cm^{-3}, $2\theta_{max} = 55.0°$, $R1 = 0.077$ (2107 reflections with $I > 2\sigma(I)$), $wR_2 = 0.151$ (2565 unique reflections). Programs used: SHELXS97, SHELXL97 and ORTEP. CCDC deposition number: 221543.

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REFERENCES

1. Constable EC, Housecroft CE, Kariuki BM, Kelly N, Smith CB. *Chem. Commun.* 2001; 2134.
2. Bock H, Lehn J-M, Pauls J, Holl S, Krenzel V. *Angew. Chem. Int. Ed. Engl.* 1999; **38**: 952.