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The crystal structure of poly[μ_2 -chlorido-(μ_2 -1,2-bis(4-pyridyl)ethane- $\kappa^2 N:N'$ silver(I)], $C_{12}H_{12}AgClN_2$

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Abstract

$\text{C}_{12}\text{H}_{12}\text{AgClN}_2$, orthorhombic, $P2_12_12_1$ (no. 19),
 $a = 9.007(2)$ Å, $b = 9.493(2)$ Å, $c = 13.642(3)$ Å,
 $V = 1166.5(4)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0160$, $wR_{\text{ref}}(F^2) = 0.0370$,
 $T = 295$ K.

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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.

Source of material

An amount of 0.1435 g (1.0 mmol) AgCl and 0.1842 g (1.0 mmol) 1,2-bis(4-pyridyl)ethane were successively added to a 25 mL Teflon-lined stainless-steel autoclave charged with 20 mL DMF/H₂O (v:v = 1:1) solution. The mixture was heated at 160 °C for three days and subsequently cooled to

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.55 × 0.52 × 0.24 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.93 mm ⁻¹
Diffractometer, scan mode:	Rigaku R-Axis RAPID, ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9156, 2052, 0.019
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2020
$N(\text{param})_{\text{refined}}$:	145
Programs:	Rigaku [1], SHELX [2, 3]

room at a rate of 5 °C h⁻¹. Colorless block crystals were obtained.

Experimental details

All H-atoms from C atoms were positioned with idealized geometry ($U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and methylene H atoms, respectively), using a riding model with C–H = 0.93 or 0.97 Å.

Comment

In recent years, coordination polymers have attracted extensive attention owing to their structural diversities and potential application as functional materials [4–8]. Structural properties of the ligands are one of the main factors which influence the topology and composition of the coordination polymers. Bipyridyl-based ligands are effective

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

Atom	x	y	z	U _{iso} [*] /U _{eq}
Ag	0.41144 (3)	0.30479 (3)	0.73973 (2)	0.04277 (9)
Cl	0.36205 (9)	0.01797 (8)	0.74438 (6)	0.04137 (18)
N1	0.4073 (3)	0.3213 (3)	0.57538 (16)	0.0346 (6)
N2	0.3370 (3)	0.3376 (3)	−0.10415 (19)	0.0354 (6)
C1	0.3401 (4)	0.2229 (4)	0.5219 (2)	0.0376 (8)
H1A	0.289203	0.151694	0.554422	0.045 [*]
C2	0.3420 (4)	0.2209 (4)	0.4208 (2)	0.0424 (9)
H2A	0.291264	0.151024	0.386823	0.051 [*]
C3	0.4862 (4)	0.4278 (4)	0.4256 (3)	0.0453 (9)
H3A	0.537365	0.500395	0.394731	0.054 [*]
C4	0.4765 (4)	0.4241 (4)	0.5268 (3)	0.0403 (8)
H4A	0.520135	0.496509	0.562488	0.048 [*]
C5	0.4196 (4)	0.3231 (4)	0.3705 (2)	0.0415 (8)
C6	0.4313 (4)	0.3189 (5)	0.2597 (2)	0.0568 (10)
H6A	0.510608	0.381284	0.238941	0.068 [*]
H6B	0.457135	0.224134	0.239352	0.068 [*]
C7	0.2895 (4)	0.3621 (4)	0.2097 (2)	0.0422 (8)
H7A	0.264630	0.457682	0.228685	0.051 [*]
H7B	0.209611	0.300923	0.231172	0.051 [*]
C8	0.3028 (4)	0.3543 (4)	0.0995 (2)	0.0341 (7)
C9	0.2475 (4)	0.2419 (4)	0.0466 (2)	0.0374 (7)
H9A	0.197363	0.169676	0.078608	0.045 [*]
C10	0.2666 (4)	0.2367 (4)	−0.0534 (2)	0.0379 (8)
H10A	0.228922	0.159640	−0.087384	0.046 [*]
C11	0.3879 (4)	0.4477 (3)	−0.0531 (2)	0.0372 (8)
H11A	0.434919	0.520047	−0.086957	0.045 [*]
C12	0.3740 (4)	0.4591 (4)	0.0468 (2)	0.0381 (8)
H12A	0.412427	0.537317	0.079120	0.046 [*]

building blocks for the construction of coordination polymers [9–12]. Silver is an extremely soft Lewis acid and has a good affinity to N-based ligands. Various coordination polymers can be produced by the self-assembly of silver with pyridine derivative ligands, but the self-assembling process is affected by the solvent system, the ratio of metal to ligand, the template and the presence of counter ions [13–18]. Here, we report the title two-dimensional coordination polymer, [AgCl(bpe)_n] (bpe = 1,2-bis(4-pyridyl)ethane), with (4,4) net topology.

The asymmetric unit of the title compound consists of one Ag(I) cation, one Cl[−] anion and one bpe ligand. The four-coordinated Ag⁺ center adopts a distorted tetrahedral geometry, which is completed by two symmetry-related Cl atoms and two N atoms from two dependent bpe ligands (Cl–Ag–Cl = 143.63(2)°; N–Ag–N = 158.09(9)°; N–Ag–Cl = 92.17(8) and 95.11(7)°). The Ag–Cl bond lengths are 2.760(1) and 2.882(1) Å, the Ag–N bond lengths are 2.248(2) and 2.254(2) Å, which are within normal ranges [19]. The

interaction between Ag⁺ and Cl[−] forms zigzag chains along [100]. The Ag–Cl chains are further linked by bpe ligands to form an order (4,4) net framework parallel to (100). The two-pyridyl rings of the bpe ligand are almost coplanar with the dihedral angle at 6.9(2)°.

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