Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

Xiu-Ling Zhang,^a Yue Qiu^a and Seik Weng Ng^b*

^aDepartment of Chemistry, Dezhou University, Dezhou 253011, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study T = 294 K Mean σ (C–C) = 0.007 Å R factor = 0.036 wR factor = 0.092 Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

catena-Poly[silver(I)- μ_3 -5-phenyl-1,2,3,4-tetrazolato- $\kappa^3 N^1: N^2: N^3$]

The 5-phenyltetrazolate anion in the title compound, $[Ag(C_7H_5N_4)]_n$, uses three of its four N atoms to link silver cations into a linear ribbon structure; the Ag atom shows a trigonal planar coordination.

Received 16 November 2006 Accepted 22 November 2006

Comment

Although metal tetrazolates are now emerging as a class of useful materials (Gaponik et al., 2006), there are few crystal structure reports of such compounds in the literature. Among the organic tetrazolates, the crystal structure is known only for dimethylammonium 5-phenyltetrazolate (Guzei & Bikzhanova, 2002). The 5-phenyltetrazolate anion is monodentate in the titanium and niobium (Yelamos et al., 2001) complexes. In the potassium derivative, it binds as a bidentate chelate (Zheng et al., 2003), whereas in the copper derivative it functions as a bridging ligand (Shao et al., 2004). The dicvclopentadienvllanthanum derivative has the ligand binding in a bridging mode (Zhou et al., 2000); other lanthanide complexes show similar bonding features (Zhou et al., 1998). On the other hand, the diphenylthallium derivative has a complex composition (Bhandari et al., 2000), as does the dicyclopentadienylholonium derivative (Huang et al., 1998). The zinc derivative is known to be SHG-active (Ye et al., 2005); the only other inorganic main-group compound appears to be the aluminium derivative (Munoz-Hernandez et al., 1998).



Silver 5-phenyltetrazolate, (I), was first mentioned in the context of the photolysis of 2-alkenyl-5-phenyl-substituted tetrazoles (Padwa *et al.*, 1978). In (I), the anion uses three of its four Lewis basic sites to bind to three different Ag atoms; the metal atom shows a trigonal planar coordination (Fig. 1

© 2006 International Union of Crystallography All rights reserved

metal-organic papers

and Table 1). The binding mode gives rise to the formation of a ribbon motif; the backbone of the ribbon, which propagates along the b axis, is essentially flat.

Experimental

Silver perchlorate (41 mg, 0.2 mmol) and 5-phenyltetrazole (30 mg, 0.2 mmol) were dissolved in 10% aqueous ammonia (10 ml). The solution was filtered and then allowed to stand in the dark for three weeks. Crystals were isolated in 60% yield.

Crystal data

 $\begin{bmatrix} Ag(C_7H_5N_4) \end{bmatrix} \\ M_r = 253.02 \\ Monoclinic, P2_1/c \\ a = 10.433 (2) Å \\ b = 6.275 (1) Å \\ c = 11.894 (2) Å \\ \beta = 110.388 (2)^{\circ} \\ V = 729.9 (2) Å^3$

Z = 4 D_x = 2.303 Mg m⁻³ Mo K α radiation μ = 2.70 mm⁻¹ T = 294 (2) K Block, colorless 0.20 × 0.18 × 0.10 mm

3709 measured reflections

 $R_{\rm int} = 0.047$

 $\theta_{\rm max} = 26.4^\circ$

1459 independent reflections 1138 reflections with $I > 2\sigma(I)$

Data collection

Bruker SMART 1K area-detector diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.446, T_{\max} = 0.774$

Refinement

Refinement on F^2 H-atom parameters constrained $R[F^2 > 2\sigma(F^2)] = 0.036$ $w = 1/[\sigma^2(F_o^2) + (0.0544P)^2]$ $wR(F^2) = 0.092$ where $P = (F_o^2 + 2F_c^2)/3$ S = 0.98 $(\Delta/\sigma)_{max} = 0.001$ 1459 reflections $\Delta\rho_{max} = 1.16$ e Å⁻³109 parameters $\Delta\rho_{min} = -1.37$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1-N1	2.251 (3)	Ag1-N3 ⁱⁱ	2.256 (3)
Ag1-N2 ⁱ	2.299 (3)		
N1-Ag1-N2 ⁱ	114.4 (1)	N2 ⁱ -Ag1-N3 ⁱⁱ	110.4 (1)
N1-Ag1-N3 ⁱⁱ	134.5 (1)		

Symmetry codes: (i) -x + 1, $y - \frac{1}{2}$, $-z + \frac{3}{2}$; (ii) x, y - 1, z.

H atoms were positioned geometrically (C-H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The final difference Fourier map had a large peak/hole at about 1 Å from Ag1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X*-



Figure 1

A fragment of the ribbon structure of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii. Symmetry codes are as given in Table 1.

SEED (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

We thank Dezhou University and the University of Malaya for supporting this study.

References

- Barbour, L. J. (2001). J. Supramol. Chem. 1, 189-191.
- Bhandari, S., Mahon, M. F., Molloy, K. C., Palmer, J. S. & Sayers, S. F. (2000). *Dalton Trans.* pp. 1053–1060.
- Bruker (1998). SMART (Version 5.051) and SAINT (Version V6.28A). Bruker AXS Inc., Madison, Wisconsin USA.
- Gaponik, P. N., Voitekhovich, S. V. & Ivashkevich, O. A. (2006). Russ. Chem. Rev. 75, 507–539.
- Guzei, I. A. & Bikzhanova, G. A. (2002). Acta Cryst. E58, 0937-0939.
- Huang, X.-Y., Zhou, X.-G., Zhang, L.-X., Feng, X.-J., Cai, R.-F. & Huang, Z.-E.
- (1998). Chin. J. Struct. Chem., 17, 449–453.
 Munoz-Hernandez, M.-A., Hill, M. S. & Atwood, D. A. (1998). Polyhedron, 17, 2237–2242.
- Padwa, A., Nahm, S. & Sato, E. (1978). J. Org. Chem. 43, 1664-01671.
- Shao, Z.-H., Luo, J., Cai, R.-F., Zhou, X.-G., Weng, L.-H. & Chen, Z.-X. (2004). Acta Cryst. E60, m225–m227.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Westrip, S. P. (2006). publCIF. In preparation.
- Yelamos, C., Gust, K. R., Baboul, A. G. & Heeg, M. J. (2001). *Inorg. Chem.* 40, 6451–6462.
- Ye, Q., Li, Y.-H., Song, Y.-M., Huang, X.-F., Xiong, R.-G. & Xue, Z.-L. (2005). *Inorg. Chem.* 44, 3618–3625.
- Zheng, W.-J., Heeg, M. J. & Winter, C. H. (2003). Angew. Chem. Int. Ed. Engl. 42, 2761–2764.
- Zhou, X.-G., Huang, Z.-E., Cai, R.-F., Zhang, L.-X., Hou, X.-F., Feng, X.-J. & Huang, X.-Y. (1998). J. Organomet. Chem. 563, 101–112.
- Zhou, X.-G., Zhang, L.-X., Huang, Z.-E., Cai, R.-F. & Huang, X.-Y. (2000). Synth. React. Inorg. Met.-Org. Chem. 30, 965–978.