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Aqua(2,2′-bipyridyl-*N*,*N*′)(thiodiacetato-*O*,*O*′,*S*)zinc(II) Tetrahydrate

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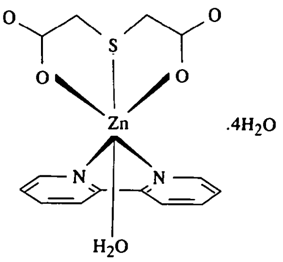
Abstract

The title complex, aqua(2,2′-bipyridyl-*N*,*N*′)(3-thiapentanedioate-*O*,*S*,*O*′)zinc(II) tetrahydrate, $[Zn(C_4H_4O_4S)(C_{10}H_8N_2)(H_2O)].4H_2O$, is mononuclear with a coordination sphere consisting of one S, two N and three O atoms. The Zn atom is linked to a tridentate thiodiacetate ligand, a bidentate 2,2′-bipyridine ligand and an aqua ligand resulting in a slightly distorted octahedral coordination geometry. The molecular units are linked together in the crystal by an extensive hydrogen-bonding network and by intermolecular S···S interactions.

Comment

Current interest in zinc compounds with thioether sulfur ligands is due in part to their relevance as structural models in biological systems (Bouwman, Evans, de Graaff, Kooijman, Poinsot, Rabu, Reedijk & Spek, 1995; Haanstra, Driessen, Reedijk, Turpeinen & Hämäläinen, 1989). Very few crystal structures of zinc complexes with acyclic ligands having thioether groups as coordinating agents have been reported so far (Drew, Rice & Timewell, 1975; Teixidor, Escriche, Casabo, Molins & Miravitlles, 1986; Mangia, Nardelli, Palmieri & Pellizzi, 1972). Among these, triaquazinc(II) thiodiacetate monohydrate, $[Zn\{S(CH_2COO)_2\}(H_2O)_3].H_2O$, was found to be monomeric, with a distorted octahedral ZnO_5S core and a Zn—S bond length of 2.601 (2) Å (Drew *et al.*, 1975). The results of the present study include the preparation, characterization and X-ray structure determination of the title complex, $[Zn\{S(CH_2COO)_2\}(2,2'\text{-bpy})(H_2O)].4H_2O$ (bpy is bipyridine), hereafter (1). It was of interest to further examine the coordination behaviour of the thiodiacetate ligand towards the 'hard' Zn^{II} metal ion and to study its dependence on the ligands associated with the metal centre.



(1)

The structure of (1) and the atomic numbering scheme are shown in Fig. 1. The Zn atom has octahedral geometry to a reasonably good approximation, comprised of the two carboxylate O atoms of the thiodiacetate [Zn—O1 2.047 (2), Zn—O5 2.067 (2) Å and O1—Zn—O5 95.94 (6)°], the thioether S atom of the thiodiacetate [Zn—S3 2.618 (1) Å], two N atoms of the 2,2′-bpy ligand [Zn—N1 2.124 (2), Zn—N2 2.167 (2) Å and

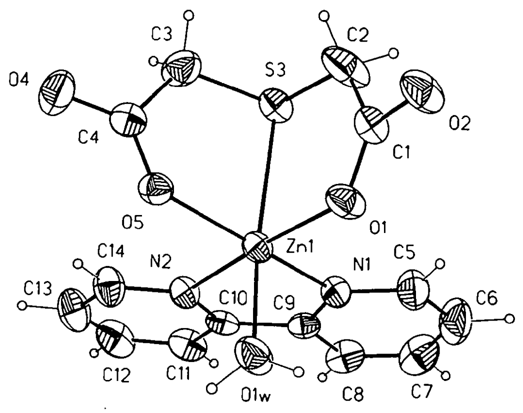


Fig. 1. Molecular diagram showing the labelling scheme used. Displacement ellipsoids are drawn at the 50% probability level.

N1—Zn—N2 76.52 (7)°] and the O atom of the aqua ligand [Zn—O1W 2.064 (2) Å].

The S3 and O1W atoms occupy the axial sites with respect to the basal plane defined by the O1, O5, N1 and N2 atoms [maximum/mean deviations from the least-squares plane are 0.100 (2)/0.080(2) Å; deviations of the axial bonds from the normal for S3 and O1W are 10.12 (4) and 5.32 (5)°, respectively; out-of-plane displacement of the cation is 0.11 Å towards O1W].

Comparison of the Zn coordination sphere in (1) with that found in the related $[Zn\{O(CH_2COO)_2\}(2,2'\text{-}bpy)(H_2O)].3H_2O$ complex (Baggio, Garland & Perec, 1996), confirms the larger flexibility of the sulfur site in the thiodiacetate ligand as compared with the homologous and rather rigid oxydiacetate. In fact, the bending along S3—Zn1 of the two planar wings, O1—C1—C2—S3—Zn1 and O5—C4—C3—S3—Zn1, to a dihedral angle of 99.43 (4)° allows a cation environment with significantly smaller distortions from an ideal regular geometry.

The Zn—S bond distance of 2.618 (1) Å is comparable to the value of 2.601 (2) Å found in $[Zn\{S(CH_2COO)_2\}(H_2O)_3].H_2O$. These values are significantly longer than the sum of the covalent radii (2.33 Å) but shorter than the van der Waals distance (3.27 Å) and indicative of weak bonding interactions. In molecule (1), the two inner carboxylate bonds [C1—O1 1.255 (3) and C4—O5 1.273 (3) Å] are only slightly longer than the outer carboxylate bonds [C1—O2 1.244 (3) and C4—O4 1.233 (3) Å]. This suggests that the negative charges of the ligand are preferentially localized on the O atoms bound to Zn^{II}. Other bond lengths and angles within the ligand are consistent with the values reported for $[Zn\{S(CH_2COO)_2\}(H_2O)_3].H_2O$.

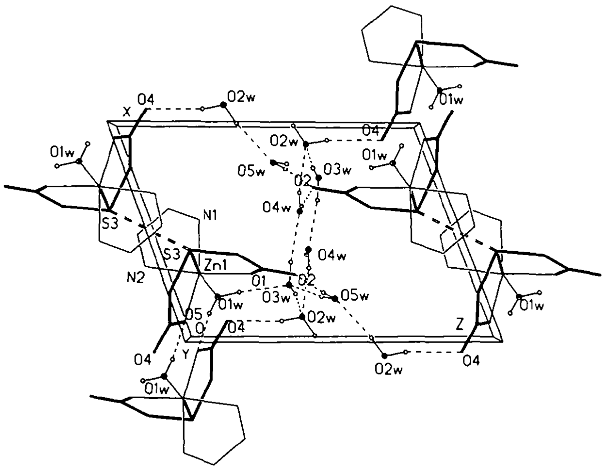


Fig. 2. Simplified packing diagram viewed down [010] showing direct S···S contacts (double dashes), as well as the hydrogen-bonding network involving the water molecules (single dashes). For clarity, bipyridyl groups are schematically represented with the rings removed and a comprehensive labelling of the water molecules in the diagram has been adopted.

The crystal structure of (1) is a rather complex three-dimensional network of octahedra connected by hydrogen bonds involving all coordinated and non-coordinated water molecules in the structure (Fig. 2). A summary of bond distances and angles involving hydrogen-bonding contacts is given in Table 3.

An interesting feature in the structure of (1) is the presence of an additional short intermolecular interaction between the two centrosymmetrically related thioether S atoms. The S3···S3($1-x$, $1-y$, $-z$) non-bonding distance of 3.307 (2) Å is significantly shorter than the sum of the van der Waals radii (*ca.* 3.60 Å). A similar S···S intermolecular contact of 3.34 Å is found in the reported structure of the homologous copper(II) complex $[Cu\{S(CH_2COO)_2\}(2,2'\text{-}bpy)(H_2O)].4H_2O$ (Bonomo, Rizzarelli, Bresciani-Pahor & Nardin, 1982).

Experimental

Zinc acetate dihydrate (0.44 g, 0.20 mmol) was added to a solution of thiodiacetic acid (0.30 g, 0.20 mmol) and 2,2'-bipyridine (0.30 g, 0.20 mmol) in water (50 ml). After stirring for 6 h at 313 K, the resultant solution was cooled to room temperature, passed through a glass filter and concentrated to *ca.* 25 ml on a rotary evaporator. After 12 h, the white solid product was collected, washed with small amounts of cold water and air dried. The title product was recrystallized by dissolving a small portion in warm water and allowing the solution to cool slowly. After 24 h, colourless crystals of (1) were isolated by filtration and dried *in vacuo*. Yield 0.45 g (70%). Analysis found: C 36.70, H 4.75, N 6.20, S 7.35, Zn 14.5%; $C_{14}H_{22}N_2O_9SZn$ requires C 36.55, H 4.80, N 6.10, S 7.00, Zn 14.20%; IR (KBr disk, cm^{-1}): 3391 (*vs*), 1607 (*vs*), 1576 (*vs*), 1493 (*m*), 1476 (*m*), 1445 (*s*), 1402 (*s*), 1377 (*s*), 1319 (*m*), 1254 (*m*), 1236 (*m*), 1180 (*w*), 1159 (*w*), 1024 (*m*), 935 (*m*), 766 (*s*), 737 (*m*), 696 (*m*), 652 (*m*), 631 (*w*), 416 (*m*), 347 (*w*).

Crystal data

$[Zn(C_4H_4O_4S)(C_{10}H_8N_2)$-
$(H_2O)].4H_2O$
$M_r = 459.77$
Triclinic
$P\bar{1}$
$a = 9.162$ (2) Å
$b = 10.808$ (3) Å
$c = 11.627$ (3) Å
$\alpha = 102.01$ (1)°
$\beta = 103.27$ (1)°
$\gamma = 113.63$ (1)°
$V = 966.8$ (4) Å^3
$Z = 2$
$D_x = 1.579$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 7.5$–12.5°
$\mu = 1.427$ mm^{-1}
$T = 293$ (2) K
Polyhedron
0.26 × 0.22 × 0.18 mm
Colourless

Data collection

Siemens $R3m$ diffractometer
$\omega/2\theta$ scans

2332 observed reflections
$[I > 2\sigma(I)]$

Absorption correction: semi-empirical *via* ψ scan (*XEMP* in *SHELXTL/PC*; Sheldrick, 1991)
$T_{\min} = 0.870$, $T_{\max} = 0.940$
3101 measured reflections
2528 independent reflections
$R_{\rm int} = 0.0083$
$\theta_{\max} = 22.54°$
$h = -1 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$
2 standard reflections monitored every 98 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0221$
$wR(F^2) = 0.0583$
$S = 1.036$
2528 reflections
244 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0320P)^2 + 0.5598P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.187$ e Å^{-3}
$\Delta\rho_{\min} = -0.261$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Zn1	0.29789 (3)	0.23965 (3)	0.10434 (2)	0.02557 (10)
O1	0.2981 (2)	0.3342 (2)	0.27638 (14)	0.0358 (4)
O2	0.2968 (2)	0.5060 (2)	0.4170 (2)	0.0432 (4)
S3	0.40952 (7)	0.50488 (6)	0.10746 (5)	0.0312 (2)
O4	−0.0662 (2)	0.2967 (2)	−0.1310 (2)	0.0478 (5)
O5	0.0734 (2)	0.2275 (2)	0.00125 (14)	0.0300 (4)
O1*W*	0.1873 (2)	0.0478 (2)	0.1357 (2)	0.0414 (4)
O2*W*	−0.0863 (3)	0.2117 (2)	−0.3878 (2)	0.0629 (6)
O3*W*	−0.2425 (3)	−0.0664 (2)	−0.3846 (2)	0.0566 (5)
O4*W*	−0.4091 (3)	−0.8000 (2)	−0.4919 (2)	0.0582 (5)
O5*W*	−0.1829 (3)	−0.2850 (2)	−0.5196 (2)	0.0696 (6)
N1	0.5501 (2)	0.2690 (2)	0.1662 (2)	0.0295 (4)
N2	0.3291 (2)	0.1494 (2)	−0.0674 (2)	0.0277 (4)
C1	0.3220 (3)	0.4599 (2)	0.3202 (2)	0.0315 (5)
C2	0.3892 (4)	0.5683 (3)	0.2556 (3)	0.0540 (8)
C3	0.2145 (3)	0.4674 (3)	−0.0060 (3)	0.0452 (7)
C4	0.0621 (3)	0.3194 (2)	−0.0482 (2)	0.0301 (5)
C5	0.6554 (3)	0.3308 (3)	0.2860 (2)	0.0431 (6)
C6	0.8142 (4)	0.3395 (3)	0.3227 (3)	0.0574 (8)
C7	0.8660 (3)	0.2813 (3)	0.2331 (3)	0.0528 (7)
C8	0.7586 (3)	0.2185 (3)	0.1094 (3)	0.0406 (6)
C9	0.6016 (3)	0.2144 (2)	0.0785 (2)	0.0278 (5)
C10	0.4805 (3)	0.1531 (2)	−0.0530 (2)	0.0275 (5)
C11	0.5229 (3)	0.1080 (3)	−0.1557 (2)	0.0398 (6)
C12	0.4053 (4)	0.0567 (3)	−0.2749 (2)	0.0485 (7)
C13	0.2504 (4)	0.0516 (3)	−0.2896 (2)	0.0477 (7)
C14	0.2170 (3)	0.0989 (3)	−0.1840 (2)	0.0395 (6)

Table 2. *Selected geometric parameters (Å, °)*

Zn1—O1	2.047 (2)	N2—C14	1.340 (3)
Zn1—O1*W*	2.064 (2)	N2—C10	1.341 (3)
Zn1—O5	2.067 (2)	C1—C2	1.521 (3)
Zn1—N1	2.124 (2)	C3—C4	1.522 (3)
Zn1—N2	2.167 (2)	C5—C6	1.377 (4)
Zn1—S3	2.618 (1)	C6—C7	1.379 (4)
O1—C1	1.255 (3)	C7—C8	1.381 (4)
O2—C1	1.244 (3)	C8—C9	1.380 (3)
S3—C3	1.792 (3)	C9—C10	1.489 (3)
S3—C2	1.797 (3)	C10—C11	1.391 (3)
O4—C4	1.233 (3)	C11—C12	1.380 (4)
O5—C4	1.273 (3)	C12—C13	1.367 (4)
N1—C5	1.341 (3)	C13—C14	1.379 (4)
N1—C9	1.343 (3)		
O1—Zn1—O1*W*	86.25 (6)	O5—Zn1—N2	90.23 (7)
O1—Zn1—O5	95.94 (6)	N1—Zn1—N2	76.52 (7)
O1*W*—Zn1—O5	96.16 (6)	O1—Zn1—S3	80.20 (5)
O1—Zn1—N1	96.96 (7)	O1*W*—Zn1—S3	165.52 (5)
O1*W*—Zn1—N1	95.60 (7)	O5—Zn1—S3	80.33 (4)
O5—Zn1—N1	163.06 (7)	N1—Zn1—S3	91.08 (5)
O1—Zn1—N2	173.37 (7)	N2—Zn1—S3	98.51 (5)
O1*W*—Zn1—N2	95.53 (7)		

Table 3. *Hydrogen-bonding geometry (Å, °)*

Values are normalized following Jeffrey & Lewis (1978) and Taylor & Kennard (1983).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1W*A*···O3*W*$^{\rm i}$	0.94	1.84	2.770 (3)	171
O1*W*—H1W*B*···O5$^{\rm i}$	0.94	1.84	2.771 (2)	171
O2*W*—H2W*A*···O4	0.94	1.99	2.875 (3)	156
O2*W*—H2W*B*···O5*W*$^{\rm ii}$	0.94	1.89	2.807 (4)	166
O3*W*—H3W*A*···O4*W*$^{\rm iii}$	0.94	1.84	2.771 (3)	173
O3*W*—H3W*B*···O2*W*	0.94	1.85	2.776 (3)	171
O4*W*—H4W*A*···O2$^{\rm i}$	0.94	1.85	2.780 (3)	169
O4*W*—H4W*B*···O2*W*$^{\rm iv}$	0.94	1.94	2.867 (4)	168
O5*W*—H5W*A*···O3*W*	0.94	1.94	2.869 (4)	173
O5*W*—H5W*B*···O2$^{\rm i}$	0.94	1.89	2.824 (3)	175

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, -y, -1-z$; (iii) $-1-x, -1-y, -1-z$; (iv) $x, y-1, z$.

The title structure was solved through a combination of direct methods and difference Fourier synthesis, using the *SHELXTL/PC* (Sheldrick, 1991) package. Refinement was performed with *SHELXL*93 (Sheldrick, 1993) on F^2 using the whole data set and anisotropic displacement parameters for non-H atoms. H atoms attached to C atoms were placed at their idealized positions and allowed to ride. Those corresponding to water molecules were located in a difference Fourier synthesis and subsequently refined with restrained O—H and H···H distances, and isotropic displacement parameters 1.3 times the equivalent isotropic displacement parameters of the host atoms. In all cases, distance and angle calculations involving H atoms were performed using the normalized positions after Jeffrey & Lewis (1978) and Taylor & Kennard (1983).

Data collection: *P3/P4-PC* (Siemens, 1991). Cell refinement: *P3/P4-PC*. Data reduction: *XDISK* in *SHELXTL/PC*. Molecular graphics: *XP* in *SHELXTL/PC*. Software used to prepare material for publication: *CIFTAB* in *SHELXL*93, *PARST* (Nardelli, 1983) and the Cambridge Structural Database (Allen, Kennard & Taylor, 1983).

The purchase of the single crystal diffractometer currently operating at the Universidad de Chile by Fundación Andes is gratefully acknowledged. This work was supported by the Universidad de Buenos Aires and by the Consejo Nacional de Investigaciones Cientificas y Tecnicas (CONICET). MP is a member of CONICET.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: FG1160). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Diphenylcyclopropene Complex of Tungsten, $[WCl_2O(PMePh_2)_2(\eta^2$-3,3-diphenylcyclopropene)], Precursor to a Tungsten–Oxo–Olefin Metathesis Catalyst

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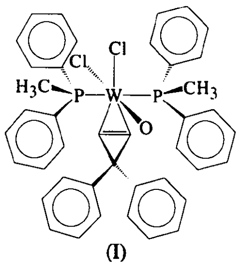
Abstract

The title compound, dichlorobis(methyldiphenylphosphine-*P*)[(1,2-η)-3,3-diphenylcyclopropene]oxotungsten, $[WCl_2O(C_{15}H_{12})(C_{13}H_{13}P)_2]$, is a mononuclear complex with an approximately octahedral environment around the metal atom. The 3,3-diphenylcyclopropene ligand is bonded to the W atom in a η^2-geometry, with effectively identical metal-to-carbon bond distances [W—C1 2.133 (7) and W—C2 2.131 (7) Å].

Comment

The development of well defined tungsten alkylidene-based metathesis catalysts has been an area of interest. In sharp contrast to the large number of arylimido-based metathesis catalysts that have been reported, there has been only one report of a tungsten–oxo–alkylidene metathesis catalyst (de la Mata & Grubbs, 1996). The title compound, (I), is a precursor to that catalyst. The active tungsten–oxo–vinyl-alkylidene is obtained from the title compound by ring opening of the cyclopropene, facilitated by the addition of lithium alkoxide salts (de la Mata & Grubbs, 1996).



(I)

Drawings of the tungsten complex are shown in Figs. 1 and 2, with a packing diagram shown in Fig. 3. The ligands are arranged around the W atom in a distorted octahedron. The phosphine ligands are *trans* with respect to one another and the P—W—P angle [154.99 (7)°] suggests there is significant steric crowding between the phosphine and olefin ligands. This steric effect is also observed in $[W(PMePh_2)_2Cl_2O(\eta^2$-ethylene)] (Su, Cooper, Geib, Rheingold & Mayer, 1986). The P—W bond distances are nearly identical; P1—W 2.590 (2) and P2—W 2.598 (2) Å. Three of the remaining coordination sites are occupied by two *cis*-chloride ligands [Cl2—W—Cl1 85.76 (7)°] and an oxo O atom [O—W—Cl1 174.3 (2) and O—W—Cl2 88.7 (2)°]. The tungsten–chloride bond *trans* to the oxo ligand (Cl1) is longer than the *cis* bond distance [Cl1—W 2.487 (2) and Cl2—W 2.471 (2) Å], consistent with the *trans* influence observed in other dichloride–tungsten–oxo complexes (Churchill & Rheingold, 1982; Chiu, Lyons, Wilkinson, Thornton-Pett & Hursthouse, 1983; Su *et al.*, 1986; Bryan, Geib, Rheingold & Mayer, 1987; Yoon, Parkin, Hughes & Leigh, 1992). The W—O distance of 1.692 (4) Å is identical to the average terminal W—O bond length reported for 22 other tungsten–oxo complexes (Orpen, Brammer, Allen, Kennard, Watson & Taylor, 1989). The last site is occupied by 3,3-diphenylcyclopropene, with the C=C bond parallel (within 0.4°) to the P···P vector. The W—C distances are identical within their e.s.d.'s [C1—W 2.133 (7) and C2—W 2.131 (7) Å] and the C=C bond is long [C1=C2 1.447 (9) Å]. Similar lengthening of the C=C bond is found in the crystal structures of other η^2-cyclopropene complexes (Johnson, Grubbs & Ziller, 1993; Li, Nguyen, Grubbs & Ziller, 1994). The two single bonds of the cyclopropene ring are slightly shortened, averaging 1.502 (6) Å. The P—C distances range from 1.800 to 1.825 Å, with an average value of 1.817 (4) Å. The C—C distances in the phenyl rings

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