

Table 4. Hydrogen-bonding geometry (Å, °) for (2)

D—H...A	D—H	H...A	D...A	D—H...A
O3—H3A...Cl	1.02	2.27	3.127 (6)	140
O4—H4A...Br	0.85	2.70	3.451 (6)	148
O4—H4B...O2 ^l	1.04	1.74	2.754 (6)	164
O5—H5A...Cl ^{ll}	0.92	2.24	3.142 (6)	152
O5—H5B...Br ^{ll}	1.05	2.41	3.367 (6)	163
O6—H6A...Br ^l	1.07	2.32	3.321 (7)	163
O6—H6B...Cl ^{ll}	1.11	2.01	3.057 (6)	157
O7—H7A...Cl	1.05	2.17	3.093 (7)	146
O8—H8...Br	1.11	2.11	3.219 (6)	173

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

For both structures, H atoms attached to carbon were placed in calculated positions (*SHELXL HFIX* 23 instruction; C—H = 0.97 Å) and allowed to ride with isotropic displacement parameters 20% larger than those of the attached C atom. Locations of H atoms bound to oxygen were obtained from difference maps. For (1), reasonable locations for all H atoms could be found but, for (2), one H atom each on O3 and O7 could not be located with confidence. Attempts to refine H atoms attached to oxygen were unsuccessful so they were positioned in the locations indicated by the difference maps and allowed to ride with isotropic displacement parameters 20% larger than those of the attached O atoms.

For both compounds, data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*. Data reduction: *PROCESS* in *MolEN* (Fair, 1990) for (1); *XCAD4* (Harms & Wocadlo, 1987) for (2). Program(s) used to solve structures: *SIR88* (Burla *et al.*, 1989) for (1); *SHELXS86* (Sheldrick, 1990) for (2). Program(s) used to refine structures: *LSFM* in *MolEN* for (1); *SHELXL93* (Sheldrick, 1993) for (2). For both compounds, molecular graphics: *SHELXTL-Plus* (Sheldrick, 1994); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1475). Services for accessing these data are described at the back of the journal.

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Bis{(μ -acetato)[μ -bis(salicylidene)-1,3-propanediaminato]copper(II)}cadmium(II) Dioxane Solvate†

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Abstract

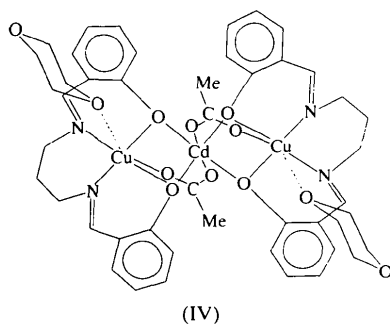
The title compound, [Cd{Cu(CH₃CO₂)(C₁₇H₁₆N₂O₂)₂]₂·C₄H₈O₂, is a linear hetero-trinuclear complex with a central Cd^{II} ion and lies on an inversion centre. This central Cd^{II} ion has an irregular octahedral coordination. The coordination around the Cd^{II} ion involves four O atoms from two *N,N'*-bis(salicylidene)-1,3-propanediaminato (SALPD²⁻) and two acetate ligands. The terminal Cu^{II} ions have an irregular square-pyramidal coordination. The coordination of the terminal Cu^{II} atom is provided by the two O and two N atoms from an SALPD²⁻ ligand and one O atom from an acetate ligand. The Cd...Cu bridging distance is 3.244 (3) Å.

Comment

Syntheses and structures of oxygen-bridged trimeric linear homometal and heterometal complexes based on Schiff base ligands, such as [Cd{Ni(SALPD)(CH₃CO₂)-

† Alternative name: bis(μ -acetato)-1:2 κ^2 O':1:3 κ^2 O':O'-bis{ μ -2,2'-[1,3-propanediy]bis(nitrilomethylidene)diphenolato}-1 κ^2 O,O':2 κ^4 N,N'.O.O':1 κ^2 O,O':3 κ^4 N,N'.O.O'-cadmium(II)dicopper(II) dioxane solvate.

(dmf)₂] (dmf is dimethylformamide; Ülkü, Tahir *et al.*, 1997), [Ni₃{(SALPD)(CH₃CO₂)(dmso)}₂] (dmso is dimethyl sulfoxide; Ülkü, Ercan *et al.*, 1997) and [Mn{Ni(SALPD)(CH₃CO₂)(dmf)}₂] (Ercan & Atakol, 1998), have been the subject of interest in this laboratory owing to their magnetic superexchange interactions between the bridged metal ions. Structural details for [Zn{(CH₃CO₂)₂(SALPD)Cu}₂] (Fukuhara *et al.*, 1990) and [M₃(SALPN)₂(CH₃CO₂)₂].2dmf [*M* = Co²⁺ or Fe²⁺, and SALPN is *N,N'*-bis(salicylidene)-2,2-dimethylpropylenediamine; Gerli *et al.*, 1991] are also available. We report here a new linear heterometal trinuclear complex, [Cd{Cu(SALPD)(CH₃CO₂)₂}₂].C₄H₈O₂, (IV).



The structure consists of a centrosymmetric trinuclear species with the central Cd ion occupying an inversion centre. The coordination around cadmium (Fig. 1) is a distorted octahedron involving four bridging O atoms from two SALPD²⁻ ligands in the equatorial plane and an O atom from each of the two bridging acetate groups in the apical positions.

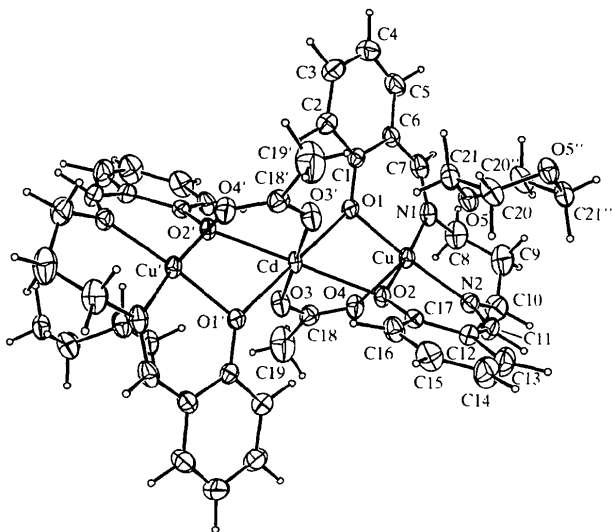


Fig. 1. The molecular structure of the title compound with the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, -y, 1-z$.]

The two inversion-related Cu^{II} ions have irregular square-pyramidal coordination polyhedra, with the four equatorial positions occupied by the two N and the two O atoms of the SALPD²⁻ ligand. There is an O atom from the bridging acetate group in the axial positions of these irregular square-pyramidal polyhedra. The substantial distortion of the square pyramids is revealed by the bond angles between apical and equatorial donor atoms: O4—Cu—N1 94.6(3), O4—Cu—N2 96.5(3), O4—Cu—O1 93.5(2) and O4—Cu—O2 90.8(3)°. The average of these bond angles is 93.8(3)°, greater than the normal angle (90°) in a regular square pyramid. There is less distortion in equatorial positions. The bond angles between the donor atoms in this direction are defined as O1—Cu—O2 84.4(1), O1—Cu—N1 89.5(1), N1—Cu—N2 94.4(2) and O2—Cu—N2 90.8(3)°. The dihedral angle between the equatorial planes [O1, O2, O1ⁱ, O2ⁱ and O1, O2, N1, N2; symmetry code: (i) $-x, -y, -z$] of the neighbouring polyhedra sharing atoms O1 and O2 is 21.51(8)°. The Cu atom is $-0.1353(4)$ Å out of the equatorial best plane defined by O1, O2, N2 and N1. The Cd...Cu distance is 3.244(3) Å.

The SALPD²⁻ ligand is not planar. The dihedral angles between the equatorial plane (O1, O2, N1, N2) and the two salicylaldimine residues (N2, C11, C12—C17, O2 and N1, C7, C1—C6, O1) are 31.24(10) and 37.24(6)°, respectively. These angles are similar to those reported by Ülkü, Ercan *et al.* (1997), Ülkü, Tahir *et al.* (1997) and Ercan & Atakol (1998). The six-membered chelate ring (Cu, N1, C8, C9, C10, N2) has a chair conformation. The distances of the two *para*-positioned chair atoms, Cu and C9, from the best plane of the six atoms are $-0.0937(4)$ and $0.277(5)$ Å, respectively. In the Cd^{II} coordination sphere, the Cd—O_{SALPD²⁻} bond lengths [2.280(3)—2.310(3) Å] are longer than the Cd—O_{acetate} distances [2.238(2) Å]. The Cu—O bond lengths are in the range 1.953(3)—2.324(2) Å, the longest distance being to the acetate O atom. The Cu—N1 and Cu—N2 bond lengths are 1.972(3) and 1.993(3) Å, respectively. The bond lengths are shorter than the Ni—N distances [average 2.018(2) Å] reported by Gerli *et al.* (1991), Ülkü, Tahir *et al.* (1997), Ülkü, Ercan *et al.* (1997) and Ercan & Atakol (1998).

A comparison of the dihedral angles between the two equatorial planes of the neighbouring polyhedra (φ) and between the *M*(Ni, Cu)—O—*M*(Ni, Cu, Mn)—O bridging plane and the coordination plane around the central atom (κ), along with the related distance ranges and bridging angles, are given in Table 2 for the four trimeric metal complexes recently studied in this laboratory. Although the type of metal ions and some of the coordinating groups are different in the complexes mentioned above, the coordination around the metal ions is very similar in the first three trimeric metal complexes recently studied in this laboratory. However, the coordination of the inversion-related terminal Cu

ions observed in (IV) is slightly different from these compounds. Dioxane solvate bridges between the two trimeric complexes of the neighbouring unit cell. The Cu...O5ⁱ distance is 2.627 (3) Å. In this state, it can be thought that the two terminal Cu^{II} ions also have an approximate irregular octahedral coordination. The dioxane solvate has a chair conformation and lies on an inversion centre. Atoms O5 and O5ⁱⁱ [symmetry code: (ii) $-x, -y, 1-z$] of the dioxane lie ± 0.6622 (3) Å from the plane of the C atoms. The shortest intramolecular H...H contacts, H7...H81 and H82...H101, are 1.92 and 2.11 Å, respectively.

The magnetic behaviour of these compounds is currently under investigation.

Experimental

To a solution of *N,N'*-bis(salicylidene)-1,3-propanediamine (0.840 g, 3 mmol) in hot ethanol (50 ml), ammonia solution (20%, 10 ml) was added and the mixture was heated to boiling point. A solution of CuCl₂·2H₂O (0.510 g, 3 mmol) in hot water (20 ml) was added and the resulting mixture was set aside for 6 to 7 h. The green Cu complex was filtered and dried at 383 K for 3 h. This complex (0.344 g, 1 mmol) was dissolved in hot dioxane (50 ml). Dropwise addition of Cd(AcO)₂ (0.115 g, 0.5 mmol) solution in hot methanol (20 ml) to the final mixture resulted in the formation of green crystals after 4 d. The green crystals were filtered off and dried in air.

Crystal data

[CdCu₂(C₂H₃O₂)₂(C₁₇H₁₆-N₂O₂)₂].C₄H₈O₂
M_r = 1016.42
 Triclinic
 $P\bar{1}$
 $a = 10.2266$ (9) Å
 $b = 10.7507$ (11) Å
 $c = 11.0355$ (8) Å
 $\alpha = 64.400$ (7)°
 $\beta = 70.297$ (7)°
 $\gamma = 78.614$ (8)°
 $V = 1028.2$ (2) Å³
 $Z = 1$
 $D_x = 1.64$ Mg m⁻³
 D_m not measured

Mo $K\alpha$ radiation
 $\lambda = 0.71073$ Å
 Cell parameters from 25 reflections
 $\theta = 10-18^\circ$
 $\mu = 1.60$ mm⁻¹
 $T = 295$ K
 Prismatic
 $0.32 \times 0.24 \times 0.16$ mm
 Green

Data collection

Enraf-Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: empirical *via* ψ scans (North *et al.*, 1968)
 $T_{\min} = 0.680, T_{\max} = 0.774$
 4415 measured reflections
 4173 independent reflections

3017 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$
 $\theta_{\max} = 26.3^\circ$
 $h = -12 \rightarrow 0$
 $k = -13 \rightarrow 13$
 $l = -13 \rightarrow 12$
 3 standard reflections
 frequency: 120 min
 intensity decay: 1.4%

Refinement

Refinement on F
 $R = 0.033$
 $wR = 0.042$
 $S = 1.08$
 3017 reflections
 268 parameters
 H atoms: see below
 $w = 1/[\sigma F^2 + (0.02F)^2 + 0.10]$

$(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.92$ e Å⁻³
 $\Delta\rho_{\min} = -0.14$ e Å⁻³
 Extinction correction: none
 Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. Selected geometric parameters (Å, °)

Cd—Cu	3.244 (3)	O5—C20	1.428 (7)
Cd—O1	2.280 (3)	O5—C21	1.440 (5)
Cd—O2	2.310 (3)	N1—C7	1.284 (5)
Cd—O3	2.238 (2)	N1—C8	1.473 (6)
Cu—O1	1.970 (3)	N2—C10	1.479 (6)
Cu—O2	1.953 (3)	N2—C11	1.270 (5)
Cu—N1	1.972 (3)	C6—C7	1.429 (6)
Cu—N2	1.993 (3)	C8—C9	1.479 (7)
O1—C1	1.319 (4)	C9—C10	1.503 (7)
O2—C17	1.317 (4)	C11—C12	1.445 (7)
O3—C18	1.249 (6)	C18—C19	1.521 (6)
O4—C18	1.230 (6)		
O1—Cd—O2	70.06 (9)	C7—N1—C8	117.3 (4)
O1—Cd—O3	87.1 (1)	Cu—N2—C10	121.6 (2)
O2—Cd—O3	89.3 (1)	Cu—N2—C11	122.2 (3)
O1—Cu—O2	84.4 (1)	C10—N2—C11	116.2 (4)
O1—Cu—N1	89.5 (1)	O1—C1—C2	120.6 (4)
O1—Cu—N2	168.93 (9)	O1—C1—C6	121.7 (4)
O2—Cu—N1	172.1 (1)	N1—C7—C6	127.3 (4)
N1—Cu—N2	94.4 (2)	N1—C8—C9	112.4 (3)
Cd—O1—C1	132.6 (3)	C8—C9—C10	115.9 (5)
Cu—O1—C1	123.1 (3)	N2—C10—C9	114.3 (3)
Cd—O2—Cu	98.7 (1)	N2—C11—C12	128.0 (4)
Cd—O2—C17	131.9 (3)	O2—C17—C12	122.3 (4)
Cu—O2—C17	124.9 (3)	O2—C17—C16	120.0 (4)
Cd—O3—C18	131.9 (3)	O3—C18—O4	128.0 (3)
C20—O5—C21	109.3 (3)	O3—C18—C19	112.4 (5)
Cu—N1—C7	122.9 (3)	O4—C18—C19	119.6 (5)
Cu—N1—C8	119.7 (2)		

Table 2. Structural data, bridging angles and dihedral angles (φ and κ) for four homo- or hetero-trinuclear complexes

M_{terminal} atoms are Ni²⁺ and Cu²⁺, and M_{central} atoms are Ni²⁺, Cd²⁺ and Mn²⁺.

Complex	$M_{\text{terminal}}-\text{O}$ (Å)	$M_{\text{central}}-\text{O}$ (Å)	$M-M$ (Å)	O— M_{central} —O (°)	O— M_{terminal} —N (°)	φ (°)	κ (°)
(I)	2.010 (3)–2.254 (3)	2.024 (3)–2.098 (3)	3.043 (2)	79.4 (1)	89.8 (2)–90.6 (2)	21.9 (1)	33.1 (1)–35.06 (7)
(II)	2.012 (1)–2.190 (2)	2.260 (1)–2.293 (2)	3.227 (5)	73.66 (5)	88.09 (7)–89.76 (6)	23.10 (7)	26.38 (6)–32.80 (7)
(III)	2.017 (2)–2.184 (2)	2.163 (1)–2.194 (2)	3.133 (2)	76.66 (6)	88.93 (8)–90.38 (7)	23.68 (8)	26.91 (7)–32.36 (9)
(IV)	1.953 (3)–2.324 (2)	2.280 (3)–2.310 (3)	3.244 (3)	70.06 (9)	89.5 (1)–90.8 (1)	21.51 (8)	31.24 (10)–37.24 (6)

Notes: (I) is [Ni₃(CH₃CO₂)₂(SALPD)₂(dmsO)₂] (Ülkü, Ercan *et al.*, 1997), (II) is [CdNi₂(CH₃CO₂)₂(SALPD)₂(dmf)₂] (Ülkü, Tahir *et al.*, 1997), (III) is [MnNi₂(CH₃CO₂)₂(SALPD)₂(dmf)₂] (Ercan & Atakol, 1998) and (IV) is [CdCu₂(CH₃CO₂)₂(SALPD)₂].C₄H₈O₂ (title compound).

All non-H atoms were refined with anisotropic displacement parameters. H-atom positions were taken from difference maps. For all H atoms, $U_{\text{iso}}(\text{H}) = 1.3U_{\text{eq}}(\text{C})$ of the parent atom and a riding model was used.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1993). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SIMPEL* in *MolEN*. Program(s) used to refine structure: *LSFM* in *MolEN*. Molecular graphics: *MolEN* version of *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *MolEN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1131). Services for accessing these data are described at the back of the journal.

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Di-*n*-butylbis(2-phenylquinazoline-4-thiolato-*N*³,*S*)tin(IV)

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Abstract

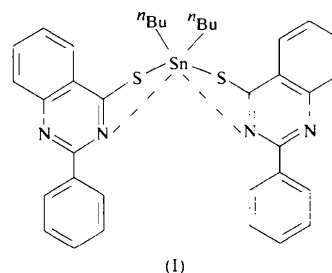
The central Sn atom in the title complex, [Sn(C₄H₉)₂(C₁₄H₉N₂S)₂], is located on a twofold axis. The coordination polyhedron about the Sn atom is a skew-

trapezoidal bipyramid. The trapezoidal plane is formed by the two 2-phenylquinazoline-4-thiolate residues, which act as bidentate ligands with *cis*-Sn—S and *cis*-Sn—N bonds. The axial C atoms are shifted towards the half-sphere occupied by two N atoms, resulting in a C—Sn—C angle of 131.1 (2)°. Each phenyl substituent is twisted with respect to the mean plane of the quinazoline system.

Comment

For diorganotin(IV) bis-chelates, the coordination polyhedron around the Sn atom is either a regular *trans* or *cis* octahedron, or a distorted skew-trapezoidal bipyramid (STB), depending on the nature of the C- and heteroatom-donor ligands (Kumar Das *et al.*, 1987). Distortion from an octahedron to an STB is especially favoured if the chelate bite angle is small (Kepert, 1976, 1977).

The structure of the title compound, (I), consists of discrete molecules. The shortest intermolecular contact [3.504 (7) Å] is N1...C16(−*x*, −*y*, 1 − *z*).



The coordination about Sn is skew-trapezoidal bipyramidal, with two S [Sn—S1 2.469 (2) Å] and two N atoms of the chelating groups occupying the trapezoidal plane, and the butyl groups [Sn—C 2.107 (4) Å] occupying the axial positions. The bond distance Sn—N3 [2.724 (4) Å] is appreciably shorter than the sum of the appropriate van der Waals radii (3.75 Å; Bondi, 1964) and indicates the bidentate nature of the ligand. These bonds draw the quinazoline groups closer together, but result in severe steric repulsion between these groups (Kepert, 1976). Similar distances have been reported for Me₂Sn(NO₃)₂ (2.70 Å; Hilton *et al.*, 1973), Bu₂Sn(2-SPy-5-NO₂)₂ (2.77 Å; SPy is pyridinethiolate; Domazetis *et al.*, 1979), Me₂Sn(2-SPy)₂ (2.70 Å; Castano *et al.*, 1990), Cyhex₂Sn(2-SPy)₂ (2.72 Å; Cyhex is cyclohexyl; Boualam *et al.*, 1992) and Ph₂Sn(2-SPy)₂ [2.634 (4) and 2.698 (4) Å; Schmiedgen *et al.*, 1993].

Each quinazoline ring adopts an almost planar conformation with maximum deviations from the mean planes through each half of the ring system exhibited by C5 [−0.005 (6) Å] and C4 [0.017 (5) Å]; the dihedral angle between the planes is 2.8 (2)°. The phenyl ring is not