

- Sutton, L. E. (1965). *Tables of Interatomic Distances and Configurations in Molecules and Ions*, Supplement. London: The Chemical Society.
- Tian, Y.-P., Duan, C.-Y., Zhao, C.-Y., You, X.-Z., Mak, T. C. W. & Zhang, Z.-Y. (1997). *Inorg. Chem.* **36**, 1247–1252.
- Togni, A. & Rihs, G. (1993). *Organometallics*, **12**, 3368–3376.
- Williams, D. J. (1984). *Angew. Chem. Int. Ed. Engl.* **23**, 690–695.

Acta Cryst. (1999). **C55**, 2060–2061

[N,N'-Bis(salicylidene)ethylenediaminato-N,N',O,O']platinum(II)

WOLFGANG SAWODNY,^a ULF THEWALT,^b EDITH POTTHOFF^a AND REINHARD OHL^a

^aAbteilung Anorganische Chemie I, Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany, and ^bSektion für Röntgen- und Elektronenbeugung, Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany. E-mail: ulf.thewalt@chemie.uni-ulm.de

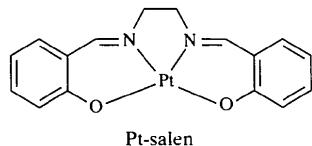
(Received 17 February 1999; accepted 5 August 1999)

Abstract

The title compound, [Pt(C₁₆H₁₄N₂O₂)], is nearly planar. There is pairing of two molecules with a Pt···Pt distance of 3.277(1) Å indicating weak interaction. The pairs form puckered layers in the (010) planes.

Comment

A great number of structures of Schiff base complexes of divalent first row transition metal ions are well known. They exhibit either planar (Akhtar & Drew, 1982) or tetrahedral (Fox *et al.*, 1964) coordination around the central atom. Also, widening of the coordination sphere by additional metal–metal (Shkol'nikova *et al.*, 1970) or metal–base (Hall *et al.*, 1968) interactions can occur. No complete structural data of heavier transition metals, especially of group ten metals, are known so far. Only the point group and unit-cell dimensions of the Pd-salen complex have been reported (Shkol'nikova *et al.*, 1963), though this complex exhibits interesting catalytic properties (Henrici-Olivé & Olivé, 1974). The structure of Pt-salen described here is the first one reported for this type of complex.



The whole molecule is nearly planar with a hardly perceptible arch-like deviation from the long axis (Fig. 1). The tetrahedral distortion around the Pt ion is very small, as indicated by the deviations of the ligating atoms from the best plane defined by them: O1 0.015(2), O2 –0.015(2), N1 –0.016(2) and N2 0.016(2) Å. The Pt atom deviates by 0.007(2) Å and the maximum deviation from the plane is shown by C15 [0.373(9) Å], giving the PtN₂(CH₂)₂ ring an envelope form.

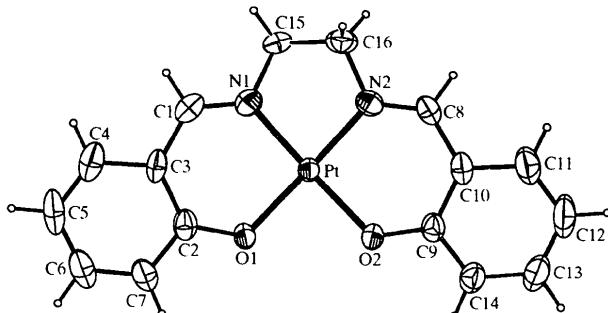


Fig. 1. The molecular structure of Pt-salen showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

The arrangement of the molecules within the crystal lattice (Fig. 2) is in pairs with a rotation of 180° and a Pt···Pt distance of 3.277(1) Å indicating metal–metal interaction as in the analogous Ni-salen complex (3.21 Å; Gaetani Manfredotti & Guastini, 1983). These pairs form puckered layers with an alternate tilt angle of ±24.4(3)° from the (010) plane. The analogy of the lattice constants of Pd-salen to Pt-salen suggests a similarity of the structures with only slightly different geometrical data.

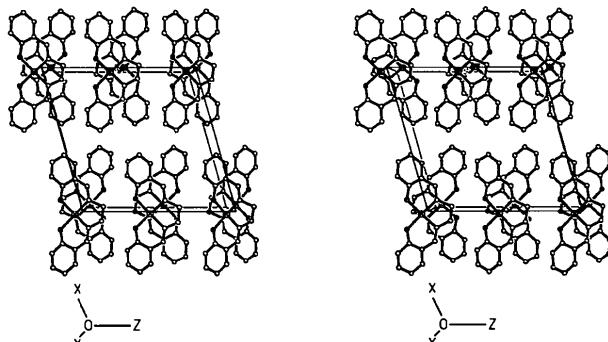


Fig. 2. Stereoscopic view of the crystal structure of Pt-salen down the y axis.

Experimental

Pt-salen was prepared by stirring a mixture of Pt(en)Cl₂ (0.5 g) and the Tl salt of salicylaldehyde (1 g) in absolute *N,N'*-dimethylformamide (70 ml) for 20 d at 333 K. Vine-red

crystals of Pt-salen crystallize from the solution together with TlCl and can be separated mechanically because of the colour. The product can be recrystallized from chloroform. Elemental analysis (%): C 41.21 (41.65), H 3.06 (3.06), N 6.07 (6.07), Pt 42.04 (42.28) (theoretical values in brackets).

Crystal data

[Pt(C₁₆H₁₄N₂O₂)]

$M_r = 461.39$

Monoclinic

$P2_1/c$

$a = 13.788$ (2) Å

$b = 7.3827$ (12) Å

$c = 14.0672$ (17) Å

$\beta = 105.66$ (2)°

$V = 1378.8$ (4) Å³

$Z = 4$

$D_x = 2.223$ Mg m⁻³

D_m not measured

Mo K α radiation

$\lambda = 0.71069$ Å

Cell parameters from 16 reflections

$\theta = 15.1-18.4^\circ$

$\mu = 10.182$ mm⁻¹

$T = 293$ (2) K

Fragment cut from a larger crystal

0.38 × 0.24 × 0.15 mm

Red

Data collection

Stoe-modified Philips PW1100 diffractometer

ω -2θ scans

Absorption correction:

ψ scan (X-RED; Stoe & Cie, 1994a)

$T_{\min} = 0.048$, $T_{\max} = 0.217$

4850 measured reflections

2425 independent reflections

2195 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 24.99^\circ$

$h = -16 \rightarrow 16$

$k = 0 \rightarrow 8$

$l = -16 \rightarrow 16$

3 standard reflections frequency: 60 min intensity decay: 3%

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.068$

$S = 1.051$

2425 reflections

191 parameters

H atoms constrained

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.570$ e Å⁻³ (0.89 Å from Pt)

$\Delta\rho_{\min} = -2.026$ e Å⁻³ (0.93 Å from Pt)

Extinction correction:

SHELXL97 (Sheldrick, 1997a)

Extinction coefficient: 0.0071 (3)

Scattering factors from International Tables for Crystallography (Vol. C)

Table 1. Selected geometric parameters (Å, °)

Pt—N1	1.938 (5)	C8—N2	1.276 (8)
Pt—N2	1.950 (5)	C9—O2	1.310 (7)
Pt—O2	2.002 (4)	C15—C16	1.468 (9)
Pt—O1	2.006 (4)	C15—N1	1.497 (7)
C1—N1	1.288 (9)	C16—N2	1.483 (7)
C2—O1	1.305 (7)		
N1—Pt—N2	84.2 (2)	N1—Pt—O1	94.5 (2)
N2—Pt—O2	94.27 (19)	O2—Pt—O1	87.02 (15)

Data collection: STAD14 (Stoe & Cie, 1994b). Cell refinement: STAD14. Data reduction: X-RED (Stoe & Cie, 1994a). Program(s) used to solve structure: SHELXS97 (Sheldrick, 1997b). Program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a). Molecular graphics: PLATON (Spek, 1998) and ORTEPIII (Johnson & Burnett, 1996). Software used to prepare material for publication: SHELXL97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GS1038). Services for accessing these data are described at the back of the journal.

References

- Akhtar, F. & Drew, M. G. B. (1982). *Acta Cryst.* **B38**, 1149–1154.
- Fox, M. R., Orioli, P. L., Lingafelter, E. C. & Sacconi, L. (1964). *Acta Cryst.* **17**, 1159–1166.
- Gaetani Manfredotti, A. & Gaustini, C. (1983). *Acta Cryst.* **C39**, 863–865.
- Hall, D., Sheat, S. V. & Waters, T. N. (1968). *J. Chem. Soc. A*, pp. 460–463.
- Henrici-Olivé, G. & Olivé, S. (1974). *Angew. Chem.* **86**, 561–562.
- Johnson, C. K. & Burnett, M. N. (1996). ORTEPIII. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Sheldrick, G. M. (1997a). SHELXL97. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXS97. *Program for the Solution of Crystal Structures*. University of Göttingen, Germany.
- Shkol'nikova, L. M., Shugam, E. A. & Makarevich, L. G. (1963). *J. Struct. Chem.* **4**, 854–855.
- Shkol'nikova, L. M., Yumal, E. M., Shugam, E. A. & Voblikova, V. A. (1970). *J. Struct. Chem.* **11**, 819–823.
- Spek, A. L. (1998). PLATON. *Program for Calculations on X-ray Data*. University of Utrecht, The Netherlands.
- Stoe & Cie (1994a). X-RED. *Data Reduction Program*. Version 1.04. Stoe & Cie, Darmstadt, Germany.
- Stoe & Cie (1994b). STAD14. *Diffractometer Control Program*. Version 1.04. Stoe & Cie, Darmstadt, Germany.

Acta Cryst. (1999). **C55**, 2061–2063

Bis[μ -(hydrogen benzene-1,2-dicarboxylato)-O:O']bis[bis(1,10-phenanthroline-N,N')cobalt(II)] bis(hydrogen benzene-1,2-dicarboxylate) dihydrate

DEJAN POLETI,^a LJILJANA KARANOVIĆ,^b GORAN A. BOGDANOVIĆ^{c†} AND ANNE SPASOJEVIĆ-DE BIRÉ^c

^aDepartment of General and Inorganic Chemistry, Faculty of Technology and Metallurgy, PO Box 494, 11001 Belgrade, Yugoslavia, ^bLaboratory of Crystallography, Faculty of Mining and Geology, Djušina 7, 11000 Belgrade, Yugoslavia, and ^cÉcole Centrale Paris, Laboratoire de Physico-Chimie Moléculaire et Minérale, URA 1907 du CNRS, Grande Voie des Vignes, 92295 Châtenay-Malabry CEDEX, France

(Received 24 June 1999; accepted 6 August 1999)

Abstract

The structure of the title compound, [Co₂(C₈H₅O₄)₂·(C₁₂H₈N₂)₄](C₈H₅O₄)₂·2H₂O, consists of centrosym-

† Current address: Laboratory of Theoretical Physics and Condensed Matter Physics, Institute of Nuclear Sciences 'Vinča', 11001 Belgrade, PO Box 522, Yugoslavia.