

Na—O12	2.565 (2)	O1—C1	1.443 (3)
Na—O1 <sup>1</sup>	2.580 (2)	C1—C2	1.542 (4)
P1—O12	1.498 (2)	C2—C3	1.528 (4)
P1—O11	1.502 (2)	C3—C4	1.508 (4)
P1—O13	1.576 (2)	C4—N	1.489 (4)
P1—C1	1.860 (3)		
O12—P1—O11	117.2 (1)	O21—P2—C1	106.5 (1)
O12—P1—O13	106.0 (1)	O1—C1—C2	111.0 (2)
O11—P1—O13	111.3 (1)	O1—C1—P2	107.8 (2)
O12—P1—C1	110.3 (1)	C2—C1—P2	111.5 (2)
O11—P1—C1	106.0 (1)	O1—C1—P1	105.1 (2)
O13—P1—C1	105.4 (1)	C2—C1—P1	111.2 (2)
O22—P2—O23	116.8 (1)	P2—C1—P1	110.0 (1)
O22—P2—O21	110.9 (1)	C3—C2—C1	113.9 (2)
O23—P2—O21	106.6 (1)	C4—C3—C2	112.0 (2)
O22—P2—C1	108.4 (1)	N—C4—C3	110.7 (2)
O23—P2—C1	107.3 (1)		

Symmetry code: (i)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$ .

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

Normalized values are according to Jeffrey & Lewis (1978) and Taylor & Kennard (1983).

D—H...A	D—H	H...A	D...A	D—H...A
O1W—H1WA...O11 <sup>i</sup>	0.94	1.76	2.687 (3)	169
O1W—H1WB...O22 <sup>ii</sup>	0.94	1.87	2.767 (2)	159
O2W—H2WA...O1W	0.94	1.84	2.777 (3)	176
O2W—H2WB...O21 <sup>iii</sup>	0.94	2.04	2.945 (3)	163
O3W—H3WA...O11 <sup>iv</sup>	0.94	1.81	2.735 (3)	168
O3W—H3WB...O2W	0.94	2.00	2.932 (3)	172
N—HC...O11 <sup>v</sup>	1.03	1.96	2.866 (3)	145
N—HC...O1 <sup>v</sup>	1.03	2.33	3.023 (3)	124
N—HA...O2W <sup>vi</sup>	1.03	1.84	2.868 (3)	172
N—HB...O22 <sup>vii</sup>	1.03	1.87	2.879 (3)	166
O1—H1...O3W <sup>viii</sup>	0.94	1.74	2.677 (3)	173
O21—H21...O12 <sup>viii</sup>	0.94	1.70	2.619 (2)	164
O13—H13...O23 <sup>viii</sup>	0.94	1.59	2.520 (2)	170

Symmetry codes: (i)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (ii)  $1 + x, y, z$ ; (iii)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (iv)  $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$ ; (v)  $1 - x, 1 - y, 2 - z$ ; (vi)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (vii)  $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} + z$ ; (viii)  $x - 1, y, z$ .

Data collection: *P3/P4-PC Diffractometer Program* (Siemens, 1991). Cell refinement: *P3/P4-PC Diffractometer Program*. Data reduction: *XDISK* in *SHELXTL/PC* (Sheldrick, 1991). Program(s) used to solve structure: *XS* in *SHELXTL/PC*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XP* in *SHELXTL/PC*. Software used to prepare material for publication: *CIFTAB* in *SHELXL93*, *PARST* (Nardelli, 1983), *CSD* (Allen, Kennard & Taylor, 1983).

The authors would like to thank Dr Dora Tombari for suggesting the problem as well as for helpful discussions. The purchase of the single-crystal diffractometer currently operating at the Universidad de Chile by Fundación Andes is gratefully acknowledged. This work has been partially funded through project FONDECYT No. 1940515.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and indexed X-ray powder diffraction peaks have been deposited with the IUCr (Reference: FG1158). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1996). **C52**, 2201–2204

## Bis(acetato-*O*)bis(pyridine-*N*)palladium(II) Monohydrate and Bis(acetato-*O*)bis-(diethylamine-*N*)palladium(II)

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(Received 23 November 1994; accepted 2 May 1996)

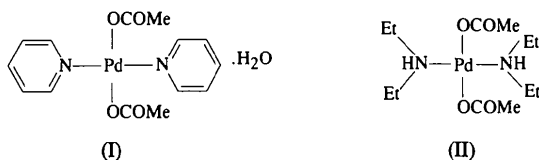
## Abstract

The title complexes, [Pd(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub>].H<sub>2</sub>O, (I), and [Pd(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>4</sub>H<sub>11</sub>N)<sub>2</sub>], (II), are typical of metal acetates with additional N-donor coordination. In both structures, the central Pd atom has a centrosymmetric square-planar environment. In the pyridine complex (I), carbonyl O atoms are involved in intermolecular O—H...O hydrogen bonds with water molecules and in the amine complex (II), they participate in intramolecular N—H...O hydrogen bonds. Owing to the latter, the Pd—N bond lengths are different with values of 2.010 (4) for complex (I) and 2.066 (2) Å for complex (II).

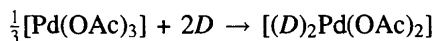
## Comment

In the course of our work on the relationship between the geometry of molecular complexes and

their formation enthalpies (Guryanova, Goldstein & Romm, 1975; Guryanova, 1975; Guryanova & Romm, 1992), we began to provide missing information on platinum metal complexes. We began recently to investigate systematically the structures and physico-chemical properties of palladium(II) diacetates with N-donor ligands (Romm, Buslayeva, Lyalina, Shifrina & Sinitsin, 1992; Lyalina, Dargina, Sobolev, Buslayeva & Romm, 1993). The present work reports the results of X-ray structure analyses of two such complexes, namely, [Pd(OCOCH<sub>3</sub>)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub>].H<sub>2</sub>O, (I), and [Pd(OCOCH<sub>3</sub>)<sub>2</sub>{NH(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>}<sub>2</sub>], (II).



In both title complexes, the Pd atom has square-planar coordination because it is sited on a symmetry centre (Figs. 1 and 2). An interesting feature is that the Pd—N bond is longer in (II) [2.066(2) Å] than in (I) [2.010(4) Å]. The formation enthalpy of complex (I) (93.7 kJ mol<sup>-1</sup>; measured calorimetrically in benzene solution) is substantially less than that of (II) (123.8 kJ mol<sup>-1</sup>) in the reaction



where all components are in solution, OAc is acetate and *D* is the N-donor molecule. This is due to the additional heat evolution when the two intramolecular hydrogen bonds are formed between the carbonyl O atoms and the amino groups (Fig. 2); N—H 0.71(3), H...O 2.13(3), N...O 2.785(4) Å and N—H...O 156(2)°. The N—Pd coordination bond in complex (II) decreases the electron density on the amino H atom and increases its ability to participate in hydrogen-bond formation.

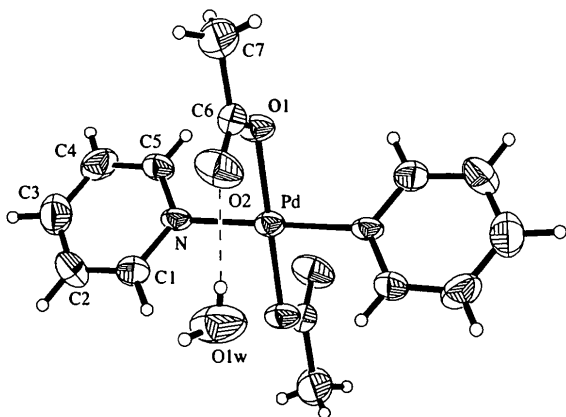


Fig. 1. The molecular structure of complex (I) with displacement ellipsoids shown at the 50% probability level.

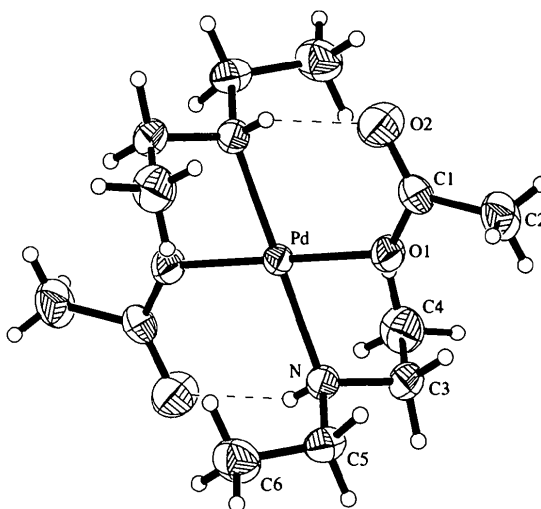


Fig. 2. The molecular structure of complex (II) with displacement ellipsoids shown at the 50% probability level.

This also affects the Pd coordination square. Owing to additional six-membered planar ring formation, the O—Pd—N bond angles in (II) are different [83.8(1) and 96.2(1)°], while in (I), where such intramolecular interactions are absent, these angles are practically equal [89.4(2) and 90.6(2)°]. In complex (I), the dihedral angle between the central square plane and the pyridine ring plane is 49.8°.

In complex (I), there are intermolecular O—H...O bonds between carbonyl O atoms and water molecules; O—H 0.72(6), H...O 2.13(8), O...O 2.824(6) Å, O—H...O 162(7)°. In (II), intermolecular contacts are of the usual van der Waals type.

## Experimental

The synthesis of palladium diacetate was carried out according to the method of Stephenson, Morehouse, Powell, Heffer & Wilkinson (1965). The complexes were obtained by slow evaporation of a benzene solution of the palladium salt and the corresponding amine (molar ratio 1:2).

### Complex (I)

#### Crystal data

[Pd(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub>].H<sub>2</sub>O

*M<sub>r</sub>* = 400.70

Monoclinic

*C*2/*c*

*a* = 12.383(2) Å

*b* = 11.802(3) Å

*c* = 11.373(5) Å

β = 94.57(3)°

*V* = 1656.8(9) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.606 Mg m<sup>-3</sup>

Mo *K*α radiation

λ = 0.71069 Å

Cell parameters from 12 reflections

θ = 10.0–12.5°

μ = 1.143 mm<sup>-1</sup>

*T* = 293(2) K

Prism

0.12 × 0.12 × 0.07 mm

Colourless

**Data collection**

Syntex P1 diffractometer  
 $\theta$ -2 $\theta$  scans  
 Absorption correction:  
 none  
 732 measured reflections  
 682 independent reflections  
 682 observed reflections  
 $[I > 2\sigma(I)]$

**Refinement**

Refinement on  $F^2$   
 $R(F) = 0.0269$   
 $wR(F^2) = 0.0499$   
 $S = 1.093$   
 682 reflections  
 139 parameters  
 H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0362P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = -0.006$

**Complex (II)****Crystal data**

$[\text{Pd}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_4\text{H}_{11}\text{N})_2]$   
 $M_r = 370.76$   
 Triclinic  
 $P\bar{1}$   
 $a = 8.089 (1) \text{ \AA}$   
 $b = 7.173 (1) \text{ \AA}$   
 $c = 8.480 (1) \text{ \AA}$   
 $\alpha = 88.70 (1)^\circ$   
 $\beta = 65.76 (1)^\circ$   
 $\gamma = 80.80 (1)^\circ$   
 $V = 442.4 (1) \text{ \AA}^3$   
 $Z = 1$   
 $D_x = 1.392 \text{ Mg m}^{-3}$

**Data collection**

Nicolet P3 diffractometer  
 $\theta/2\theta$  scans  
 Absorption correction:  
 none  
 1671 measured reflections  
 1569 independent reflections  
 1569 observed reflections  
 $[I > 2\sigma(I)]$

**Refinement**

Refinement on  $F^2$   
 $R(F) = 0.0188$   
 $wR(F^2) = 0.0480$   
 $S = 1.080$   
 1569 reflections  
 144 parameters  
 H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 0.0174P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$\theta_{\max} = 24.97^\circ$   
 $h = -14 \rightarrow 14$   
 $k = 0 \rightarrow 14$   
 $l = 0 \rightarrow 8$   
 3 standard reflections  
 monitored every 100  
 reflections  
 intensity decay: none

$\Delta\rho_{\max} = 0.371 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.466 \text{ e \AA}^{-3}$   
 Extinction correction:  
 SHELXL93  
 Extinction coefficient:  
 0.0009 (3)  
 Atomic scattering factors  
 from *International Tables*  
 for *Crystallography* (1992),  
 Vol. C, Tables 4.2.6.8 and  
 6.1.1.4)

Mo  $K\alpha$  radiation  
 $\lambda = 0.71069 \text{ \AA}$   
 Cell parameters from 12  
 reflections  
 $\theta = 10\text{--}12.5^\circ$   
 $\mu = 1.059 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 Prism  
 $0.25 \times 0.20 \times 0.15 \text{ mm}$   
 Colourless

$\theta_{\max} = 25.05^\circ$   
 $h = -8 \rightarrow 9$   
 $k = -8 \rightarrow 8$   
 $l = 0 \rightarrow 10$   
 3 standard reflections  
 monitored every 100  
 reflections  
 intensity decay: 1%

$(\Delta/\sigma)_{\max} = 0.011$   
 $\Delta\rho_{\max} = 0.310 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.254 \text{ e \AA}^{-3}$   
 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 ( $\text{\AA}^2$ )**

$$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\cdot a_j.$$

	x	y	z	$U_{\text{eq}}$
<b>Complex (I)</b>				
Pd	1/2	0	0	0.0318 (2)
O1	0.4375 (3)	0.1280 (3)	0.0892 (3)	0.0400 (9)
O2	0.4143 (3)	0.2372 (3)	-0.0703 (4)	0.0595 (12)
N	0.6495 (3)	0.0598 (4)	0.0454 (4)	0.0328 (11)
C1	0.7208 (5)	0.0741 (5)	-0.0351 (6)	0.046 (2)
C2	0.8249 (5)	0.1115 (6)	-0.0062 (8)	0.061 (2)
C3	0.8559 (6)	0.1365 (7)	0.1085 (9)	0.062 (2)
C4	0.7830 (5)	0.1223 (6)	0.1910 (8)	0.055 (2)
C5	0.6808 (4)	0.0838 (5)	0.1568 (6)	0.040 (2)
C6	0.4116 (4)	0.2204 (4)	0.0351 (6)	0.038 (2)
C7	0.3736 (8)	0.3120 (8)	0.1149 (11)	0.063 (3)
O1W	1/2	0.1080 (7)	-1/4	0.088 (3)
<b>Complex (II)</b>				
Pd	1/2	1/2	1/2	0.04155 (9)
O1	0.4807 (2)	0.6215 (3)	0.2910 (2)	0.0602 (4)
O2	0.1943 (3)	0.6148 (4)	0.3288 (3)	0.0979 (8)
N	0.7633 (3)	0.5630 (3)	0.3915 (3)	0.0488 (4)
C1	0.3457 (4)	0.6558 (4)	0.2484 (3)	0.0569 (6)
C2	0.3844 (7)	0.7570 (6)	0.0829 (5)	0.0844 (9)
C3	0.8772 (4)	0.4681 (4)	0.2200 (3)	0.0624 (6)
C4	0.8965 (5)	0.2584 (5)	0.2234 (5)	0.0842 (9)
C5	0.7655 (4)	0.7682 (4)	0.3895 (4)	0.0624 (6)
C6	0.6820 (5)	0.8588 (5)	0.5682 (5)	0.0830 (9)

**Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )**

<b>Complex (I)</b>		<b>Complex (II)</b>	
Pd—O1	2.009 (3)	Pd—O1	2.010 (2)
Pd—N	2.010 (4)	Pd—N	2.066 (2)
O1—C6	1.281 (6)	O1—C1	1.272 (3)
O2—C6	1.219 (7)	O2—C1	1.213 (3)
N—C5	1.325 (7)	N—C3	1.474 (3)
N—C1	1.333 (7)	N—C5	1.475 (3)
C1—C2	1.377 (8)	C1—C2	1.504 (4)
C2—C3	1.362 (11)	C3—C4	1.488 (5)
C3—C4	1.362 (10)	C5—C6	1.496 (4)
C4—C5	1.372 (8)	C6—C7	1.510 (10)
O1—Pd—N <sup>i</sup>	90.6 (2)	O1—Pd—N	83.79 (7)
O1—Pd—N	89.4 (2)	O1—Pd—N <sup>ii</sup>	96.21 (7)
C6—O1—Pd	119.3 (4)	C1—O1—Pd	130.7 (2)
C5—N—C1	118.1 (5)	C3—N—C5	111.9 (2)
C5—N—Pd	120.9 (4)	C3—N—Pd	113.4 (2)
C1—N—Pd	121.0 (4)	C5—N—Pd	112.5 (2)
N—C1—C2	122.3 (7)	O2—C1—O1	125.8 (2)
C3—C2—C1	119.0 (7)	O2—C1—C2	119.5 (3)
C2—C3—C4	118.8 (7)	O1—C1—C2	114.7 (3)
C3—C4—C5	119.5 (7)	N—C3—C4	112.9 (2)
N—C5—C4	122.3 (6)	N—C5—C6	112.0 (2)
O2—C6—O1	125.8 (5)		
O2—C6—C7	120.6 (6)		
O1—C6—C7	113.5 (6)		

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

For both compounds, program(s) used to solve structures: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993).

SVK and IPR are grateful to the Russian Foundation for Fundamental Research for a grant.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: VS1019). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1996). **C52**, 2204–2206

### Aqua[bis(salicylidene)ethylenediaminato]-(isobutyl)cobalt(III)

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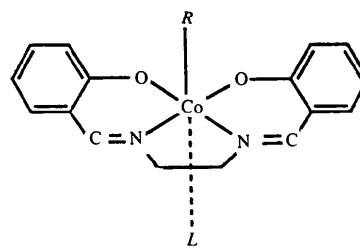
(Received 24 February 1993; accepted 4 July 1996)

## Abstract

The title B<sub>12</sub> model compound, aqua{2,2'-[1,2-ethanediybis(nitrilomethylidene)]diphenolato-*N,N',O,O'*}(isobutyl)cobalt(III), [Co(C<sub>4</sub>H<sub>9</sub>)(C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>)(H<sub>2</sub>O)], has distorted octahedral stereochemistry around the Co<sup>III</sup> ion. The equatorial salen ligand displays a 'stepped' conformation, which is the preferred conformation in penta- and hexacoordinate organocobalt-salen complexes. The axial Co—C bond length is close to that of coenzyme B<sub>12</sub> and in accordance with those of other B<sub>12</sub> models, but the difference in the axial Co—O bond length as well as the deviation from the ideal tetrahedral value of the Co—C—C angle are due to the *trans* influence of the axial isobutyl group, which has stronger  $\sigma$ -donor power.

## Comment

The title compound, (1), was studied as a coenzyme B<sub>12</sub> model compound (Halpern, 1982).



(1)  $R = i\text{Bu}$ ,  $L = \text{H}_2\text{O}$

The X-ray analysis of (1) showed that the crystal consists of discrete molecules with distorted octahedral stereochemistry (Fig. 1). The salen ligand, coordinated to the Co<sup>III</sup> ion *via* its two N and two O atoms, is in the equatorial plane, the atoms of which are coplanar to within  $\pm 0.014$  Å. One isobutyl group and one H<sub>2</sub>O molecule occupy the two axial positions. The Co<sup>III</sup> ion lies above the N<sub>2</sub>O<sub>2</sub> mean plane by 0.078 Å, towards the isobutyl group. The isobutyl group is oriented with respect to the equatorial salen plane in such a way that it lies above and towards the plane through O1, N1, C1, C12, C16 and C11. As a result, the O1—Co—C5 and N1—Co—C5 angles are slightly larger than the O2—Co—C5 and N2—Co—C5 angles. The Co(salen) unit is significantly distorted from planarity, with an asymmetric 'stepped' conformation ( $\alpha \neq \gamma$ ), while the ethylenediamine bridge assumes an asymmetric half-chair conformation,

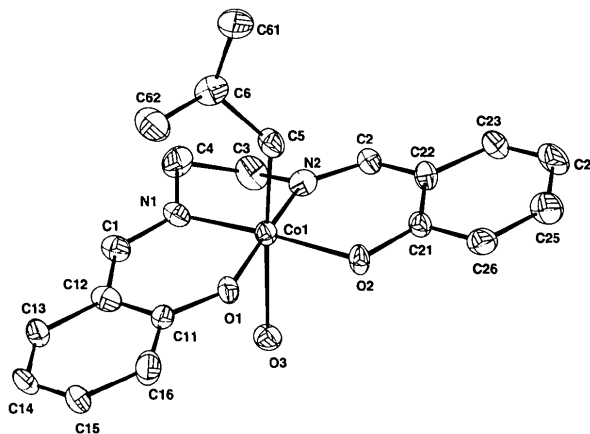


Fig. 1. A displacement ellipsoid (50% probability) plot of the title complex, with H atoms omitted for clarity.

The bond lengths between the Co<sup>III</sup> ion and the salen ligand donor atoms are in agreement with the values found in other hexacoordinate organocobalt(III)-salen complexes. The bond lengths and angles of the equatorial salen ligand as well as the axial C—Co—O(H<sub>2</sub>O)