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Structure of Bromo(diphenylphosphinoacetato)(diphenylphosphinoacetic acid)platinum(II) Monohydrate

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Abstract. $C_{28}H_{25}BrO_4P_2Pt.H_2O$, $[PtBr(C_{14}H_{12}O_2P)(C_{14}H_{13}O_2P)].H_2O$, monoclinic, $P2_1/c$, $a = 11{\cdot}154$ (3), $b = 15{\cdot}673$ (4), $c = 18{\cdot}097$ (4) Å, $\beta = 116{\cdot}78$ (2)°, $Z = 4$, $V = 2824{\cdot}3$ Å^3, $D_m = 1{\cdot}82$, $D_c = 1{\cdot}79$ Mg m^{-3}, μ(Mo $K\alpha$) = 6·71 mm^{-1}. $R = 0{\cdot}024$ for 3594 reflexions $[I > 3\sigma(I)]$ and 369 parameters. The Pt atom is surrounded in a distorted *cis* square-planar arrangement by two P [Pt—P = 2·225 (2) and 2·229 (2) Å], Br [Pt—Br = 2·456 (1) Å] and an O of an acetato group [Pt—O = 2·079 (4) Å]. The other O of the acetato group is hydrogen bonded to an O of the acetic acid of the neighbouring molecule; thus the molecules are linked to form chains parallel to **b**.

Introduction. Spectral and other indirect evidence (Růžičková & Podlahová, 1978; Podlahová & Podlaha, 1979) indicate that phosphinoacetic acids and their anions, here diphenylphosphinoacetate (dppa), can bond to transition-metal ions as unidentate (P or O) or chelating (P,O) ligands. Crystal structure determinations have confirmed the unidentate P coordination in dibromobis(diphenylphosphinoacetic acid)palladium(II) (Podlahová, Loub & Ječný, 1979) and the bidentate (P and O) coordination in bis(diphenylphosphinoacetato)palladium(II) (Civiš, Podlahová, Loub & Ječný, 1980). The title compound, $[Pt^{II}Br(dppa)(Hdppa)].H_2O$, should contain both monodentate and bidentate ligands (Pangrác & Podlahová, 1981). We have therefore determined its crystal structure for comparison with those of $[Pd^{II}Br_2(Hdppa)_2]$ and $[Pd^{II}(dppa)_2]$.

Single crystals were grown on slowly cooling the solution of an authentic sample of $[Pt^{II}Br(dppa)(Hdppa)]$ (Pangrác & Podlahová, 1981) in 60% aqueous acetic acid. The crystals, m.p. 509–511 K (dec.), contain water of solvation as demonstrated by the IR spectrum: ν(OH) (cm^{-1}) 3560 *w*, 3640 *w*. The water is evolved at 353 K/1 kPa without any noticeable change of the powder pattern.

The crystals are prismatic, bounded by {100} and {110} and terminated by {001} and {011}. Weissenberg and precession photographs showed systematic absences ($h0l$: $l = 2n + 1$ and $0k0$: $k = 2n + 1$) indicating the space group $P2_1/c$. A single crystal 0·11 × 0·25 × 0·63 mm was mounted on a Picker FACS-1 diffractometer. The cell dimensions were refined from the setting angles of 15 reflexions measured at $\pm 2\theta$ with Cu $K\alpha$ radiation. Intensities were measured out to $2\theta = 50°$ with Zr-filtered Mo $K\alpha$ radiation. The ω–2θ step-scanning technique was used with a step length of 0·04° and a scan width of $(3{\cdot}0 + 0{\cdot}692 \tan \theta)°$; each step was counted for 1 s. 5569 independent reflexions were obtained, of which 3594 had $I > 3\sigma(I)$ according to counting statistics. Data were corrected for Lorentz and polarization factors, absorption and for dead-time losses. The density was determined pycnometrically in xylene.

The coordinates of Pt and Br were found from the Patterson map. Difference Fourier syntheses enabled the location of the light atoms. Least-squares refinement of a scale factor, atomic coordinates, thermal parameters (anisotropic for non-hydrogen atoms and isotropic for H) gave $R = 0{\cdot}042$. A difference map revealed the presence of the O and one H of a water molecule. Further refinement, including an isotropic extinction parameter, g, reduced R to 0·025. As the H atoms were poorly determined a refinement was carried out in which the H atoms, other than H(O4) and H(O5), were kept fixed in positions calculated assuming C—H = 0·95 Å. The final R was 0·024 and $R_w = 0{\cdot}030$ for 369 parameters and 3594 reflexions.† The extinction parameter, $g = 0{\cdot}24\ (2) \times 10^{-4}$, corresponded

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† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36171 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional coordinates* ($\times 10^5$ *for* Pt *and* Br, $\times 10^4$ *for* P, O, *and* C, *and* $\times 10^3$ *for* H) *and* $U_{\rm iso}$($Å^2 \times 10^{-3}$)

For atoms other than H, $U_{\rm iso}$ is calculated from the U_{ij} by $U_{\rm iso} = \frac{1}{3}\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$, with the mean standard deviation of the U_{ii}'s in parentheses.

	x	y	z	$U_{\rm iso}$
Pt	7348 (2)	19347 (1)	39885 (1)	26 (0·1)
Br	−17188 (7)	20623 (5)	33886 (5)	55 (0·5)
P(1)	2874 (2)	1602 (1)	4377 (1)	32 (1)
P(2)	909 (2)	2624 (1)	5110 (1)	26 (1)
O(1)	447 (4)	1348 (3)	2891 (3)	39 (3)
O(2)	1310 (6)	707 (3)	2157 (3)	61 (4)
O(3)	437 (5)	4083 (3)	3859 (3)	58 (4)
O(4)	−1422 (5)	4570 (3)	3871 (3)	50 (3)
O(5)	−2063 (10)	576 (7)	1441 (7)	176 (11)
C(1)	1398 (7)	953 (4)	2827 (4)	41 (5)
C(2)	2648 (7)	770 (5)	3619 (4)	52 (5)
C(3)	3910 (6)	2384 (4)	4209 (4)	37 (4)
C(4)	3329 (7)	3115 (5)	3760 (4)	52 (5)
C(5)	4144 (9)	3700 (5)	3608 (5)	70 (7)
C(6)	5489 (8)	3555 (6)	3912 (5)	79 (7)
C(7)	6058 (9)	2814 (6)	4338 (6)	76 (7)
C(8)	5265 (7)	2231 (5)	4477 (5)	56 (5)
C(9)	3833 (6)	1119 (4)	5386 (4)	35 (4)
C(10)	4910 (7)	1516 (4)	6022 (4)	47 (5)
C(11)	5572 (8)	1137 (5)	6798 (5)	59 (6)
C(12)	5139 (8)	372 (5)	6944 (5)	62 (6)
C(13)	4047 (8)	−28 (5)	6330 (5)	63 (7)
C(14)	3395 (7)	339 (5)	5544 (5)	54 (5)
C(15)	2549 (6)	3057 (4)	5800 (4)	31 (3)
C(16)	3147 (7)	3632 (4)	5478 (4)	42 (5)
C(17)	4420 (7)	3949 (4)	5970 (5)	52 (5)
C(18)	5104 (7)	3705 (5)	6786 (5)	54 (5)
C(19)	4528 (7)	3151 (5)	7118 (4)	54 (5)
C(20)	3251 (7)	2824 (4)	6628 (4)	44 (4)
C(21)	429 (6)	1974 (4)	5757 (3)	32 (3)
C(22)	593 (8)	1100 (4)	5767 (4)	51 (5)
C(23)	358 (10)	588 (5)	6312 (5)	70 (6)
C(24)	−84 (9)	951 (5)	6834 (5)	67 (6)
C(25)	−270 (8)	1809 (5)	6825 (5)	60 (6)
C(26)	−12 (8)	2327 (5)	6297 (5)	54 (6)
C(27)	−213 (6)	3552 (3)	4873 (4)	32 (4)
C(28)	−354 (6)	4079 (4)	4146 (4)	34 (4)
H(1)	257	23	383	79 (23)
H(2)	341	76	351	92 (25)
H(4)	239	322	356	33 (16)
H(5)	376	420	329	84 (25)
H(6)	605	396	383	117 (29)
H(7)	699	271	453	118 (29)
H(8)	565	171	476	53 (20)
H(10)	520	206	593	43 (17)
H(11)	633	141	723	68 (21)
H(12)	560	11	748	74 (22)
H(13)	374	−55	644	85 (24)
H(14)	265	6	512	80 (24)
H(16)	268	380	491	52 (18)
H(17)	482	434	575	81 (24)
H(18)	598	392	712	88 (25)
H(19)	500	299	768	72 (23)
H(20)	286	244	686	48 (23)
H(22)	87	84	539	62 (23)
H(23)	50	−1	632	68 (24)
H(24)	−26	60	720	79 (28)
H(25)	−58	205	719	69 (23)
H(26)	−13	293	630	92 (30)
H(27)	−108	335	476	33 (17)
H(28)	12	391	535	73 (25)
H(O4)	−145 (7)	498 (4)	353 (4)	84 (24)
H(O5)	−200 (12)	121 (7)	130 (8)	219 (57)

to a minimum value of F_o^2/F_c^2(corrected) of 0·80. The maximum residual electron density on the final difference map was 0·3 e $Å^{-3}$. The weighting scheme used was $w = \{[\sigma(F_o^2) + 1{\cdot}02F_o^2]^{1/2} - |F_o|\}^{-2}$. Scattering factors were those of *International Tables for X-ray Crystallography* (1974) for Pt, of Cromer & Mann (1968) for Br, P, O, and C, and of Stewart, Davidson & Simpson (1965) for H. Corrections were made for the anomalous dispersion of Pt (Cromer & Liberman, 1970). The final fractional coordinates are given in Table 1.

Calculations were carried out on a Cyber 173 computer with the following programs: *PROFILE*, *DATAP* and *DSORTH* (State University of New York at Buffalo) (data reduction, including absorption correction); *ZALKINS* (A. Zalkin, Lawrence Radiation Laboratory) (Fourier synthesis); *LINUS* (Coppens & Hamilton, 1970) (least-squares refinement); *ORFFE* (Busing, Martin & Levy, 1964) (calculation of molecular geometry); *ORTEP* (Johnson, 1965) (drawings).

Discussion. The final atomic parameters are listed in Table 1, bond distances in Table 2, and angles in Table 3.

Table 2. *Bond lengths* (Å)

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

Pt–Br	2·456 (1)	P(2)–C(15)	1·819 (6)
Pt–O(1)	2·079 (4)	C(15)–C(16)	1·395 (8)
Pt–P(1)	2·225 (2)	C(16)–C(17)	1·384 (9)
Pt–P(2)	2·229 (2)	C(17)–C(18)	1·376 (10)
O(1)–C(1)	1·277 (7)	C(18)–C(19)	1·370 (10)
O(2)–C(1)	1·233 (7)	C(19)–C(20)	1·392 (9)
C(1)–C(2)	1·510 (10)	C(20)–C(15)	1·391 (8)
C(2)–P(1)	1·826 (6)	P(2)–C(21)	1·805 (6)
P(1)–C(3)	1·802 (6)	C(21)–C(22)	1·383 (8)
C(3)–C(4)	1·386 (9)	C(22)–C(23)	1·384 (9)
C(4)–C(5)	1·403 (10)	C(23)–C(24)	1·372 (11)
C(5)–C(6)	1·364 (11)	C(24)–C(25)	1·360 (10)
C(6)–C(7)	1·379 (12)	C(25)–C(26)	1·379 (10)
C(7)–C(8)	1·371 (10)	C(26)–C(21)	1·391 (9)
C(8)–C(3)	1·384 (9)	P(2)–C(27)	1·838 (6)
P(1)–C(9)	1·814 (6)	C(27)–C(28)	1·502 (8)
C(9)–C(10)	1·382 (9)	C(28)–O(3)	1·209 (7)
C(10)–C(11)	1·391 (10)	C(28)–O(4)	1·313 (7)
C(11)–C(12)	1·363 (10)	O(4)–H(O4)	0·87 (7)
C(12)–C(13)	1·375 (11)	H(O4)–O(2$^{\rm i}$)	1·76 (7)
C(13)–C(14)	1·397 (10)	O(5)–H(O5)	1·05 (10)
C(14)–C(9)	1·393 (9)	O(4)–O(2$^{\rm i}$)	2·620 (6)

The structure (Fig. 1) consists of molecules linked by H bonds to form chains parallel to **b**. The Pt atom is located in a distorted *cis* square-planar environment formed by a P,O-chelating dppa, the P of the monodentate dppa and Br. The deviations from planarity are of the order of 0·05 Å. As in $[Pd^{II}(dppa)_2]$, overcrowding of the bulky diphenylphosphine groups leads to an opening out of the PPtP angle. The geometry of the bidentate ligand is similar to that in $[Pd^{II}(dppa)_2]$ and that of the monodentate ligand is similar to that of $[Pd^{II}Br_2(Hdppa)_2]$ (see Table 4). The chelate ring Pt–P(1)–C(2)–C(1)–O(1)– adopts the λ-envelope conformation. O(3) is at the apex of the pyramid the base of which is defined by P(1), P(2), O(1), and Br; the Pt–O(3) distance is 3·381 (5) Å and must be considered as non-bonded {*cf.* $[Pd^{II}Br_2(Hdppa)_2]$ where Pd–O(2) = 3·171 (6) Å}.

Table 3. *Bond angles* (°)

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

Br–Pt–P(1)	169·06 (4)	C(12)–C(13)–C(14)	120·1 (8)
Br–Pt–P(2)	89·17 (4)	C(13)–C(14)–C(9)	120·0 (7)
P(1)–Pt–P(2)	100·66 (6)	Pt–P(2)–C(15)	117·0 (2)
Br–Pt–O(1)	87·3 (1)	Pt–P(2)–C(21)	112·8 (2)
O(1)–Pt–P(1)	83·1 (1)	Pt–P(2)–C(27)	113·6 (2)
O(1)–Pt–P(2)	175·7 (1)	C(15)–P(2)–C(21)	105·4 (3)
Pt–O(1)–C(1)	121·6 (4)	C(15)–P(2)–C(27)	103·5 (3)
O(1)–C(1)–O(2)	122·6 (7)	C(21)–P(2)–C(27)	103·2 (3)
O(1)–C(1)–C(2)	117·1 (5)	P(2)–C(15)–C(16)	118·4 (5)
O(2)–C(1)–C(2)	120·3 (6)	P(2)–C(15)–C(20)	123·1 (5)
C(1)–C(2)–P(1)	109·5 (5)	C(20)–C(15)–C(16)	118·5 (6)
C(2)–P(1)–Pt	99·5 (2)	C(15)–C(16)–C(17)	120·6 (6)
C(2)–P(1)–C(3)	103·9 (3)	C(16)–C(17)–C(18)	120·2 (7)
C(2)–P(1)–C(9)	106·1 (3)	C(17)–C(18)–C(19)	120·3 (7)
Pt–P(1)–C(3)	117·7 (2)	C(18)–C(19)–C(20)	120·1 (7)
Pt–P(1)–C(9)	118·6 (2)	C(19)–C(20)–C(15)	120·4 (7)
C(3)–P(1)–C(9)	108·7 (3)	P(2)–C(21)–C(22)	119·5 (5)
P(1)–C(3)–C(4)	119·7 (5)	P(2)–C(21)–C(26)	122·2 (5)
P(1)–C(3)–C(8)	120·4 (5)	C(26)–C(21)–C(22)	118·1 (6)
C(8)–C(3)–C(4)	119·8 (6)	C(21)–C(22)–C(23)	121·2 (7)
C(3)–C(4)–C(5)	118·8 (7)	C(22)–C(23)–C(24)	119·5 (7)
C(4)–C(5)–C(6)	120·2 (8)	C(23)–C(24)–C(25)	120·1 (7)
C(5)–C(6)–C(7)	120·8 (8)	C(24)–C(25)–C(26)	120·8 (7)
C(6)–C(7)–C(8)	119·3 (8)	C(25)–C(26)–C(21)	120·2 (7)
C(7)–C(8)–C(3)	120·9 (8)	P(2)–C(27)–C(28)	115·6 (4)
P(1)–C(9)–C(10)	123·2 (5)	C(27)–C(28)–O(3)	124·8 (6)
P(1)–C(9)–C(14)	118·1 (5)	C(27)–C(28)–O(4)	111·9 (5)
C(14)–C(9)–C(10)	118·5 (6)	O(3)–C(28)–O(4)	123·3 (6)
C(9)–C(10)–C(11)	121·0 (7)	C(28)–O(4)–H(O4)	116 (5)
C(10)–C(11)–C(12)	119·9 (8)	O(4)–H(O4)–O(2^i)	171 (7)
C(11)–C(12)–C(13)	120·4 (8)	H(O4)–O(2^i)–C(1^i)	156 (2)

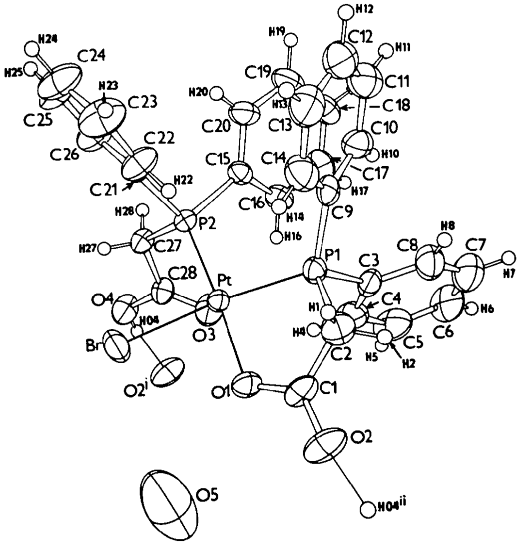

Fig. 1. A perspective drawing of the molecule showing the numbering of the atoms. Symmetry code: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-x, y-\frac{1}{2}, \frac{1}{2}-z$. H(O5) is hidden behind O(5).

Unlike $[Pd^{II}Br_2(Hdppa)_2]$, the intermolecular H bonds are of the acetato–acetic acid type [O(4)–H(O4)···O(2^i)] which seems to be preferred in structures containing both protonated and dissociated (uncoordinated) carboxyl groups (Podlahová, Kratochvíl & Langer, 1981).

The water molecule is located in the structure at O–H···O distances and angles which are safely outside the range of hydrogen bonding (Falk & Knop, 1973). Among stoichiometric hydrates, this situation is uncommon, especially when there are many potential acceptor atoms in the compound. In accord with the large thermal vibrations of O(5) the water is bonded very loosely and the dehydration taking place at mild conditions has little if any effect on the remaining structure. One hydrogen, H(O5), was found near the direction to the nearest oxygen, O(1), 3·09 Å away, but the position of the other H atom could not be established, possibly because the water is disordered or rotating about the O(5)–H(O5) axis. Two ν(OH) bands at high wave numbers indicate that the H atoms are differently but very weakly affected by the surroundings.

Table 4. *Comparison of dppa complexes of* Pd *and* Pt

		M–P (Å)	*M*–O (Å)	*M*–P–C (°)	P–*M*–P (°)	$P–CH_2$ (Å)	$P–C_6H_5$ (Å)
$[Pd^{II}Br_2(Hdppa)_2]$	Unidentate	2·322 (2)	—	112·5 (2)	180	1·831 (8)	1·826 (6)
$[Pd^{II}(dppa)_2]$	Bidentate	2·235 (2)	2·076 (4)	98·8 (2)	104·1 (1)	1·829 (6)	1·814 (4)
$[Pt^{II}Br(dppa)(Hdppa)].H_2O$	Unidentate	2·229 (2)	—	113·6 (2)	100·66 (6)	1·832 (4)	1·810 (4)
	Bidentate	2·225 (2)	2·079 (4)	99·8 (3)			

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Die Struktur des *gem*-Diols Natriumglyoxylathydrat

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Abstract. $C_2H_3O_4^-.Na^+$, sodium salt of 1,1-dihydroxyacetic acid: orthorhombic, *Pbcm*, $a = 5{\cdot}320\,(2)$, $b = 6{\cdot}807\,(3)$, $c = 10{\cdot}592\,(4)$ Å, $V = 383{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}97$ Mg m^{-3}, $\mu = 0{\cdot}3$ mm^{-1}, $F(000) = 232$; 534 reflexions; $R = 0{\cdot}031$, $R' = 0{\cdot}044$. The title compound belongs to the rare species of stable *gem*-diols. The $(OH)_2HCCO_2^-$ anions are situated on crystallographic mirror planes. They form infinite chains by hydrogen bonds with the carboxylic oxygens as acceptors. The bond distances are similar to the values found in other *gem*-diols.

Einleitung. Nur wenige einfach aufgebaute Carbonylverbindungen bilden unter Wasseranlagerung stabile *gem*-Dihydroxyverbindungen. Ausser Chloral- und Cyclopropanon gehört auch das Na-Salz der Glyoxylsäure, OHC—COOH, zu dieser Gruppe. Im Zusammenhang mit Studien über die Schwingungsspektren von *gem*-Diolen, zur Konformation von Oxalsäurederivaten und zu Wasserstoffbrückenbindungen in kleinen Molekülen haben wir jetzt die Struktur von $Na[CH(OH)_2COO]$ aufgeklärt. Strukturbestimmungen an Chloralhydrat (Brown & Levy, 1973), sowie einigen weiteren vielatomigen *gem*-Diolen wie Ninhydrin (Medrud, 1969; siehe auch dort zitierte Literatur) liegen bereits vor, ebenso Untersuchungen zur Struktur und Konformation von Glyoxylsäure im Gaszustand (van Eijck & van Duijneveldt, 1977; siehe auch dort zitierte Literatur).

Die Intensitäten von 1104 Reflexen eines Kristalls der Grösse 0,25 × 0,3 × 0,5 mm wurden bei Zimmertemperatur mittels eines Syntex $P2_1$-Diffraktometers gemessen (Graphitmonochromator, Mo $K\alpha$-Strahlung, $\theta/2\theta$ Scantechnik, Scan-Geschwindigkeit 4,86–29,3° min^{-1}, $\theta_{max} = 30°$, Messzeit Reflex:

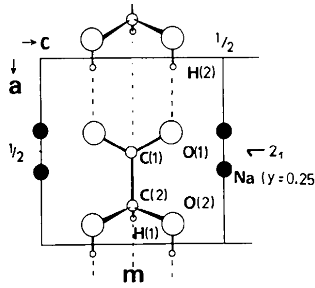

Fig. 1. Ausschnitt aus der Elementarzelle von $Na[O_2CCH(OH)_2]$. Zur Vereinfachung ist nur eine der vier Anionenketten eingezeichnet, die die Elementarzelle durchlaufen.

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