Table 3. *Shape characteristics for coordination polyhedron of the title compound in comparison with hard sphere model (HSM) and most favourable polyhedron (MFP)*

Δ_{SAP}	Δ_{BCTP}	σ				φ	θ	l/s	t	v_1	h_1	h_3	v_2	c_2	c_1	h_2
0·023	0·073	4·6	16·8	55·4	56·8	29·9	57·3	1·05	4·22	3·69	3·09	3·02	2·85	2·89	2·82	2·81
HSM_{SAP}		0·0	0·0	52·4	52·4	24·5	59·2	1·10								
HSM_{BCTP}		0·0	21·8	48·2	48·2	14·1										
MFP_{BCTP}									1·78	1·50	1·36	1·36	1·25	1·21	1·18	1·13

The Δ values (Å) are calculated by the equation $\Delta = \sum_{i=1}^{i=8} d_i^2/8$, where d_i is distance between comparable points in the observed and ideal polyhedron. SAP: square antiprism; BCTP: bicapped trigonal prism. (σ, φ and θ are in °; t, v_1, h_1, h_3, v_2, c_2, c_1 and h_2 are in Å.)

difference between the structure of the present threonine compound and the hydroxyacetate compounds is that the former consists of one-dimensional polymeric chains, while the latter consist of three-dimensional polymeric networks.

The Ho ion is eight-coordinated. The coordination polyhedron (Fig. 2) is so distorted that it can be described as intermediate between a square antiprism and a bicapped trigonal prism. The 'square' faces of the antiprism are made up of O(1), O(3), O(8), O(6) and O(2^{i}), O(4), O(5), O(7). The dihedral angle between the 'square' faces is 4·9 (8)°. The Δ value, defined as $\sum d_i^2/8$ for $i = 1$–8, is 0·023 Å. Here d_i is the distance between the observed position of the ith atom (vertex) and the relevant one in the ideal, least-squares-fitted polyhedron (Drew, 1977). The triangular faces of the trigonal prism comprise the atoms O(1), O(5), O(7) and O(2^{i}), O(4), O(8). The dihedral angle between these faces is 18·1 (9)°. The hydroxyl oxygen O(3) and water oxygen O(6) form the caps of the prism. In this case $\Delta = 0{\cdot}073$ Å. The other shape characteristics of the coordination polyhedron calculated in comparison with ideal polyhedra are given in Table 3.

The bond distances and angles of L-threonine in the present structure do not show any significant differences in comparison with those in free (zwitterionic) L-threonine (Shoemaker, Donohue, Schomaker & Corey, 1950). The torsion angles Ho—O(1)—C(1)—C(2) and Ho—O(2)—C(1)—C(2) are 1·3 (12) and −141·5 (8)°, respectively. Other torsion angles have been deposited.* Each threonine–Ho chelate forms a six-membered ring which has a twist-boat conformation [$Q = 0{\cdot}659$ (9), $q_2 = 0{\cdot}623$ (9) Å, $\theta = 71{\cdot}0$ (8), $\varphi = 202{\cdot}5$ (9)°]. The crystal structure is stabilized by hydrogen bonds of the type O—H···O, O—H···Cl and N—H···Cl.

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* See deposition footnote.

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Carbonatobis(triphenylphosphine)platinum(II) Tetrahydrofuran Solvate

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Abstract. $[Pt(CO_3)\{P(C_6H_5)_3\}_2].C_4H_8O$, $M_r = 851{\cdot}8$, triclinic, $P\bar{1}$, $a = 10{\cdot}666$ (2), $b = 12{\cdot}359$ (2), $c = 15{\cdot}525$ (4) Å, $\alpha = 83{\cdot}73$ (2), $\beta = 70{\cdot}48$ (3), $\gamma = 69{\cdot}76$ (2)°, $V = 1810$ Å^3, $Z = 2$, $D_x = 1{\cdot}56$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 40{\cdot}4$ cm^{-1}, $F(000) = 848$, $T = 298$ K, $R = 0{\cdot}029$ for 5493 reflections with $I > 3\sigma(I)$. Structure is essentially a redetermination of that originally published by Cariati, Mason, Robertson & Ugo [*J. Chem. Soc. Chem. Commun.* (1967), p. 408] but with tetrahydrofuran instead of benzene solvent in the lattice. Features not observed or commented upon in the original include the presence of

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agostic Pt···H interactions of lengths 2·79 and 2·85 Å and some asymmetry in the Pt—P bond lengths [2·254 (2) and 2·228 (1) Å].

Introduction. Crystals of the title compound were isolated as a side-product of reactions aimed at the synthesis and study of the reactivity of simple heterobimetallic systems containing platinum (Powell, Gregg & Sawyer, 1984; Powell, Sawyer & Smith, 1985; Powell, Sawyer & Stainer, 1985).

Experimental. Yellow plate-shaped crystal, described by the faces {001}, (010), (0$\bar{1}$0), (111) and ($\bar{2}\bar{1}\bar{1}$) which were 0·0045, 0·0150, 0·0100, 0·0140 and 0·0185 cm respectively from an origin within the crystal, was used throughout. Unit-cell dimensions were obtained by least-squares fit of diffracting positions of 25 reflections ($11\cdot1 < \theta < 15\cdot9°$) on an Enraf–Nonius CAD-4 diffractometer using graphite-monochromatized Mo $K\alpha$ radiation. Intensity data collected using ω–2θ scans over ω-scan ranges $(0\cdot70 + 0\cdot35 \tan\theta)°$. Scan rates conditional on information collected in prescans (at 10° min^{-1}) selected to give $I/\sigma(I) \geq 25$ within a max. scan time of 55 s. Three standard reflections monitored every 6500 s of exposure time showed no significant losses in intensity over data-collection period. Backgrounds by extending scan by 25% on either side of peak measured for half the time taken to collect the peak. 6375 reflections (excluding standards) in octants $h, \pm k, \pm l$ with $2\theta \leq 50°$ measured. Lorentz, polarization and, at a later stage of refinement, absorption [*ABSCOR, SDP* package (Frenz, 1981): 10 × 10 × 6 grid, min. T: 0·41, max. T: 0·70] corrections applied to all data and 193 reflections with $F_{obs} = 0\cdot0$ rejected to give final data set of 6182 reflections (h −11→12, k ±14, l 0→18).

Structure solution: Patterson for Pt, least squares, Fourier and difference Fourier synthesis for non-H atoms. With the composition of the crystal ascertained a literature check revealed a previously published description of the present structure with benzene instead of tetrahydrofuran solvent in the lattice (Cariati, Mason, Robertson & Ugo, 1967).*† Completion of the structure was with H atoms in calculated positions ($U = 0\cdot09$ Å^2) and anisotropic thermal parameters for all non-H atoms except those in the solvent. Blocked least-squares refinement minimizing $\sum w\Delta F^2$ then converged (max. $\Delta/\sigma = 0\cdot18$) to final agreement indices $R = 0\cdot0290$, $wR = 0\cdot0341$ for 5493 data with $I \geq 3\sigma(I)$. Weights given by $w = [\sigma^2(F) + 0\cdot01008F^2]^{-1}$. Most significant features in a final ΔF map were some peaks up to 1·16 e Å^{-3} near Pt and peaks ≤ 0·85 e Å^{-3} near atoms in the solvent. Programs: Enraf–Nonius *SDP* package (Frenz, 1981) and *SHELX*76 (Sheldrick, 1976) on PDP 11/23 and Gould 9705 computers. Scattering factors from *International Tables for X-ray Crystallography* (1974). The final atomic positional and thermal parameters and selected bond lengths and bond angles are given in Tables 1 and 2.*

Table 1. *Final atomic positional* (×10^4) *and thermal* (×10^3) *parameters*

	x	y	z	U_{eq}*(Å^2)
Pt	1809·4 (2)	1115·8 (1)	2177·5 (1)	29·2 (1)
P(1)	2966 (1)	1745 (1)	2884 (1)	33·3 (4)
P(2)	1169 (1)	2666 (1)	1342 (1)	30·9 (3)
O(1)	2178 (4)	−509 (3)	2726 (2)	40·1 (12)
O(2)	1445 (5)	−1762 (3)	2219 (3)	56 (2)
O(3)	1000 (4)	70 (3)	1752 (3)	42·5 (12)
C(1)	1526 (5)	−817 (4)	2225 (4)	42 (2)
C(111)	2389 (5)	1398 (4)	4089 (3)	39 (2)
C(112)	1030 (6)	1371 (6)	4491 (4)	59 (2)
C(113)	547 (7)	1166 (9)	5437 (4)	81 (3)
C(114)	1421 (7)	966 (8)	5938 (4)	76 (3)
C(115)	2781 (8)	955 (8)	5536 (5)	75 (3)
C(116)	3260 (6)	1160 (6)	4616 (4)	55 (2)
C(121)	2854 (6)	3258 (4)	2880 (4)	47 (2)
C(122)	2031 (8)	3921 (6)	3656 (7)	76 (3)
C(123)	1916 (10)	5112 (7)	3609 (9)	99 (5)
C(124)	2620 (11)	5540 (7)	2854 (9)	93 (5)
C(125)	3424 (10)	4896 (7)	2084 (8)	89 (4)
C(126)	3542 (7)	3735 (5)	2091 (6)	62 (3)
C(131)	4854 (5)	958 (4)	2501 (3)	37 (2)
C(132)	5843 (6)	1439 (5)	2518 (4)	49 (2)
C(133)	7268 (7)	807 (6)	2251 (4)	57 (2)
C(134)	7711 (6)	−338 (7)	1982 (4)	59 (2)
C(135)	6739 (7)	−810 (6)	1964 (5)	65 (3)
C(136)	5298 (6)	−171 (5)	2225 (4)	50 (2)
C(211)	338 (5)	4057 (4)	1915 (4)	39 (2)
C(212)	568 (6)	5070 (5)	1539 (4)	47 (2)
C(213)	−148 (8)	6089 (5)	2001 (6)	64 (3)
C(214)	−1164 (9)	6144 (6)	2850 (6)	76 (3)
C(215)	−1406 (8)	5139 (7)	3245 (5)	75 (3)
C(216)	−660 (7)	4080 (5)	2788 (4)	55 (2)
C(221)	2616 (5)	2728 (4)	317 (3)	32·4 (14)
C(222)	3958 (5)	1944 (4)	214 (4)	39 (2)
C(223)	5078 (6)	1901 (5)	−579 (4)	47 (2)
C(224)	4836 (7)	2670 (6)	−1273 (4)	54 (2)
C(225)	3543 (7)	3421 (5)	−1182 (4)	51 (2)
C(226)	2417 (6)	3468 (5)	−402 (4)	44 (2)
C(231)	−144 (5)	2591 (4)	857 (3)	36 (2)
C(232)	157 (6)	1693 (5)	299 (4)	42 (2)
C(233)	−809 (7)	1644 (6)	−101 (4)	54 (2)
C(234)	−2079 (7)	2504 (7)	73 (5)	68 (3)
C(235)	−2436 (7)	3398 (6)	664 (6)	71 (3)
C(236)	−1468 (6)	3444 (5)	1053 (5)	50 (2)
C(1*S*)	3764 (27)	7067 (20)	5675 (16)	234 (9)†
C(2*S*)	2824 (23)	7180 (20)	5195 (17)	237 (9)†
C(3*S*)	3583 (30)	8023 (23)	4453 (19)	268 (11)†
C(4*S*)	4634 (24)	7076 (22)	4014 (17)	237 (9)†
C(5*S*)	5062 (28)	6608 (22)	4898 (20)	266 (10)†

* $U_{eq} = \frac{1}{3}$ trace **U**.
† Refined isotropically.

Discussion. The improved accuracy of the present determination of the $[(Ph_3P)_2Pt(CO_3)]$ molecule over

* Rotation [0,0,1/1,0,0/0,1,−1] of their cell gives $a = 10\cdot56$, $b = 12\cdot49$, $c = 15\cdot48_3$ Å, $\alpha = 84\cdot8_1$, $\beta = 71\cdot3_2$, $\gamma = 70\cdot0°$.

† As noted by Bhaduri, Johnson, Pickard, Raithby, Sheldrick & Zuccaro (1977), all the compounds $[(Ph_3P)_2PtL]$ with $L = CO_3$, S_2CO and N_2O_2 crystallize in space group $P\bar{1}$ with closely similar cell dimensions and contain disordered solvent molecules.

* Lists of structure-factor amplitudes, least-squares mean planes, bond lengths/bond angles in the phenyl rings and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44364 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

that previously published (Cariati *et al.*, 1967) allows several further observations on the structure to be made. Thus, in addition to isolated molecules (Fig. 1), the lattice also contains tetrahydrofuran solvent which is only weakly held. [The high thermal parameters did not allow the O atom to be identified.] In the molecule the Pt—P distances are significantly different [2·254 (2) and 2·228 (1) Å, $\Delta/\sigma \sim 13$], the Pt—O distances are equivalent [2·047 (5) and 2·053 (3) Å] and the PPtP angle has opened out to 99·25 (5)° due to the steric size of the PPh_3 ligands and the small bite of the carbonato ligand [64·5 (2)°].

Table 2. *Selected bond lengths* (Å), *bond angles* (°) *and intramolecular contacts* (Å,°)

Pt—P(1)	2·254 (2)	P(1)—C(111)	1·816 (5)
—P(2)	2·228 (1)	—C(121)	1·831 (6)
—O(1)	2·053 (3)	—C(131)	1·824 (5)
···C(1)	2·501 (6)	P(2)—C(211)	1·813 (5)
—O(3)	2·047 (5)	—C(221)	1·826 (4)
···H(222)	2·79	—C(231)	1·828 (7)
···H(112)	2·85	C(1*S*)—C(2*S*)	1·40 (4)
···H(136)	2·95	—C(5*S*)	1·48 (3)
O(1)—C(1)	1·358 (8)	C(2*S*)—C(3*S*)	1·66 (4)
O(2)—C(1)	1·201 (7)	C(3*S*)—C(4*S*)	1·36 (3)
O(3)—C(1)	1·315 (6)	C(4*S*)—C(5*S*)	1·58 (4)
P(1)—Pt—P(2)	99·25 (5)	Pt—P(1)—C(111)	108·0 (2)
—O(1)	97·1 (1)	—C(121)	122·9 (2)
—O(3)	161·5 (1)	—C(131)	111·8 (2)
···H(222)	76·0	C(111)—P(1)—C(121)	104·1 (3)
···H(112)	67·7	—C(131)	104·2 (2)
P(2)—Pt—O(1)	163·5 (1)	C(121)—P(1)—C(131)	104·1 (3)
—O(3)	99·2 (1)	Pt—P(2)—C(211)	117·6 (2)
···H(222)	69·1	—C(221)	111·8 (1)
···H(112)	112·6	—C(231)	111·4 (2)
O(1)—Pt—O(3)	64·5 (2)	C(211)—P(2)—C(221)	109·7 (2)
···H(222)	113·1	—C(231)	102·8 (2)
···H(112)	75·9	C(221)—P(2)—C(231)	102·0 (2)
O(3)—Pt···H(222)	109·3	C(5*S*)—C(1*S*)—C(2*S*)	96 (2)
···H(112)	106·3	C(1*S*)—C(2*S*)—C(3*S*)	89 (2)
Pt—O(1)—C(1)	92·0 (3)	C(2*S*)—C(3*S*)—C(4*S*)	90 (2)
Pt—O(3)—C(1)	93·6 (4)	C(3*S*)—C(4*S*)—C(5*S*)	93 (2)
O(1)—C(1)—O(2)	124·7 (5)	C(4*S*)—C(5*S*)—C(1*S*)	105 (2)
—O(3)	109·8 (5)	Pt···H(222)—C(222)	119
O(2)—C(1)—O(3)	125·5 (7)		

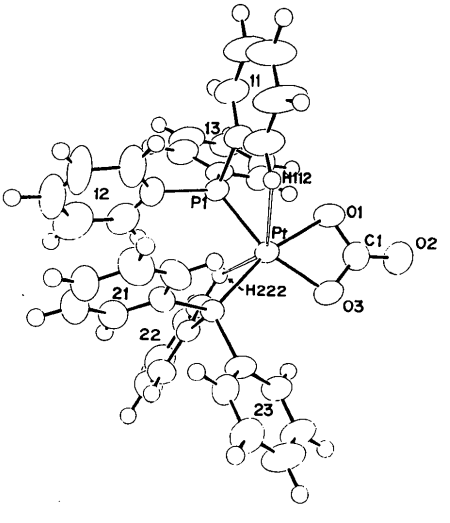

Fig. 1. *ORTEP* view (Johnson, 1976) of the molecule showing the numbering of selected atoms and phenyl rings. The shortest Pt···H interactions are indicated as unfilled bonds. Thermal ellipsoids are drawn at the 50% probability level, H atoms with uniform isotropic temperature factors.

The observed Pt—P distances are fairly typical for Pt^{II}—P bonds [*e.g.* Kin-Chee, McLaughlin, McPartlin & Robertson (1982); Bhaduri *et al.* (1977); Russell & Tucker (1975)] which have values in the range 2·218–2·362 Å according to the influence of the *trans* ligands. The observed Pt—O distances are close to the sum of the covalent radii of Pt and O (2·01 Å) and distances in $[(Ph_3P)_2Pt(N_2O_2)]$ [2·00 (2) and 2·03 (3) Å; Bhaduri *et al.* (1977)], and some related compounds (Immirzi & Musco, 1977). The carbonato ligand is completely planar and makes an angle of *ca* 6·5° with the PtPP plane. A least-squares mean plane through Pt, P(1), P(2) and the CO_3^{2-} ligand shows a maximum deviation of 0·074 (5) Å for O(2).*

The inequivalence in the Pt—P distances is related to the different arrangements of the phenyl rings on each P atom which are oriented so that some of the *ortho* H atoms form short Pt···H contacts (2·79, 2·85 Å). Similar contacts have been described as agostic (Crabtree, Holt, Lavin & Morehouse, 1985) or non-primary valence interactions (Bennett, Donaldson, Hitchcock & Mason, 1975) and have been the subject of theoretical calculations (Gritsenko, Vysotskaya, Bagaturyants & Kazanskii, 1984) in comparable Pd systems. As has been noted elsewhere (Alcock, Kemp & Wimmer, 1981), the PtPC angles involving the adjacent 'interior' phenyl rings 12 (122·9°) and 21 (117·6°) are somewhat enlarged [$\Delta\theta = ca$ 11° at P(1) and *ca* 6° at P(2)] over the remaining angles. These two rings are, notably, approximately parallel to each other ($\theta \sim 8°$) although the displacements of the two rings from the PtP(1)P(2) plane are significantly different.*

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* See deposition footnote.

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Structure of Calcium Bis(4-fluorobenzoate) Trihydrate

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Abstract. $Ca^{2+}.2C_7H_4FO_2^-.3H_2O$, $M_r = 372{\cdot}3$, monoclinic, $P2_1/c$, $a = 7{\cdot}239$ (2), $b = 33{\cdot}173$ (6), $c = 6{\cdot}534$ (1) Å, $\beta = 92{\cdot}27$ (2)°, $V = 1568$ Å^3, $Z = 4$, $D_m = 1{\cdot}56$, $D_x = 1{\cdot}58$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 4{\cdot}5$ cm^{-1}, $F(000) = 768$, $T \simeq 293$ K, final $R = 0{\cdot}048$ for 3070 observed unique reflections. Only one of the two independent 4-fluorobenzoate ions in the asymmetric unit is coordinated to Ca^{2+} ions. The eightfold-coordinated Ca^{2+} is linked to four carboxylate O atoms from three different 4-fluorobenzoate ions and four O atoms from three different water molecules. Both the carboxylate group and one of the coordinated water molecules bridge adjacent Ca^{2+} ions to form a polymeric network.

Introduction. Recently, we reported the crystal structure of calcium bis(2-fluorobenzoate) dihydrate where the aromatic F atom was found to participate in a rather short hydrogen bond with a coordinated water molecule (Karipides & Miller, 1984). Continuing our studies to investigate the structural characteristics of fluorine interactions in crystalline metal salts of fluorine-containing carboxylic acids, we have determined the crystal structure of calcium bis(4-fluorobenzoate) trihydrate.

Experimental. Colorless prismatic crystals of the title compound were grown from an aqueous solution of the 1:1 salt by slow evaporation. Crystal size: 0·18 × 0·32 × 0·60 mm. The density was determined by flotation in a bromobenzene/iodoethane mixture. Cell parameters obtained from 15 centered reflections ($2\theta > 25°$) at 293 ±1 K. Intensity data out to $\sin\theta/\lambda = 0{\cdot}6168$ Å^{-1} collected on a Nicolet diffractometer equipped with a graphite monochromator using an ω-scan technique. Each of six check reflections recorded every 300 reflections showed no change in intensity. Index range: h 0 to 8; k 0 to 40; l −8 to 8. Total number of unique reflections measured was 3070. E.s.d.'s calculated from $\sigma(F) = \{[\sigma(F_o)]^2 + (0{\cdot}02F_o)^2\}^{1/2}$ with $\sigma(F_o)$ obtained from counting statistics. All reflections had $F_o > \sigma(F_o)$ and no reflections were taken as unobserved. Absorption and secondary-extinction corrections were not applied. Structure was solved by Patterson and difference Fourier methods and refined by a full-matrix least-squares procedure. H atoms were located from difference maps but hydrogen parameters were not refined. Scattering factors and anomalous-dispersion corrections were from *International Tables for X-ray Crystallography* (1974). All calculations were performed on an IBM 4341 using established programs (Karipides, 1979). Anisotropic refinement (on F) of all non-H atoms (217 variable parameters) converged to $R = 0{\cdot}048$, $wR = 0{\cdot}048$ and goodness-of-fit of 1·47. Maximum shift/e.s.d. in final least-squares cycle was 0·03. Maxima and minima in the final difference Fourier maps: 0·36, −0·38 e Å^{-3}. Final atom coordinates are given in Table 1.*

Discussion. Bond distances and angles are given in Table 2. A view of a portion of the polymeric structural unit with atom-numbering scheme is presented in Fig. 1. There are no symmetry conditions imposed on the structure.

* Lists of structure factors, H-atom coordinates, anisotropic thermal parameters and hydrogen-bonding parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44345 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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