des angles dièdres avec le programme *BEST PLANES* (Ito & Sugawara, 1983). Dessins de la structure à l'aide du programme *ORTEPII* (Johnson, 1976).

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Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des coordonnées des atomes d'hydrogène, des distances et angles des atomes d'hydrogène et des plans moyens, ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 71483: 16 pp.). On peut en obtenir des copies en s'adressant à: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre. [Référence de CIF: PA1052]

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## Références

Carruthers, B. & Watkin, D. W. J. (1986). *CRYSTALS*. Chemical Crystallography Laboratory, Univ. d'Oxford, Angleterre.

Davies, G., El-Kady, N., Onan, K. D., Shomaly, W., El-Sayed, M. A. & El-Toukhy, A. (1988). *Inorg. Chim. Acta*, **149**, 21–30.

Ito, T. & Sugawara, Y. (1983). *Best Plane Program*, 3ième version. Institut de Recherche en Physique et Chemie, Wako-Shi, Saitama 351, Japon.

Johnson, C. K. (1976). *ORTEPII*. Rapport ORNL-5138. Oak Ridge National Laboratory, Tennessee, EU.

Lehuede, J. & Vierfond, J.-M. (1990). Communication aux quatrièmes journées de pharmacochimie de Caen, France.

Orpen, A. G., Brammer, L., Allen, H. F., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* **12**, S1–S83.

Viossat, B., Rodier, N., Lehuede, J. & Vierfond, J.-M. (1986). *Acta Cryst.* C**42**, 227–230.

Viossat, B., Nguyen-Huy, D. & Robert, F. (1993). *Acta Cryst.* C**49**, 84–85.

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# [2,3-Bis(3,4-dimethoxyphenyl)-3-oxopropanalato-*O*,*O*′]difluoroboron(III)

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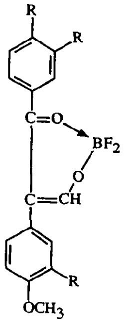
## Abstract

In the title compound, $C_{19}H_{19}BF_2O_6$ (1), boron is tetrahedrally coordinated to two F atoms and to the two O atoms of the bidentate 2,3-bis(3,4-dimethoxyphenyl)-3-oxopropanalato ligand. Average B—O and B—F bond distances are 1.478 (12) and 1.337 (7) Å, respectively. The 3-oxopropanalato group is planar to within 0.05 Å and the B atom is displaced by only 0.13 Å from this plane.

## Comment

Certain difluoroboron complexes of 1,3-dicarbonyl compounds are of interest as intermediates in the synthesis of lignin model compounds (Kristersson & Lundquist, 1980; Ahvonen, Brunow, Kristersson & Lundquist, 1983; Ralph, Ede, Robinson & Main, 1987; Stomberg & Lundquist, 1991; Li, Lundquist & Stomberg, 1993). A recent synthesis of a naturally occurring flavonolignan also proceeded *via* such a difluoroboron complex (Tanaka, Hiroo, Ichino & Ito, 1989). Similar difluoroboron complexes are intermediates in the synthesis of 1,3-diketones by boron trifluoride catalysed acylation of ketones (Sagredos, 1966). Some difluoroboron complexes of 1,3-dicarbonyl compounds exhibit interesting photochemical properties (Chow, Cheng & Johansson, 1991; Chow & Cheng, 1991). This paper describes the crystal structure of the difluoroboron complex (1). The compound was synthesized (Li, Lundquist & Stomberg, 1993) by treatment of *trans*-1,3-bis(3,4-dimethoxyphenyl)-2,3-epoxy-1-propanone with boron trifluoride etherate according to a method used by House & Ryerson (1961) for the preparation of analogous compounds. The compound was crystallized from benzene (m.p. 444–446 K).



(1) R = $OCH_3$
(2) R = H

The structure was solved initially using room-temperature data [collected by a Syntex $P2_1$ diffractometer (Cu $K\alpha$ radiation); $a = 8.832\,(1)$, $b = 19.247\,(3)$, $c = 11.057\,(1)$ Å, $\beta = 92.08\,(1)°$, $V = 1878.3\,(4)$ Å$^3$]. The F atoms showed very large thermal anisotropy. To diminish the thermal motions a new data set was collected at 133 K and this has been used to derive the results presented here.

A perspective view of the molecule is shown in Fig. 1. Boron is tetrahedrally coordinated to two F atoms and to the two O atoms of the bidentate 2,3-bis(3,4-dimethoxyphenyl)-3-oxopropanalato ligand. The mean bond angle at boron is 109.5 (10)°.

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The 3-oxopropanalato group is almost planar [the maximum deviation of 0.053 (3) Å is shown by C(7)]. H(C9) is situated in the plane defined by the 3-oxopropanalato group and B(1) is displaced by 0.131 (3) Å from this plane. An analogous structural arrangement was observed in difluoro[2-(4-methoxyphenyl)-3-oxo-3-phenylpropanalato-*O*,*O'*]boron(III) (2) (Stomberg & Lundquist, 1991) as well as in 2,2-difluoro-4,6-dimethyl-5-(4-nitrophenyl)-1,3,2-dioxaborinane (Emsley, Freeman, Bates & Hursthouse, 1989). In all the hitherto mentioned complexes, the 1,3-dicarbonyl–boron ring has an envelope conformation with the B atom as the flap. In (1) and (2), these flaps point in the same direction relative to the rest of the molecule. The conformations of (1) and (2) are very similar. The angle between the benzene ring planes is 66.5 (3) in (1) and 61° in (2). In (1), the angles between the 3-oxopropanalato group and the benzene ring planes are 28.3 [C(1)–C(6)] and 55.4° [C(10)–C(15)]. In (2), the corresponding angles are 33.5 and 58.2°. In 2,2-difluoro-4,6-dimethyl-5-(4-nitrophenyl)-1,3,2-dioxaborinane the angle between the 1,3-dicarbonyl group and the benzene ring plane is as large as 81° (Emsley, Freeman, Bates & Hursthouse, 1989). It is noteworthy that the conformations of the difluoroboron complexes discussed above differ in certain respects from that reported for benzoylacetonatodifluoroboron(III) (Hanson & Macaulay, 1972), *e.g.* the aromatic ring is coplanar with the 1,3-dicarbonyl group in this latter compound.

The twists between the 3-oxopropanalato group and the benzene rings in (1) diminish the repulsion between H(C9) and H(C11), and between H(C2) and O(1), which is reflected by the H(C9)···H(C11) [2.66 (4) Å] and H(C2)···O(1) [2.37 (2) Å] distances. The C—O bond distances in the 3-oxopropanalato group are somewhat longer than in metal–1,3-dicarbonyl chelates (Lingafelter & Braun, 1966). The C—C bond distances in the 1,3-dicarbonyl group are similar to the corresponding bond distances in metal chelates of acetylacetone (Lingafelter & Braun, 1966; Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The average C—C bond distance within the benzene rings is 1.390 (12) Å.

The benzylic C(7) atom is twisted out of the benzene ring plane by as much as 0.159 (3) Å; the corresponding distance for C(8) is only 0.024 (3) Å. Among the shortest intermolecular distances are: 2.909 (5) Å [C(9)···F(2)], 2.36 (3) Å [F(2)···H(C11)], 2.38 (3) Å [O(5)···H(C9)] and 2.54 (5) Å [HC(16)···H2(C18)].

The investigations of the difluoroboron complexes discussed above seem to be the only structure determinations performed on such compounds in which the C atoms in the 1,3-dicarbonyl–boron ring are bonded solely to C or H atoms. Crystal structures of a second type of 1,3-dicarbonyl–difluoroboron complex have been reported (Jones & Peterson, 1983; Jones, Begley, Peterson & Sumaria, 1990; Boeyens, Denner, Painter & Staskun, 1987). A characteristic of this latter series of difluoroboron complexes is that an N atom is linked to the 1,3-dicarbonyl moiety. Nevertheless, they exhibit striking structural similarities to the difluoroboron complex investigated in this paper.

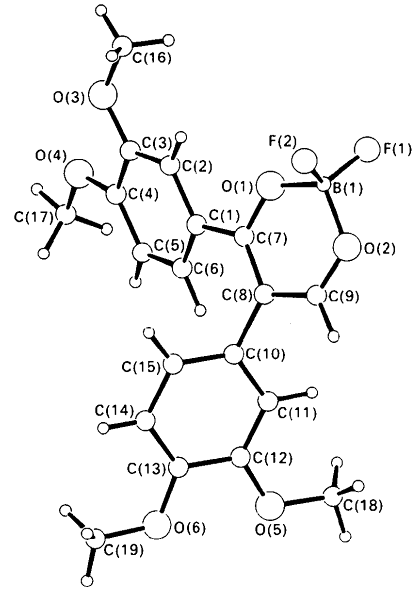

Fig. 1. A perspective drawing (*ORTEP*II; Johnson, 1976) of the title molecule. Atoms are represented by spheres of arbitrary size.

## Experimental

### *Crystal data*

$[BF_2(C_{19}H_{19}O_6)]$
$M_r = 392.16$
Monoclinic
$P2_1/a$
$a = 8.745$ (4) Å
$b = 19.207$ (3) Å
$c = 10.981$ (3) Å
$\beta = 92.23$ (3)°
$V = 1843$ (1) Å$^3$
$Z = 4$
$D_x = 1.413$ Mg m$^{-3}$

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 23 reflections
$\theta = 20.0$–$23.2°$
$\mu = 0.109$ mm$^{-1}$
$T = 133$ K
Whisker fragment
0.55 × 0.23 × 0.13 mm
Orange

### *Data collection*

Rigaku AFC-6*R* diffractometer
$\omega$-2$\theta$ scans
Absorption correction: none
3580 measured reflections
3351 independent reflections
1894 observed reflections $[I > 3\sigma(I)]$

$R_{\rm int} = 0.030$
$\theta_{\rm max} = 25°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 22$
$l = -13 \rightarrow 13$
3 standard reflections monitored every 150 reflections intensity variation: ±3%

### *Refinement*

Refinement on *F*
$R = 0.040$
$wR = 0.045$
$S = 1.69$
1894 reflections
330 parameters
All H-atom parameters refined

$w = [\sigma^2(F_o) + 0.03(F_o)^2]^{-1}$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.38$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.33$ e Å$^{-3}$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å$^2$)

$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

| | *x* | *y* | *z* | $B_{eq}$ |
|---|---|---|---|---|
| C(1) | −0.0063 (3) | 0.7801 (1) | 0.2829 (2) | 1.8 (1) |
| C(2) | −0.0471 (3) | 0.8466 (2) | 0.2384 (3) | 2.0 (1) |
| C(3) | −0.0009 (3) | 0.8683 (1) | 0.1266 (3) | 1.9 (1) |
| C(4) | 0.0895 (3) | 0.8247 (2) | 0.0560 (2) | 2.0 (1) |
| C(5) | 0.1286 (3) | 0.7592 (2) | 0.0996 (3) | 2.1 (1) |
| C(6) | 0.0811 (3) | 0.7367 (2) | 0.2117 (3) | 2.0 (1) |
| C(7) | −0.0444 (3) | 0.7624 (2) | 0.4082 (2) | 2.0 (1) |
| C(8) | −0.0520 (3) | 0.6953 (1) | 0.4582 (3) | 2.0 (1) |
| C(9) | −0.0625 (4) | 0.6906 (2) | 0.5824 (3) | 3.2 (2) |
| C(10) | −0.0438 (3) | 0.6293 (1) | 0.3858 (2) | 1.9 (1) |
| C(11) | 0.0702 (4) | 0.5804 (1) | 0.4146 (3) | 1.9 (1) |
| C(12) | 0.0771 (3) | 0.5190 (1) | 0.3499 (2) | 1.9 (1) |
| C(13) | −0.0301 (3) | 0.5054 (2) | 0.2540 (3) | 2.2 (1) |
| C(14) | −0.1415 (4) | 0.5541 (2) | 0.2255 (3) | 2.4 (1) |
| C(15) | −0.1485 (4) | 0.6161 (2) | 0.2919 (3) | 2.3 (1) |
| C(16) | −0.1043 (5) | 0.9822 (2) | 0.1529 (4) | 3.5 (2) |
| C(17) | 0.2380 (5) | 0.8128 (2) | −0.1218 (3) | 3.3 (2) |
| C(18) | 0.2984 (4) | 0.4818 (2) | 0.4659 (3) | 2.6 (2) |
| C(19) | −0.1274 (6) | 0.4245 (3) | 0.1066 (5) | 5.1 (3) |
| O(1) | −0.0662 (3) | 0.8167 (1) | 0.4773 (2) | 2.6 (1) |
| O(2) | −0.0722 (3) | 0.7427 (1) | 0.6567 (2) | 3.7 (1) |
| O(3) | −0.0314 (3) | 0.9321 (1) | 0.0770 (2) | 2.7 (1) |
| O(4) | 0.1360 (3) | 0.8525 (1) | −0.0492 (2) | 2.8 (1) |
| O(5) | 0.1845 (2) | 0.4682 (1) | 0.3710 (2) | 2.3 (1) |
| O(6) | −0.0124 (3) | 0.4429 (1) | 0.1967 (2) | 3.1 (1) |
| F(1) | 0.0066 (3) | 0.8561 (1) | 0.6680 (2) | 6.9 (1) |
| F(2) | −0.2371 (3) | 0.8336 (1) | 0.6289 (2) | 6.6 (1) |
| B(1) | −0.0925 (5) | 0.8138 (2) | 0.6105 (3) | 2.5 (2) |

Table 2. *Selected geometric parameters* (Å, °)

| | | | |
|---|---|---|---|
| C(1)—C(7) | 1.468 (4) | C(13)—O(6) | 1.368 (3) |
| C(3)—O(3) | 1.364 (3) | C(16)—O(3) | 1.439 (4) |
| C(4)—O(4) | 1.350 (3) | C(17)—O(4) | 1.439 (4) |
| C(7)—C(8) | 1.404 (4) | C(18)—O(5) | 1.437 (4) |
| C(7)—O(1) | 1.309 (3) | C(19)—O(6) | 1.427 (5) |
| C(8)—C(9) | 1.373 (4) | B(1)—O(1) | 1.490 (4) |
| C(8)—C(10) | 1.498 (4) | B(1)—O(2) | 1.466 (4) |
| C(9)—O(2) | 1.296 (4) | B(1)—F(1) | 1.330 (4) |
| C(12)—O(5) | 1.368 (3) | B(1)—F(2) | 1.343 (4) |
| C(2)—C(1)—C(7) | 118.2 (3) | C(13)—C(12)—O(5) | 115.3 (3) |
| C(6)—C(1)—C(7) | 122.4 (3) | C(12)—C(13)—O(6) | 115.1 (3) |
| C(2)—C(3)—O(3) | 124.8 (3) | C(14)—C(13)—O(6) | 125.7 (3) |
| C(4)—C(3)—O(3) | 114.9 (2) | C(7)—O(1)—B(1) | 124.8 (2) |
| C(3)—C(4)—O(4) | 115.5 (3) | C(9)—O(2)—B(1) | 120.7 (3) |
| C(5)—C(4)—O(4) | 125.3 (3) | C(3)—O(3)—C(16) | 117.0 (2) |
| C(1)—C(7)—C(8) | 126.6 (3) | C(4)—O(4)—C(17) | 118.5 (3) |
| C(1)—C(7)—O(1) | 113.6 (2) | C(12)—O(5)—C(18) | 116.5 (2) |
| C(8)—C(7)—O(1) | 119.7 (2) | C(13)—O(6)—C(19) | 116.5 (3) |
| C(7)—C(8)—C(9) | 117.0 (3) | O(1)—B(1)—O(2) | 110.7 (3) |
| C(7)—C(8)—C(10) | 124.3 (2) | O(1)—B(1)—F(1) | 108.7 (3) |
| C(9)—C(8)—C(10) | 118.6 (3) | O(1)—B(1)—F(2) | 108.6 (3) |
| C(8)—C(9)—O(2) | 125.7 (3) | O(2)—B(1)—F(1) | 109.7 (3) |
| C(8)—C(10)—C(11) | 119.8 (3) | O(2)—B(1)—F(2) | 108.3 (3) |
| C(8)—C(10)—C(15) | 120.7 (3) | F(1)—B(1)—F(2) | 110.8 (3) |
| C(11)—C(12)—O(5) | 124.5 (3) | | |
| C(1)—C(7)—C(8)—C(9) | 168.6 (3) | | |
| C(1)—C(7)—C(8)—C(10) | −9.2 (5) | | |
| C(1)—C(7)—O(1)—B(1) | −174.3 (3) | | |
| C(2)—C(1)—C(7)—C(8) | 161.6 (3) | | |
| C(2)—C(1)—C(7)—O(1) | −21.4 (4) | | |
| C(2)—C(3)—O(3)—C(16) | 6.4 (5) | | |
| C(5)—C(4)—O(4)—C(17) | −1.8 (4) | | |
| C(7)—C(8)—C(9)—O(2) | 2.9 (5) | | |
| C(7)—C(8)—C(9)—H(C9) | −177 (2) | | |
| C(7)—C(8)—C(10)—C(11) | 122.3 (3) | | |
| C(7)—O(1)—B(1)—O(2) | 6.9 (4) | | |
| C(8)—C(7)—O(1)—B(1) | 2.9 (4) | | |
| C(8)—C(9)—O(2)—B(1) | 7.9 (6) | | |
| C(9)—C(8)—C(7)—O(1) | −8.3 (4) | | |
| C(9)—C(8)—C(10)—C(11) | −55.5 (4) | | |
| C(9)—O(2)—B(1)—O(1) | −12.1 (5) | | |
| C(10)—C(8)—C(7)—O(1) | 174.0 (3) | | |
| C(10)—C(8)—C(9)—O(2) | −179.2 (3) | | |
| C(11)—C(12)—O(5)—C(18) | −1.4 (4) | | |
| C(14)—C(13)—O(6)—C(19) | −5.5 (5) | | |

Symmetry and approximate cell dimensions were derived from rotation and Weissenberg photographs (Cu $K\alpha$ radiation). The *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985), including *SHELXS*86 (Sheldrick, 1985), was used to solve and refine the structure. The F atoms show rather large anisotropy even at 133 K. The remaining peaks in the electron density difference map, both 0.38 e Å$^{-3}$, could be due to disordered F atoms or may indicate that the model does not describe the thermal motion correctly. A disordered model, with the $BF_2$ group in two positions, was refined and an *R* value of 0.035 was obtained. The bond distances and angles arrived at, however, were not convincing. Therefore, we prefer to describe the structure as ordered.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71512 (30 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU1058]

---

## References

Ahvonen, T., Brunow, G., Kristersson, P. & Lundquist, K. (1983). *Acta Chem. Scand. Ser. B*, **37**, 845–849.

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–S19.

Boeyens, J. C. A., Denner, L., Painter, S. & Staskun, B. (1987). *S. Afr. J. Chem.* **40**, 60–64.

Chow, Y. L. & Cheng, X. (1991). *Can J. Chem.* **69**, 1575–1583.

Chow, Y. L., Cheng, X. & Johansson, C. I. (1991). *J. Photochem. Photobiol. A*, **57**, 247–255.

Emsley, J., Freeman, N. J., Bates, P. A. & Hursthouse, M. B. (1989). *J. Mol. Struct.* **196**, 249–255.

Hanson, A. W. & Macaulay, E. W. (1972). *Acta Cryst.* **B28**, 1961–1967.

House, H. O. & Ryerson, G. D. (1961). *J. Am. Chem. Soc.* **83**, 979–983.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Jones, R. C. F., Begley, M. J., Peterson, G. E. & Sumaria, S. (1990). *J. Chem. Soc. Perkin Trans.* 1, pp. 1959–1968.

Jones, R. C. F. & Peterson, G. E. (1983). *Tetrahedron Lett.* **24**, 4757–4760.

Kristersson, P. & Lundquist, K. (1980). *Acta Chem. Scand. Ser. B*, **34**, 213–215.

Li, S., Lundquist, K. & Stomberg, R. (1993). *Acta Chem. Scand.* **47**, 867–871.
Lingafelter, E. C. & Braun, R. L. (1966). *J. Am. Chem. Soc.* **88**, 2951–2956.
Molecular Structure Corporation. (1985). *TEXSAN. TEXRAY Structure Analysis Package.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Ralph, J., Ede, R. M., Robinson, N. P. & Main, L. J. (1987). *J. Wood Chem. Technol.* **7**, 133–160.
Sagredos, A. N. (1966). *Liebigs Ann. Chem.* **700**, 30–31.
Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures.* Univ. of Göttingen, Germany.
Stomberg, R. & Lundquist, K. (1991). *J. Crystallogr. Spectrosc. Res.* **21**, 701–710.
Tanaka, H., Hiroo, M., Ichino, K. & Ito, K. (1989). *Chem. Pharm. Bull.* **37**, 1441–1445.

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*Acta Cryst.* (1994). **C50**, 217–219

# *cis*-Dichloro[1,2-bis(dicyclohexylphosphino)ethane]palladium(II)

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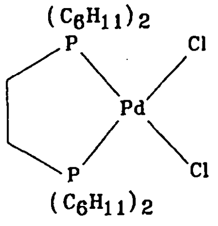
## Abstract

The structure of *cis*-$\mathrm{PdCl_2}$(dcpe), where dcpe is 1,2-bis(dicyclohexylphosphino)ethane, $[\mathrm{PdCl_2(C_{26}H_{48}P_2)}]$, consists of an approximately square planar $\mathrm{Pd^{II}}$ ion coordinated by a chelating dcpe ligand and two $\mathrm{Cl^-}$ ions. The coordination sphere of the Pd shows a slight tetrahedral distortion. A significant *trans* influence of the dcpe ligand on the Pd—Cl distances is evident.

## Comment

Recently, we have employed hydroxy-bridged dinuclear $\mathrm{Pd^{II}}$ complexes such as $[\mathrm{Pd}(\mu\text{-OH})(\mathrm{dppe})]_2(\mathrm{BF_4})_2$ [dppe is 1,2-bis(diphenylphosphino)ethane] as catalysts for the homogeneous hydration of alkenes (Ganguly & Roundhill, 1991). As part of continuing studies to assess the effect of changes in the electronic and steric properties of the phosphine ligand(s) on the catalysis, the related species $[\mathrm{Pd}(\mu\text{-OH})(\mathrm{dcpe})]_2(\mathrm{BF_4})_2$ was prepared from *cis*-$\mathrm{PdCl_2}$(dcpe) (Ganguly, Mague & Roundhill, 1992). Recent studies have indicated that the analogous platinum complex *cis*-$\mathrm{PtCl_2}$(dcpe) is a precursor to a wide variety of species containing the [Pt(dcpe)] moiety (Mague, Fink & Recatto, 1993) and suggest that *cis*-$\mathrm{PdCl_2}$(dcpe) can similarly be the source of a broad range of palladium complexes containing the chelated dcpe ligand. Therefore, we have determined the structure of $\mathrm{PdCl_2}$(dcpe) (I).



(I)

The coordination sphere of the Pd atom is approximately square planar but with a small tetrahedral distortion, as can be seen from the dihedral angle of 5.3 (2)° between the plane defined by Pd, P(1) and P(2), and that defined by Pd, Cl(1) and Cl(2). A similar distortion [dihedral angle of 5.9 (5)°] was found in the Pt analogue (Mague, Fink & Recatto, 1993). The Pd—P distances are equal, within experimental error, and essentially the same as found in *cis*-$\mathrm{PdCl_2}$(dppe) [2.226 (2) and 2.233 (2) Å (Steffen & Palenik, 1976)] and in *cis*-$\mathrm{PdCl_2}$(DH), where DH is 1,2-bis(diisopropylphosphino)benzene [2.233 (1) and 2.234 (1) Å (Liu, Cheu, Peng, Hsiao & Cheng, 1990)]. The contraction of the P(1)—Pd—P(2) angle from the ideal value of 90° is greater than that found in the Pt analogue but not as great as that found in *cis*-$\mathrm{PdCl_2}$(dppe). The Pd—Cl distances in (I) differ by an amount which is possibly significant; an even greater difference [2.398 (2) *versus* 2.417 (2) Å] is seen in *cis*-$\mathrm{PdCl_2(P^nPr_3)_2}$ (Alcock, Kemp & Wimmer, 1981). By contrast, the Pd—Cl distances in *cis*-$\mathrm{PdCl_2}$(dppe) and *cis*-$\mathrm{PdCl_2}$(DH) are equal within experimental error. The inequality seen in the triisopropylphos-

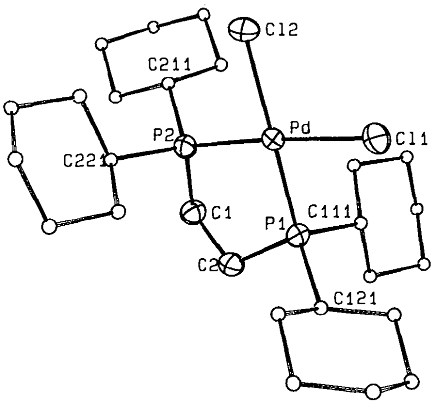


Fig. 1. A perspective view of $\mathrm{PdCl_2}$(dcpe); displacement ellipsoids are drawn at the 50% contour level, cyclohexyl C atoms are drawn arbitrarily small and H atoms are omitted for clarity.

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