

N(2)—Yb—O(3)	97.3 (7)	C(19)—C(20)—C(24)	120 (3)
N(2)—Yb—O(4)	157.5 (7)	C(20)—C(24)—C(23)	122 (2)
O(1)—Yb—O(2)	87.6 (6)	C(21)—C(13)—C(14)	119 (3)
O(1)—Yb—O(3)	164.8 (5)	C(21)—C(22)—C(23)	108 (2)
O(1)—Yb—O(4)	99.0 (6)	C(22)—C(21)—C(13)	121 (3)
O(2)—Yb—O(3)	87.1 (6)	C(22)—C(23)—C(17)	141 (3)
O(2)—Yb—O(4)	77.1 (6)	C(22)—C(23)—C(24)	106 (2)
O(3)—Yb—O(4)	65.8 (5)	C(23)—C(17)—C(18)	122 (3)
Yb—N(1)—C(9)	126 (1)	C(23)—C(24)—N(2)	109 (3)
Yb—N(1)—C(12)	128 (2)	C(24)—N(2)—C(21)	105 (2)
Yb—N(2)—C(21)	131 (2)	C(24)—C(23)—C(17)	114 (3)
Yb—N(2)—C(24)	119 (2)	C(25)—O(1)—C(28)	108 (2)
N(1)—C(9)—C(1)	127 (2)	C(25)—C(26)—C(27)	100 (3)
N(1)—C(9)—C(10)	114 (2)	C(26)—C(27)—C(28)	107 (3)
N(1)—C(12)—C(8)	129 (3)	C(27)—C(28)—O(1)	107 (3)
N(2)—C(21)—C(13)	127 (3)	C(4)—C(10)—C(11)	135 (2)
N(2)—C(21)—C(22)	112 (3)	C(5)—C(6)—C(7)	122 (3)
N(2)—C(24)—C(20)	130 (3)	C(6)—C(7)—C(8)	123 (3)
O(1)—C(25)—C(26)	107 (3)	C(7)—C(8)—C(12)	117 (3)
O(2)—C(29)—C(30)	108 (3)	C(8)—C(12)—C(11)	119 (2)
C(1)—C(2)—C(3)	120 (3)	C(9)—C(1)—C(2)	120 (3)
C(2)—C(3)—C(4)	122 (3)	C(9)—C(10)—C(11)	103 (2)
C(3)—C(4)—C(10)	117 (3)	C(10)—C(9)—C(1)	118 (2)
C(4)—C(10)—C(9)	122 (2)	C(10)—C(11)—C(5)	130 (2)
C(10)—C(11)—C(12)	107 (2)	C(29)—O(2)—C(32)	107 (2)
C(11)—C(5)—C(6)	117 (3)	C(29)—C(30)—C(31)	104 (3)
C(11)—C(12)—N(1)	112 (2)	C(30)—C(31)—C(32)	108 (3)
C(12)—N(1)—C(9)	103 (2)	C(31)—C(32)—O(2)	109 (3)
C(12)—C(11)—C(5)	123 (2)		

A representative crystal was mounted in a Lindemann glass capillary tube under Ar in a dry box. The crystal was fixed to the side of the tube with a small amount of dry liquid paraffin. Intensity data were measured on an automatic four-circle diffractometer equipped with a graphite monochromator, as described previously (Canty, Chaichit & Gatehouse, 1980). Three standard reflections decreased in intensity by 52 (2)%; a correction for decomposition was applied. It is believed that the high *R* value arises as a result of the decomposition. Data were processed using a program written specifically for the PW1100 diffractometer (Hornstra & Stubbe, 1972). Scattering factors for neutral atoms and corrections for anomalous dispersion were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations were performed on the Monash University VAX11/780 computer system. Programs used: *SHELX76* (Sheldrick, 1976) and *ORFFE* (Busing, Martin & Levy, 1964).

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 71623 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL1064]

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## A New Orthorhombic Crystal Form of Dichloro[(-)-(R,R)-2,2-dimethyl-4,5-bis(diphenylphosphinomethyl)-1,3-dioxolane-P,P']platinum, [{(R,R)-diop}PtCl<sub>2</sub>]

CHRISTIAN GANTER AND A. GUY ORPEN\*

*School of Chemistry, University of Bristol, Bristol BS8 1TS, England*

PAOLA BERGAMINI AND EMILIANA COSTA

*Dipartimento di Chimica dell'Università di Ferrara e Centro di Fotochimica CNR, Via L. Borsari 46, 44100 Ferrara, Italy*

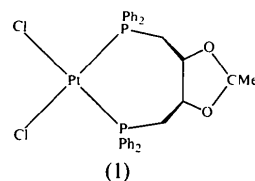
(Received 1 February 1993; accepted 22 September 1993)

## Abstract

In the orthorhombic form of the title compound, [PtCl<sub>2</sub>(C<sub>31</sub>H<sub>32</sub>O<sub>2</sub>P<sub>2</sub>)], the geometry at Pt is approximately square planar and the molecular conformation observed is qualitatively similar to that of one of the two independent molecules in a triclinic polymorph determined previously. The crystal and molecular structures are pseudo-isomorphous with those of [(S,S)-diop}PtMeCl].

## Comment

Crystals of dichloro[(-)-(R,R)-2,2-dimethyl-4,5-bis(diphenylphosphinomethyl)-1,3-dioxolane-P,P']-



platinum, [(*R,R*)-diop}PtCl<sub>2</sub>] (1), were serendipitously isolated from the attempted preparation of the insertion product of a functionalized carbene into a Pt—Cl bond. The molecular and crystal structure of [(*R,R*)-diop}PtCl<sub>2</sub>] was originally determined more than ten years ago together with those of the analogous Ni and Pd compounds (Gramlich & Consiglio, 1979). The structure was found to be triclinic with two molecules in the unit cell of space group *P*1. We intended to compare the geometric parameters of the previously unknown orthorhombic modification with those exhibited by the triclinic polymorph. A perspective view of the molecular structure is presented in Fig. 1.

The space group and crystal structure found in our determination differs clearly from that reported earlier in the literature (triclinic, *P*1, *a* = 10.381, *b* = 11.127, *c* = 14.643 Å,  $\alpha$  = 98.20,  $\beta$  = 85.32,  $\gamma$  = 118.30°, *Z* = 2). The two structures are not related by simple transformations. The analogous compound [(*R,R*)-diop}NiCl<sub>2</sub>] has the same space group (*P*2<sub>1</sub>2<sub>1</sub>) as the title crystal; however, the cell dimensions are completely different (*a* = 10.785, *b* = 14.441, *c* = 19.396 Å, *Z* = 4). The known structures of the Pt and Pd analogues are isomorphous, having space group *P*1 and *Z* = 2 (Gramlich & Consiglio, 1979). In contrast, the published (Payne & Stephan, 1982) crystal structure of [(*S,S*)-diop}PtClMe] (*a* = 16.282, *b* = 16.995, *c* = 10.973 Å, space group *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, *Z* = 4) is isostructural with that of the orthorhombic form of [(*R,R*)-diop}PtCl<sub>2</sub>], although the absolute structure is, of course, inverted. The similarity of the spatial requirements of methyl and chlorine substituents in organic and organometallic species has been noted and exploited in studies of molecular packing (Gavezzotti & Simonetta, 1975; Aime, Braga, Gobetto, Grepioni & Orlandi, 1991). The bond distances and angles for the present molecular structure lie in the same range as found

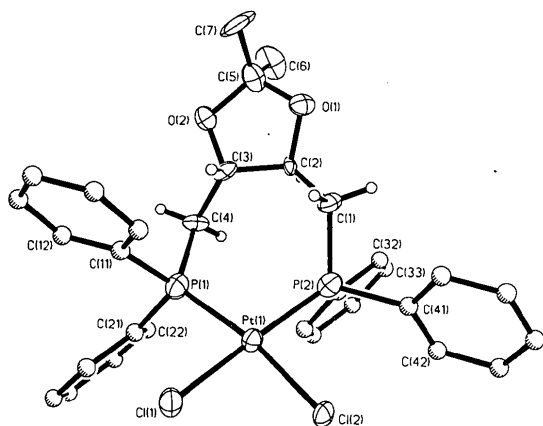


Fig. 1. The molecular structure of [(*R,R*)-diop}PtCl<sub>2</sub>] with methyl and phenyl H atoms omitted for clarity. Ellipsoids are drawn to enclose 30% probability density.

for the two independent molecules in the triclinic structure of (1). The differences are more pronounced for the torsion angles which describe the conformation of the molecule. As can be seen from Fig. 2, the conformation of (1) in the *P*2<sub>1</sub>2<sub>1</sub> structure qualitatively resembles that of one of the two molecules in the triclinic structure, but is completely different from the second one. Even for the similar conformations, however, the differences between individual intra-five- and seven-membered ring torsion-angle values are as much as 15°.

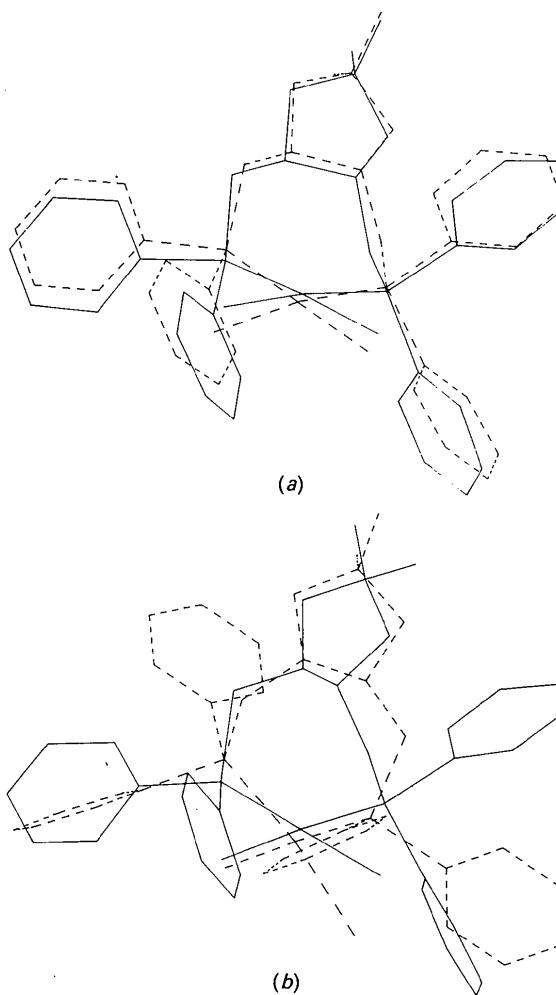


Fig. 2. Least-squares superpositions (based on all non-H atoms except phenyl C atoms) of the molecular structure of orthorhombic [(*R,R*)-diop}PtCl<sub>2</sub>] with those of the two independent molecules (a) and (b) from the triclinic form; full line: triclinic, dashed line: orthorhombic.

## Experimental

### Crystal data

[PtCl<sub>2</sub>(C<sub>31</sub>H<sub>32</sub>O<sub>2</sub>P<sub>2</sub>)]  
*M<sub>r</sub>* = 764.5

Mo *K*α radiation  
 $\lambda$  = 0.71073 Å

Orthorhombic  
 $P2_12_12_1$   
 $a = 16.382$  (8) Å  
 $b = 16.796$  (7) Å  
 $c = 10.926$  (3) Å  
 $V = 3006$  (2) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.69$  Mg m<sup>-3</sup>

Cell parameters from 33 reflections  
 $\theta = 3-12^\circ$   
 $\mu = 4.98$  mm<sup>-1</sup>  
 $T = 293$  K  
 Multi-faceted block  
 $0.3 \times 0.2 \times 0.1$  mm  
 Pale yellow  
 Crystal source: Et<sub>2</sub>O/CH<sub>2</sub>-Cl<sub>2</sub>/N<sub>2</sub>CHCO<sub>2</sub>Et solution

## Data collection

Siemens P3m diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction: empirical azimuthal scan  
 $T_{\min} = 0.535$ ,  $T_{\max} = 0.676$   
 3791 measured reflections  
 3172 independent reflections  
 1817 observed reflections  
 $[I > 2\sigma(I)]$

$R_{\text{int}} = 0.026$   
 $\theta_{\text{max}} = 25^\circ$   
 $h = 0 \rightarrow 19$   
 $k = 0 \rightarrow 20$   
 $l = 0 \rightarrow 13$   
 3 standard reflections monitored every 50 reflections  
 intensity variation:  $\pm 3\%$

## Refinement

Refinement on  $F^2$   
 $R = 0.063$   
 $wR = 0.056$   
 $S = 1.19$   
 1817 reflections  
 175 parameters  
 $w = [\sigma^2(F) + 0.0005F^2]^{-1}$

$(\Delta/\sigma)_{\text{max}} = 0.028$   
 $\Delta\rho_{\text{max}} = 1.5$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.5$  e Å<sup>-3</sup>  
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)
$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}$
Pt(1)	0.1027 (1)	0.2049 (1)	0.1868 (1)	0.040 (1)
Cl(1)	0.1721 (6)	0.3248 (4)	0.1656 (9)	0.073 (4)
Cl(2)	0.0430 (5)	0.2621 (4)	0.3603 (7)	0.048 (3)
P(1)	0.1621 (5)	0.1697 (4)	0.0083 (7)	0.054 (3)
P(2)	0.0385 (5)	0.0893 (4)	0.2244 (7)	0.063 (3)
O(1)	0.1642 (11)	-0.1106 (10)	0.1341 (16)	0.047 (7)
O(2)	0.2117 (12)	-0.0584 (11)	-0.0509 (17)	0.055 (8)
C(1)	0.1025 (19)	0.0010 (13)	0.231 (2)	0.044 (9)
C(2)	0.1256 (15)	-0.0373 (14)	0.111 (2)	0.029 (10)
C(3)	0.1812 (18)	0.0049 (15)	0.026 (2)	0.048 (12)
C(4)	0.1468 (16)	0.0695 (12)	-0.056 (2)	0.039 (10)
C(5)	0.202 (2)	-0.1300 (19)	0.020 (3)	0.063 (15)
C(6)	0.149 (2)	-0.1890 (16)	-0.055 (3)	0.094 (17)
C(7)	0.282 (2)	-0.164 (2)	0.054 (4)	0.16 (2)
C(11)	0.2713 (8)	0.1737 (9)	0.0101 (18)	0.041 (8)
C(12)	0.3161 (8)	0.1816 (9)	-0.0978 (18)	0.058 (9)
C(13)	0.4010 (8)	0.1755 (9)	-0.0951 (18)	0.053 (8)
C(14)	0.4411 (8)	0.1616 (9)	0.0155 (18)	0.061 (9)
C(15)	0.3963 (8)	0.1537 (9)	0.1234 (18)	0.076 (9)
C(16)	0.3114 (8)	0.1597 (9)	0.1207 (18)	0.047 (8)
C(21)	0.1294 (9)	0.2335 (9)	-0.1190 (11)	0.020 (6)
C(22)	0.0706 (9)	0.2078 (9)	-0.2025 (11)	0.038 (6)
C(23)	0.0512 (9)	0.2548 (9)	-0.3037 (11)	0.058 (8)
C(24)	0.0907 (9)	0.3275 (9)	-0.3214 (11)	0.060 (8)
C(25)	0.1495 (9)	0.3531 (9)	-0.2379 (11)	0.062 (9)
C(26)	0.1689 (9)	0.3061 (9)	-0.1368 (11)	0.054 (9)
C(31)	-0.0444 (9)	0.0641 (10)	0.1217 (15)	0.044 (8)
C(32)	-0.0687 (9)	0.1195 (10)	0.0337 (15)	0.047 (8)
C(33)	-0.1352 (9)	0.1032 (10)	-0.0420 (15)	0.061 (10)
C(34)	-0.1775 (9)	0.0315 (10)	-0.0296 (15)	0.063 (10)

C(35)	-0.1533 (9)	-0.0238 (10)	0.0584 (15)	0.073 (11)
C(36)	-0.0867 (9)	-0.0075 (10)	0.1340 (15)	0.050 (8)
C(41)	-0.0136 (15)	0.0830 (11)	0.3733 (16)	0.054 (9)
C(42)	-0.0947 (15)	0.1083 (11)	0.3787 (16)	0.087 (11)
C(43)	-0.1382 (15)	0.1021 (11)	0.4880 (16)	0.136 (18)
C(44)	-0.1007 (15)	0.0707 (11)	0.5919 (16)	0.108 (13)
C(45)	-0.0196 (15)	0.0454 (11)	0.5865 (16)	0.096 (13)
C(46)	0.0239 (15)	0.0516 (11)	0.4772 (16)	0.092 (13)

Table 2. Selected bond lengths (Å), bond angles (°) and torsion angles (°)

Pt(1)—Cl(1)	2.324 (8)	O(1)—C(2)	1.41 (3)
Pt(1)—P(2)	2.246 (8)	O(2)—C(5)	1.44 (4)
P(1)—C(21)	1.836 (15)	C(3)—C(4)	1.52 (4)
P(2)—C(41)	1.84 (2)	Pt(1)—P(1)	2.258 (8)
O(2)—C(3)	1.44 (3)	P(1)—C(11)	1.790 (15)
C(2)—C(3)	1.48 (4)	P(2)—C(31)	1.812 (18)
C(5)—C(7)	1.47 (5)	O(1)—C(5)	1.43 (4)
Pt(1)—Cl(2)	2.339 (8)	C(1)—C(2)	1.51 (3)
P(1)—C(4)	1.84 (2)	C(5)—C(6)	1.55 (5)
P(2)—C(1)	1.82 (3)		
Cl(1)—Pt(1)—Cl(2)	86.0 (3)	Cl(1)—Pt(1)—P(1)	86.0 (3)
Cl(2)—Pt(1)—P(1)	171.0 (3)	Cl(1)—Pt(1)—P(2)	175.1 (3)
Cl(2)—Pt(1)—P(2)	90.6 (3)	P(1)—Pt(1)—P(2)	97.6 (3)
Pt(1)—P(1)—C(4)	120.7 (8)	Pt(1)—P(2)—C(1)	116.3 (10)
C(2)—O(1)—C(5)	104 (2)	C(3)—O(2)—C(5)	105 (2)
P(2)—C(1)—C(2)	117.2 (17)	O(1)—C(2)—C(1)	109.0 (19)
O(1)—C(2)—C(3)	105 (2)	C(1)—C(2)—C(3)	120 (2)
O(2)—C(3)—C(2)	103 (2)	O(2)—C(3)—C(4)	108 (2)
C(2)—C(3)—C(4)	119 (2)	P(1)—C(4)—C(3)	112.2 (17)
O(1)—C(5)—O(2)	109 (2)	O(1)—C(5)—C(6)	111 (3)
O(2)—C(5)—C(6)	108 (3)	O(1)—C(5)—C(7)	105 (3)
O(2)—C(5)—C(7)	111 (3)	C(6)—C(5)—C(7)	113 (3)
P(2)—Pt(1)—P(1)—C(4)	0.0 (10)		
Pt(1)—P(1)—C(4)—C(3)	-64 (2)		
Pt(1)—P(1)—C(11)—C(16)	29.9 (6)		
Pt(1)—P(1)—C(21)—C(26)	83.6 (4)		
Pt(1)—P(2)—C(31)—C(32)	-5.7 (7)		
Pt(1)—P(2)—C(41)—C(42)	89.5 (6)		
C(5)—O(1)—C(2)—C(3)	-36 (3)		
C(5)—O(2)—C(3)—C(2)	-24 (3)		
P(2)—C(1)—C(2)—C(3)	68 (3)		
C(1)—C(2)—C(3)—C(4)	-81 (3)		
P(1)—Pt(1)—P(2)—C(1)	56.7 (9)		
Pt(1)—P(1)—C(11)—C(12)	-157.1 (2)		
Pt(1)—P(1)—C(21)—C(22)	-101.2 (4)		
Pt(1)—P(2)—C(1)—C(2)	-82 (2)		
Pt(1)—P(2)—C(31)—C(36)	177.9 (2)		
Pt(1)—P(2)—C(41)—C(46)	-93.0 (6)		
C(2)—O(1)—C(5)—O(2)	21 (3)		
C(3)—O(2)—C(5)—O(1)	2 (3)		
O(1)—C(3)—C(3)—O(2)	37 (2)		
C(2)—C(4)—C(4)—P(1)	97 (2)		

Some additional reflections with  $k < 0$  were measured. The absolute configuration was established by refinement of an  $\eta$  parameter (Rogers, 1981);  $\eta = 1.11$  (4). H atoms were placed with idealized geometries (C—H = 0.96 Å), riding on their respective C atoms with fixed  $U$ . *SHELXTL-Plus* (Sheldrick, 1990) was used for calculations.

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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 71658 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HU1050]

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*Acta Cryst.* (1994). **C50**, 510–512

### Dichlorobis(5,7-dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine-*N*<sup>3</sup>)zinc(II)

JUAN MANUEL SALAS, MARÍA ANGUSTIAS ROMERO,  
AND ABDERRAHMAN RAHMANI

*Departamento de Química Inorgánica,  
Universidad de Granada 18071, Granada, Spain*

RENÉ FAURE

*Laboratoire de Chimie Analytique II, Université Claude  
Bernard, Lyon I, 69622 Villeurbanne CEDEX, France*

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## Abstract

The synthesis and crystal structure of the title compound, [ZnCl<sub>2</sub>(C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>)<sub>2</sub>], obtained by the reaction of zinc(II) chloride with 5,7-dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine (dmtp), are reported. The Zn atom is tetrahedrally coordinated by two Cl atoms at distances of 2.197 (1) and 2.2499 (8) Å and to two N3 atoms of two independent molecules of dmtp at distances of 2.058 (2) and 2.020 (2) Å. One of the dmtp ligand types is associated in couples by stacking interactions with an interplanar distance of 3.36 (1) Å.

## Comment

5,7-Dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine (dmtp) is a ligand especially suited to mimicking purine rings, from which it differs mainly in having a pyrimidine N atom in a bridgehead position. Crystallographic studies carried out on metal–dmtp complexes have indicated that the N3 atom in the monodentate form is the most preferred binding site. This coordination mode has been found for [Cd(dmtp)<sub>2</sub>(NCS)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] and [Hg(dmtp)<sub>2</sub>(SCN)<sub>2</sub>]

(Dillen, Lenstra, Haasnoot & Reedijk, 1983), [Cu(dmtp)<sub>2</sub>(SCN)<sub>2</sub>]<sub>2</sub> and [Pt(dmtp)<sub>4</sub>][Pt(SCN)<sub>6</sub>] (Biagini-Cingi, Manotti-Lanfredi, Tiripicchio, Haasnoot & Reedijk, 1983), β-[Cu(dmtp)<sub>2</sub>(SCN)<sub>2</sub>]<sub>2</sub> (Haasnoot, Driessen & Reedijk, 1984), [CoHg(dmtp)<sub>3</sub>(SCN)<sub>4</sub>(H<sub>2</sub>O)]<sub>2</sub> (Biagini-Cingi, Manotti-Lanfredi, Tiripicchio, Haasnoot & Reedijk, 1984), [FeHg(dmtp)<sub>2</sub>(NCS)<sub>4</sub>(H<sub>2</sub>O)<sub>1.5</sub>], [FeHg(dmtp)<sub>2</sub>(NCS)<sub>4</sub>(H<sub>2</sub>O)] and [FeHg(dmtp)(NCS)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>(Me<sub>2</sub>CO)] (Biagini-Cingi, Manotti-Lanfredi, Tiripicchio, Haasnoot & Reedijk, 1985), [Cu(dmtp)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>][PF<sub>6</sub>]<sub>2</sub> (Favre, Haasnoot & Reedijk, 1986), [CuHg(dmtp)<sub>2</sub>(μ-SCN)<sub>3</sub>] (Biagini-Cingi, Manotti-Lanfredi, Tiripicchio, Haasnoot & Reedijk, 1986), [Ni(dmtp)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>](H<sub>2</sub>O)<sub>2</sub>I<sub>2</sub> and [Ni(dmtp)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>](dmtp)<sub>2</sub>(I<sub>3</sub>)<sub>2</sub> (Lenstra, Bruins, Beurskens, Haasnoot & Reedijk, 1989) and [Pd(dmtp)<sub>2</sub>Br<sub>2</sub>][CH<sub>3</sub>OH] (Hage, Graaff, Haasnoot, Kieler & Reedijk, 1990). A different coordination mode *via* N3 and N4 has been found in the cluster [Cu<sub>4</sub>(dmtp)<sub>4</sub>Cl<sub>2</sub>][Cu<sub>2</sub>Cl<sub>4</sub>] (Haasnoot, Favre, Hinrichs & Reedijk, 1988).

As part of our work on the coordination chemistry of purine analogues (Sirera, Romero, Salas, Sánchez & Moreno, 1991; Salas *et al.*, 1992; Romero, Salas, Quirós, Williams & Molina, 1993), we report here the synthesis and crystal structure of the metal complex [Zn(dmtp)<sub>2</sub>Cl<sub>2</sub>] (I).

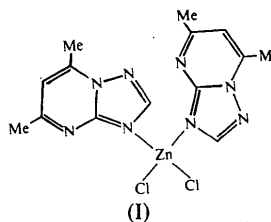


Fig. 1 shows a projection of the molecule with the atomic numbering scheme. The crystal structure of the title compound consists of monomeric Zn(dmtp)<sub>2</sub>Cl<sub>2</sub> units. The coordination polyhedron around the Zn atom is a distorted tetrahedron which involves two N atoms of two independent dmtp ligands and two Cl atoms. The dmtp ligands act in a monodentate manner through N3. The Zn–N3 distances of 2.058 (2) (N3A) and 2.020 (2) Å (N3B) are in agreement with those found for the analogous complex dibromobis([1,2,4]triazolo[1,5-*a*]pyrimidine-*N*<sup>3</sup>)zinc(II) hemihydrate (Sanni *et al.*, 1986). The Zn–Cl distances of 2.197 (1) (Zn–Cl1) and 2.2499 (8) Å (Zn–Cl2) are in the expected range for metal complexes with ZnN<sub>2</sub>Cl<sub>2</sub> distorted tetrahedral environments (Preston & Kennard, 1969; Baenziger & Schultz, 1971; Steffen & Palenik, 1977; Beauchamp, 1984; Cariati *et al.*, 1983; Bharadwaj, Schugar & Potenza, 1991).

The structural parameters of the two independent dmtp molecules are quite regular; both are planar