

Dibromido(η^5, η^5 -propane-2,2-diyl-dicyclopentadienyl)titanium(IV)

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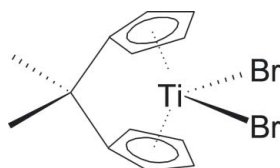
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.052; wR factor = 0.147; data-to-parameter ratio = 19.4.

In the molecule of the title compound, $[\text{TiBr}_2(\text{C}_{13}\text{H}_{14})]$, the Ti^{IV} centre is in a distorted tetrahedral environment involving two η^5 -bonded cyclopentadienyl rings of a propane-2,2-diyl-dicyclopentadienyl ligand [$\text{Ti}-\text{Cg} = 2.045$ (2) Å; Cg is the centroid of the cyclopentadienyl ring] and two Br atoms [$\text{Ti}-\text{Br} = 2.5115$ (7) Å]. The presence of the short 2,2-propylidene bridge between the two cyclopentadienyl rings constrains the $\text{Cg}-\text{Ti}-\text{Cg}$ angle to a value of 121.32 (9)°. The Ti and central C atoms are located on a crystallographic C_2 axis.

Related literature

For related structures, see: Koch *et al.* (2000); Picka *et al.* (2005).



Experimental

Crystal data

$[\text{TiBr}_2(\text{C}_{13}\text{H}_{14})]$

$M_r = 377.96$

Monoclinic, $C2/c$

$a = 13.1890$ (4) Å

$b = 9.7180$ (3) Å

$c = 10.8200$ (3) Å

$\beta = 112.0801$ (18)°

$V = 1285.10$ (7) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 6.85$ mm⁻¹

$T = 150$ (2) K

$0.22 \times 0.15 \times 0.08$ mm

Data collection

Nonius KappaCCD area-detector diffractometer

Absorption correction: integration (Gaussian; Coppens, 1970)

$T_{\min} = 0.274$, $T_{\max} = 0.721$

10067 measured reflections

1475 independent reflections

1333 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.079$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.147$

$S = 1.17$

1475 reflections

76 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 3.38$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.50$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cg1 and Cg1^i are the centroids defined by atoms $\text{C1}-\text{C5}$ and $\text{C1}^i-\text{C5}^i$, respectively. P_1 and P_1^i are the ring planes defined by atoms $\text{C1}-\text{C5}$ and $\text{C1}^i-\text{C5}^i$, respectively.

Ti—Cg1	2.045 (2)	C1—C6—C1 ⁱ	96.8 (4)
Ti—Br1	2.5115 (7)	C7—C6—C7 ⁱ	110.8 (4)
Cg1—Ti—Cg1 ⁱ	121.32 (9)	P ₁ —C1—C6	15.5 (3)
Br1—Ti—Br1 ⁱ	96.87 (3)	P ₁ —P ₁ ⁱ	65.8 (3)

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

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2334).

References

- Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
- Altomare, A., Casciarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–436.
- Coppens, P. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 255–270. Copenhagen: Munksgaard.
- Hooft, R. W. (1998). *COLLECT*. Nonius, Delft, The Netherlands.
- Koch, T., Blaurock, S., Somoza, F. B. Jr, Voigt, A., Kirmse, R. & Hey-Hawkins, E. (2000). *Organometallics*, **19**, 2556–2563.
- Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol. Part A*, **276**, 307–326.
- Picka, M., Císařová, I., Vinklárek, J. & Erben, M. (2005). *Acta Cryst.* **E61**, m1266–m1268.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

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Dibromido(η^5, η^5 -propane-2,2-diyl)dicyclopentadienyl)titanium(IV)

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Comment

Group 4 cyclopentadienyl complexes belong to important class of catalysts for methylalumoxane-promoted polymerization of olefines. In order to find a relationship between the structure and catalytic activity, large series of variously substituted derivatives have been synthesized. It was found that incorporation of short interannular bridge connecting both cyclopentadienyl rings leads to disclosing of electronically unsaturated central metal atom that is better accessible to be attacked by electron-rich olefin. We prepared the title complex, (I), in the framework of our investigation of catalytically active cyclopentadienyl complexes and we report herein its crystal structure.

In the molecule of the title compound, (I), Ti1 and C6 atoms are located on a crystallographic C_2 axis (Fig. 1). It is a typical ansa-metallocene structure with two cyclopentadienyl rings interconnected together with propylidene bridge. The Ti^{IV} centre is in a distorted tetrahedral environment involving two η^5 -bonded cyclopentadienyl rings of $(C_{13}H_{14})^{2-}$ ligand and two Br atoms (Table 1).

In (I), the angle between the planes of cyclopentadienyl rings is $65.8(3)^\circ$, in which it reflects the degree of the disclosure of the central C6 atom. In the analogous dichloride $\{TiCl_2[(C_5H_4)_2C(CH_3)_2]\}$, (II), (Koch *et al.*, 2000) and difluoride $\{TiF_2[(C_5H_4)_2C(CH_3)_2]\}$, (III), (Pícka *et al.*, 2005) complexes, the observed angles are $66.8(10)^\circ$ in (II) and $65.76(9)^\circ$ in (III).

The $Ti1-Cg$ [2.045(2) Å; Cg is the centroid of cyclopentadienyl ring] distance in (I) is shorter than the reported value [$Ti-Cg = 2.193$ Å] in (II), but it is nearly the same with the corresponding values [$Ti1-Cg1 = 2.0558(7)$ Å and $Ti1-Cg2 = 2.0567(8)$ Å] in (III). In (I), the $Ti1-Br1$ distance is $2.5115(7)$ Å. The constraining of the $Cg-Ti-Cg$ angle to a value of $121.32(9)^\circ$ is caused by the presence of the short 2,2-propylidene bridge between the two cyclopentadienyl rings.

On the inspection of ascertained geometric parameters, it is evident that the substitution of halide ligands in ansa-complexes of this type has no significant impact on the structure of $[Ti(C_{13}H_{14})]^{2+}$ unit.

Experimental

Compound (I) was prepared from the chloride derivative (II) by the reaction with boron tribromide in dichloromethane. Starting complex (II) (0.22 g, 0.69 mmol) was dissolved in dry dichloromethane (20 ml) and boron tribromide (0.47 mmol, 0.045 ml) was added. The green-coloured reaction mixture was stirred for 2 h at room temperature and volatiles were evaporated *in vacuo*. The solid residue was washed three times with hexane (10 ml) and dried *in vacuo* (yield; 0.2 g, 75%). Upon slow evaporation of saturated chloroform solution at 270 K, green crystals of (I) suitable for X-ray analysis were obtained.

Refinement

The highest peak in the final difference electron-density map is located 1.05 Å from the Br1 atom. H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms.

Figures

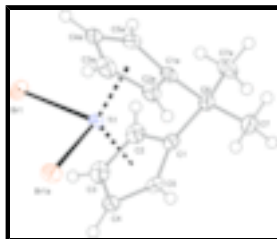


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code (a): $2 - x, y, 3/2 - z$].

Dibromido(η^5, η^5 -propane-2,2-diyl)dicyclopentadienyl)titanium(IV)

Crystal data

[TiBr₂(C₁₃H₁₄)]

$M_r = 377.96$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 13.1890$ (4) Å

$b = 9.7180$ (3) Å

$c = 10.8200$ (3) Å

$\beta = 112.0801$ (18)°

$V = 1285.10$ (7) Å³

$Z = 4$

$F_{000} = 736$

$D_x = 1.954$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5340 reflections

$\theta = 1-27.5^\circ$

$\mu = 6.85$ mm⁻¹

$T = 150$ (2) K

Prism, green

$0.22 \times 0.15 \times 0.08$ mm

Data collection

Nonius KappaCCD area-detector diffractometer

Monochromator: graphite

Detector resolution: 9.091 pixels mm⁻¹

$T = 150$ (2) K

φ and ω scans

Absorption correction: integration (Gaussian; Coppens, 1970)

$T_{\text{min}} = 0.274$, $T_{\text{max}} = 0.721$

10067 measured reflections

1475 independent reflections

1333 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.079$

$\theta_{\text{max}} = 27.5^\circ$

$\theta_{\text{min}} = 2.7^\circ$

$h = -17 \rightarrow 17$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0967P)^2 + 2.0144P]$
$wR(F^2) = 0.147$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{\max} < 0.001$
1475 reflections	$\Delta\rho_{\max} = 3.38 \text{ e } \text{\AA}^{-3}$
76 parameters	$\Delta\rho_{\min} = -1.50 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0032 (9)

Special details

Experimental. *M.p.*: 610 K (dec.) Spectroscopic analysis: ^1H NMR (CDCl_3 , δ , p.p.m.): 6.98 (m, 4H), 5.72 (m, 4H), 1.83 (s, 6H). ^{13}C NMR (CDCl_3 , δ , p.p.m.): 23.3, 36.8, 114.2, 115.5, 131.3. IR (KBr disc, cm^{-1}): 3124 (m), 3101 (m), 3087 (m), 2980 (m), 2967 (m), 2855 (w), 1479 (w), 1465 (m), 1442 (w), 1416 (m), 1383 (m), 1374 (w), 1271 (s), 1225 (w), 1152 (m), 1074 (w), 1048 (m), 947 (w), 907 (m), 885 (w), 875 (m), 845 (w), 829 (s), 817 (s), 733 (s), 733 (s), 706 (m), 608 (w), 464 (m), 424 (m), 319 (m); Raman (quartz capillary, cm^{-1}): 2123 (m), 3100 (m), 3086 (w), 2988 (w), 2941(w), 2918(w), 2870 (w), 1481 (w), 1465 (w), 1447 (w), 1408 (m), 1339 (w), 1348 (w), 1271 (m), 1225 (w), 1152 (m), 1082 (w), 1065 (w), 950 (w), 875 (m), 847 (w), 826 (w), 733 (w), 548 (w), 462 (m) 424 (m), 367 (m), 334 (w), 323 (w), 262 (s), 207 (w), 169 (s), 157 (m), 116 (s), 84 (s); UV-Vis (CH_2Cl_2 , maxima at nm): 593, 406, 319(sh), 271; Elemental analysis, calculated for $\text{C}_{13}\text{H}_{14}\text{Br}_2\text{Ti}$: C 41.31, H 3.73; found: C 41.12, H 3.75.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ti1	1.0000	0.31726 (9)	0.7500	0.0164 (3)
Br1	1.15259 (4)	0.48873 (4)	0.84124 (4)	0.0255 (3)
C1	1.0122 (4)	0.1080 (4)	0.6515 (4)	0.0208 (8)
C2	1.1089 (4)	0.1829 (4)	0.6708 (4)	0.0229 (9)
H2	1.1787	0.1604	0.7305	0.027*
C3	1.0818 (4)	0.2977 (5)	0.5840 (5)	0.0283 (10)
H3	1.1311	0.3615	0.5749	0.034*

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C4	0.9700 (4)	0.2992 (4)	0.5152 (4)	0.0276 (10)
H4	0.9308	0.3643	0.4525	0.033*
C5	0.9253 (4)	0.1831 (4)	0.5574 (4)	0.0235 (9)
H5	0.8515	0.1604	0.5281	0.028*
C6	1.0000	0.0042 (5)	0.7500	0.0210 (13)
C7	0.8971 (4)	-0.0858 (5)	0.6889 (5)	0.0302 (10)
H7A	0.8859	-0.1378	0.7581	0.045*
H7B	0.9065	-0.1476	0.6248	0.045*
H7C	0.8347	-0.0281	0.6456	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0165 (5)	0.0176 (5)	0.0146 (5)	0.000	0.0053 (4)	0.000
Br1	0.0183 (4)	0.0283 (3)	0.0276 (4)	-0.00664 (14)	0.0059 (3)	-0.00450 (15)
C1	0.028 (2)	0.0198 (18)	0.017 (2)	0.0003 (16)	0.0108 (17)	-0.0039 (15)
C2	0.026 (2)	0.025 (2)	0.024 (2)	0.0030 (16)	0.0167 (19)	-0.0037 (16)
C3	0.037 (3)	0.028 (2)	0.030 (2)	-0.0029 (19)	0.025 (2)	-0.0050 (19)
C4	0.048 (3)	0.021 (2)	0.016 (2)	0.0031 (19)	0.014 (2)	-0.0008 (16)
C5	0.028 (2)	0.025 (2)	0.015 (2)	-0.0020 (16)	0.0046 (18)	-0.0031 (16)
C6	0.021 (3)	0.018 (3)	0.021 (3)	0.000	0.005 (3)	0.000
C7	0.040 (3)	0.024 (2)	0.027 (2)	-0.0103 (19)	0.014 (2)	-0.0057 (18)

Geometric parameters (\AA , $^\circ$)

Ti1—C1 ⁱ	2.329 (4)	C1—C6	1.520 (5)
Ti1—C1	2.329 (4)	C2—C3	1.415 (6)
Ti1—C2 ⁱ	2.330 (4)	C2—H2	0.9300
Ti1—C2	2.330 (4)	C3—C4	1.380 (7)
Ti1—C5	2.339 (4)	C3—H3	0.9300
Ti1—C5 ⁱ	2.339 (4)	C4—C5	1.425 (6)
Ti1—C3	2.425 (4)	C4—H4	0.9300
Ti1—C3 ⁱ	2.425 (4)	C5—H5	0.9300
Ti1—C4	2.426 (4)	C6—C1 ⁱ	1.520 (5)
Ti1—C4 ⁱ	2.426 (4)	C6—C7	1.539 (5)
Ti1—Br1	2.5116 (7)	C6—C7 ⁱ	1.539 (5)
Ti1—Br1 ⁱ	2.5116 (7)	C7—H7A	0.9600
C1—C2	1.414 (6)	C7—H7B	0.9600
C1—C5	1.415 (6)	C7—H7C	0.9600
C1 ⁱ —Ti1—C1	58.40 (18)	C4 ⁱ —Ti1—Br1	81.10 (12)
C1 ⁱ —Ti1—C2 ⁱ	35.34 (15)	C1 ⁱ —Ti1—Br1 ⁱ	125.18 (11)
C1—Ti1—C2 ⁱ	80.63 (14)	C1—Ti1—Br1 ⁱ	125.60 (11)
C1 ⁱ —Ti1—C2	80.63 (14)	C2 ⁱ —Ti1—Br1 ⁱ	90.16 (11)
C1—Ti1—C2	35.34 (15)	C2—Ti1—Br1 ⁱ	137.81 (11)
C2 ⁱ —Ti1—C2	111.8 (2)	C5—Ti1—Br1 ⁱ	90.74 (11)
C1 ⁱ —Ti1—C5	80.95 (15)	C5 ⁱ —Ti1—Br1 ⁱ	136.63 (11)

C1—Ti1—C5	35.29 (15)	C3—Ti1—Br1 ⁱ	105.95 (12)
C2 ⁱ —Ti1—C5	84.49 (16)	C3 ⁱ —Ti1—Br1 ⁱ	80.16 (12)
C2—Ti1—C5	58.06 (16)	C4—Ti1—Br1 ⁱ	81.10 (12)
C1 ⁱ —Ti1—C5 ⁱ	35.29 (15)	C4 ⁱ —Ti1—Br1 ⁱ	104.53 (12)
C1—Ti1—C5 ⁱ	80.95 (15)	Br1—Ti1—Br1 ⁱ	96.87 (4)
C2 ⁱ —Ti1—C5 ⁱ	58.06 (16)	C2—C1—C5	106.4 (4)
C2—Ti1—C5 ⁱ	84.49 (16)	C2—C1—C6	124.4 (4)
C5—Ti1—C5 ⁱ	112.2 (2)	C5—C1—C6	125.2 (3)
C1 ⁱ —Ti1—C3	113.39 (14)	C2—C1—Ti1	72.4 (2)
C1—Ti1—C3	57.75 (14)	C5—C1—Ti1	72.7 (2)
C2 ⁱ —Ti1—C3	137.38 (15)	C6—C1—Ti1	102.4 (2)
C2—Ti1—C3	34.55 (15)	C1—C2—C3	108.6 (4)
C5—Ti1—C3	56.78 (16)	C1—C2—Ti1	72.3 (2)
C5 ⁱ —Ti1—C3	117.42 (16)	C3—C2—Ti1	76.4 (2)
C1 ⁱ —Ti1—C3 ⁱ	57.75 (14)	C1—C2—H2	125.7
C1—Ti1—C3 ⁱ	113.39 (14)	C3—C2—H2	125.7
C2 ⁱ —Ti1—C3 ⁱ	34.55 (15)	Ti1—C2—H2	117.5
C2—Ti1—C3 ⁱ	137.38 (15)	C4—C3—C2	108.5 (4)
C5—Ti1—C3 ⁱ	117.42 (16)	C4—C3—Ti1	73.5 (2)
C5 ⁱ —Ti1—C3 ⁱ	56.78 (16)	C2—C3—Ti1	69.0 (2)
C3—Ti1—C3 ⁱ	171.0 (2)	C4—C3—H3	125.7
C1 ⁱ —Ti1—C4	113.82 (14)	C2—C3—H3	125.7
C1—Ti1—C4	57.97 (14)	Ti1—C3—H3	123.3
C2 ⁱ —Ti1—C4	117.65 (16)	C3—C4—C5	107.8 (4)
C2—Ti1—C4	56.95 (16)	C3—C4—Ti1	73.5 (2)
C5—Ti1—C4	34.74 (15)	C5—C4—Ti1	69.3 (2)
C5 ⁱ —Ti1—C4	137.81 (15)	C3—C4—H4	126.1
C3—Ti1—C4	33.06 (18)	C5—C4—H4	126.1
C3 ⁱ —Ti1—C4	145.77 (18)	Ti1—C4—H4	122.8
C1 ⁱ —Ti1—C4 ⁱ	57.97 (14)	C1—C5—C4	108.6 (4)
C1—Ti1—C4 ⁱ	113.82 (14)	C1—C5—Ti1	72.0 (2)
C2 ⁱ —Ti1—C4 ⁱ	56.95 (16)	C4—C5—Ti1	76.0 (2)
C2—Ti1—C4 ⁱ	117.65 (16)	C1—C5—H5	125.7
C5—Ti1—C4 ⁱ	137.81 (15)	C4—C5—H5	125.7
C5 ⁱ —Ti1—C4 ⁱ	34.74 (15)	Ti1—C5—H5	118.2
C3—Ti1—C4 ⁱ	145.77 (18)	C1—C6—C1 ⁱ	96.8 (4)
C3 ⁱ —Ti1—C4 ⁱ	33.06 (18)	C1—C6—C7	112.6 (2)
C4—Ti1—C4 ⁱ	171.7 (2)	C1 ⁱ —C6—C7	111.7 (2)
C1 ⁱ —Ti1—Br1	125.60 (11)	C1—C6—C7 ⁱ	111.7 (2)
C1—Ti1—Br1	125.18 (11)	C1 ⁱ —C6—C7 ⁱ	112.6 (2)
C2 ⁱ —Ti1—Br1	137.81 (11)	C7—C6—C7 ⁱ	110.8 (5)
C2—Ti1—Br1	90.16 (11)	C6—C7—H7A	109.5

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C5—Ti1—Br1	136.63 (11)	C6—C7—H7B	109.5
C5 ⁱ —Ti1—Br1	90.74 (11)	H7A—C7—H7B	109.5
C3—Ti1—Br1	80.16 (12)	C6—C7—H7C	109.5
C3 ⁱ —Ti1—Br1	105.95 (12)	H7A—C7—H7C	109.5
C4—Ti1—Br1	104.53 (12)	H7B—C7—H7C	109.5

Symmetry codes: (i) $-x+2, y, -z+3/2$.

Table 1

Selected geometric parameters (Å, °).

Ti—Cg1	2.045 (2)	C1—C6—C1a	96.8 (4)
Ti—Br1	2.5115 (7)	C7—C6—C7a	110.8 (4)
Cg1—Ti—Cg1a	121.32 (9)	P _r 1—C1—C6	15.5 (3)
Br1—Ti—Br1a	96.87 (3)	P _r 1—P _r 1a	65.8 (3)

Cg1 and Cg1a are the centroids defined by atoms C1–C5 and C1a–C5a, respectively. P_r1 and P_r1a are the ring planes defined by atoms C1–C5 and C1a–C5a, respectively [Symmetry code: (a) $2 - x, y, 3/2 - z$].

Fig. 1

