

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

# Tetracarbonyl[bis(diphenylphosphanyl)tetramethyldisiloxane- $\kappa^2 P, P'$ ]chromium(0)

### Normen Peulecke,\* Bernd H. Müller, Anke Spannenberg and Uwe Rosenthal

Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany

Correspondence e-mail: normen.peulecke@catalysis.de

Received 19 December 2011; accepted 3 January 2012

Key indicators: single-crystal X-ray study; T = 150 K; mean  $\sigma$ (C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.059; data-to-parameter ratio = 17.2.

The title compound,  $[Cr(C_{28}H_{32}OP_2Si_2)(CO)_4]$ , was obtained by the ligand-exchange reaction of  $Cr(CO)_6$  with  $(Ph_2PSiMe_2)_2O$  in refluxing toluene. The  $CrC_4P_2$  coordination geometry is distorted octahedral, with a P-Cr-P bite angle of 99.22 (4)°.

### **Related literature**

For the synthesis of  $(Ph_2PSiMe_2)_2O$ , using  $(SiMe_2Cl)_2O$ instead of  $SiMe_2Cl_2$ , see: Hassler & Seidl (1988). For the structures of complexes of group III metals with  $(H_2PSi^iPr_2)_2O$ , see: von Hänisch & Stahl (2006, 2007), and for group II metals, see: Kopecky *et al.* (2010). For the structure of a chromium complex with a silicon-bridged bisphosphine, see: Peulecke *et al.* (2010).



### **Experimental**

### Crystal data

 $\begin{bmatrix} Cr(C_{28}H_{32}OP_2Si_2)(CO)_4 \end{bmatrix} \\ M_r = 666.70 \\ Monoclinic, Cc \\ a = 9.2722 (5) Å \\ b = 21.4148 (15) Å \\ c = 16.5695 (8) Å \\ \beta = 95.200 (4)^\circ \end{bmatrix}$ 

### Data collection

Stoe IPDS II diffractometer Absorption correction: numerical (X-SHAPE and X-RED32; Stoe & Cie, 2005)  $T_{min} = 0.830, T_{max} = 0.952$ 

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	
$wR(F^2) = 0.059$	
S = 0.79	
5756 reflections	
335 parameters	
2 restraints	

 $V = 3276.5 \text{ (3) } \text{\AA}^{3}$ Z = 4 Mo K\alpha radiation  $\mu = 0.56 \text{ mm}^{-1}$ T = 150 K  $0.30 \times 0.21 \times 0.12 \text{ mm}$ 

21143 measured reflections 5756 independent reflections 4303 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.071$ 

H-atom parameters constrained  $\Delta \rho_{\text{max}} = 0.32 \text{ e} \text{ Å}^{-3}$   $\Delta \rho_{\text{min}} = -0.20 \text{ e} \text{ Å}^{-3}$ Absolute structure: Flack (1983), 2799 Friedel pairs Flack parameter: -0.021 (19)

Data collection: X-AREA (Stoe & Cie, 2005); cell refinement: X-AREA; data reduction: X-AREA; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97.

This work was supported by the Leibniz-Institut für Katalyse e·V. an der Universität Rostock.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YK2038).

### References

- Flack, H. D. (1983). Acta Cryst. A39, 876-881.
- Hänisch, C. von & Stahl, S. (2006). Angew. Chem. Int. Ed. 45, 2302-2305.
- Hänisch, C. von & Stahl, S. (2007). J. Organomet. Chem. 692, 2780-2783.
- Hassler, K. & Seidl, S. (1988). Monatsh. Chem. 119, 1241-1244.
- Kopecky, P., von Hänisch, C., Weigend, F. & Kracke, A. (2010). Eur. J. Inorg. Chem. pp. 258–265.
- Peulecke, N., Peitz, S., Müller, B. H., Spannenberg, A. & Rosenthal, U. (2010). Acta Cryst. E66, m1494.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Stoe & Cie (2005). X-SHAPE, X-RED32 and X-AREA. Stoe & Cie, Darmstadt, Germany.

# supporting information

Acta Cryst. (2012). E68, m119 [doi:10.1107/S1600536812000219]

# Tetracarbonyl[bis(diphenylphosphanyl)tetramethyldisiloxane- $\kappa^2 P, P'$ ]chromium(0)

# Normen Peulecke, Bernd H. Müller, Anke Spannenberg and Uwe Rosenthal

# S1. Comment

Diphosphines (like diphenylphosphanylpropane) are widely used as chelating ligands for the complex formation. Among them the siloxane-bridged ligands and their complexes with transition metals are not known. The few examples were made for  $(H_2PSi^{1}Pr_2)_2O$  coordinated with Al, Ga or In yielding polycyclic structures (von Hänisch *et al.*, 2006, 2007) or with Mg, Ca, Sr or Ba yielding only in the case of Mg a monomeric structure (Kopecky *et al.*, 2010). During our studies on the selective oligomerization of ethene *via* transition metal-catalyzed tri- or tetramerization we became interested in chromium complexes with ligands of this class (*e.g.* (Ph<sub>2</sub>P)<sub>2</sub>SiMe<sub>2</sub>: Peulecke *et al.*, 2010). In the present publication, we report the preparation and crystal structure of  $C_{32}H_{32}CrO_3P_2Si_2$ , which was observed to be the single product of a reaction of (Ph<sub>2</sub>PSiMe<sub>2</sub>)<sub>2</sub>O with Cr(CO)<sub>6</sub>. The coordination geometry at the chromium centre is distorted octahedral. The observed bite-angle P—Cr—P is 99.22 (4)°.

# S2. Experimental

 $Cr(CO)_6$  (175 mg, 0.8 mmol) was added to a solution of  $(Ph_2PSiMe_2)_2O$  (321 mg, 0.75 mmol) in 20 ml toluene and the resulting mixture was stirred at reflux temperature for 72 h. Subsequently, the formed yellow solution was cooled down to 0°C and filtered. Toluene was removed and the product was extracted with dichloromethane. The major part of dichloromethane was removed and the remaining solution was over-layered with *n*-hexane to get single crystals of the title compound, which were suitable for X-ray crystal structure analysis. The pale yellow compound was fully characterized by standard analytical methods, <sup>31</sup>P-NMR: (CD<sub>2</sub>Cl<sub>2</sub>): 5,9 p.p.m..

# S3. Refinement

H atoms were placed in idealized positions with d(C-H) = 0.95 Å (CH) and 0.98 Å (CH<sub>3</sub>) and refined using a riding model with  $U_{iso}(H)$  fixed at 1.2  $U_{eq}(C)$  for CH and 1.5  $U_{eq}(C)$  for CH<sub>3</sub>.



## Figure 1

The molecular structure of the title compound with atom labels and 30% displacement ellipsoids. Hydrogen atoms are omitted for clarity.

### Tetracarbonyl[bis(diphenylphosphanyl)tetramethyldisiloxane- $\kappa^2 P, P'$ ]chromium(0)

Crystal data	
$[Cr(C_{28}H_{32}OP_{2}Si_{2})(CO)_{4}]$	F(000) = 1384
$M_r = 666.70$	$D_{\rm x} = 1.352 {\rm Mg} {\rm m}^{-3}$
Monoclinic. Cc	Mo K $\alpha$ radiation. $\lambda = 0.71073$ Å
Hall symbol: C -2vc	Cell parameters from 4413 reflections
a = 9.2722 (5) Å	$\theta = 1.9 - 28.3^{\circ}$
b = 21.4148 (15) Å	$\mu = 0.56 \text{ mm}^{-1}$
c = 16.5695(8)Å	T = 150  K
$\beta = 95.200 (4)^{\circ}$	Prism, yellow
V = 3276.5 (3) Å <sup>3</sup>	$0.30 \times 0.21 \times 0.12 \text{ mm}$
Z=4	
Data collection	
Stoe IPDS II	21143 measured reflections
diffractometer	5756 independent reflections
Radiation source: fine-focus sealed tube	4303 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.071$
ωscans	$\theta_{\text{max}} = 25.3^{\circ}, \ \theta_{\text{min}} = 1.9^{\circ}$
Absorption correction: numerical	$h = -11 \rightarrow 11$
(X-SHAPE and X-RED32; Stoe & Cie, 2005)	$k = -25 \rightarrow 25$
$T_{\min} = 0.830, T_{\max} = 0.952$	$l = -19 \rightarrow 19$
Refinement	
Refinement on $F^2$	335 parameters
Least-squares matrix: full	2 restraints
$R[F^2 > 2\sigma(F^2)] = 0.035$	Primary atom site location: structure-in

 2 restraints
 Primary atom site location: structure-invariant direct methods
 Secondary atom site location: difference Fourier map

 $wR(F^2) = 0.059$ 

5756 reflections

S = 0.79

Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained  $w = 1/[\sigma^2(F_o^2) + (0.0178P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{max} < 0.001$ 

# Special details

 $\begin{aligned} \Delta \rho_{\text{max}} &= 0.32 \text{ e } \text{\AA}^{-3} \\ \Delta \rho_{\text{min}} &= -0.20 \text{ e } \text{\AA}^{-3} \\ \text{Absolute structure: Flack (1983),$ **2799 Friedelpairs** $\\ \text{Absolute structure parameter: -0.021 (19)} \end{aligned}$ 

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

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
C1	0.7971 (2)	0.47102 (10)	0.89997 (14)	0.0260 (8)
C2	0.9455 (2)	0.46252 (10)	0.91594 (14)	0.0323 (9)
H2	0.9816	0.4315	0.9534	0.039*
C3	1.04124 (19)	0.49949 (13)	0.87708 (16)	0.0404 (11)
Н3	1.1427	0.4937	0.8880	0.048*
C4	0.9885 (3)	0.54495 (12)	0.82225 (15)	0.0464 (12)
H4	1.0539	0.5702	0.7957	0.056*
C5	0.8400 (3)	0.55345 (11)	0.80628 (14)	0.0445 (11)
Н5	0.8039	0.5845	0.7688	0.053*
C6	0.7443 (2)	0.51649 (12)	0.84514 (15)	0.0358 (10)
H6	0.6428	0.5223	0.8342	0.043*
C7	0.5653 (2)	0.48049 (10)	1.00308 (14)	0.0284 (9)
C8	0.6274 (2)	0.53733 (11)	1.02723 (14)	0.0339 (9)
H8	0.7233	0.5468	1.0154	0.041*
C9	0.5493 (3)	0.58024 (9)	1.06870 (15)	0.0424 (10)
H9	0.5917	0.6191	1.0852	0.051*
C10	0.4089 (3)	0.56631 (11)	1.08601 (15)	0.0433 (12)
H10	0.3555	0.5956	1.1144	0.052*
C11	0.3468 (2)	0.50947 (13)	1.06186 (16)	0.0407 (11)
H11	0.2509	0.4999	1.0737	0.049*
C12	0.4249 (2)	0.46656 (10)	1.02039 (16)	0.0330 (9)
H12	0.3825	0.4277	1.0039	0.040*
C13	0.6284 (4)	0.36230 (18)	0.7687 (2)	0.0311 (9)
H13A	0.5700	0.3395	0.7261	0.047*
H13B	0.6998	0.3340	0.7963	0.047*
H13C	0.6784	0.3969	0.7445	0.047*
C14	0.3937 (4)	0.45715 (19)	0.7988 (2)	0.0378 (10)
H14A	0.3678	0.4848	0.8424	0.057*
H14B	0.3055	0.4396	0.7706	0.057*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(Å^2)$ 

H14C	0.4463	0.4810	0.7604	0.057*
C15	0.2877 (4)	0.3024 (2)	1.0248 (3)	0.0391 (10)
H15A	0.2035	0.3285	1.0080	0.059*
H15B	0.3546	0.3257	1.0628	0.059*
H15C	0.2557	0.2645	1.0512	0.059*
C16	0.2766 (4)	0.2188 (2)	0.8767 (3)	0.0420 (11)
H16A	0.3063	0.2172	0.8215	0.063*
H16B	0.1730	0.2283	0.8748	0.063*
H16C	0.2956	0.1784	0.9033	0.063*
C17	0.5663 (3)	0.19242 (10)	1.05885 (13)	0.0303 (9)
C18	0.5334 (3)	0.13181 (12)	1.03342 (11)	0.0312 (9)
H18	0.5345	0.1210	0.9779	0.037*
C19	0.4989 (3)	0.08701 (9)	1.08926 (16)	0.0406 (11)
H19	0.4764	0.0456	1.0719	0.049*
C20	0.4973 (3)	0.10283 (12)	1.17053 (14)	0.0457 (11)
H20	0.4737	0.0722	1.2087	0.055*
C21	0.5302 (3)	0.16344 (14)	1.19597 (11)	0.0542 (12)
H21	0.5291	0.1742	1.2515	0.065*
C22	0.5646 (3)	0.20824 (10)	1.14013 (15)	0.0443 (11)
H22	0.5871	0.2497	1.1575	0.053*
C23	0.6851 (2)	0.20647 (11)	0.90486 (12)	0.0255 (9)
C24	0.8044 (2)	0.16907 (12)	0.92776 (11)	0.0345 (9)
H24	0.8388	0.1655	0.9833	0.041*
C25	0.8732 (2)	0.13685 (11)	0.86935 (16)	0.0436 (11)
H25	0.9547	0.1113	0.8850	0.052*
C26	0.8228 (3)	0.14204 (12)	0.78803 (14)	0.0438 (11)
H26	0.8698	0.1200	0.7481	0.053*
C27	0.7035 (3)	0.17944 (12)	0.76513 (10)	0.0371 (10)
H27	0.6691	0.1830	0.7096	0.045*
C28	0.6347 (2)	0.21165 (11)	0.82354 (13)	0.0310 (9)
H28	0.5532	0.2372	0.8079	0.037*
C29	0.9060 (4)	0.39081 (19)	1.0826 (2)	0.0300 (9)
C30	0.8865 (4)	0.31736 (18)	0.9509 (2)	0.0273 (9)
C31	0.8607 (4)	0.27757 (19)	1.0996 (2)	0.0337 (9)
C32	0.6494 (4)	0.36119 (18)	1.1135 (2)	0.0284 (9)
Cr1	0.76936 (6)	0.33701 (3)	1.03423 (4)	0.02284 (14)
01	0.4032 (2)	0.34064 (12)	0.87633 (15)	0.0311 (6)
O2	0.9939 (3)	0.42194 (14)	1.11716 (16)	0.0440 (8)
O3	0.9613 (3)	0.30592 (13)	0.90084 (16)	0.0384 (7)
O4	0.9272 (3)	0.24106 (14)	1.14056 (18)	0.0548 (9)
05	0.5824 (3)	0.37908 (14)	1.16462 (17)	0.0469 (8)
P1	0.66695 (9)	0.42154 (5)	0.95043 (6)	0.0236 (2)
P2	0.60852 (10)	0.25311 (5)	0.98419 (6)	0.0247 (2)
Si1	0.50981 (10)	0.39322 (5)	0.84235 (6)	0.0283 (3)
Si2	0.38082 (10)	0.28057 (5)	0.93478 (6)	0.0288 (3)

Atomic displacement parameters  $(Å^2)$ 

$\begin{array}{cccccccccccccccccccccccccccccccccccc$		$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	<i>U</i> <sup>13</sup>	<i>U</i> <sup>23</sup>
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	0.038 (2)	0.021 (2)	0.019 (2)	0.0002 (17)	0.0021 (16)	-0.0045 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	0.036 (2)	0.035 (3)	0.026 (2)	-0.0021 (19)	0.0065 (17)	0.0034 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3	0.038 (2)	0.049 (3)	0.035 (3)	-0.009 (2)	0.0054 (19)	-0.002 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4	0.069 (3)	0.043 (3)	0.029 (2)	-0.021 (2)	0.015 (2)	0.004 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5	0.063 (3)	0.033 (3)	0.036 (3)	-0.004 (2)	-0.003 (2)	0.007 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.044 (2)	0.030 (2)	0.032 (2)	0.003 (2)	-0.0028 (19)	0.0019 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7	0.033 (2)	0.031 (2)	0.020 (2)	0.0103 (18)	-0.0037 (16)	0.0010 (17)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8	0.038 (2)	0.035 (2)	0.027 (2)	0.0046 (19)	-0.0038 (17)	-0.0067 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9	0.056 (3)	0.041 (3)	0.029 (2)	0.009 (2)	-0.004 (2)	-0.012 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10	0.059 (3)	0.051 (3)	0.019 (2)	0.029 (2)	-0.001 (2)	-0.003 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11	0.040 (2)	0.051 (3)	0.031 (2)	0.010(2)	0.0019 (19)	-0.003 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	0.036 (2)	0.032 (2)	0.032 (2)	0.0053 (18)	0.0060 (18)	-0.0047 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13	0.037 (2)	0.034 (2)	0.021 (2)	0.0009 (18)	-0.0046 (17)	0.0011 (17)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C14	0.032 (2)	0.043 (3)	0.036 (2)	0.0092 (19)	-0.0067 (18)	0.001 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15	0.027 (2)	0.048 (3)	0.043 (3)	-0.003 (2)	0.0073 (18)	-0.009 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C16	0.028 (2)	0.043 (3)	0.055 (3)	-0.004 (2)	0.0000 (19)	-0.012 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C17	0.027 (2)	0.032 (2)	0.031 (2)	-0.0007 (18)	0.0014 (17)	0.0025 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C18	0.030 (2)	0.034 (2)	0.029 (2)	-0.0039 (18)	0.0021 (17)	0.0017 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19	0.034 (2)	0.041 (3)	0.047 (3)	-0.004 (2)	0.0019 (19)	0.011 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C20	0.041 (2)	0.051 (3)	0.045 (3)	-0.014 (2)	0.006 (2)	0.018 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C21	0.074 (3)	0.057 (3)	0.033 (3)	-0.012 (3)	0.014 (2)	0.005 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C22	0.061 (3)	0.041 (3)	0.032 (3)	-0.012 (2)	0.011 (2)	-0.001 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C23	0.026 (2)	0.022 (2)	0.029 (2)	-0.0021 (16)	0.0024 (16)	-0.0007 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C24	0.038 (2)	0.032 (2)	0.034 (2)	0.0066 (19)	0.0033 (17)	-0.0038 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C25	0.039 (2)	0.040 (3)	0.052 (3)	0.010 (2)	0.009 (2)	-0.004 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C26	0.049 (3)	0.039 (3)	0.047 (3)	-0.004 (2)	0.024 (2)	-0.012 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C27	0.046 (2)	0.038 (3)	0.028 (2)	-0.002(2)	0.0095 (19)	-0.0052 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C28	0.035 (2)	0.031 (2)	0.027 (2)	-0.0007 (18)	0.0044 (17)	0.0023 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C29	0.035 (2)	0.032 (2)	0.023 (2)	0.004 (2)	0.0045 (17)	0.0058 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C30	0.025 (2)	0.026 (2)	0.030(2)	0.0028 (17)	-0.0065 (18)	0.0000 (18)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C31	0.042 (2)	0.032 (2)	0.026 (2)	-0.003(2)	-0.0026 (18)	-0.001 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C32	0.032 (2)	0.027 (2)	0.025 (2)	-0.0029 (19)	-0.0030 (19)	0.0018 (18)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Cr1	0.0245 (3)	0.0260 (3)	0.0177 (3)	0.0008 (3)	0.0004 (2)	0.0006 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01	0.0225 (13)	0.0387 (16)	0.0310 (15)	0.0027 (13)	-0.0036 (11)	-0.0031 (13)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O2	0.0440 (17)	0.0467 (19)	0.0393 (18)	-0.0202 (15)	-0.0076 (14)	-0.0015 (15)
O4         0.066 (2)         0.047 (2)         0.047 (2)         0.0058 (16)         -0.0199 (16)         0.0163 (16)           O5         0.0479 (18)         0.067 (2)         0.0275 (17)         0.0013 (16)         0.0121 (14)         -0.0112 (16)           P1         0.0252 (5)         0.0252 (5)         0.0201 (5)         0.0034 (5)         0.0005 (4)         -0.0011 (4)           P2         0.0271 (5)         0.0257 (5)         0.0213 (5)         -0.0002 (5)         0.0032 (4)         -0.0007 (4)           Si1         0.0296 (6)         0.0309 (6)         0.0234 (6)         0.0001 (5)         -0.0030 (5)         -0.0015 (5)           Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	O3	0.0333 (15)	0.0500 (19)	0.0332 (17)	0.0070 (13)	0.0097 (13)	-0.0023 (14)
O5         0.0479 (18)         0.067 (2)         0.0275 (17)         0.0013 (16)         0.0121 (14)         -0.0112 (16)           P1         0.0252 (5)         0.0252 (5)         0.0201 (5)         0.0034 (5)         0.0005 (4)         -0.0011 (4)           P2         0.0271 (5)         0.0257 (5)         0.0213 (5)         -0.0002 (5)         0.0032 (4)         -0.0007 (4)           Si1         0.0296 (6)         0.0309 (6)         0.0234 (6)         0.0046 (5)         -0.0030 (5)         -0.0015 (5)           Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	O4	0.066 (2)	0.047 (2)	0.047 (2)	0.0058 (16)	-0.0199 (16)	0.0163 (16)
P1         0.0252 (5)         0.0252 (5)         0.0201 (5)         0.0034 (5)         0.0005 (4)         -0.0011 (4)           P2         0.0271 (5)         0.0257 (5)         0.0213 (5)         -0.0002 (5)         0.0032 (4)         -0.0007 (4)           Si1         0.0296 (6)         0.0309 (6)         0.0234 (6)         0.0046 (5)         -0.0030 (5)         -0.0015 (5)           Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	05	0.0479 (18)	0.067 (2)	0.0275 (17)	0.0013 (16)	0.0121 (14)	-0.0112 (16)
P2         0.0271 (5)         0.0257 (5)         0.0213 (5)         -0.0002 (5)         0.0032 (4)         -0.0007 (4)           Si1         0.0296 (6)         0.0309 (6)         0.0234 (6)         0.0046 (5)         -0.0030 (5)         -0.0015 (5)           Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	P1	0.0252 (5)	0.0252 (5)	0.0201 (5)	0.0034 (5)	0.0005 (4)	-0.0011 (4)
Si1         0.0296 (6)         0.0309 (6)         0.0234 (6)         0.0046 (5)         -0.0030 (5)         -0.0015 (5)           Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	P2	0.0271 (5)	0.0257 (5)	0.0213 (5)	-0.0002 (5)	0.0032 (4)	-0.0007 (4)
Si2         0.0241 (5)         0.0326 (6)         0.0298 (6)         0.0001 (5)         0.0023 (5)         -0.0048 (5)	Si1	0.0296 (6)	0.0309 (6)	0.0234 (6)	0.0046 (5)	-0.0030 (5)	-0.0015 (5)
	Si2	0.0241 (5)	0.0326 (6)	0.0298 (6)	0.0001 (5)	0.0023 (5)	-0.0048 (5)

Geometric parameters (Å, °)

C1—C2	1.3900	C16—H16C	0.9800	
C1—C6	1.3900	C17—C18	1.3900	
C1—P1	1.860(2)	C17—C22	1.3900	
C2—C3	1.3900	C17—P2	1.860 (2)	
С2—Н2	0.9500	C18—C19	1.3900	
C3—C4	1.3900	C18—H18	0.9500	
С3—Н3	0.9500	C19—C20	1.3900	
C4—C5	1.3900	C19—H19	0.9500	
C4—H4	0.9500	C20—C21	1.3900	
С5—С6	1.3900	C20—H20	0.9500	
С5—Н5	0.9500	C21—C22	1.3900	
С6—Н6	0.9500	C21—H21	0.9500	
С7—С8	1.3900	C22—H22	0.9500	
C7—C12	1.3900	C23—C24	1.3900	
C7—P1	1.8419 (19)	C23—C28	1.3900	
С8—С9	1.3900	C23—P2	1.8437 (19)	
С8—Н8	0.9500	C24—C25	1.3900	
C9—C10	1.3900	C24—H24	0.9500	
С9—Н9	0.9500	C25—C26	1.3900	
C10-C11	1.3900	C25—H25	0.9500	
C10—H10	0.9500	C26—C27	1.3900	
C11—C12	1.3900	C26—H26	0.9500	
C11—H11	0.9500	C27—C28	1.3900	
C12—H12	0.9500	C27—H27	0.9500	
C13—Si1	1.838 (4)	C28—H28	0.9500	
C13—H13A	0.9800	C29—O2	1.163 (4)	
C13—H13B	0.9800	C29—Cr1	1.841 (4)	
С13—Н13С	0.9800	C30—O3	1.155 (4)	
C14—Si1	1.847 (4)	C30—Cr1	1.881 (4)	
C14—H14A	0.9800	C31—O4	1.173 (4)	
C14—H14B	0.9800	C31—Cr1	1.829 (4)	
C14—H14C	0.9800	C32—O5	1.161 (4)	
C15—Si2	1.849 (4)	C32—Cr1	1.869 (4)	
C15—H15A	0.9800	Cr1—P1	2.4223 (11)	
C15—H15B	0.9800	Cr1—P2	2.4322 (11)	
С15—Н15С	0.9800	O1—Si1	1.632 (3)	
C16—Si2	1.854 (4)	O1—Si2	1.635 (3)	
C16—H16A	0.9800	P1—Si1	2.2856 (13)	
C16—H16B	0.9800	P2—Si2	2.2716 (13)	
$C^2$ $C^1$ $C^6$	120.0	C21 C20 U20	120.0	
$C_2 = C_1 = C_0$	120.0	$C_{21}$ $-C_{20}$ $-H_{20}$	120.0	
$C_2 \rightarrow C_1 \rightarrow r_1$	120.70(14)	C19 - C20 - H20	120.0	
$C_1 = C_1 = C_2$	119.24 (14)	$C_{20}$ $C_{21}$ $C_{22}$	120.0	
C1 = C2 = U3	120.0	$C_{20}$ $C_{21}$ $H_{21}$	120.0	
C1 - C2 - H2	120.0	$C_{22}$ — $C_{21}$ — $H_{21}$	120.0	
U3-U2-H2	120.0	$C_{21} - C_{22} - C_{17}$	120.0	

C4—C3—C2	120.0	C21—C22—H22	120.0
С4—С3—Н3	120.0	C17—C22—H22	120.0
С2—С3—Н3	120.0	C24—C23—C28	120.0
C3—C4—C5	120.0	C24—C23—P2	117.76 (13)
C3—C4—H4	120.0	C28—C23—P2	122.03 (13)
С5—С4—Н4	120.0	C23—C24—C25	120.0
C6—C5—C4	120.0	C23—C24—H24	120.0
С6—С5—Н5	120.0	C25—C24—H24	120.0
C4—C5—H5	120.0	C24—C25—C26	120.0
C5—C6—C1	120.0	C24—C25—H25	120.0
С5—С6—Н6	120.0	C26—C25—H25	120.0
С1—С6—Н6	120.0	C27—C26—C25	120.0
C8-C7-C12	120.0	$C_{27}$ $C_{26}$ $H_{26}$	120.0
C8-C7-P1	121.32 (14)	$C_{25}$ $C_{26}$ $H_{26}$	120.0
$C_{12} - C_{7} - P_{1}$	118 66 (14)	$C_{26} = C_{27} = C_{28}$	120.0
C7 - C8 - C9	120.0	$C_{26} = C_{27} = H_{27}$	120.0
C7 C8 H8	120.0	$C_{20} = C_{27} = H_{27}$	120.0
$C_{1} = C_{2} = 118$	120.0	$C_{20} = C_{27} = C_{127}$	120.0
$C_{2} = C_{2} = C_{2}$	120.0	$C_{27} = C_{28} = C_{23}$	120.0
$C_{10} = C_{9} = C_{8}$	120.0	$C_{2} = C_{2} = C_{2$	120.0
$C_{10} - C_{9} - H_{9}$	120.0	$C_{23} = C_{28} = H_{28}$	120.0
$C_{8}$	120.0	02-029-011	175.5 (3)
	120.0	03	1/8.3 (3)
С9—С10—Н10	120.0	04—C31—Cr1	175.9 (4)
C11—C10—H10	120.0	O5—C32—Cr1	175.3 (3)
C12—C11—C10	120.0	C31—Cr1—C29	85.09 (17)
C12—C11—H11	120.0	C31—Cr1—C32	92.86 (17)
C10—C11—H11	120.0	C29—Cr1—C32	87.19 (16)
C11—C12—C7	120.0	C31—Cr1—C30	90.68 (17)
C11—C12—H12	120.0	C29—Cr1—C30	92.24 (16)
C7—C12—H12	120.0	C32—Cr1—C30	176.35 (18)
Si1—C13—H13A	109.5	C31—Cr1—P1	174.94 (13)
Si1—C13—H13B	109.5	C29—Cr1—P1	90.02 (12)
H13A—C13—H13B	109.5	C32—Cr1—P1	88.19 (12)
Si1—C13—H13C	109.5	C30—Cr1—P1	88.20 (12)
H13A—C13—H13C	109.5	C31—Cr1—P2	85.67 (13)
H13B—C13—H13C	109.5	C29—Cr1—P2	170.75 (12)
Si1—C14—H14A	109.5	C32—Cr1—P2	93.36 (12)
Si1—C14—H14B	109.5	C30—Cr1—P2	87.78 (12)
H14A—C14—H14B	109.5	P1—Cr1—P2	99.22 (4)
Sil—Cl4—Hl4C	109.5	Si1-01-Si2	149.42 (16)
H14A— $C14$ — $H14C$	109.5	C7 - P1 - C1	101.72(12)
H14B $C14$ $H14C$	109.5	$C7$ _P1_Sil	103.63 (9)
Si2 C15 H15A	109.5	$C_1 = P_1 = S_1$	103.03(9)
Si2 C15 H15P	109.5	$C_1 \longrightarrow 1 \longrightarrow 0$	115 56 (0)
$\begin{array}{c} 512 \\ \mathbf{-} \mathbf{C13} \\ \mathbf{-} \mathbf{113D} \\ \mathbf{-} \mathbf{115D} \\ \mathbf{-} \mathbf$	109.5	$C_1 = D_1 = C_{r1}$	116 54 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	107.3	$C_1 - F_1 - C_{11}$	110.34(0)
512—С15—Н15С	109.3	SII = rI = CII	110.09 (3)
HIDA-UID-HIDU	109.5	$C_{23}$ $P_{2}$ $C_{1}$	102.33 (12)
H15B—C15—H15C	109.5	C23—P2—S12	106.78 (9)

Si2—C16—H16A	109.5	C17—P2—Si2	100.11 (9)
Si2—C16—H16B	109.5	C23—P2—Cr1	112.29 (9)
H16A—C16—H16B	109.5	C17—P2—Cr1	116.68 (9)
Si2—C16—H16C	109.5	Si2—P2—Cr1	116.92 (5)
H16A—C16—H16C	109.5	O1—Si1—C13	113.43 (16)
H16B—C16—H16C	109.5	O1—Si1—C14	107.24 (16)
C18—C17—C22	120.0	C13—Si1—C14	111.74 (18)
C18—C17—P2	120.29 (14)	O1—Si1—P1	106.01 (10)
C22—C17—P2	119.69 (14)	C13—Si1—P1	103.80 (12)
C19—C18—C17	120.0	C14—Si1—P1	114.63 (14)
C19—C18—H18	120.0	O1—Si2—C15	111.88 (17)
C17—C18—H18	120.0	O1—Si2—C16	110.00 (17)
C18—C19—C20	120.0	C15—Si2—C16	109.82 (19)
C18—C19—H19	120.0	O1—Si2—P2	104.67 (10)
С20—С19—Н19	120.0	C15—Si2—P2	105.15 (14)
C21—C20—C19	120.0	C16—Si2—P2	115.21 (14)