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Tetrachlorido[(diphenylphosphino)- diphenylphosphine oxide- κ O]- zirconium(IV) benzene monosolvate. Corrigendum

Takahiko Ogawa, Yuji Kajita and Hideki Masuda*

Department of Applied Chemistry, Nagoya Institute of Technology, Showa-ku,
Nagoya 466-8555, Japan

Correspondence e-mail: masuda.hideki@nitech.ac.jp

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The chemical name of the title compound in the paper by Ogawa, Kajita & Masuda [*Acta Cryst.* (2009), **E65**, m1129] is corrected.

In the paper by Ogawa *et al.* (2009), the chemical name given in the *Title* should be 'Tetrachloridobis[(diphenylphosphino)diphenylphosphine oxide- κ O]zirconium(IV) benzene monosolvate'.

References

Ogawa, T., Kajita, Y. & Masuda, H. (2009). *Acta Cryst.* **E65**, m1129.

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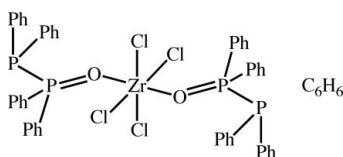
Received 10 August 2009; accepted 12 August 2009

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.045; wR factor = 0.151; data-to-parameter ratio = 19.2.

In the title centrosymmetric mononuclear Zr^{IV} compound, $[\text{ZrCl}_4\{\text{P}(\text{O})(\text{C}_6\text{H}_5)_2\text{P}(\text{C}_6\text{H}_5)_2\}_2]\cdot\text{C}_6\text{H}_6$, the central Zr^{IV} ion is coordinated by two O atoms from two symmetry-related (diphenylphosphino)diphenylphosphine ligands and four Cl atoms in a distorted octahedral geometry with the four Cl atoms in the equatorial positions. The molecule lies about a center of inversion and the benzene solvent molecule about another center of inversion. The $\text{P}=\text{O}$ bond [1.528 (2) Å] is slightly longer than a typical $\text{P}=\text{O}$ double bond (average 1.500 Å).

Related literature

For general background to the structure and coordination mode of (diphenylphosphino)diphenylphosphine (DPDP), see: Ferguson *et al.* (1990); Kuramshin & Khramov (1983). For a Zr^{IV} complex with a DPDP ligand, see: Muratova *et al.* (1980). For comparison P–O bond distances, see: Berners-Price *et al.* (2009).



Experimental

Crystal data

 $[\text{ZrCl}_4(\text{C}_{24}\text{H}_{20}\text{OP}_2)_2]\cdot\text{C}_6\text{H}_6$ $M_r = 1083.81$

Triclinic, $P\bar{1}$
 $a = 9.6073$ (3) Å
 $b = 10.1521$ (4) Å
 $c = 14.0204$ (10) Å
 $\alpha = 79.027$ (13)°
 $\beta = 87.269$ (13)°
 $\gamma = 73.096$ (11)°

$V = 1284.42$ (11) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.59$ mm⁻¹
 $T = 173$ K
 $0.30 \times 0.15 \times 0.13$ mm

Data collection

Rigaku Mercury diffractometer
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\text{min}} = 0.900$, $T_{\text{max}} = 0.927$

10324 measured reflections
 5669 independent reflections
 4497 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.151$
 $S = 1.02$
 5669 reflections

296 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.04$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.81$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|---------|------------|--------|-------------|
| Zr1—Cl1 | 2.4450 (9) | Zr1—O1 | 2.0820 (18) |
| Zr1—Cl2 | 2.4627 (7) | | |

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2007); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

We gratefully acknowledge the support of this work by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2624).

References

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supplementary materials

Acta Cryst. (2009). E65, m1129 [doi:10.1107/S1600536809031882]

Tetrachlorido[(diphenylphosphino)diphenylphosphine oxide- κ O]zirconium(IV) benzene monosolvate

T. Ogawa, Y. Kajita and H. Masuda

Comment

The phosphinoyl derivative, (diphenylphosphino)diphenylphosphine (DPDP), has a unique structure and coordination mode (Ferguson 1990 and Muratova *et al.*, 1980). The complex which contains DPDP ligands is very rare and is a novel Zr^{IV} complex with DPDP ligand (Kuramshin & Khramov *et al.*, 1983). The centrosymmetric unit of the title compound, [ZrCl₄(C₂₄H₂₀P₂O)₂] C₆H₆, contains a neutral Zr^{IV} complex and a solvent benzene molecule (Fig. 1). The compound crystallized in the triclinic space group *P* $\bar{1}$. In the complex, the Zr^{IV} ion is six-coordinated in a slightly distorted octahedral environment by two O atoms of DPDP ligand and four Cl ions. The P atoms do not coordinate to the Zr^{IV} atom. The Zr—Cl(1) [2.4450 (9) Å] and Zr—Cl(2) [2.4627 (9) Å] bond lengths are slightly different each other (Table 1). The P—O bond length [1.5281 (19) Å] is slightly longer compared with a typical double bond (Berners-Price *et al.*, 2009). The P—P bond length [2.2057 (10) Å] is similar to several P^{III}—P^V derivatives.

Experimental

The title compound was prepared by the reaction of ZrCl₄ (0.03 g, 0.13 mmol) and (diphenylphosphino)diphenylphosphine (0.10 g, 0.26 mmol) in benzene (5 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving colorless single crystals.

Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

The final difference Fourier map had a peak near the Zr1 atom.

Figures

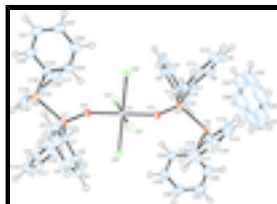


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator ((i) $-x + 2, -y, -z + 2$; (ii) $-x + 1, -y + 1, -z + 1$).

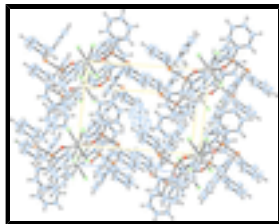


Fig. 2. A partial packing diagram of the title compound.

Tetrachlorido[(diphenylphosphino)diphenylphosphine oxide- κ O]zirconium(IV) benzene monosolvate

Crystal data

$[\text{ZrCl}_4(\text{C}_{24}\text{H}_{20}\text{OP}_2)_2] \cdot \text{C}_6\text{H}_6$

$M_r = 1083.81$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 9.6073$ (3) Å

$b = 10.1521$ (4) Å

$c = 14.0204$ (10) Å

$\alpha = 79.027$ (13)°

$\beta = 87.269$ (13)°

$\gamma = 73.096$ (11)°

$V = 1284.42$ (11) Å³

$Z = 1$

$F_{000} = 554.00$

$D_x = 1.401$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å

Cell parameters from 3589 reflections

$\theta = 3.2$ – 27.5 °

$\mu = 0.59$ mm⁻¹

$T = 173$ K

Chip, colorless

$0.30 \times 0.15 \times 0.13$ mm

Data collection

Rigaku Mercury
diffractometer

Detector resolution: 7.31 pixels mm⁻¹

$T = 173$ K

ω scans

Absorption correction: Multi-scan
(Jacobson, 1998)

$T_{\min} = 0.900$, $T_{\max} = 0.927$

10324 measured reflections

5669 independent reflections

4497 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 27.5$ °

$h = -12 \rightarrow 12$

$k = -11 \rightarrow 13$

$l = -13 \rightarrow 18$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.151$

$S = 1.02$

5669 reflections

296 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 1.04$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.81$ e Å⁻³

Extinction correction: none

Special details

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 was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|--------------|----------------------------------|
| Zr1 | 1 | 0 | 1 | 0.01849 (13) |
| Cl1 | 1.14353 (9) | 0.14927 (8) | 1.03401 (6) | 0.0305 (2) |
| Cl2 | 0.79704 (8) | 0.12426 (8) | 1.09344 (6) | 0.02711 (18) |
| P1 | 0.79655 (8) | 0.24267 (8) | 0.80566 (5) | 0.01964 (17) |
| P2 | 0.87015 (9) | 0.33171 (9) | 0.66302 (6) | 0.0249 (2) |
| O1 | 0.9163 (2) | 0.1442 (2) | 0.87498 (15) | 0.0212 (4) |
| C1 | 0.6603 (3) | 0.1623 (3) | 0.7861 (2) | 0.0239 (6) |
| C2 | 0.6455 (4) | 0.1237 (4) | 0.6987 (2) | 0.0404 (9) |
| C3 | 0.5388 (4) | 0.0607 (5) | 0.6859 (3) | 0.0509 (11) |
| C4 | 0.4473 (4) | 0.0343 (4) | 0.7626 (2) | 0.0377 (8) |
| C5 | 0.4620 (3) | 0.0716 (3) | 0.8512 (2) | 0.0346 (7) |
| C6 | 0.5688 (3) | 0.1353 (3) | 0.8631 (2) | 0.0301 (7) |
| C7 | 0.7107 (3) | 0.3971 (3) | 0.8540 (2) | 0.0245 (6) |
| C8 | 0.5776 (3) | 0.4851 (3) | 0.8158 (2) | 0.0339 (7) |
| C9 | 0.5195 (4) | 0.6137 (4) | 0.8442 (3) | 0.0471 (10) |
| C10 | 0.5940 (4) | 0.6522 (4) | 0.9110 (3) | 0.0482 (10) |
| C11 | 0.7256 (4) | 0.5653 (3) | 0.9496 (2) | 0.0401 (9) |
| C12 | 0.7856 (3) | 0.4366 (3) | 0.9215 (2) | 0.0288 (7) |
| C13 | 0.9801 (3) | 0.4239 (3) | 0.7122 (2) | 0.0284 (7) |
| C14 | 0.9168 (4) | 0.5667 (3) | 0.7125 (2) | 0.0375 (8) |
| C15 | 0.9878 (5) | 0.6405 (4) | 0.7568 (3) | 0.0476 (10) |
| C16 | 1.1218 (5) | 0.5752 (4) | 0.7984 (3) | 0.0513 (11) |
| C17 | 1.1876 (4) | 0.4354 (4) | 0.7969 (3) | 0.0484 (10) |
| C18 | 1.1170 (4) | 0.3584 (4) | 0.7553 (2) | 0.0358 (8) |
| C19 | 1.0058 (3) | 0.1844 (3) | 0.6233 (2) | 0.0276 (6) |
| C20 | 1.0628 (5) | 0.2151 (4) | 0.5313 (3) | 0.0552 (12) |
| C21 | 1.1635 (5) | 0.1132 (5) | 0.4917 (3) | 0.0686 (15) |
| C22 | 1.2062 (4) | -0.0226 (4) | 0.5424 (2) | 0.0423 (9) |
| C23 | 1.1486 (4) | -0.0549 (4) | 0.6320 (2) | 0.0410 (9) |
| C24 | 1.0484 (4) | 0.0476 (3) | 0.6725 (2) | 0.0358 (8) |
| C25 | 0.4088 (12) | 0.5582 (15) | 0.5682 (6) | 0.165 (7) |
| C26 | 0.5127 (14) | 0.6167 (11) | 0.5268 (8) | 0.167 (5) |
| C27 | 0.6047 (12) | 0.5579 (14) | 0.4560 (7) | 0.171 (6) |
| H1 | 0.7090 | 0.1403 | 0.6467 | 0.049* |
| H2 | 0.5285 | 0.0358 | 0.6252 | 0.061* |

supplementary materials

| | | | | |
|-----|--------|---------|--------|--------|
| H3 | 0.3746 | -0.0093 | 0.7543 | 0.045* |
| H4 | 0.3994 | 0.0537 | 0.9034 | 0.041* |
| H5 | 0.5794 | 0.1603 | 0.9237 | 0.036* |
| H6 | 0.5267 | 0.4573 | 0.7704 | 0.041* |
| H7 | 0.4292 | 0.6746 | 0.8179 | 0.056* |
| H8 | 0.5540 | 0.7399 | 0.9307 | 0.058* |
| H9 | 0.7753 | 0.5936 | 0.9954 | 0.048* |
| H10 | 0.8763 | 0.3765 | 0.9477 | 0.035* |
| H11 | 0.8247 | 0.6134 | 0.6823 | 0.045* |
| H12 | 0.9430 | 0.7368 | 0.7582 | 0.057* |
| H13 | 1.1700 | 0.6262 | 0.8285 | 0.061* |
| H14 | 1.2819 | 0.3914 | 0.8245 | 0.058* |
| H15 | 1.1616 | 0.2615 | 0.7562 | 0.043* |
| H16 | 1.0318 | 0.3079 | 0.4953 | 0.066* |
| H17 | 1.2033 | 0.1364 | 0.4296 | 0.082* |
| H18 | 1.2752 | -0.0933 | 0.5153 | 0.051* |
| H19 | 1.1776 | -0.1486 | 0.6668 | 0.049* |
| H20 | 1.0088 | 0.0235 | 0.7345 | 0.043* |
| H21 | 0.3452 | 0.6006 | 0.6148 | 0.199* |
| H22 | 0.5231 | 0.6982 | 0.5461 | 0.200* |
| H23 | 0.6756 | 0.6003 | 0.4258 | 0.205* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|--------------|---------------|
| Zr1 | 0.0175 (2) | 0.0156 (2) | 0.0215 (2) | -0.00302 (15) | 0.00179 (15) | -0.00429 (15) |
| Cl1 | 0.0292 (4) | 0.0249 (3) | 0.0416 (4) | -0.0116 (3) | -0.0023 (3) | -0.0096 (3) |
| Cl2 | 0.0237 (3) | 0.0243 (3) | 0.0309 (4) | -0.0023 (3) | 0.0078 (3) | -0.0082 (3) |
| P1 | 0.0202 (3) | 0.0174 (3) | 0.0200 (3) | -0.0032 (2) | 0.0018 (2) | -0.0041 (2) |
| P2 | 0.0277 (4) | 0.0234 (4) | 0.0211 (3) | -0.0051 (3) | 0.0007 (3) | -0.0013 (3) |
| O1 | 0.0228 (10) | 0.0185 (9) | 0.0204 (10) | -0.0038 (8) | -0.0003 (8) | -0.0020 (8) |
| C1 | 0.0240 (14) | 0.0194 (14) | 0.0268 (15) | -0.0042 (12) | 0.0027 (12) | -0.0045 (12) |
| C2 | 0.043 (2) | 0.063 (2) | 0.0286 (17) | -0.032 (2) | 0.0102 (15) | -0.0183 (17) |
| C3 | 0.057 (2) | 0.075 (3) | 0.042 (2) | -0.042 (2) | 0.0090 (19) | -0.029 (2) |
| C4 | 0.0338 (18) | 0.044 (2) | 0.042 (2) | -0.0189 (17) | -0.0023 (15) | -0.0118 (17) |
| C5 | 0.0272 (16) | 0.0403 (19) | 0.0376 (19) | -0.0138 (15) | 0.0068 (14) | -0.0054 (15) |
| C6 | 0.0313 (17) | 0.0321 (17) | 0.0274 (16) | -0.0106 (14) | 0.0035 (13) | -0.0057 (13) |
| C7 | 0.0252 (15) | 0.0184 (14) | 0.0291 (15) | -0.0046 (12) | 0.0053 (12) | -0.0064 (12) |
| C8 | 0.0274 (16) | 0.0271 (16) | 0.045 (2) | -0.0015 (14) | -0.0034 (15) | -0.0106 (15) |
| C9 | 0.036 (2) | 0.033 (2) | 0.063 (2) | 0.0057 (16) | 0.0071 (19) | -0.0124 (19) |
| C10 | 0.060 (2) | 0.0254 (18) | 0.055 (2) | -0.0007 (18) | 0.014 (2) | -0.0178 (17) |
| C11 | 0.063 (2) | 0.0270 (17) | 0.0353 (19) | -0.0181 (18) | 0.0053 (17) | -0.0107 (15) |
| C12 | 0.0389 (18) | 0.0210 (15) | 0.0262 (15) | -0.0097 (14) | 0.0031 (13) | -0.0026 (12) |
| C13 | 0.0317 (16) | 0.0284 (16) | 0.0237 (15) | -0.0091 (14) | 0.0075 (13) | -0.0025 (12) |
| C14 | 0.049 (2) | 0.0249 (17) | 0.0371 (19) | -0.0130 (16) | 0.0107 (16) | 0.0007 (14) |
| C15 | 0.072 (3) | 0.0304 (19) | 0.047 (2) | -0.026 (2) | 0.019 (2) | -0.0107 (17) |
| C16 | 0.070 (3) | 0.053 (2) | 0.049 (2) | -0.041 (2) | 0.012 (2) | -0.019 (2) |
| C17 | 0.046 (2) | 0.060 (2) | 0.049 (2) | -0.028 (2) | -0.0003 (19) | -0.015 (2) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C18 | 0.0355 (18) | 0.0371 (19) | 0.0354 (18) | -0.0113 (16) | 0.0031 (15) | -0.0074 (15) |
| C19 | 0.0296 (16) | 0.0298 (16) | 0.0247 (15) | -0.0089 (13) | 0.0026 (12) | -0.0080 (13) |
| C20 | 0.077 (3) | 0.036 (2) | 0.045 (2) | -0.008 (2) | 0.030 (2) | -0.0062 (18) |
| C21 | 0.085 (3) | 0.056 (2) | 0.046 (2) | 0.003 (2) | 0.039 (2) | -0.009 (2) |
| C22 | 0.050 (2) | 0.041 (2) | 0.0311 (18) | -0.0035 (18) | 0.0114 (16) | -0.0136 (16) |
| C23 | 0.051 (2) | 0.0328 (18) | 0.0328 (18) | -0.0020 (17) | 0.0065 (17) | -0.0076 (15) |
| C24 | 0.047 (2) | 0.0298 (17) | 0.0247 (16) | -0.0032 (15) | 0.0104 (15) | -0.0053 (13) |
| C25 | 0.142 (9) | 0.180 (11) | 0.057 (4) | 0.105 (9) | 0.007 (4) | 0.026 (6) |
| C26 | 0.168 (10) | 0.152 (9) | 0.091 (6) | 0.074 (8) | -0.027 (6) | 0.014 (6) |
| C27 | 0.146 (8) | 0.169 (10) | 0.084 (6) | 0.082 (8) | 0.016 (5) | 0.048 (6) |

Geometric parameters (Å, °)

| | | | |
|------------------------------|-------------|----------------------------|------------|
| Zr1—C11 | 2.4450 (9) | C19—C24 | 1.380 (4) |
| Zr1—C11 ⁱ | 2.4450 (9) | C20—C21 | 1.379 (6) |
| Zr1—C12 | 2.4627 (7) | C21—C22 | 1.377 (5) |
| Zr1—C12 ⁱ | 2.4627 (7) | C22—C23 | 1.369 (5) |
| Zr1—O1 | 2.0820 (18) | C23—C24 | 1.386 (5) |
| Zr1—O1 ⁱ | 2.0820 (18) | C25—C26 | 1.358 (19) |
| P1—P2 | 2.2057 (10) | C25—C27 ⁱⁱ | 1.33 (2) |
| P1—O1 | 1.5281 (19) | C26—C27 | 1.399 (16) |
| P1—C1 | 1.787 (3) | C2—H1 | 0.950 |
| P1—C7 | 1.788 (3) | C3—H2 | 0.950 |
| P2—C13 | 1.833 (4) | C4—H3 | 0.950 |
| P2—C19 | 1.833 (3) | C5—H4 | 0.950 |
| C1—C2 | 1.382 (5) | C6—H5 | 0.950 |
| C1—C6 | 1.397 (4) | C8—H6 | 0.950 |
| C2—C3 | 1.391 (7) | C9—H7 | 0.950 |
| C3—C4 | 1.392 (6) | C10—H8 | 0.950 |
| C4—C5 | 1.390 (6) | C11—H9 | 0.950 |
| C5—C6 | 1.394 (6) | C12—H10 | 0.950 |
| C7—C8 | 1.393 (4) | C14—H11 | 0.950 |
| C7—C12 | 1.397 (5) | C15—H12 | 0.950 |
| C8—C9 | 1.387 (5) | C16—H13 | 0.950 |
| C9—C10 | 1.382 (7) | C17—H14 | 0.950 |
| C10—C11 | 1.379 (5) | C18—H15 | 0.950 |
| C11—C12 | 1.389 (5) | C20—H16 | 0.950 |
| C13—C14 | 1.400 (4) | C21—H17 | 0.950 |
| C13—C18 | 1.397 (4) | C22—H18 | 0.950 |
| C14—C15 | 1.388 (7) | C23—H19 | 0.950 |
| C15—C16 | 1.366 (6) | C24—H20 | 0.950 |
| C16—C17 | 1.379 (6) | C25—H21 | 0.950 |
| C17—C18 | 1.390 (7) | C26—H22 | 0.950 |
| C19—C20 | 1.392 (5) | C27—H23 | 0.950 |
| Cl(1)···C(11) ⁱⁱⁱ | 3.525 (4) | H(7)···H(3) ^{xi} | 3.057 |
| Cl(2)···C(4) ^{iv} | 3.562 (4) | H(7)···H(13) ^{ix} | 2.668 |
| Cl(2)···C(5) ^{iv} | 3.585 (4) | H(7)···H(14) ^{ix} | 3.540 |

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| C(4)···Cl(2) ^{iv} | 3.562 (4) | H(7)···H(19) ^{xiii} | 3.174 |
| C(5)···Cl(2) ^{iv} | 3.585 (4) | H(7)···H(21) | 3.273 |
| C(11)···Cl(1) ⁱⁱⁱ | 3.525 (4) | H(8)···Cl(1) ⁱⁱⁱ | 3.494 |
| Cl(1)···H(4) ^v | 3.032 | H(8)···Cl(2) ^{vi} | 3.258 |
| Cl(1)···H(8) ⁱⁱⁱ | 3.494 | H(8)···C(4) ^{xi} | 3.362 |
| Cl(1)···H(9) ⁱⁱⁱ | 2.887 | H(8)···C(5) ^{xi} | 3.208 |
| Cl(1)···H(12) ⁱⁱⁱ | 3.318 | H(8)···C(6) ^{vi} | 3.398 |
| Cl(2)···H(3) ^{iv} | 2.911 | H(8)···H(3) ^{xi} | 3.321 |
| Cl(2)···H(4) ^{iv} | 2.961 | H(8)···H(4) ^{xi} | 3.055 |
| Cl(2)···H(7) ^{vi} | 2.927 | H(8)···H(4) ^{vi} | 3.535 |
| Cl(2)···H(8) ^{vi} | 3.258 | H(8)···H(5) ^{vi} | 2.572 |
| Cl(2)···H(13) ⁱⁱⁱ | 3.045 | H(9)···Cl(1) ⁱⁱⁱ | 2.887 |
| C(2)···H(17) ^{vii} | 3.413 | H(9)···C(16) ⁱⁱⁱ | 3.110 |
| C(2)···H(18) ^{vii} | 3.110 | H(9)···C(17) ⁱⁱⁱ | 2.899 |
| C(3)···H(17) ^{vii} | 3.277 | H(9)···H(10) ⁱⁱⁱ | 3.588 |
| C(3)···H(18) ^{vii} | 3.282 | H(9)···H(13) ⁱⁱⁱ | 2.949 |
| C(3)···H(23) ⁱⁱ | 3.560 | H(9)···H(14) ⁱⁱⁱ | 2.582 |
| C(4)···H(8) ^{viii} | 3.362 | H(10)···H(9) ⁱⁱⁱ | 3.588 |
| C(4)···H(15) ^{ix} | 3.020 | H(10)···H(13) ⁱⁱⁱ | 3.143 |
| C(5)···H(8) ^{viii} | 3.208 | H(11)···C(20) ^x | 3.460 |
| C(5)···H(14) ^{ix} | 3.164 | H(11)···C(21) ^x | 3.354 |
| C(5)···H(15) ^{ix} | 3.157 | H(11)···H(16) ^x | 2.879 |
| C(6)···H(4) ^{iv} | 3.442 | H(11)···H(17) ^x | 2.667 |
| C(6)···H(8) ^{vi} | 3.398 | H(11)···H(22) | 3.352 |
| C(6)···H(14) ^{ix} | 3.176 | H(12)···Cl(1) ⁱⁱⁱ | 3.318 |
| C(8)···H(14) ^{ix} | 3.237 | H(12)···C(23) ^{xi} | 3.490 |
| C(8)···H(21) | 3.481 | H(12)···C(24) ^{xi} | 3.568 |
| C(9)···H(13) ^{ix} | 3.339 | H(12)···H(17) ^x | 2.930 |
| C(10)···H(5) ^{vi} | 3.352 | H(12)···H(19) ^{xi} | 2.960 |
| C(11)···H(13) ⁱⁱⁱ | 3.366 | H(12)···H(20) ^{xi} | 3.109 |
| C(11)···H(14) ⁱⁱⁱ | 3.275 | H(13)···Cl(2) ⁱⁱⁱ | 3.045 |
| C(12)···H(13) ⁱⁱⁱ | 3.465 | H(13)···C(9) ^v | 3.339 |
| C(13)···H(16) ^x | 3.566 | H(13)···C(11) ⁱⁱⁱ | 3.366 |
| C(14)···H(16) ^x | 3.027 | H(13)···C(12) ⁱⁱⁱ | 3.465 |
| C(14)···H(17) ^x | 3.209 | H(13)···H(6) ^v | 3.492 |
| C(15)···H(16) ^x | 3.479 | H(13)···H(7) ^v | 2.668 |
| C(15)···H(17) ^x | 3.335 | H(13)···H(9) ⁱⁱⁱ | 2.949 |
| C(15)···H(19) ^{xi} | 3.244 | H(13)···H(10) ⁱⁱⁱ | 3.143 |
| C(16)···H(7) ^v | 3.426 | H(13)···H(19) ^{xi} | 2.912 |
| C(16)···H(9) ⁱⁱⁱ | 3.110 | H(13)···H(21) ^v | 3.382 |
| C(16)···H(19) ^{xi} | 3.220 | H(14)···C(5) ^v | 3.164 |

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| C(16)···H(21) ^v | 3.293 | H(14)···C(6) ^v | 3.176 |
| C(17)···H(6) ^v | 3.327 | H(14)···C(8) ^v | 3.237 |
| C(17)···H(9) ⁱⁱⁱ | 2.899 | H(14)···C(11) ⁱⁱⁱ | 3.275 |
| C(17)···H(21) ^v | 3.332 | H(14)···H(4) ^v | 3.268 |
| C(17)···H(23) ^x | 3.371 | H(14)···H(5) ^v | 3.293 |
| C(18)···H(23) ^x | 3.192 | H(14)···H(6) ^v | 2.665 |
| C(20)···H(11) ^x | 3.460 | H(14)···H(7) ^v | 3.540 |
| C(21)···H(1) ^{vii} | 3.425 | H(14)···H(9) ⁱⁱⁱ | 2.582 |
| C(21)···H(2) ^{vii} | 3.408 | H(14)···H(21) ^v | 3.424 |
| C(21)···H(11) ^x | 3.354 | H(14)···H(23) ^x | 3.500 |
| C(22)···H(1) ^{vii} | 3.091 | H(15)···C(4) ^v | 3.020 |
| C(22)···H(2) ^v | 3.600 | H(15)···C(5) ^v | 3.157 |
| C(22)···H(2) ^{vii} | 3.375 | H(15)···H(3) ^v | 2.914 |
| C(22)···H(3) ^v | 3.494 | H(15)···H(4) ^v | 3.149 |
| C(22)···H(22) ^{xii} | 3.500 | H(15)···H(23) ^x | 3.233 |
| C(23)···H(3) ^v | 3.020 | H(16)···C(13) ^x | 3.566 |
| C(23)···H(12) ^{viii} | 3.490 | H(16)···C(14) ^x | 3.027 |
| C(23)···H(21) ^{xii} | 3.506 | H(16)···C(15) ^x | 3.479 |
| C(24)···H(3) ^v | 3.242 | H(16)···H(11) ^x | 2.879 |
| C(24)···H(12) ^{viii} | 3.568 | H(16)···H(23) ^x | 3.494 |
| C(25)···H(6) | 2.983 | H(17)···C(2) ^{vii} | 3.413 |
| C(25)···H(18) ^{xiii} | 3.342 | H(17)···C(3) ^{vii} | 3.277 |
| C(26)···H(1) ⁱⁱ | 3.419 | H(17)···C(14) ^x | 3.209 |
| C(26)···H(6) | 3.481 | H(17)···C(15) ^x | 3.335 |
| C(26)···H(18) ^{xiii} | 3.138 | H(17)···H(1) ^{vii} | 3.071 |
| C(27)···H(6) ⁱⁱ | 3.518 | H(17)···H(2) ^{vii} | 2.827 |
| H(1)···C(21) ^{vii} | 3.425 | H(17)···H(11) ^x | 2.667 |
| H(1)···C(22) ^{vii} | 3.091 | H(17)···H(12) ^x | 2.930 |
| H(1)···C(26) ⁱⁱ | 3.419 | H(17)···H(22) ^x | 3.566 |
| H(1)···H(17) ^{vii} | 3.071 | H(18)···C(2) ^{vii} | 3.110 |
| H(1)···H(18) ^{vii} | 2.397 | H(18)···C(3) ^{vii} | 3.282 |
| H(1)···H(22) ⁱⁱ | 3.424 | H(18)···C(25) ^{xii} | 3.342 |
| H(2)···C(21) ^{vii} | 3.408 | H(18)···C(26) ^{xii} | 3.138 |
| H(2)···C(22) ^{ix} | 3.600 | H(18)···H(1) ^{vii} | 2.397 |
| H(2)···C(22) ^{vii} | 3.375 | H(18)···H(2) ^{vii} | 2.762 |
| H(2)···H(17) ^{vii} | 2.827 | H(18)···H(21) ^{xii} | 3.046 |
| H(2)···H(18) ^{vii} | 2.762 | H(18)···H(22) ^{xii} | 2.675 |
| H(2)···H(22) ⁱⁱ | 3.190 | H(19)···C(15) ^{viii} | 3.244 |
| H(2)···H(23) ⁱⁱ | 3.595 | H(19)···C(16) ^{viii} | 3.220 |
| H(3)···Cl(2) ^{iv} | 2.911 | H(19)···H(3) ^v | 3.088 |
| H(3)···C(22) ^{ix} | 3.494 | H(19)···H(7) ^{xii} | 3.174 |

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| H(3)···C(23) ^{ix} | 3.020 | H(19)···H(12) ^{viii} | 2.960 |
| H(3)···C(24) ^{ix} | 3.242 | H(19)···H(13) ^{viii} | 2.912 |
| H(3)···H(7) ^{viii} | 3.057 | H(19)···H(21) ^{xii} | 2.796 |
| H(3)···H(8) ^{viii} | 3.321 | H(20)···H(3) ^v | 3.452 |
| H(3)···H(15) ^{ix} | 2.914 | H(20)···H(12) ^{viii} | 3.109 |
| H(3)···H(19) ^{ix} | 3.088 | H(21)···C(8) | 3.481 |
| H(3)···H(20) ^{ix} | 3.452 | H(21)···C(16) ^{ix} | 3.293 |
| H(4)···Cl(1) ^{ix} | 3.032 | H(21)···C(17) ^{ix} | 3.332 |
| H(4)···Cl(2) ^{iv} | 2.961 | H(21)···C(23) ^{xiii} | 3.506 |
| H(4)···C(6) ^{iv} | 3.442 | H(21)···H(6) | 2.756 |
| H(4)···H(4) ^{iv} | 3.226 | H(21)···H(7) | 3.273 |
| H(4)···H(5) ^{iv} | 2.901 | H(21)···H(13) ^{ix} | 3.382 |
| H(4)···H(8) ^{viii} | 3.055 | H(21)···H(14) ^{ix} | 3.424 |
| H(4)···H(8) ^{vi} | 3.535 | H(21)···H(18) ^{xiii} | 3.046 |
| H(4)···H(14) ^{ix} | 3.268 | H(21)···H(19) ^{xiii} | 2.796 |
| H(4)···H(15) ^{ix} | 3.149 | H(22)···C(22) ^{xiii} | 3.500 |
| H(5)···C(10) ^{vi} | 3.352 | H(22)···H(1) ⁱⁱ | 3.424 |
| H(5)···H(4) ^{iv} | 2.901 | H(22)···H(2) ⁱⁱ | 3.190 |
| H(5)···H(8) ^{vi} | 2.572 | H(22)···H(6) | 3.593 |
| H(5)···H(14) ^{ix} | 3.293 | H(22)···H(11) | 3.352 |
| H(6)···C(17) ^{ix} | 3.327 | H(22)···H(17) ^x | 3.566 |
| H(6)···C(25) | 2.983 | H(22)···H(18) ^{xiii} | 2.675 |
| H(6)···C(26) | 3.481 | H(23)···C(3) ⁱⁱ | 3.560 |
| H(6)···C(27) ⁱⁱ | 3.518 | H(23)···C(17) ^x | 3.371 |
| H(6)···H(13) ^{ix} | 3.492 | H(23)···C(18) ^x | 3.192 |
| H(6)···H(14) ^{ix} | 2.665 | H(23)···H(2) ⁱⁱ | 3.595 |
| H(6)···H(21) | 2.756 | H(23)···H(14) ^x | 3.500 |
| H(6)···H(22) | 3.593 | H(23)···H(15) ^x | 3.233 |
| H(7)···Cl(2) ^{vi} | 2.927 | H(23)···H(16) ^x | 3.494 |
| H(7)···C(16) ^{ix} | 3.426 | | |
| Cl(1)—Zr(1)—Cl(1) ⁱ | 180 | C(20)—C(21)—C(22) | 119.9 (4) |
| Cl(1)—Zr(1)—Cl(2) | 89.73 (2) | C(21)—C(22)—C(23) | 119.6 (3) |
| Cl(1)—Zr(1)—Cl(2) ⁱ | 90.27 (2) | C(22)—C(23)—C(24) | 120.7 (3) |
| Cl(1)—Zr(1)—O(1) | 90.01 (7) | C(19)—C(24)—C(23) | 120.5 (3) |
| Cl(1)—Zr(1)—O(1) ⁱ | 89.99 (7) | C(26)—C(25)—C(27) ⁱⁱ | 120.6 (10) |
| Cl(1) ⁱ —Zr(1)—Cl(2) | 90.27 (2) | C(25)—C(26)—C(27) | 120.5 (13) |
| Cl(1) ⁱ —Zr(1)—Cl(2) ⁱ | 89.73 (2) | C(25) ⁱⁱ —C(27)—C(26) | 118.9 (12) |
| Cl(1) ⁱ —Zr(1)—O(1) | 89.99 (7) | C(1)—C(2)—H(1) | 119.6 |
| Cl(1) ⁱ —Zr(1)—O(1) ⁱ | 90.01 (7) | C(3)—C(2)—H(1) | 119.6 |
| Cl(2)—Zr(1)—Cl(2) ⁱ | 180 | C(2)—C(3)—H(2) | 120.2 |
| Cl(2)—Zr(1)—O(1) | 89.43 (5) | C(4)—C(3)—H(2) | 120.2 |

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| Cl(2)—Zr(1)—O(1) ⁱ | 90.57 (5) | C(3)—C(4)—H(3) | 119.9 |
| Cl(2) ⁱ —Zr(1)—O(1) | 90.57 (5) | C(5)—C(4)—H(3) | 119.9 |
| Cl(2) ⁱ —Zr(1)—O(1) ⁱ | 89.43 (5) | C(4)—C(5)—H(4) | 120.1 |
| O(1)—Zr(1)—O(1) ⁱ | 180 | C(6)—C(5)—H(4) | 120.1 |
| P(2)—P(1)—O(1) | 115.79 (9) | C(1)—C(6)—H(5) | 120.0 |
| P(2)—P(1)—C(1) | 108.46 (10) | C(5)—C(6)—H(5) | 120.0 |
| P(2)—P(1)—C(7) | 101.63 (10) | C(7)—C(8)—H(6) | 120.1 |
| O(1)—P(1)—C(1) | 111.99 (13) | C(9)—C(8)—H(6) | 120.1 |
| O(1)—P(1)—C(7) | 109.97 (14) | C(8)—C(9)—H(7) | 120.3 |
| C(1)—P(1)—C(7) | 108.32 (15) | C(10)—C(9)—H(7) | 120.3 |
| P(1)—P(2)—C(13) | 95.26 (11) | C(9)—C(10)—H(8) | 119.4 |
| P(1)—P(2)—C(19) | 105.04 (10) | C(11)—C(10)—H(8) | 119.5 |
| C(13)—P(2)—C(19) | 103.65 (16) | C(10)—C(11)—H(9) | 119.9 |
| Zr(1)—O(1)—P(1) | 155.63 (13) | C(12)—C(11)—H(9) | 119.9 |
| P(1)—C(1)—C(2) | 122.1 (2) | C(7)—C(12)—H(10) | 120.5 |
| P(1)—C(1)—C(6) | 118.3 (2) | C(11)—C(12)—H(10) | 120.5 |
| C(2)—C(1)—C(6) | 119.6 (3) | C(13)—C(14)—H(11) | 119.8 |
| C(1)—C(2)—C(3) | 120.7 (3) | C(15)—C(14)—H(11) | 119.8 |
| C(2)—C(3)—C(4) | 119.7 (4) | C(14)—C(15)—H(12) | 119.9 |
| C(3)—C(4)—C(5) | 120.1 (4) | C(16)—C(15)—H(12) | 119.9 |
| C(4)—C(5)—C(6) | 119.8 (3) | C(15)—C(16)—H(13) | 119.8 |
| C(1)—C(6)—C(5) | 120.1 (3) | C(17)—C(16)—H(13) | 119.8 |
| P(1)—C(7)—C(8) | 119.6 (2) | C(16)—C(17)—H(14) | 119.8 |
| P(1)—C(7)—C(12) | 119.5 (2) | C(18)—C(17)—H(14) | 119.8 |
| C(8)—C(7)—C(12) | 120.4 (3) | C(13)—C(18)—H(15) | 120.1 |
| C(7)—C(8)—C(9) | 119.8 (3) | C(17)—C(18)—H(15) | 120.1 |
| C(8)—C(9)—C(10) | 119.4 (3) | C(19)—C(20)—H(16) | 119.4 |
| C(9)—C(10)—C(11) | 121.1 (3) | C(21)—C(20)—H(16) | 119.4 |
| C(10)—C(11)—C(12) | 120.2 (4) | C(20)—C(21)—H(17) | 120.1 |
| C(7)—C(12)—C(11) | 119.0 (3) | C(22)—C(21)—H(17) | 120.1 |
| P(2)—C(13)—C(14) | 117.1 (2) | C(21)—C(22)—H(18) | 120.2 |
| P(2)—C(13)—C(18) | 124.0 (2) | C(23)—C(22)—H(18) | 120.2 |
| C(14)—C(13)—C(18) | 118.8 (3) | C(22)—C(23)—H(19) | 119.6 |
| C(13)—C(14)—C(15) | 120.4 (3) | C(24)—C(23)—H(19) | 119.6 |
| C(14)—C(15)—C(16) | 120.2 (3) | C(19)—C(24)—H(20) | 119.8 |
| C(15)—C(16)—C(17) | 120.3 (5) | C(23)—C(24)—H(20) | 119.8 |
| C(16)—C(17)—C(18) | 120.5 (4) | C(26)—C(25)—H(21) | 119.7 |
| C(13)—C(18)—C(17) | 119.8 (3) | C(27) ⁱⁱ —C(25)—H(21) | 119.7 |
| P(2)—C(19)—C(20) | 115.2 (2) | C(25)—C(26)—H(22) | 119.7 |
| P(2)—C(19)—C(24) | 126.5 (2) | C(27)—C(26)—H(22) | 119.8 |
| C(20)—C(19)—C(24) | 118.2 (3) | C(25) ⁱⁱ —C(27)—H(23) | 120.6 |
| C(19)—C(20)—C(21) | 121.1 (3) | C(26)—C(27)—H(23) | 120.6 |
| Cl(1)—Zr(1)—O(1)—P(1) | -126.6 (3) | C(19)—P(2)—C(13)—C(18) | -30.0 (3) |
| Cl(1)—Zr(1)—O(1) ⁱ —P(1) ⁱ | -53.4 (3) | P(1)—C(1)—C(2)—C(3) | 179.7 (2) |
| Cl(1) ⁱ —Zr(1)—O(1)—P(1) | 53.4 (3) | P(1)—C(1)—C(6)—C(5) | -179.4 (2) |
| Cl(1) ⁱ —Zr(1)—O(1) ⁱ —P(1) ⁱ | 126.6 (3) | C(2)—C(1)—C(6)—C(5) | -1.0 (4) |
| Cl(2)—Zr(1)—O(1)—P(1) | -36.8 (3) | C(6)—C(1)—C(2)—C(3) | 1.3 (5) |

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| Cl(2)—Zr(1)—O(1) ⁱ —P(1) ⁱ | -143.2 (3) | C(1)—C(2)—C(3)—C(4) | -1.0 (5) |
| Cl(2) ⁱ —Zr(1)—O(1)—P(1) | 143.2 (3) | C(2)—C(3)—C(4)—C(5) | 0.4 (5) |
| Cl(2) ⁱ —Zr(1)—O(1) ⁱ —P(1) ⁱ | 36.8 (3) | C(3)—C(4)—C(5)—C(6) | -0.1 (4) |
| P(2)—P(1)—O(1)—Zr(1) | -171.5 (3) | C(4)—C(5)—C(6)—C(1) | 0.4 (4) |
| O(1)—P(1)—P(2)—C(13) | -61.58 (14) | P(1)—C(7)—C(8)—C(9) | -171.8 (3) |
| O(1)—P(1)—P(2)—C(19) | 44.08 (17) | P(1)—C(7)—C(12)—C(11) | 172.2 (2) |
| P(2)—P(1)—C(1)—C(2) | 19.8 (2) | C(8)—C(7)—C(12)—C(11) | -0.2 (5) |
| P(2)—P(1)—C(1)—C(6) | -161.7 (2) | C(12)—C(7)—C(8)—C(9) | 0.6 (5) |
| C(1)—P(1)—P(2)—C(13) | 171.56 (13) | C(7)—C(8)—C(9)—C(10) | -0.7 (6) |
| C(1)—P(1)—P(2)—C(19) | -82.77 (16) | C(8)—C(9)—C(10)—C(11) | 0.4 (6) |
| P(2)—P(1)—C(7)—C(8) | 72.2 (2) | C(9)—C(10)—C(11)—C(12) | -0.0 (6) |
| P(2)—P(1)—C(7)—C(12) | -100.3 (2) | C(10)—C(11)—C(12)—C(7) | -0.1 (4) |
| C(7)—P(1)—P(2)—C(13) | 57.55 (15) | P(2)—C(13)—C(14)—C(15) | 173.9 (3) |
| C(7)—P(1)—P(2)—C(19) | 163.22 (17) | P(2)—C(13)—C(18)—C(17) | -175.3 (2) |
| O(1)—P(1)—C(1)—C(2) | -109.2 (2) | C(14)—C(13)—C(18)—C(17) | -0.4 (5) |
| O(1)—P(1)—C(1)—C(6) | 69.2 (2) | C(18)—C(13)—C(14)—C(15) | -1.4 (5) |
| C(1)—P(1)—O(1)—Zr(1) | -46.5 (4) | C(13)—C(14)—C(15)—C(16) | 1.6 (6) |
| O(1)—P(1)—C(7)—C(8) | -164.6 (2) | C(14)—C(15)—C(16)—C(17) | -0.1 (5) |
| O(1)—P(1)—C(7)—C(12) | 22.9 (3) | C(15)—C(16)—C(17)—C(18) | -1.6 (6) |
| C(7)—P(1)—O(1)—Zr(1) | 74.0 (3) | C(16)—C(17)—C(18)—C(13) | 1.9 (6) |
| C(1)—P(1)—C(7)—C(8) | -41.9 (3) | P(2)—C(19)—C(20)—C(21) | -178.6 (4) |
| C(1)—P(1)—C(7)—C(12) | 145.6 (2) | P(2)—C(19)—C(24)—C(23) | 177.4 (3) |
| C(7)—P(1)—C(1)—C(2) | 129.4 (2) | C(20)—C(19)—C(24)—C(23) | 1.9 (6) |
| C(7)—P(1)—C(1)—C(6) | -52.2 (2) | C(24)—C(19)—C(20)—C(21) | -2.5 (7) |
| P(1)—P(2)—C(13)—C(14) | -98.1 (2) | C(19)—C(20)—C(21)—C(22) | 1.8 (8) |
| P(1)—P(2)—C(13)—C(18) | 76.9 (2) | C(20)—C(21)—C(22)—C(23) | -0.3 (7) |
| P(1)—P(2)—C(19)—C(20) | 177.0 (3) | C(21)—C(22)—C(23)—C(24) | -0.4 (7) |
| P(1)—P(2)—C(19)—C(24) | 1.3 (3) | C(22)—C(23)—C(24)—C(19) | -0.5 (6) |
| C(13)—P(2)—C(19)—C(20) | -83.7 (3) | C(26)—C(25)—C(27) ⁱⁱ —C(26) ⁱⁱ | -1.8 (15) |
| C(13)—P(2)—C(19)—C(24) | 100.6 (3) | C(27) ⁱⁱ —C(25)—C(26)—C(27) | 1.8 (16) |
| C(19)—P(2)—C(13)—C(14) | 155.0 (2) | C(25)—C(26)—C(27)—C(25) ⁱⁱ | -1.8 (15) |

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+2$; (iv) $-x+1, -y, -z+2$; (v) $x+1, y, z$; (vi) $-x+1, -y+1, -z+2$; (vii) $-x+2, -y, -z+1$; (viii) $x, y-1, z$; (ix) $x-1, y, z$; (x) $-x+2, -y+1, -z+1$; (xi) $x, y+1, z$; (xii) $x+1, y-1, z$; (xiii) $x-1, y+1, z$.

Fig. 2

