

## (*R,R*)-Ethylenebis[(2-methylphenyl)-phenylphosphine oxide] ('*o*-Tolyl DiPAMPO')

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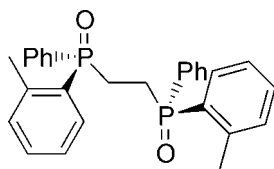
Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;

$R$  factor = 0.047;  $wR$  factor = 0.113; data-to-parameter ratio = 23.2.

In the course of studies on the synthesis of P-chiral phosphine ligands, a simple route to enantiopure DiPAMP analogues has been developed. The crystal structure of the title compound,  $\text{C}_{28}\text{H}_{28}\text{O}_2\text{P}_2$ , shows it to be the *R,R* enantiomer of the bisphosphine oxide, prior to reduction to the corresponding bisphosphine. This is believed to be the first example of a crystal structure of an enantiopure DiPAMPO-type compound.

### Related literature

For related literature, see: Bergin *et al.* (2007); Gilheany (1992).



### Experimental

#### Crystal data

$\text{C}_{28}\text{H}_{28}\text{O}_2\text{P}_2$

$M_r = 458.44$

Orthorhombic,  $P2_12_12_1$

$a = 5.7941$  (5) Å

$b = 17.2455$  (15) Å

$c = 23.012$  (2) Å

$V = 2299.4$  (3) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 0.21$  mm<sup>-1</sup>

$T = 100$  (2) K

$0.50 \times 0.50 \times 0.05$  mm

#### Data collection

Bruker APEX CCD area-detector diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.717$ ,  $T_{\max} = 0.989$

24918 measured reflections

6693 independent reflections

5820 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.113$

$S = 1.09$

6693 reflections

289 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.56$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>

Absolute structure: Flack (1983)

Flack parameter:  $-0.02$  (8), 2860

Friedel pairs

Data collection: *SMART* (Bruker, 2003); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank James Morey for help with the structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2065).

### References

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**supplementary materials**

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**(*R,R*)-Ethylenebis[(2-methylphenyl)phenylphosphine oxide] (*o*-Tolyl DiPAMPO')**

**G. King, E. Bergin, H. Müller-Bunz and D. G. Gilheany**

**Comment**

This crystal structure establishes that in our recently developed method for the construction of P-stereogenic phosphine oxides (Bergin *et al.*, 2007), the use of (-)-menthol gives rise to the *R*-configured phosphine oxide.

The PO and PC bond lengths are both at the high ends of the ranges expected for phosphine oxides, (147.5–149) and (179–181) pm respectively (Gilheany, 1992). The bond angles at phosphorus (CPO 111–113.5° and CPC 106–106.5°) show the expected deviation from the tetrahedral values consistent with the shorter PO distance (Gilheany, 1992).

**Experimental**

The title compound was synthesized by our recently developed method for the generation of P-stereogenic phosphorus compounds (Bergin *et al.*, 2007). The corresponding monophosphine oxide was produced in good ee (80%) from the reaction of the racemic phosphine with (-)-menthol in the presence of hexachloroacetone. It was subsequently oxidatively coupled to yield the bisphosphine oxide in 98% ee. X-ray quality crystals were obtained by crystallizing from benzene. To the best of our knowledge this is the first crystal structure of an enantiomerically pure DiPAMPO analogue.

**Figures**

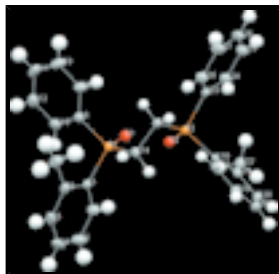


Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-hydrogen atoms.

**(*R,R*)-Ethylenebis[(2-methylphenyl)phenylphosphine oxide]**

*Crystal data*

C<sub>28</sub>H<sub>28</sub>O<sub>2</sub>P<sub>2</sub>

*M<sub>r</sub>* = 458.44

Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

*a* = 5.7941 (5) Å

*b* = 17.2455 (15) Å

*c* = 23.012 (2) Å

*D<sub>x</sub>* = 1.324 Mg m<sup>-3</sup>

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 5179 reflections

θ = 2.5–30.8°

μ = 0.21 mm<sup>-1</sup>

*T* = 100 (2) K

# supplementary materials

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$$V = 2299.4 (3) \text{ \AA}^3$$

$$Z = 4$$

$$F_{000} = 968$$

Lath, colourless

$$0.50 \times 0.50 \times 0.05 \text{ mm}$$

## Data collection

Bruker APEX CCD area-detector  
diffractometer

6693 independent reflections

Radiation source: fine-focus sealed tube

5820 reflections with  $I > 2\sigma(I)$

Monochromator: graphite

$$R_{\text{int}} = 0.054$$

$$T = 100(2) \text{ K}$$

$$\theta_{\text{max}} = 30.0^\circ$$

$\varphi$  and  $\omega$  scans

$$\theta_{\text{min}} = 1.8^\circ$$

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$$h = -8 \rightarrow 8$$

$$T_{\text{min}} = 0.717, T_{\text{max}} = 0.989$$

$$k = -24 \rightarrow 24$$

24918 measured reflections

$$l = -32 \rightarrow 32$$

## Refinement

Refinement on  $F^2$

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

$$R[F^2 > 2\sigma(F^2)] = 0.047$$

$$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$$

$$wR(F^2) = 0.113$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$S = 1.09$$

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

6693 reflections

$$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$$

289 parameters

$$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Secondary atom site location: difference Fourier map

Absolute structure: Flack (1983)

Flack parameter:  $-0.02 (8)$

## 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 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.33886 (9)	0.29398 (3)	0.21588 (2)	0.01480 (11)

O1	0.5851 (3)	0.29881 (9)	0.19807 (6)	0.0211 (3)
C1	0.2408 (4)	0.19598 (11)	0.22940 (9)	0.0171 (4)
C2	0.0501 (4)	0.16736 (13)	0.19982 (10)	0.0265 (5)
H2A	-0.0349	0.2006	0.1748	0.032*
C3	-0.0176 (5)	0.09058 (14)	0.20643 (12)	0.0350 (6)
H3A	-0.1479	0.0714	0.1859	0.042*
C4	0.1036 (4)	0.04265 (13)	0.24256 (11)	0.0318 (6)
H4A	0.0591	-0.0101	0.2465	0.038*
C5	0.2907 (5)	0.07055 (13)	0.27351 (10)	0.0308 (6)
H5A	0.3714	0.0369	0.2991	0.037*
C6	0.3631 (4)	0.14753 (12)	0.26775 (9)	0.0223 (4)
C7	0.5636 (5)	0.17576 (14)	0.30295 (11)	0.0333 (6)
H7A	0.6237	0.1331	0.3267	0.050*
H7B	0.5132	0.2181	0.3283	0.050*
H7C	0.6851	0.1945	0.2769	0.050*
C8	0.2867 (3)	0.34813 (11)	0.28190 (9)	0.0174 (4)
C9	0.4561 (4)	0.39914 (12)	0.30008 (10)	0.0251 (5)
H9A	0.5929	0.4052	0.2778	0.030*
C10	0.4266 (5)	0.44147 (14)	0.35085 (12)	0.0338 (6)
H10A	0.5431	0.4766	0.3631	0.041*
C11	0.2307 (5)	0.43278 (14)	0.38321 (11)	0.0315 (6)
H11A	0.2124	0.4612	0.4183	0.038*
C12	0.0594 (5)	0.38282 (13)	0.36513 (10)	0.0303 (5)
H12A	-0.0768	0.3772	0.3877	0.036*
C13	0.0843 (4)	0.34061 (13)	0.31418 (10)	0.0244 (5)
H13A	-0.0352	0.3069	0.3014	0.029*
C14	0.1437 (4)	0.33385 (12)	0.16196 (9)	0.0185 (4)
H14A	0.1397	0.2991	0.1277	0.022*
H14B	-0.0140	0.3362	0.1784	0.022*
C15	0.2170 (4)	0.41508 (11)	0.14268 (9)	0.0161 (4)
H15A	0.3778	0.4134	0.1282	0.019*
H15B	0.2120	0.4507	0.1764	0.019*
P2	0.02887 (8)	0.45118 (3)	0.08600 (2)	0.01335 (11)
O2	-0.2200 (2)	0.44574 (9)	0.10142 (6)	0.0188 (3)
C16	0.1036 (3)	0.39833 (11)	0.02016 (8)	0.0141 (4)
C17	0.2915 (3)	0.34797 (11)	0.01890 (9)	0.0169 (4)
H17A	0.3940	0.3461	0.0511	0.020*
C18	0.3312 (4)	0.30052 (12)	-0.02873 (9)	0.0209 (4)
H18A	0.4604	0.2666	-0.0291	0.025*
C19	0.1830 (4)	0.30256 (12)	-0.07545 (9)	0.0224 (4)
H19A	0.2045	0.2681	-0.1072	0.027*
C20	0.0026 (4)	0.35514 (12)	-0.07596 (9)	0.0204 (4)
H20A	-0.0940	0.3581	-0.1093	0.024*
C21	-0.0409 (3)	0.40357 (11)	-0.02912 (9)	0.0171 (4)
C22	-0.2408 (4)	0.45922 (12)	-0.03249 (9)	0.0212 (4)
H22A	-0.3182	0.4535	-0.0701	0.032*
H22B	-0.1839	0.5125	-0.0284	0.032*
H22C	-0.3503	0.4479	-0.0012	0.032*
C23	0.1147 (3)	0.55056 (11)	0.07362 (8)	0.0151 (4)

## supplementary materials

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C24	0.3295 (4)	0.57026 (12)	0.05179 (10)	0.0236 (4)
H24A	0.4410	0.5310	0.0448	0.028*
C25	0.3826 (4)	0.64718 (13)	0.04011 (10)	0.0265 (5)
H25A	0.5286	0.6603	0.0241	0.032*
C26	0.2232 (4)	0.70479 (13)	0.05178 (10)	0.0253 (5)
H26A	0.2609	0.7574	0.0442	0.030*
C27	0.0107 (4)	0.68623 (12)	0.07428 (11)	0.0281 (5)
H27A	-0.0982	0.7260	0.0823	0.034*
C28	-0.0452 (4)	0.60876 (12)	0.08534 (10)	0.0225 (4)
H28A	-0.1923	0.5958	0.1008	0.027*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
P1	0.0144 (2)	0.0150 (2)	0.0149 (2)	-0.00059 (19)	-0.00002 (19)	0.0026 (2)
O1	0.0179 (7)	0.0223 (7)	0.0233 (7)	-0.0003 (6)	0.0016 (6)	0.0029 (6)
C1	0.0193 (9)	0.0163 (9)	0.0155 (9)	-0.0014 (8)	0.0032 (7)	-0.0003 (7)
C2	0.0242 (11)	0.0252 (11)	0.0302 (12)	-0.0040 (9)	-0.0034 (10)	-0.0015 (9)
C3	0.0314 (13)	0.0284 (12)	0.0452 (15)	-0.0101 (10)	0.0038 (12)	-0.0093 (11)
C4	0.0398 (14)	0.0168 (10)	0.0387 (13)	-0.0074 (10)	0.0160 (11)	-0.0048 (10)
C5	0.0485 (15)	0.0187 (10)	0.0253 (12)	0.0056 (10)	0.0111 (11)	0.0037 (9)
C6	0.0302 (12)	0.0193 (9)	0.0175 (9)	0.0037 (9)	0.0033 (9)	0.0000 (8)
C7	0.0459 (15)	0.0262 (11)	0.0279 (12)	0.0052 (11)	-0.0154 (11)	0.0025 (9)
C8	0.0189 (9)	0.0139 (8)	0.0194 (9)	0.0021 (7)	-0.0022 (8)	0.0031 (8)
C9	0.0210 (10)	0.0240 (10)	0.0302 (11)	-0.0036 (9)	-0.0033 (9)	-0.0046 (9)
C10	0.0341 (13)	0.0286 (12)	0.0386 (13)	0.0017 (10)	-0.0104 (11)	-0.0124 (11)
C11	0.0479 (15)	0.0266 (12)	0.0200 (11)	0.0101 (11)	-0.0042 (10)	-0.0051 (9)
C12	0.0393 (14)	0.0255 (11)	0.0261 (12)	0.0032 (11)	0.0099 (10)	0.0017 (9)
C13	0.0277 (12)	0.0181 (9)	0.0274 (11)	-0.0025 (8)	0.0056 (9)	-0.0001 (9)
C14	0.0206 (10)	0.0187 (9)	0.0161 (9)	-0.0008 (8)	-0.0015 (8)	0.0049 (7)
C15	0.0182 (10)	0.0147 (9)	0.0153 (9)	-0.0005 (7)	-0.0011 (7)	0.0016 (7)
P2	0.0129 (2)	0.0126 (2)	0.0145 (2)	0.00024 (18)	0.00076 (18)	0.00101 (18)
O2	0.0156 (7)	0.0192 (7)	0.0217 (7)	0.0000 (6)	0.0028 (5)	-0.0001 (6)
C16	0.0153 (9)	0.0119 (8)	0.0151 (9)	-0.0020 (7)	0.0023 (7)	0.0012 (7)
C17	0.0175 (9)	0.0155 (9)	0.0177 (9)	0.0004 (7)	0.0007 (7)	0.0018 (8)
C18	0.0192 (9)	0.0186 (9)	0.0250 (10)	0.0026 (8)	0.0057 (9)	-0.0016 (8)
C19	0.0261 (11)	0.0217 (10)	0.0192 (10)	-0.0036 (9)	0.0067 (8)	-0.0044 (8)
C20	0.0214 (10)	0.0245 (10)	0.0152 (9)	-0.0056 (8)	0.0004 (8)	-0.0005 (8)
C21	0.0151 (9)	0.0173 (8)	0.0188 (9)	-0.0019 (7)	0.0016 (8)	0.0024 (7)
C22	0.0187 (10)	0.0248 (10)	0.0202 (10)	0.0020 (8)	-0.0026 (8)	0.0033 (9)
C23	0.0190 (9)	0.0128 (8)	0.0133 (8)	-0.0011 (8)	-0.0022 (7)	0.0005 (7)
C24	0.0227 (10)	0.0186 (9)	0.0296 (11)	0.0007 (9)	0.0045 (9)	-0.0008 (8)
C25	0.0269 (12)	0.0216 (10)	0.0309 (12)	-0.0042 (9)	0.0025 (9)	0.0022 (9)
C26	0.0310 (12)	0.0143 (9)	0.0307 (11)	-0.0020 (9)	-0.0093 (9)	0.0051 (9)
C27	0.0281 (12)	0.0177 (9)	0.0384 (13)	0.0069 (9)	-0.0040 (10)	-0.0009 (9)
C28	0.0179 (9)	0.0198 (9)	0.0296 (11)	0.0026 (8)	0.0002 (9)	0.0002 (9)

*Geometric parameters (Å, °)*

P1—O1	1.4870 (15)	C15—P2	1.810 (2)
P1—C8	1.809 (2)	C15—H15A	0.9900
P1—C1	1.810 (2)	C15—H15B	0.9900
P1—C14	1.814 (2)	P2—O2	1.4878 (14)
C1—C2	1.388 (3)	P2—C16	1.820 (2)
C1—C6	1.407 (3)	P2—C23	1.807 (2)
C2—C3	1.389 (3)	C16—C17	1.393 (3)
C2—H2A	0.9500	C16—C21	1.413 (3)
C3—C4	1.367 (4)	C17—C18	1.387 (3)
C3—H3A	0.9500	C17—H17A	0.9500
C4—C5	1.383 (4)	C18—C19	1.376 (3)
C4—H4A	0.9500	C18—H18A	0.9500
C5—C6	1.398 (3)	C19—C20	1.384 (3)
C5—H5A	0.9500	C19—H19A	0.9500
C6—C7	1.498 (3)	C20—C21	1.387 (3)
C7—H7A	0.9800	C20—H20A	0.9500
C7—H7B	0.9800	C21—C22	1.506 (3)
C7—H7C	0.9800	C22—H22A	0.9800
C8—C13	1.394 (3)	C22—H22B	0.9800
C8—C9	1.383 (3)	C22—H22C	0.9800
C9—C10	1.388 (3)	C23—C24	1.384 (3)
C9—H9A	0.9500	C23—C28	1.392 (3)
C10—C11	1.366 (4)	C24—C25	1.388 (3)
C10—H10A	0.9500	C24—H24A	0.9500
C11—C12	1.379 (4)	C25—C26	1.383 (3)
C11—H11A	0.9500	C25—H25A	0.9500
C12—C13	1.387 (3)	C26—C27	1.374 (3)
C12—H12A	0.9500	C26—H26A	0.9500
C13—H13A	0.9500	C27—C28	1.398 (3)
C14—C15	1.530 (3)	C27—H27A	0.9500
C14—H14A	0.9900	C28—H28A	0.9500
C14—H14B	0.9900		
O1—P1—C8	111.28 (9)	C14—C15—P2	110.90 (13)
O1—P1—C1	113.64 (9)	C14—C15—H15A	109.5
C8—P1—C1	106.57 (9)	P2—C15—H15A	109.5
O1—P1—C14	112.86 (9)	C14—C15—H15B	109.5
C8—P1—C14	105.93 (9)	P2—C15—H15B	109.5
C1—P1—C14	106.01 (9)	H15A—C15—H15B	108.0
C2—C1—C6	119.8 (2)	O2—P2—C15	112.96 (9)
C2—C1—P1	119.83 (16)	O2—P2—C16	113.42 (9)
C6—C1—P1	120.29 (16)	C15—P2—C16	106.51 (9)
C1—C2—C3	120.7 (2)	O2—P2—C23	111.36 (9)
C1—C2—H2A	119.7	C15—P2—C23	105.90 (9)
C3—C2—H2A	119.7	C16—P2—C23	106.15 (9)
C4—C3—C2	119.9 (2)	C17—C16—C21	119.10 (18)
C4—C3—H3A	120.1	C17—C16—P2	121.03 (15)

## supplementary materials

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C2—C3—H3A	120.1	C21—C16—P2	119.68 (14)
C3—C4—C5	120.4 (2)	C18—C17—C16	120.91 (19)
C3—C4—H4A	119.8	C18—C17—H17A	119.5
C5—C4—H4A	119.8	C16—C17—H17A	119.5
C4—C5—C6	121.1 (2)	C19—C18—C17	119.9 (2)
C4—C5—H5A	119.5	C19—C18—H18A	120.0
C6—C5—H5A	119.5	C17—C18—H18A	120.0
C5—C6—C1	118.2 (2)	C20—C19—C18	119.64 (19)
C5—C6—C7	119.3 (2)	C20—C19—H19A	120.2
C1—C6—C7	122.5 (2)	C18—C19—H19A	120.2
C6—C7—H7A	109.5	C19—C20—C21	121.68 (19)
C6—C7—H7B	109.5	C19—C20—H20A	119.2
H7A—C7—H7B	109.5	C21—C20—H20A	119.2
C6—C7—H7C	109.5	C20—C21—C16	118.55 (18)
H7A—C7—H7C	109.5	C20—C21—C22	118.90 (18)
H7B—C7—H7C	109.5	C16—C21—C22	122.55 (18)
C13—C8—C9	119.7 (2)	C21—C22—H22A	109.5
C13—C8—P1	122.69 (16)	C21—C22—H22B	109.5
C9—C8—P1	117.64 (16)	H22A—C22—H22B	109.5
C8—C9—C10	120.1 (2)	C21—C22—H22C	109.5
C8—C9—H9A	119.9	H22A—C22—H22C	109.5
C10—C9—H9A	119.9	H22B—C22—H22C	109.5
C11—C10—C9	120.2 (2)	C24—C23—C28	119.46 (18)
C11—C10—H10A	119.9	C24—C23—P2	122.50 (15)
C9—C10—H10A	119.9	C28—C23—P2	118.02 (15)
C10—C11—C12	120.2 (2)	C23—C24—C25	120.3 (2)
C10—C11—H11A	119.9	C23—C24—H24A	119.9
C12—C11—H11A	119.9	C25—C24—H24A	119.9
C11—C12—C13	120.5 (2)	C26—C25—C24	120.1 (2)
C11—C12—H12A	119.7	C26—C25—H25A	120.0
C13—C12—H12A	119.7	C24—C25—H25A	120.0
C8—C13—C12	119.3 (2)	C25—C26—C27	120.3 (2)
C8—C13—H13A	120.4	C25—C26—H26A	119.8
C12—C13—H13A	120.4	C27—C26—H26A	119.8
C15—C14—P1	111.86 (14)	C26—C27—C28	119.9 (2)
C15—C14—H14A	109.2	C26—C27—H27A	120.0
P1—C14—H14A	109.2	C28—C27—H27A	120.0
C15—C14—H14B	109.2	C23—C28—C27	120.0 (2)
P1—C14—H14B	109.2	C23—C28—H28A	120.0
H14A—C14—H14B	107.9	C27—C28—H28A	120.0
O1—P1—C1—C2	-124.41 (18)	C14—C15—P2—O2	51.52 (16)
C8—P1—C1—C2	112.66 (18)	C14—C15—P2—C16	-73.63 (15)
C14—P1—C1—C2	0.1 (2)	C14—C15—P2—C23	173.66 (14)
O1—P1—C1—C6	52.70 (19)	O2—P2—C16—C17	-131.23 (16)
C8—P1—C1—C6	-70.23 (19)	C15—P2—C16—C17	-6.35 (18)
C14—P1—C1—C6	177.22 (17)	C23—P2—C16—C17	106.19 (16)
C6—C1—C2—C3	-1.8 (3)	O2—P2—C16—C21	43.77 (17)
P1—C1—C2—C3	175.28 (19)	C15—P2—C16—C21	168.64 (15)
C1—C2—C3—C4	0.3 (4)	C23—P2—C16—C21	-78.82 (16)



C2—C3—C4—C5	1.3 (4)	C21—C16—C17—C18	-3.2 (3)
C3—C4—C5—C6	-1.3 (4)	P2—C16—C17—C18	171.82 (15)
C4—C5—C6—C1	-0.2 (3)	C16—C17—C18—C19	-0.3 (3)
C4—C5—C6—C7	178.8 (2)	C17—C18—C19—C20	3.6 (3)
C2—C1—C6—C5	1.8 (3)	C18—C19—C20—C21	-3.3 (3)
P1—C1—C6—C5	-175.33 (16)	C19—C20—C21—C16	-0.2 (3)
C2—C1—C6—C7	-177.2 (2)	C19—C20—C21—C22	-179.76 (19)
P1—C1—C6—C7	5.7 (3)	C17—C16—C21—C20	3.4 (3)
O1—P1—C8—C13	-166.69 (16)	P2—C16—C21—C20	-171.66 (15)
C1—P1—C8—C13	-42.30 (19)	C17—C16—C21—C22	-177.02 (18)
C14—P1—C8—C13	70.29 (19)	P2—C16—C21—C22	7.9 (3)
O1—P1—C8—C9	13.8 (2)	O2—P2—C23—C24	-171.85 (16)
C1—P1—C8—C9	138.15 (17)	C15—P2—C23—C24	65.00 (19)
C14—P1—C8—C9	-109.26 (18)	C16—P2—C23—C24	-47.96 (19)
C13—C8—C9—C10	1.3 (3)	O2—P2—C23—C28	6.53 (18)
P1—C8—C9—C10	-179.16 (18)	C15—P2—C23—C28	-116.62 (17)
C8—C9—C10—C11	0.2 (4)	C16—P2—C23—C28	130.42 (16)
C9—C10—C11—C12	-1.0 (4)	C28—C23—C24—C25	-1.8 (3)
C10—C11—C12—C13	0.3 (4)	P2—C23—C24—C25	176.51 (18)
C9—C8—C13—C12	-2.0 (3)	C23—C24—C25—C26	1.8 (4)
P1—C8—C13—C12	178.48 (17)	C24—C25—C26—C27	-0.8 (4)
C11—C12—C13—C8	1.2 (3)	C25—C26—C27—C28	-0.1 (4)
O1—P1—C14—C15	-50.63 (17)	C24—C23—C28—C27	0.9 (3)
C8—P1—C14—C15	71.38 (16)	P2—C23—C28—C27	-177.55 (17)
C1—P1—C14—C15	-175.64 (14)	C26—C27—C28—C23	0.1 (3)
P1—C14—C15—P2	176.78 (11)		

Fig. 1

