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A diisopropoxyphosphonate monosulfone

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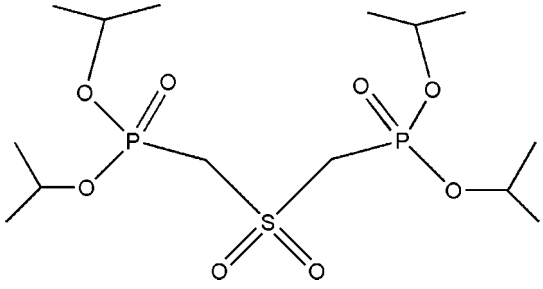
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.095; data-to-parameter ratio = 25.6.

The title compound, diisopropyl (diisopropoxyphosphoryl-methylsulfonylmethyl)phosphonate, $C_{14}H_{32}O_8P_2S$, is a monosulfone of a diphosphate ester that has been investigated as a target for chemotherapy. The molecule is in a quasi-*gauche* conformation with an approximate twofold axis. The S═O, P═O and P—O bonds average 1.444, 1.474 and 1.574 Å, respectively.

Related literature

Theoretical and conformational studies of related molecules, together with the crystal structure of a sulfonylphosphonate, have been reported by Olivato *et al.* (2001).

For related literature, see: Allen (2002); Hadd *et al.* (2001); Meadows & Gervay-Hague (2006); Meadows *et al.* (2005, 2007).



Experimental

Crystal data

$C_{14}H_{32}O_8P_2S$
M_r = 422.40
Orthorhombic, $Pna2_1$
a = 9.8124 (9) Å
b = 8.3298 (8) Å
c = 26.160 (3) Å
V = 2138.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 90 (2) K
0.47 × 0.13 × 0.08 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
T_{min} = 0.858, T_{max} = 0.974
20017 measured reflections
6014 independent reflections
5398 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
S = 1.09
6014 reflections
235 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), with 2547 Friedel pairs
Flack parameter: 0.39 (7)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2025).

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supplementary materials

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A diisopropoxyphosphonate monosulfone

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Comment

As part of our research into enzymes that are involved in the metastatic potential of tumor cells, a number of potential disulfone inhibitors for HIV-integrase have been identified (Meadows *et al.*, 2005, Meadows & Gervay-Hague, 2006, Meadows *et al.*, 2007). The monosulfone reagent reported here was envisioned and synthesized by a modification of the disulfone reaction (Hadd, *et al.*, 2001).

Molecule (I), has an approximate twofold axis that passes through the central sulfur (Fig. 1). There are no short intermolecular contacts in the packing. As expected, the P=O distances are longer than the S=O distances. A quasi-*gauche* conformation is indicated by the torsion angles O=P—C—S (−41.65 (14)]° for O2—P1—C2—S1 and −41.75 (14)° for O6—P2—C3—S1) and two of the P—C—S=O angles (−41.92 (13)° for P1—C2—S1—O4 and −42.06 (13)° for P2—C3—S—O5). This conformation is in keeping with the result of a HF/6–31G** calculation on a similar molecule (Olivato, *et al.*, 2001) that is the only other reported structure of a neutral sulfonylphosphonate in the Cambridge Structural Database (v. 5.28, Allen, 2002). The authors suggested that this conformation and the observed intramolecular P···O=S < S···O=P distances reflect a better electron- donating ability of the sulfonyl oxygen lone pair than the phosphoryl oxygen lone pair. In agreement with the previously reported structure, in (I) the P···O=S distances are 3.3094 (14) Å and 3.3082 (15) Å while the S···O=P distances are 3.1593 (16)Å and 3.1616 (15) Å.

Experimental

In the synthesis of (diisopropoxy-phosphorylmethanesulfonylmethyl)-phosphonic acid diisopropyl ester (I), to commercially available diisopropyl bromomethylphosphonate (Lancaster) (5.3 g, 20 mmol) in 15 ml of DMF were added potassium thioacetate (3.7 g, 30 mmol) and tetrabutylammonium iodide (370 mg) in sequence. The reaction mixture was heated to 358 K and stirred for 2 h. The solution was cooled and partitioned between water and ethyl acetate. The ethyl acetate layer was collected and dried over sodium sulfate and then evaporated to dryness. To the crude oil was added acetonitrile (15 ml), 3 *M* NaOH (7.4 ml) and methanol (7.4 ml) and the solution was stirred for 30 min. After 30 min, an additional 1 equiv of diisopropyl bromomethylphosphonate (4.5 g) was added to the mixture at room temperature and stirred overnight. The reaction mixture was then partitioned between water and ethyl acetate. The ethyl acetate layer was collected, dried over sodium sulfate, and evaporated to dryness. The crude oil was oxidized using oxone (24.9 g, 40 mmol) in methanol/water (*ca* 100 ml, 1:1) overnight to give a crude solid after diethyl ether/bicarbonate extraction. Recrystallization from diethyl ether/ hexane (1:1) provided 4.98 g of compound (I) as colorless, needle-like crystals (80% yield).

Refinement

The methyl H atoms were constrained to an ideal geometry with C—H distances of 0.98 \%A and *U*ĩso~(H) = 1.5*U*~eq~(C), and each group was allowed to rotate freely about its C—C bond. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.99–1.00 \%A and *U*ĩso~(H) = 1.2*U*~eq~(C). The refined value of the Flack parameter (0.37 (7)) indicated a degree of inversion twinning.

Figures

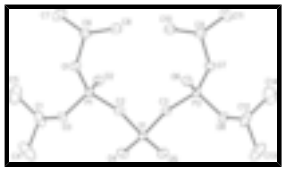


Fig. 1. A view of (I). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity.

diisopropyl (diisopropoxyphosphorylmethylsulfonylmethyl)phosphonate

Crystal data

$C_{14}H_{32}O_8P_2S$	$D_x = 1.312$ Mg m^{-3}
$M_r = 422.40$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $Pna2_1$	Cell parameters from 994 reflections
$a = 9.8124$ (9) Å	$\theta = 2.3$–20.0º
$b = 8.3298$ (8) Å	$\mu = 0.34$ mm^{-1}
$c = 26.160$ (3) Å	$T = 90$ (2) K
$V = 2138.2$ (4) Å^3	Needle, colorless
$Z = 4$	0.47 × 0.13 × 0.08 mm
$F_{000} = 904$	

Data collection

Bruker SMART 1000 diffractometer	6014 independent reflections
Radiation source: fine-focus sealed tube	5398 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
Detector resolution: 8.3 pixels mm^{-1}	$\theta_{max} = 30.5$º
$T = 90(2)$ K	$\theta_{min} = 1.6$º
ω scans	$h = -13\rightarrow13$
Absorption correction: multi-scan (SADABS; Sheldrick, 2005)	$k = -11\rightarrow11$
$T_{min} = 0.858$, $T_{max} = 0.974$	$l = -36\rightarrow31$
20017 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.3326P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.095$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.09$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
6014 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}

235 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2547 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.39 (7)
Secondary atom site location: difference Fourier map	

Special details

Experimental. ^{1}H (400 MHz, $CDCl_3$) δ 4.83 (m, 1H), 4.09 (d, J=16 Hz, 1H), 1.37 (q, 6H). ^{13}C (100 MHz, $CDCl_3$) δ 72.89 (d, J=6 Hz), 51.46 (d, J= 137 Hz), 24.29, J=4 Hz), 23.89 (d, J=5 Hz). LRMS (ESI) m/*z* calcd for $C_{14}H_{32}O_8P_2S$ $(M + H)^+$ is 423.13 and for $(M + Na)^+$ is 445.13, found $(M + H)^+$ 423.00 and $(M + Na)$+ 445.13. Anal. Calcd for $C_{14}H_{32}O_8P_2S$: C, 39.81; H, 7.64. Found: C, 39.88; H, 7.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.88344 (5)	0.34367 (4)	0.84454 (2)	0.01515 (8)
P1	0.89600 (5)	0.11641 (6)	0.933576 (18)	0.01557 (10)
P2	0.87014 (4)	0.11416 (6)	0.756060 (18)	0.01532 (10)
O1	0.80358 (14)	−0.01724 (16)	0.95810 (6)	0.0205 (3)
O2	1.02766 (13)	0.05791 (16)	0.91381 (6)	0.0192 (3)
O3	0.90314 (15)	0.24746 (18)	0.97675 (7)	0.0195 (3)
O4	0.98063 (14)	0.43243 (17)	0.87483 (6)	0.0205 (3)
O5	0.78672 (14)	0.43246 (16)	0.81398 (6)	0.0199 (3)
O6	0.73851 (13)	0.05654 (16)	0.77615 (6)	0.0190 (3)
O7	0.96206 (14)	−0.02005 (16)	0.73148 (6)	0.0201 (3)
O8	0.86268 (14)	0.24438 (17)	0.71228 (7)	0.0201 (4)
C1	1.0218 (3)	0.2557 (3)	1.01095 (12)	0.0353 (7)
H1	1.1065	0.2353	0.9907	0.042*
C2	0.79050 (17)	0.2140 (2)	0.88622 (8)	0.0166 (3)
H2A	0.7442	0.1309	0.8655	0.020*
H2B	0.7193	0.2773	0.9039	0.020*
C3	0.97566 (17)	0.2129 (2)	0.80333 (7)	0.0159 (3)
H3A	1.0217	0.1302	0.8243	0.019*
H3B	1.0471	0.2755	0.7855	0.019*
C4	1.0252 (3)	0.4245 (4)	1.03118 (14)	0.0535 (9)
H4A	0.9419	0.4455	1.0508	0.080*
H4B	1.0309	0.5001	1.0026	0.080*
H4C	1.1048	0.4380	1.0534	0.080*

C5	1.0094 (5)	0.1308 (5)	1.05165 (14)	0.0823 (15)
H5A	1.0128	0.0239	1.0361	0.123*
H5B	0.9225	0.1443	1.0696	0.123*
H5C	1.0847	0.1423	1.0760	0.123*
C6	0.8124 (2)	−0.1874 (2)	0.94238 (8)	0.0228 (4)
H6	0.9097	−0.2167	0.9358	0.027*
C7	0.7587 (3)	−0.2831 (4)	0.98725 (11)	0.0453 (7)
H7A	0.6638	−0.2529	0.9939	0.068*
H7B	0.8141	−0.2604	1.0176	0.068*
H7C	0.7635	−0.3980	0.9793	0.068*
C8	0.7292 (2)	−0.2133 (3)	0.89447 (9)	0.0260 (4)
H8A	0.7708	−0.1546	0.8660	0.039*
H8B	0.6362	−0.1740	0.9000	0.039*
H8C	0.7266	−0.3281	0.8864	0.039*
C9	0.9539 (2)	−0.1899 (2)	0.74786 (8)	0.0217 (4)
H9	0.8568	−0.2196	0.7545	0.026*
C10	1.0364 (2)	−0.2130 (3)	0.79563 (9)	0.0245 (4)
H10A	0.9948	−0.1524	0.8237	0.037*
H10B	1.1295	−0.1745	0.7899	0.037*
H10C	1.0386	−0.3273	0.8045	0.037*
C11	1.0085 (3)	−0.2872 (4)	0.70366 (10)	0.0430 (7)
H11A	1.1050	−0.2616	0.6984	0.064*
H11B	0.9570	−0.2613	0.6726	0.064*
H11C	0.9989	−0.4018	0.7113	0.064*
C12	0.7431 (2)	0.2542 (3)	0.67915 (11)	0.0321 (6)
H12	0.6593	0.2357	0.7001	0.039*
C13	0.7408 (3)	0.4223 (4)	0.65881 (13)	0.0499 (8)
H13A	0.8210	0.4400	0.6372	0.075*
H13B	0.7418	0.4984	0.6874	0.075*
H13C	0.6580	0.4384	0.6385	0.075*
C14	0.7511 (5)	0.1291 (4)	0.63869 (15)	0.0702 (11)
H14A	0.7596	0.0231	0.6546	0.105*
H14B	0.8307	0.1493	0.6170	0.105*
H14C	0.6683	0.1324	0.6178	0.105*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01363 (16)	0.01357 (15)	0.01826 (17)	0.00011 (15)	−0.00119 (14)	0.0008 (2)
P1	0.0158 (2)	0.0165 (2)	0.0145 (2)	−0.00028 (15)	−0.00081 (17)	−0.0002 (2)
P2	0.0149 (2)	0.0155 (2)	0.0155 (2)	0.00026 (15)	−0.00078 (16)	0.0012 (2)
O1	0.0239 (7)	0.0181 (6)	0.0196 (7)	−0.0029 (5)	0.0008 (5)	0.0016 (6)
O2	0.0178 (6)	0.0198 (6)	0.0200 (7)	0.0023 (5)	−0.0006 (5)	−0.0001 (5)
O3	0.0218 (7)	0.0205 (9)	0.0162 (9)	−0.0012 (5)	−0.0019 (6)	−0.0039 (5)
O4	0.0186 (6)	0.0177 (6)	0.0253 (8)	−0.0032 (5)	−0.0019 (5)	−0.0031 (6)
O5	0.0184 (6)	0.0170 (6)	0.0241 (8)	0.0036 (5)	−0.0023 (5)	0.0037 (6)
O6	0.0181 (6)	0.0200 (6)	0.0191 (7)	−0.0016 (5)	−0.0009 (5)	0.0003 (5)
O7	0.0219 (7)	0.0165 (6)	0.0218 (7)	0.0024 (5)	0.0024 (5)	0.0006 (5)

O8	0.0200 (7)	0.0215 (9)	0.0189 (10)	−0.0004 (5)	−0.0019 (5)	0.0043 (5)
C1	0.0282 (11)	0.0524 (18)	0.0253 (15)	0.0067 (10)	−0.0087 (9)	−0.0158 (11)
C2	0.0129 (7)	0.0175 (8)	0.0196 (10)	0.0009 (6)	−0.0003 (6)	0.0007 (7)
C3	0.0130 (7)	0.0180 (7)	0.0167 (9)	0.0001 (6)	−0.0006 (6)	0.0008 (7)
C4	0.0459 (16)	0.061 (2)	0.053 (2)	−0.0150 (14)	−0.0063 (14)	−0.0313 (17)
C5	0.141 (4)	0.069 (3)	0.037 (2)	0.023 (3)	−0.043 (2)	0.0053 (17)
C6	0.0265 (9)	0.0161 (9)	0.0259 (11)	0.0002 (7)	−0.0040 (7)	0.0022 (7)
C7	0.075 (2)	0.0267 (12)	0.0344 (16)	−0.0088 (13)	−0.0016 (14)	0.0128 (12)
C8	0.0320 (10)	0.0199 (9)	0.0261 (12)	−0.0022 (8)	−0.0045 (8)	−0.0003 (9)
C9	0.0235 (9)	0.0156 (8)	0.0260 (11)	−0.0011 (6)	−0.0029 (7)	0.0001 (7)
C10	0.0288 (10)	0.0184 (9)	0.0262 (12)	0.0001 (8)	−0.0046 (8)	0.0029 (9)
C11	0.075 (2)	0.0239 (11)	0.0304 (16)	0.0092 (12)	−0.0089 (13)	−0.0082 (11)
C12	0.0284 (11)	0.0445 (16)	0.0234 (15)	−0.0037 (9)	−0.0100 (9)	0.0141 (10)
C13	0.0465 (16)	0.0557 (19)	0.0474 (19)	0.0145 (13)	−0.0021 (13)	0.0302 (15)
C14	0.108 (3)	0.062 (2)	0.041 (2)	−0.023 (2)	−0.033 (2)	0.0001 (17)

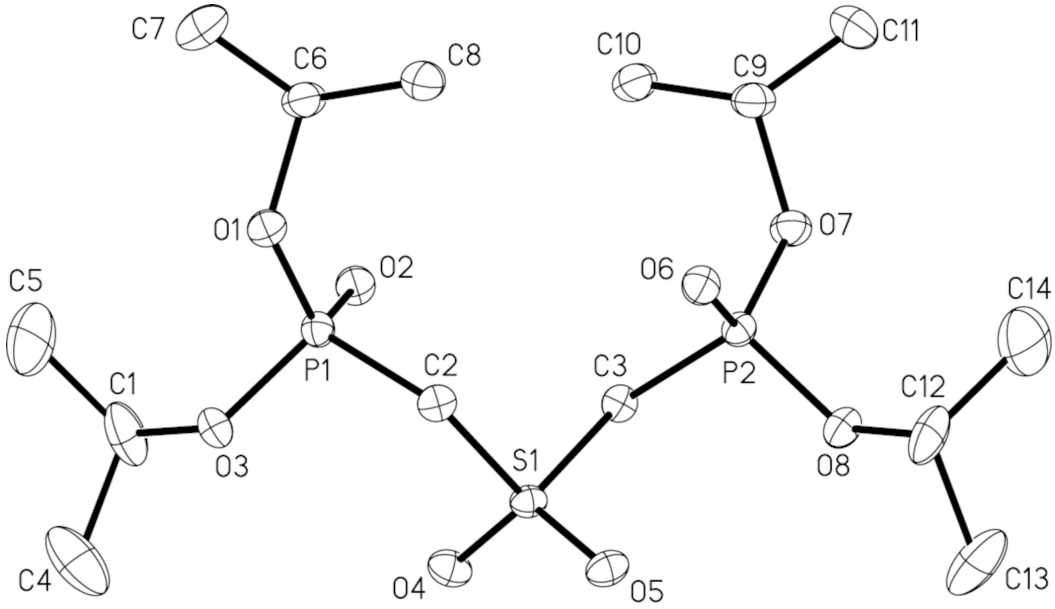
Geometric parameters (Å, °)

S1—O4	1.4435 (15)	C5—H5C	0.9800
S1—O5	1.4446 (14)	C6—C8	1.511 (3)
S1—C3	1.780 (2)	C6—C7	1.514 (3)
S1—C2	1.785 (2)	C6—H6	1.0000
P1—O2	1.4744 (14)	C7—H7A	0.9800
P1—O3	1.5722 (17)	C7—H7B	0.9800
P1—O1	1.5727 (14)	C7—H7C	0.9800
P1—C2	1.808 (2)	C8—H8A	0.9800
P2—O6	1.4747 (14)	C8—H8B	0.9800
P2—O7	1.5737 (14)	C8—H8C	0.9800
P2—O8	1.5791 (18)	C9—C10	1.501 (3)
P2—C3	1.811 (2)	C9—C11	1.510 (3)
O1—C6	1.478 (2)	C9—H9	1.0000
O3—C1	1.470 (3)	C10—H10A	0.9800
O7—C9	1.480 (2)	C10—H10B	0.9800
O8—C12	1.461 (3)	C10—H10C	0.9800
C1—C5	1.493 (5)	C11—H11A	0.9800
C1—C4	1.503 (4)	C11—H11B	0.9800
C1—H1	1.0000	C11—H11C	0.9800
C2—H2A	0.9900	C12—C14	1.487 (5)
C2—H2B	0.9900	C12—C13	1.498 (4)
C3—H3A	0.9900	C12—H12	1.0000
C3—H3B	0.9900	C13—H13A	0.9800
C4—H4A	0.9800	C13—H13B	0.9800
C4—H4B	0.9800	C13—H13C	0.9800
C4—H4C	0.9800	C14—H14A	0.9800
C5—H5A	0.9800	C14—H14B	0.9800
C5—H5B	0.9800	C14—H14C	0.9800
O4—S1—O5	118.40 (7)	O1—C6—C7	105.61 (19)
O4—S1—C3	108.06 (8)	C8—C6—C7	112.32 (19)
O5—S1—C3	108.18 (9)	O1—C6—H6	109.7

O4—S1—C2	108.19 (9)	C8—C6—H6	109.7
O5—S1—C2	108.19 (9)	C7—C6—H6	109.7
C3—S1—C2	105.04 (7)	C6—C7—H7A	109.5
O2—P1—O3	116.25 (8)	C6—C7—H7B	109.5
O2—P1—O1	114.48 (8)	H7A—C7—H7B	109.5
O3—P1—O1	102.95 (9)	C6—C7—H7C	109.5
O2—P1—C2	114.21 (9)	H7A—C7—H7C	109.5
O3—P1—C2	101.86 (9)	H7B—C7—H7C	109.5
O1—P1—C2	105.53 (8)	C6—C8—H8A	109.5
O6—P2—O7	114.61 (8)	C6—C8—H8B	109.5
O6—P2—O8	116.19 (8)	H8A—C8—H8B	109.5
O7—P2—O8	102.60 (9)	C6—C8—H8C	109.5
O6—P2—C3	113.92 (9)	H8A—C8—H8C	109.5
O7—P2—C3	105.91 (8)	H8B—C8—H8C	109.5
O8—P2—C3	102.10 (9)	O7—C9—C10	109.55 (16)
C6—O1—P1	122.11 (13)	O7—C9—C11	105.78 (18)
C1—O3—P1	120.32 (15)	C10—C9—C11	112.18 (19)
C9—O7—P2	121.98 (13)	O7—C9—H9	109.8
C12—O8—P2	120.39 (14)	C10—C9—H9	109.8
O3—C1—C5	109.7 (3)	C11—C9—H9	109.8
O3—C1—C4	106.0 (2)	C9—C10—H10A	109.5
C5—C1—C4	113.7 (3)	C9—C10—H10B	109.5
O3—C1—H1	109.1	H10A—C10—H10B	109.5
C5—C1—H1	109.1	C9—C10—H10C	109.5
C4—C1—H1	109.1	H10A—C10—H10C	109.5
S1—C2—P1	113.46 (9)	H10B—C10—H10C	109.5
S1—C2—H2A	108.9	C9—C11—H11A	109.5
P1—C2—H2A	108.9	C9—C11—H11B	109.5
S1—C2—H2B	108.9	H11A—C11—H11B	109.5
P1—C2—H2B	108.9	C9—C11—H11C	109.5
H2A—C2—H2B	107.7	H11A—C11—H11C	109.5
S1—C3—P2	113.65 (9)	H11B—C11—H11C	109.5
S1—C3—H3A	108.8	O8—C12—C14	109.9 (2)
P2—C3—H3A	108.8	O8—C12—C13	106.0 (2)
S1—C3—H3B	108.8	C14—C12—C13	113.7 (3)
P2—C3—H3B	108.8	O8—C12—H12	109.0
H3A—C3—H3B	107.7	C14—C12—H12	109.0
C1—C4—H4A	109.5	C13—C12—H12	109.0
C1—C4—H4B	109.5	C12—C13—H13A	109.5
H4A—C4—H4B	109.5	C12—C13—H13B	109.5
C1—C4—H4C	109.5	H13A—C13—H13B	109.5
H4A—C4—H4C	109.5	C12—C13—H13C	109.5
H4B—C4—H4C	109.5	H13A—C13—H13C	109.5
C1—C5—H5A	109.5	H13B—C13—H13C	109.5
C1—C5—H5B	109.5	C12—C14—H14A	109.5
H5A—C5—H5B	109.5	C12—C14—H14B	109.5
C1—C5—H5C	109.5	H14A—C14—H14B	109.5
H5A—C5—H5C	109.5	C12—C14—H14C	109.5
H5B—C5—H5C	109.5	H14A—C14—H14C	109.5

O1—C6—C8	109.63 (16)	H14B—C14—H14C	109.5
O2—P1—O1—C6	−27.16 (17)	C3—S1—C2—P1	73.30 (14)
O3—P1—O1—C6	−154.28 (14)	O2—P1—C2—S1	−41.65 (14)
C2—P1—O1—C6	99.30 (15)	O3—P1—C2—S1	84.50 (12)
O2—P1—O3—C1	−27.2 (2)	O1—P1—C2—S1	−168.27 (10)
O1—P1—O3—C1	98.8 (2)	O4—S1—C3—P2	−171.38 (10)
C2—P1—O3—C1	−152.02 (19)	O5—S1—C3—P2	−42.06 (13)
O6—P2—O7—C9	−27.84 (17)	C2—S1—C3—P2	73.30 (13)
O8—P2—O7—C9	−154.70 (14)	O6—P2—C3—S1	−41.75 (14)
C3—P2—O7—C9	98.62 (15)	O7—P2—C3—S1	−168.63 (10)
O6—P2—O8—C12	−25.8 (2)	O8—P2—C3—S1	84.33 (12)
O7—P2—O8—C12	100.08 (19)	P1—O1—C6—C8	−82.50 (19)
C3—P2—O8—C12	−150.33 (19)	P1—O1—C6—C7	156.28 (17)
P1—O3—C1—C5	−79.7 (3)	P2—O7—C9—C10	−81.56 (19)
P1—O3—C1—C4	157.1 (2)	P2—O7—C9—C11	157.34 (16)
O4—S1—C2—P1	−41.92 (13)	P2—O8—C12—C14	−80.1 (3)
O5—S1—C2—P1	−171.33 (10)	P2—O8—C12—C13	156.62 (19)

Fig. 1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C13