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1,5,6-Triphenyl-8-oxa-7-selena-6-phosphabicyclo[3.2.1]octane-6-selone

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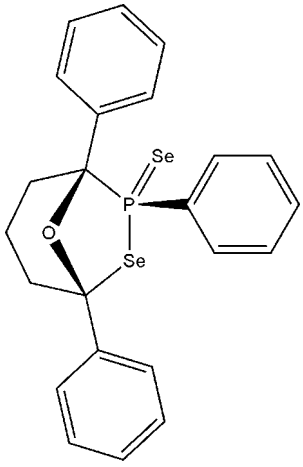
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.072; data-to-parameter ratio = 15.6.

The structure of the title compound, $C_{23}H_{21}OPSe_2$, consists of fused puckered five- and six-membered rings, $PSeC_2O$ and C_5O, respectively, with a C_2O bridgehead. The C_5O ring adopts a chair conformation, whilst the C_2PSeO ring has an envelope conformation.

Related literature

For related literature, see: An *et al.* (1998); Bhattacharyya *et al.* (2000, 2001*a*,*b*, 2002); Fitzmaurice *et al.* (1988); Gray, Bhattacharyya *et al.* (2005), Gray, Slawin *et al.* (2005); Hua & Woollins (2007); Hua, Li *et al.* (2006, 2007*a*,*b*,*c*); Shi *et al.* (2006, 2007).



Experimental

Crystal data

$C_{23}H_{21}OPSe_2$
M_r = 502.29
Triclinic, $P\overline{1}$
a = 7.6802 (9) Å
b = 9.0613 (12) Å
c = 14.9070 (16) Å
α = 84.949 (8)°
β = 75.677 (7)°
γ = 89.266 (8)°
V = 1001.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.78 mm^{-1}
T = 93 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2004)
T_{min} = 0.489, T_{max} = 0.570
7092 measured reflections
3805 independent reflections
3000 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.072
S = 1.00
3805 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick,2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2051).

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supporting information

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1,5,6-Triphenyl-8-oxa-7-selena-6-phosphabicyclo[3.2.1]octane-6-selone

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S1. Comment

2,4-bis(phenyl)-1,3-diselenadiphosphetane-2,4-diselenide $(PhPSe_2)_2$, also known as Woollins reagent, **WR**, is a selenium analogue of the well known Lawessons reagent, $(p\text{-}MeOPhPS_2)_2$. **WR** has found applications in the synthesis of selenium containing organic molecules, P—Se containing heterocycles and related compounds (Gray, Bhattacharyya *et al.*., 2005; Gray, Slawin *et al.*., 2005, Shi *et al.*, 2006, 2007, Bhattacharyya *et al.* 2000, 2001*a*, 2001*b*, 2002, Hua, Li *et al.* 2006, 2007*a*, 2007*b*, 2007*c*). We report here the synthesis and X-ray structure of a new fused [3,2,1] ring P—Se heterocycle. The title compound, (I), was generated by the reaction of Woollins′ reagent with 1,4-diketone. The P = Se bond length (2.0995 (9) Å) and the P – Se distance (2.2278 (10) Å) are consistent with the related selenides-containing P^V= Se bonds (2.08 – 2.12 Å) and P^V—Se single bonds (Fitzmaurice *et al.* 1988, An *et al.* 1998).

S2. Experimental

A red suspension of 1,3-dibenzoylpropane (0.25 g, 1 mmol) and Woollins′ reagent (0.54 g, 1 mmol) in dry toluene (10 ml) was refluxed for 16 hr. The yellow suspension was formed along with small amount of grey elemental selenium. Upon cooling to room temperature the mixture was purified by silica gel chromatography (1:9 ethyl acetate/dichloromethane as eluent) to give the title compound in 20% yield. Crystals were obtained from dichloromethane/hexane by diffusion method.

S3. Refinement

All H atoms were included in calculated positions (C—H distances are 0.98 Å for methyl H atoms, 0.99 Å for methylene H atoms and 0.95 Å for aryl H atoms) and were included in the refinement as riding atoms with Uĩso~(H) = 1.2 U~eq~ (parent atom, methylene and aryl H atoms) or Uĩso~(H) = 1.5 U~eq~ (parent atom, methyl H atoms).

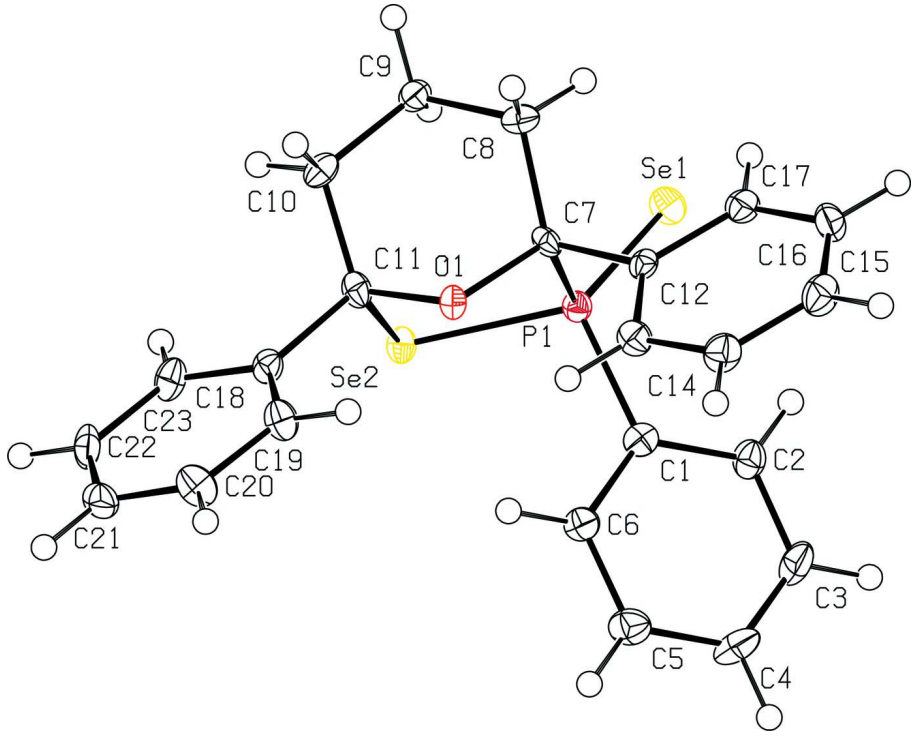

Figure 1

The structure of (**I**) with displacement ellipsoids drawn at the 50% probability level; H-atoms have been ignored for clarity.

1,5,6-Triphenyl-8-oxa-7-selena-6-phosphabicyclo[3.2.1]octane-6-selone

Crystal data

$C_{23}H_{21}OPSe_2$
$M_r = 502.29$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.6802\ (9)$ Å
$b = 9.0613\ (12)$ Å
$c = 14.9070\ (16)$ Å
$\alpha = 84.949\ (8)°$
$\beta = 75.677\ (7)°$
$\gamma = 89.266\ (8)°$
$V = 1001.2\ (2)$ Å^3
$Z = 2$
$F(000) = 500$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3344 reflections
$\theta = 2.3–28.4°$
$\mu = 3.78$ mm^{-1}
$T = 93$ K
Block, colorless
0.20 × 0.20 × 0.15 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2004)
$T_{min} = 0.489$, $T_{max} = 0.570$
7092 measured reflections
3805 independent reflections
3000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.8°$, $\theta_{min} = 2.3°$
$h = -10\rightarrow9$
$k = -10\rightarrow10$
$l = -15\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.072$
$S = 1.00$
3805 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}

Special details

Experimental. Anal. Calcd for $C_{23}H_{21}OPSe_2$: C, 55.00; H, 4.21. Found: C, 54.86; H, 4.15. ^{1}H NMR ($CDCl_3$): 7.72–7.05 (m, 15H, ArH), 2.37 (m, 4H, CH_2), 1.25 (m, 2H, CH_2). ^{31}P NMR ($CDCl_3$): 79.23 (s, J(P,Se$_{endo}$) = 430 Hz, J(P,Se$_{exo}$) = 776 Hz). ^{77}Se NMR ($CDCl_3$): 34.61 (d, J(P,Se$_{endo}$) = 430 Hz), -94.02 (d, J(P,Se$_{exo}$) = 778 Hz).

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C2	0.3921 (4)	0.3495 (4)	0.1438 (2)	0.0194 (8)
H2	0.3059	0.4106	0.1799	0.023*
Se2	0.56063 (4)	0.04366 (4)	0.35534 (2)	0.01561 (11)
Se1	0.26388 (4)	0.37283 (4)	0.37994 (2)	0.01944 (11)
P1	0.49881 (10)	0.27352 (10)	0.30698 (6)	0.0137 (2)
O1	0.8475 (3)	0.2463 (2)	0.29505 (14)	0.0147 (5)
C10	0.8065 (4)	0.1527 (4)	0.4568 (2)	0.0163 (8)
H10A	0.9283	0.1826	0.4598	0.020*
H10B	0.7710	0.0625	0.4999	0.020*
C18	0.9461 (4)	0.0000 (4)	0.3233 (2)	0.0161 (8)
C1	0.5138 (4)	0.2689 (4)	0.1839 (2)	0.0151 (7)
C12	0.7708 (4)	0.4895 (4)	0.2422 (2)	0.0133 (7)
C11	0.8112 (4)	0.1176 (4)	0.3592 (2)	0.0159 (8)
C8	0.7048 (4)	0.4071 (4)	0.4139 (2)	0.0167 (8)
H8A	0.6044	0.4773	0.4299	0.020*
H8B	0.8170	0.4596	0.4140	0.020*
C6	0.6430 (4)	0.1821 (4)	0.1293 (2)	0.0176 (8)
H6	0.7276	0.1285	0.1560	0.021*
C17	0.6750 (4)	0.6216 (4)	0.2523 (2)	0.0180 (8)
H17	0.5753	0.6289	0.3041	0.022*
C4	0.5238 (5)	0.2527 (4)	−0.0025 (2)	0.0275 (9)
H4	0.5262	0.2462	−0.0660	0.033*

C5	0.6475 (4)	0.1744 (4)	0.0366 (2)	0.0229 (9)
H5	0.7353	0.1155	−0.0004	0.027*
C21	1.1979 (4)	−0.2146 (4)	0.2626 (2)	0.0217 (9)
H21	1.2835	−0.2883	0.2412	0.026*
C9	0.6751 (4)	0.2765 (4)	0.4882 (2)	0.0165 (8)
H9A	0.6923	0.3096	0.5470	0.020*
H9B	0.5503	0.2389	0.4998	0.020*
C16	0.7245 (4)	0.7418 (4)	0.1872 (2)	0.0207 (8)
H16	0.6582	0.8310	0.1942	0.025*
C22	1.0516 (4)	−0.2490 (4)	0.3370 (2)	0.0228 (9)
H22	1.0371	−0.3465	0.3672	0.027*
C14	0.9652 (4)	0.6018 (4)	0.1018 (2)	0.0217 (8)
H14	1.0655	0.5954	0.0501	0.026*
C19	1.0923 (4)	0.0345 (4)	0.2492 (2)	0.0203 (8)
H19	1.1063	0.1316	0.2184	0.024*
C3	0.3977 (4)	0.3398 (4)	0.0505 (2)	0.0263 (9)
H3	0.3141	0.3936	0.0232	0.032*
C23	0.9267 (4)	−0.1415 (4)	0.3674 (2)	0.0212 (8)
H23	0.8271	−0.1652	0.4187	0.025*
C7	0.7176 (4)	0.3607 (4)	0.3169 (2)	0.0134 (7)
C13	0.9160 (4)	0.4807 (4)	0.1661 (2)	0.0182 (8)
H13	0.9817	0.3913	0.1582	0.022*
C15	0.8693 (4)	0.7326 (4)	0.1122 (2)	0.0231 (9)
H15	0.9035	0.8154	0.0678	0.028*
C20	1.2179 (4)	−0.0732 (4)	0.2201 (2)	0.0222 (9)
H20	1.3195	−0.0488	0.1700	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0152 (17)	0.022 (2)	0.0206 (19)	0.0026 (15)	−0.0049 (15)	0.0004 (15)
Se2	0.01333 (18)	0.0149 (2)	0.0184 (2)	−0.00064 (13)	−0.00467 (15)	0.00179 (14)
Se1	0.01320 (18)	0.0222 (2)	0.0215 (2)	0.00329 (14)	−0.00123 (15)	−0.00340 (15)
P1	0.0122 (4)	0.0142 (5)	0.0143 (4)	0.0011 (3)	−0.0029 (4)	−0.0009 (4)
O1	0.0150 (11)	0.0130 (14)	0.0160 (12)	0.0019 (9)	−0.0046 (10)	0.0014 (10)
C10	0.0132 (16)	0.022 (2)	0.0150 (17)	−0.0037 (14)	−0.0056 (14)	0.0009 (14)
C18	0.0137 (17)	0.017 (2)	0.0194 (18)	0.0013 (14)	−0.0081 (16)	−0.0017 (15)
C1	0.0130 (16)	0.015 (2)	0.0170 (18)	−0.0060 (14)	−0.0038 (15)	0.0000 (14)
C12	0.0148 (17)	0.013 (2)	0.0144 (17)	−0.0021 (13)	−0.0074 (15)	0.0001 (14)
C11	0.0109 (16)	0.015 (2)	0.0220 (19)	0.0024 (14)	−0.0047 (15)	−0.0018 (15)
C8	0.0149 (16)	0.021 (2)	0.0146 (17)	−0.0017 (14)	−0.0035 (15)	−0.0047 (15)
C6	0.0141 (17)	0.022 (2)	0.0169 (18)	0.0010 (15)	−0.0032 (15)	−0.0030 (15)
C17	0.0168 (17)	0.020 (2)	0.0191 (18)	0.0008 (15)	−0.0074 (15)	−0.0034 (15)
C4	0.029 (2)	0.041 (3)	0.0137 (19)	−0.0014 (18)	−0.0080 (17)	−0.0025 (17)
C5	0.0192 (18)	0.028 (2)	0.0196 (19)	0.0014 (16)	−0.0011 (16)	−0.0051 (16)
C21	0.0178 (18)	0.023 (2)	0.027 (2)	0.0077 (15)	−0.0098 (17)	−0.0090 (16)
C9	0.0174 (17)	0.019 (2)	0.0137 (17)	0.0009 (14)	−0.0047 (15)	−0.0009 (14)
C16	0.0237 (19)	0.014 (2)	0.025 (2)	0.0037 (15)	−0.0079 (17)	−0.0016 (15)

C22	0.026 (2)	0.016 (2)	0.030 (2)	0.0033 (15)	−0.0160 (18)	0.0037 (16)
C14	0.0199 (18)	0.025 (2)	0.0171 (18)	0.0008 (16)	−0.0005 (16)	0.0013 (15)
C19	0.0184 (18)	0.016 (2)	0.025 (2)	0.0001 (15)	−0.0035 (16)	0.0009 (15)
C3	0.027 (2)	0.032 (3)	0.023 (2)	0.0042 (17)	−0.0144 (18)	0.0028 (17)
C23	0.0163 (17)	0.025 (2)	0.0233 (19)	0.0024 (15)	−0.0087 (16)	0.0031 (16)
C7	0.0094 (15)	0.012 (2)	0.0198 (18)	0.0029 (13)	−0.0047 (14)	−0.0054 (14)
C13	0.0149 (17)	0.019 (2)	0.0201 (18)	0.0013 (15)	−0.0033 (16)	−0.0024 (15)
C15	0.026 (2)	0.021 (2)	0.0215 (19)	−0.0041 (16)	−0.0064 (17)	0.0048 (16)
C20	0.0136 (17)	0.022 (2)	0.028 (2)	0.0002 (15)	0.0006 (16)	−0.0033 (16)

Geometric parameters (Å, º)

C2—C3	1.391 (5)	C6—H6	0.9500
C2—C1	1.395 (4)	C17—C16	1.384 (5)
C2—H2	0.9500	C17—H17	0.9500
Se2—C11	2.062 (3)	C4—C3	1.377 (5)
Se2—P1	2.2278 (10)	C4—C5	1.389 (5)
Se1—P1	2.0995 (9)	C4—H4	0.9500
P1—C1	1.814 (3)	C5—H5	0.9500
P1—C7	1.909 (3)	C21—C20	1.371 (5)
O1—C11	1.425 (4)	C21—C22	1.387 (5)
O1—C7	1.432 (3)	C21—H21	0.9500
C10—C11	1.509 (4)	C9—H9A	0.9900
C10—C9	1.525 (4)	C9—H9B	0.9900
C10—H10A	0.9900	C16—C15	1.375 (4)
C10—H10B	0.9900	C16—H16	0.9500
C18—C23	1.381 (5)	C22—C23	1.383 (5)
C18—C19	1.384 (4)	C22—H22	0.9500
C18—C11	1.514 (4)	C14—C13	1.383 (4)
C1—C6	1.400 (4)	C14—C15	1.387 (5)
C12—C13	1.387 (4)	C14—H14	0.9500
C12—C17	1.396 (4)	C19—C20	1.383 (4)
C12—C7	1.525 (4)	C19—H19	0.9500
C8—C7	1.521 (4)	C3—H3	0.9500
C8—C9	1.526 (4)	C23—H23	0.9500
C8—H8A	0.9900	C13—H13	0.9500
C8—H8B	0.9900	C15—H15	0.9500
C6—C5	1.381 (4)	C20—H20	0.9500
C3—C2—C1	119.6 (3)	C5—C4—H4	119.9
C3—C2—H2	120.2	C6—C5—C4	120.1 (3)
C1—C2—H2	120.2	C6—C5—H5	120.0
C11—Se2—P1	88.68 (9)	C4—C5—H5	120.0
C1—P1—C7	106.71 (14)	C20—C21—C22	119.4 (3)
C1—P1—Se1	113.82 (10)	C20—C21—H21	120.3
C7—P1—Se1	114.85 (10)	C22—C21—H21	120.3
C1—P1—Se2	105.00 (11)	C10—C9—C8	110.4 (3)
C7—P1—Se2	95.97 (10)	C10—C9—H9A	109.6

Se1—P1—Se2	118.47 (4)	C8—C9—H9A	109.6
C11—O1—C7	113.5 (2)	C10—C9—H9B	109.6
C11—C10—C9	111.9 (3)	C8—C9—H9B	109.6
C11—C10—H10A	109.2	H9A—C9—H9B	108.1
C9—C10—H10A	109.2	C15—C16—C17	120.3 (3)
C11—C10—H10B	109.2	C15—C16—H16	119.9
C9—C10—H10B	109.2	C17—C16—H16	119.9
H10A—C10—H10B	107.9	C23—C22—C21	120.0 (3)
C23—C18—C19	119.7 (3)	C23—C22—H22	120.0
C23—C18—C11	119.6 (3)	C21—C22—H22	120.0
C19—C18—C11	120.6 (3)	C13—C14—C15	120.4 (3)
C2—C1—C6	119.7 (3)	C13—C14—H14	119.8
C2—C1—P1	119.6 (2)	C15—C14—H14	119.8
C6—C1—P1	120.7 (2)	C20—C19—C18	119.6 (3)
C13—C12—C17	119.1 (3)	C20—C19—H19	120.2
C13—C12—C7	121.7 (3)	C18—C19—H19	120.2
C17—C12—C7	119.2 (3)	C4—C3—C2	120.4 (3)
O1—C11—C10	111.8 (3)	C4—C3—H3	119.8
O1—C11—C18	108.3 (2)	C2—C3—H3	119.8
C10—C11—C18	113.8 (3)	C18—C23—C22	120.3 (3)
O1—C11—Se2	105.63 (19)	C18—C23—H23	119.9
C10—C11—Se2	109.0 (2)	C22—C23—H23	119.9
C18—C11—Se2	107.8 (2)	O1—C7—C8	110.9 (3)
C7—C8—C9	113.0 (3)	O1—C7—C12	107.9 (2)
C7—C8—H8A	109.0	C8—C7—C12	112.2 (3)
C9—C8—H8A	109.0	O1—C7—P1	104.0 (2)
C7—C8—H8B	109.0	C8—C7—P1	112.1 (2)
C9—C8—H8B	109.0	C12—C7—P1	109.4 (2)
H8A—C8—H8B	107.8	C14—C13—C12	120.2 (3)
C5—C6—C1	120.0 (3)	C14—C13—H13	119.9
C5—C6—H6	120.0	C12—C13—H13	119.9
C1—C6—H6	120.0	C16—C15—C14	119.7 (3)
C16—C17—C12	120.3 (3)	C16—C15—H15	120.1
C16—C17—H17	119.8	C14—C15—H15	120.1
C12—C17—H17	119.8	C21—C20—C19	121.0 (3)
C3—C4—C5	120.3 (3)	C21—C20—H20	119.5
C3—C4—H4	119.9	C19—C20—H20	119.5

C11—Se2—P1—C1	104.65 (14)	C23—C18—C19—C20	−0.2 (5)
C11—Se2—P1—C7	−4.46 (13)	C11—C18—C19—C20	177.3 (3)
C11—Se2—P1—Se1	−126.97 (10)	C5—C4—C3—C2	−0.4 (6)
C3—C2—C1—C6	1.6 (5)	C1—C2—C3—C4	−0.8 (5)
C3—C2—C1—P1	−176.7 (3)	C19—C18—C23—C22	−0.7 (5)
C7—P1—C1—C2	−117.1 (3)	C11—C18—C23—C22	−178.2 (3)
Se1—P1—C1—C2	10.6 (3)	C21—C22—C23—C18	0.5 (5)
Se2—P1—C1—C2	141.8 (3)	C11—O1—C7—C8	57.7 (3)
C7—P1—C1—C6	64.7 (3)	C11—O1—C7—C12	−179.0 (3)
Se1—P1—C1—C6	−167.6 (2)	C11—O1—C7—P1	−63.0 (3)

Se2—P1—C1—C6	−36.4 (3)	C9—C8—C7—O1	−52.0 (3)
C7—O1—C11—C10	−59.4 (3)	C9—C8—C7—C12	−172.7 (2)
C7—O1—C11—C18	174.3 (3)	C9—C8—C7—P1	63.7 (3)
C7—O1—C11—Se2	59.0 (3)	C13—C12—C7—O1	3.9 (4)
C9—C10—C11—O1	54.2 (3)	C17—C12—C7—O1	−173.9 (3)
C9—C10—C11—C18	177.4 (3)	C13—C12—C7—C8	126.3 (3)
C9—C10—C11—Se2	−62.2 (3)	C17—C12—C7—C8	−51.5 (4)
C23—C18—C11—O1	−172.4 (3)	C13—C12—C7—P1	−108.6 (3)
C19—C18—C11—O1	10.1 (4)	C17—C12—C7—P1	73.6 (3)
C23—C18—C11—C10	62.5 (4)	C1—P1—C7—O1	−74.6 (2)
C19—C18—C11—C10	−115.0 (3)	Se1—P1—C7—O1	158.24 (15)
C23—C18—C11—Se2	−58.5 (4)	Se2—P1—C7—O1	33.03 (19)
C19—C18—C11—Se2	124.0 (3)	C1—P1—C7—C8	165.6 (2)
P1—Se2—C11—O1	−24.59 (19)	Se1—P1—C7—C8	38.4 (3)
P1—Se2—C11—C10	95.7 (2)	Se2—P1—C7—C8	−86.8 (2)
P1—Se2—C11—C18	−140.2 (2)	C1—P1—C7—C12	40.4 (3)
C2—C1—C6—C5	−1.2 (5)	Se1—P1—C7—C12	−86.7 (2)
P1—C1—C6—C5	177.0 (3)	Se2—P1—C7—C12	148.1 (2)
C13—C12—C17—C16	−0.1 (5)	C15—C14—C13—C12	−0.6 (5)
C7—C12—C17—C16	177.8 (3)	C17—C12—C13—C14	0.6 (5)
C1—C6—C5—C4	0.0 (5)	C7—C12—C13—C14	−177.2 (3)
C3—C4—C5—C6	0.8 (6)	C17—C16—C15—C14	0.4 (5)
C11—C10—C9—C8	−48.4 (4)	C13—C14—C15—C16	0.2 (6)
C7—C8—C9—C10	47.9 (4)	C22—C21—C20—C19	−1.4 (5)
C12—C17—C16—C15	−0.4 (5)	C18—C19—C20—C21	1.3 (6)
C20—C21—C22—C23	0.5 (5)		