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

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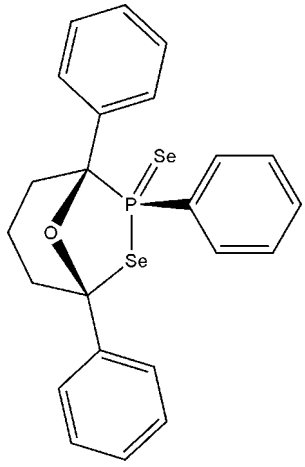
Key indicators: single-crystal X-ray study; $T$ = 93 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.039; $wR$ factor = 0.072; data-to-parameter ratio = 15.6.

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
$\alpha$ = 84.949 (8)°
$\beta$ = 75.677 (7)°
$\gamma$ = 89.266 (8)°
$V$ = 1001.2 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 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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# supplementary materials

*Acta Cryst.* (2008). E**64**, o184 [ **doi:10.1107/S1600536807063945** ]

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

**G. Hua, Y. Li, A. M. Z. Slawin and J. D. Woollins**

## 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).

## 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.

## 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).

## Figures

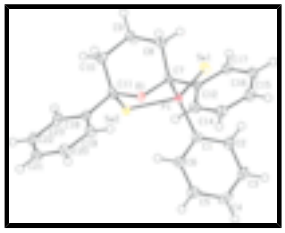


Fig. 1. The structure of (**I**) with displacement ellipsoids drawn at the 50% probability level; H-atoms have been ignored for clarity.

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

*Crystal data*

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

*Data collection*

| | |
|---|---|
| Rigaku Mercury CCD diffractometer | 3805 independent reflections |
| Radiation source: rotating anode | 3000 reflections with $I > 2\sigma(I)$ |
| Monochromator: confocal | $R_{int} = 0.031$ |
| $T = 93$(2) K | $\theta_{max} = 25.8$º |
| ω and φ scans | $\theta_{min} = 2.3$º |
| Absorption correction: multi-scan (CrystalClear; Rigaku, 2004) | $h = -10 \rightarrow 9$ |
| $T_{min} = 0.489$, $T_{max} = 0.570$ | $k = -10 \rightarrow 10$ |
| 7092 measured reflections | $l = -15 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H-atom parameters constrained |
| $wR(F^2) = 0.072$ | $w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3805 reflections | $\Delta\rho_{max} = 0.85$ e Å$^{-3}$ |
| 244 parameters | $\Delta\rho_{min} = -0.82$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

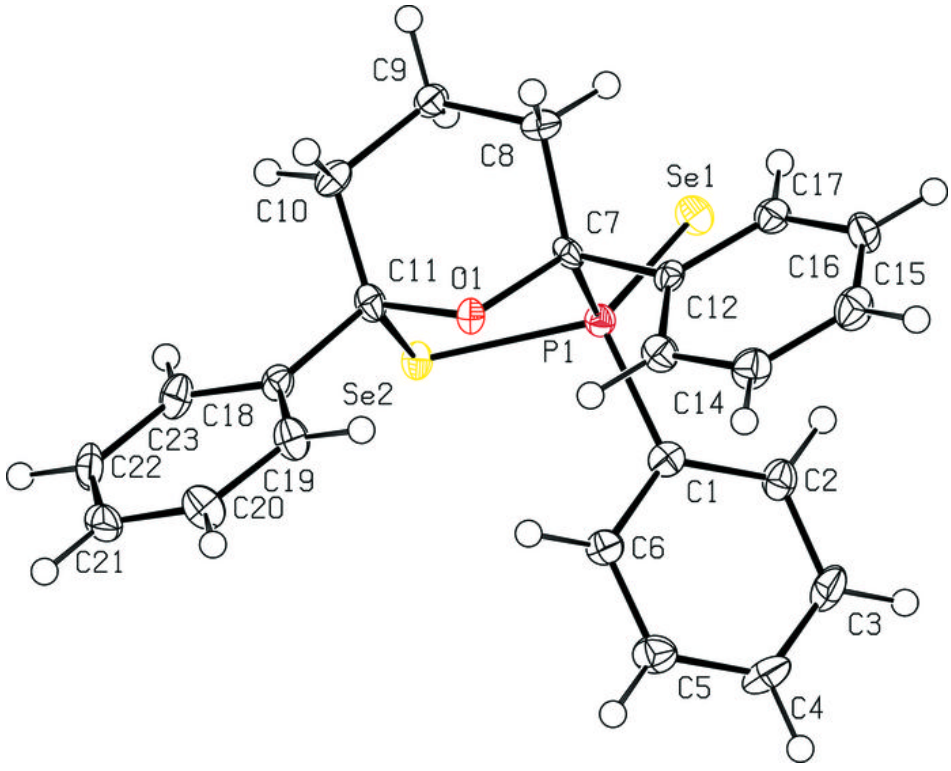
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| 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) | | |

**Fig. 1**


C9
C8
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