Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(4-fluorophenyl)phosphine selenide

Alfred Muller[a]*‡ and Reinout Meijboom[b]

[a]Department of Chemistry, University of Johannesburg, PO Box 524, Johannesburg, 2006, South Africa, and [b]Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein, 9300, South Africa
Correspondence e-mail: mulleraj.sci@ufs.ac.za

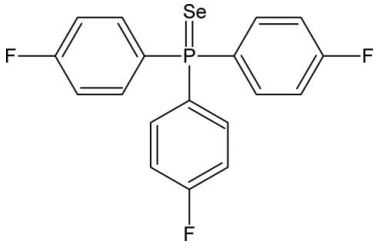
Received 10 September 2007; accepted 10 September 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.061; data-to-parameter ratio = 15.4.

The title compound, $C_{18}H_{12}F_3PSe$ or $SeP(4\text{-}FC_6H_4)_3$, where 4-FC_6H_4 is 4-fluorophenyl, crystallizes with two independent molecules in the asymmetric unit. The two independent molecules have very similar conformations and calculated cone angles of 166 and 168°.

Related literature

For general background, see: Roodt *et al.* (2003); Allen (2002). The cone angles were calculated in accordance with Tolman (1977) and Otto *et al.* (2000). For cone angles in a related structure, see: Muller *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{12}F_3PSe$
M_r = 395.21
Monoclinic, $P2_1/c$
a = 18.6554 (15) Å
b = 13.3102 (13) Å
c = 13.0653 (18) Å
β = 91.643 (9)°
V = 3242.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.44 mm^{-1}
T = 100 (2) K
0.19 × 0.14 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2003)
T_{min} = 0.654, T_{max} = 0.810
21720 measured reflections
6383 independent reflections
5419 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.061
S = 1.06
6383 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Se1—P1	2.1149 (5)	P1—C11	1.8161 (19)
Se2—P2	2.1113 (6)	P2—C61	1.8111 (19)
P1—C21	1.8116 (19)	P2—C51	1.811 (2)
P1—C31	1.8143 (19)	P2—C41	1.8161 (19)
C21—P1—C31	107.33 (9)	C61—P2—C51	104.82 (9)
C21—P1—C11	104.00 (8)	C61—P2—C41	103.70 (9)
C31—P1—C11	105.43 (8)	C51—P2—C41	108.21 (9)
C21—P1—Se1	112.67 (6)	C61—P2—Se2	111.96 (6)
C31—P1—Se1	113.79 (6)	C51—P2—Se2	113.46 (7)
C11—P1—Se1	112.87 (6)	C41—P2—Se2	113.86 (6)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The University of Pietermaritzburg (Professor O. Munroe) is thanked for the use of its diffractometer. Financial assistance by the South African National Research Foundation (grant No. 2067416), the Central Research Fund of the University of the Free State, THRIP and Sasol is gratefully acknowledged. Opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Research Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2301).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Release 3.1a. Crystal Impact, Bonn, Germany.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Muller, A., Meijboom, R. & Roodt, A. (2006). *J. Organomet. Chem.* **691**, 5794–5801.
Otto, S., Roodt, A. & Smith, J. (2000). *Inorg. Chim. Acta*, **303**, 295–299.
Oxford Diffraction (2003). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.170.32 (release 06.06.2003 CrysAlis170 VC++). Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Roodt, A., Otto, S. & Steyl, G. (2003). *Coord. Chem. Rev.* **245**, 121–137.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Tolman, C. A. (1977). *Chem. Rev.* **77**, 313–348.

‡ Current address: Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein, 9300, South Africa.

supplementary materials

Acta Cryst. (2007). E**63**, o4055 [**doi:10.1107/S1600536807044170**]

Tris(4-fluorophenyl)phosphine selenide

A. Muller and R. Meijboom

Comment

There has been extensive development in understanding the transition metal phosphorous bond by various groups, including our own (Roodt *et al.*, 2003), with various techniques utilized such as single-crystal X-ray crystallography, multi nuclear NMR and IR. As part of this systematic investigation we are now also studying selenium bonded phosphourous ligands. With this approach there is no steric crowding effect, though crystal packing effects could still be present, as normally found in transition metal complexes with bulky ligands, *e.g.* in *trans*-[Rh(CO)Cl{P(OC_6H_5)$_3$}$_2$] cone angle variation from 156° to 167° was observed for the two phosphite ligands (Muller *et al.*, 2006). The $J(^{31}P—^{77}Se)$ coupling can also be used as an additional probe to obtain more information regarding the nature of the phosphorous bond. Reported here is the selenium derivate structure of the phosphine P(4—FC_6H_4)$_3$.

The title compound, (I), crystallizes in the $P2_1/c$ (Z=8) space group with two independent molecules in the asymmetric unit. All features of the molecules are as expected (Cambridge Structural Database; Version 5.27, update of August 2006; Allen, 2002) with the selenium atom and the three aryl groups adopting a distorted arrangement about phosphorous (see Fig. 1, Table 1). An overlay (Fig. 2) of the two independent molecules shows only minor deviations, possibly due to slightly different packing enviroments (r.m.s. deviation of the all non-H atoms = 0.1297 Å). This also result in a 2° deviation in the cone angles [calculated as described by Tolman (1977) and Otto *et al.* (2000) with Se repositioned to 2.28 Å from P atom). It is also noted that transition metal complexes with P(4—FC_6H_4)$_3$ have a slightly smaller average cone angle value of 155° showing some effect of steric crowding at the metal coordination environment (data extracted and calculated from 32 useable examples in the CSD).

Experimental

P(4—FC_6H_4)$_3$ and KSeCN were bought from Sigma-Aldrich and used as received. Eqimolar amounts of KSeCN and P(4—FC_6H_4)$_3$ (*ca*. 0.04 mmol) were dissolved in the minimum amounts of methanol (*ca*. 20 ml). The KSeCN solution was added drop wise (5 min.) to the phosphine solution with stirring at room temperature. The final solution was left to evaporate slowly until dry to give crystals suitable for a single-crystal X-ray study. ^{1}H NMR ($CDCl_3$, 300 MHz, p.p.m.) 7.70 (m, 6H), 7.15 (m, 6H); ^{19}F NMR ($CDCl_3$, 282.34 MHz, p.p.m.) −107.4 (s, 3 F); ^{31}P{H}NMR ($CDCl_3$, 121.42 MHz, p.p.m.) 33.2 (t, 1P, $^1J_{(P–Se)}$ = 740 Hz)

Refinement

The aromatic H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron density was located 0.80 Å from C41.

Figures

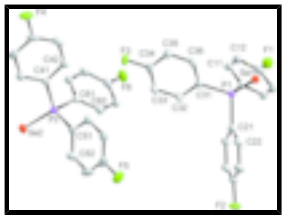


Fig. 1. The content of asymmetric unit of (I) showing atomic numbering and 50% probability displacement ellipsoids. H atoms have been omitted for clarity. For the C atoms, the first digit indicates the ring number and the second digit indicates the position of the atom in the ring.

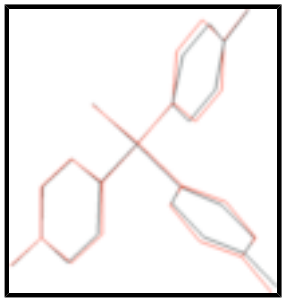


Fig. 2. Superimposed wireframe drawing of the two molecules of $SeP(4\text{-}FC_6H_4)_3$ in the asymmetric unit. H atoms have been omitted for clarity. The molecule containing P2 is indicated in red.

Tris(4-fluorophenyl)phosphine selenide

Crystal data

$C_{18}H_{12}F_3PSe$	F_{000} = 1568
M_r = 395.21	D_x = 1.619 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 812 reflections
a = 18.6554 (15) Å	θ = 4.5–26º
b = 13.3102 (13) Å	μ = 2.44 mm^{-1}
c = 13.0653 (18) Å	T = 100 (2) K
β = 91.643 (9)º	Rectangle, colourless
V = 3242.9 (6) Å^3	0.19 × 0.14 × 0.09 mm
Z = 8	

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	5419 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 100(2) K	θ_{max} = 26.1º
ω scans	θ_{min} = 4.5º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2003)	h = −23→23
T_{min} = 0.654, T_{max} = 0.810	k = −16→16
21720 measured reflections	l = −16→11
6383 independent reflections	

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.061$

$S = 1.06$

6383 reflections

415 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.38$ e Å^{-3}

$\Delta\rho_{min} = -0.33$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.621055 (10)	0.103716 (15)	0.729623 (14)	0.01947 (6)
Se2	0.897574 (11)	0.918160 (15)	0.326819 (16)	0.02365 (7)
P1	0.62681 (3)	0.19901 (4)	0.60059 (4)	0.01482 (11)
P2	0.88819 (3)	0.78304 (4)	0.41002 (4)	0.01678 (11)
F6	0.84795 (7)	0.44720 (9)	0.11754 (9)	0.0368 (3)
F3	0.88414 (6)	0.45923 (9)	0.60402 (9)	0.0291 (3)
F2	0.36650 (7)	0.44879 (10)	0.54894 (11)	0.0409 (3)
F4	1.15036 (7)	0.67567 (10)	0.65056 (9)	0.0399 (3)
F1	0.63466 (7)	−0.03582 (10)	0.21669 (9)	0.0339 (3)
F5	0.62867 (7)	0.76698 (11)	0.65890 (11)	0.0444 (4)
C41	0.96798 (10)	0.75060 (14)	0.48581 (14)	0.0167 (4)
C44	1.08909 (11)	0.70120 (17)	0.59752 (15)	0.0260 (5)
C14	0.63309 (11)	0.01933 (15)	0.30470 (14)	0.0222 (4)
C62	0.80951 (10)	0.62562 (14)	0.31662 (15)	0.0202 (4)
H62	0.771	0.6445	0.3586	0.024*
C52	0.75337 (12)	0.84151 (17)	0.46779 (17)	0.0304 (5)
H52	0.7559	0.8867	0.4117	0.037*
C51	0.81223 (10)	0.78129 (14)	0.49330 (15)	0.0189 (4)
C66	0.93154 (11)	0.64628 (15)	0.26487 (15)	0.0214 (4)
H66	0.9764	0.6799	0.2708	0.026*
C56	0.80831 (11)	0.71756 (15)	0.57794 (15)	0.0222 (4)
H56	0.8485	0.6773	0.5974	0.027*
C46	1.02144 (10)	0.82209 (15)	0.50358 (15)	0.0202 (4)
H46	1.0156	0.8881	0.477	0.024*
C36	0.76472 (10)	0.25537 (15)	0.66323 (15)	0.0215 (4)

H36	0.764	0.197	0.7051	0.026*
C15	0.56991 (11)	0.02464 (15)	0.35560 (15)	0.0231 (5)
H15	0.5282	−0.0092	0.3305	0.028*
C42	0.97688 (11)	0.65346 (15)	0.52487 (15)	0.0212 (4)
H42	0.941	0.6041	0.5117	0.025*
C11	0.63048 (10)	0.13024 (14)	0.48080 (14)	0.0155 (4)
C33	0.76667 (12)	0.42744 (16)	0.54342 (17)	0.0292 (5)
H33	0.7676	0.4868	0.5031	0.035*
C24	0.42770 (11)	0.39403 (15)	0.56057 (17)	0.0248 (5)
C54	0.68954 (11)	0.77189 (17)	0.60401 (17)	0.0290 (5)
C12	0.69356 (10)	0.12266 (15)	0.42664 (15)	0.0201 (4)
H12	0.7357	0.1561	0.4508	0.024*
C25	0.46805 (11)	0.37678 (15)	0.47605 (16)	0.0242 (5)
H25	0.4545	0.4043	0.4112	0.029*
C64	0.85697 (12)	0.52250 (15)	0.18719 (15)	0.0249 (5)
C63	0.80001 (11)	0.54816 (15)	0.24591 (16)	0.0239 (5)
H63	0.7554	0.5141	0.2386	0.029*
C31	0.70485 (10)	0.28041 (14)	0.60301 (14)	0.0164 (4)
C43	1.03771 (12)	0.62883 (16)	0.58257 (15)	0.0260 (5)
H43	1.0436	0.5636	0.611	0.031*
C16	0.56885 (11)	0.08081 (14)	0.44465 (15)	0.0202 (4)
H16	0.5258	0.0858	0.4815	0.024*
C22	0.50643 (11)	0.29953 (15)	0.66749 (15)	0.0228 (4)
H22	0.5195	0.2731	0.7329	0.027*
C34	0.82465 (11)	0.39990 (14)	0.60367 (15)	0.0210 (4)
C21	0.54847 (10)	0.27843 (14)	0.58411 (14)	0.0164 (4)
C61	0.87489 (10)	0.67566 (14)	0.32648 (14)	0.0167 (4)
C32	0.70671 (11)	0.36624 (16)	0.54298 (16)	0.0276 (5)
H32	0.6662	0.3833	0.5009	0.033*
C26	0.52904 (10)	0.31812 (14)	0.48820 (15)	0.0192 (4)
H26	0.5579	0.3048	0.431	0.023*
C45	1.08307 (11)	0.79745 (16)	0.55991 (15)	0.0247 (5)
H45	1.12	0.8455	0.5721	0.03*
C13	0.69482 (11)	0.06620 (15)	0.33732 (16)	0.0236 (5)
H13	0.7375	0.0603	0.2998	0.028*
C55	0.74655 (12)	0.71257 (16)	0.63360 (16)	0.0278 (5)
H55	0.7437	0.6691	0.691	0.033*
C35	0.82578 (11)	0.31522 (15)	0.66261 (15)	0.0244 (5)
H35	0.8673	0.2976	0.7023	0.029*
C65	0.92239 (12)	0.56852 (15)	0.19553 (16)	0.0247 (5)
H65	0.9608	0.5475	0.1545	0.03*
C23	0.44564 (12)	0.35863 (16)	0.65614 (17)	0.0284 (5)
H23	0.4172	0.3742	0.7132	0.034*
C53	0.69128 (12)	0.83648 (19)	0.52305 (18)	0.0365 (6)
H53	0.6509	0.877	0.5051	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.01902 (11)	0.02054 (11)	0.01881 (11)	0.00033 (8)	−0.00038 (8)	0.00614 (8)
Se2	0.02811 (13)	0.01797 (11)	0.02475 (12)	−0.00212 (8)	−0.00152 (9)	0.00646 (8)
P1	0.0148 (3)	0.0145 (2)	0.0151 (2)	0.00030 (19)	−0.00054 (19)	0.00088 (19)
P2	0.0172 (3)	0.0150 (2)	0.0181 (3)	−0.0003 (2)	0.0001 (2)	0.0015 (2)
F6	0.0503 (9)	0.0255 (7)	0.0350 (7)	−0.0060 (6)	0.0072 (6)	−0.0145 (6)
F3	0.0259 (7)	0.0280 (7)	0.0338 (7)	−0.0128 (5)	0.0072 (5)	−0.0049 (6)
F2	0.0266 (7)	0.0352 (8)	0.0608 (9)	0.0166 (6)	0.0015 (7)	0.0080 (7)
F4	0.0331 (8)	0.0494 (9)	0.0361 (7)	0.0166 (6)	−0.0188 (6)	−0.0110 (6)
F1	0.0375 (8)	0.0388 (8)	0.0254 (7)	−0.0020 (6)	0.0017 (6)	−0.0168 (6)
F5	0.0304 (8)	0.0546 (9)	0.0495 (9)	−0.0058 (7)	0.0223 (7)	−0.0147 (7)
C41	0.0177 (10)	0.0189 (10)	0.0136 (9)	0.0013 (8)	0.0011 (8)	−0.0005 (8)
C44	0.0233 (11)	0.0371 (13)	0.0173 (10)	0.0120 (9)	−0.0051 (9)	−0.0064 (9)
C14	0.0309 (12)	0.0196 (11)	0.0159 (10)	0.0018 (9)	−0.0004 (9)	−0.0039 (8)
C62	0.0197 (11)	0.0192 (10)	0.0218 (10)	−0.0001 (8)	0.0025 (8)	0.0012 (8)
C52	0.0289 (13)	0.0333 (13)	0.0291 (12)	0.0094 (10)	0.0025 (10)	0.0061 (10)
C51	0.0193 (10)	0.0182 (10)	0.0191 (10)	−0.0006 (8)	0.0006 (8)	−0.0041 (8)
C66	0.0194 (11)	0.0216 (11)	0.0233 (10)	−0.0019 (8)	0.0039 (9)	0.0002 (9)
C56	0.0224 (11)	0.0200 (10)	0.0243 (11)	−0.0012 (8)	0.0017 (9)	−0.0018 (9)
C46	0.0205 (11)	0.0210 (10)	0.0193 (10)	−0.0003 (8)	0.0031 (8)	−0.0009 (8)
C36	0.0221 (11)	0.0185 (10)	0.0238 (11)	−0.0024 (8)	−0.0026 (9)	0.0027 (8)
C15	0.0226 (11)	0.0232 (11)	0.0232 (11)	−0.0046 (9)	−0.0020 (9)	−0.0032 (9)
C42	0.0235 (11)	0.0198 (10)	0.0203 (10)	0.0010 (8)	0.0003 (8)	−0.0012 (8)
C11	0.0159 (10)	0.0153 (9)	0.0152 (9)	0.0003 (8)	−0.0001 (8)	0.0020 (8)
C33	0.0283 (13)	0.0210 (11)	0.0381 (13)	−0.0041 (9)	−0.0004 (10)	0.0103 (10)
C24	0.0177 (11)	0.0166 (10)	0.0400 (13)	0.0047 (8)	−0.0014 (9)	0.0027 (9)
C54	0.0223 (12)	0.0346 (13)	0.0308 (12)	−0.0056 (10)	0.0111 (10)	−0.0137 (10)
C12	0.0162 (10)	0.0212 (10)	0.0228 (10)	−0.0008 (8)	0.0008 (8)	−0.0025 (8)
C25	0.0258 (12)	0.0225 (11)	0.0237 (11)	0.0011 (9)	−0.0086 (9)	0.0039 (9)
C64	0.0361 (13)	0.0171 (10)	0.0214 (11)	0.0003 (9)	−0.0002 (9)	−0.0022 (9)
C63	0.0232 (11)	0.0200 (11)	0.0284 (11)	−0.0056 (9)	−0.0019 (9)	−0.0012 (9)
C31	0.0187 (10)	0.0147 (9)	0.0161 (9)	−0.0008 (8)	0.0028 (8)	−0.0028 (8)
C43	0.0359 (13)	0.0225 (11)	0.0194 (11)	0.0087 (9)	−0.0019 (9)	−0.0007 (9)
C16	0.0166 (10)	0.0227 (11)	0.0215 (10)	−0.0011 (8)	0.0038 (8)	−0.0020 (8)
C22	0.0278 (12)	0.0217 (11)	0.0189 (10)	0.0031 (9)	0.0030 (9)	0.0033 (8)
C34	0.0212 (11)	0.0189 (10)	0.0235 (11)	−0.0072 (8)	0.0082 (9)	−0.0067 (8)
C21	0.0167 (10)	0.0141 (9)	0.0183 (10)	−0.0008 (8)	−0.0002 (8)	−0.0014 (8)
C61	0.0205 (10)	0.0153 (9)	0.0143 (9)	−0.0008 (8)	−0.0016 (8)	0.0031 (8)
C32	0.0245 (12)	0.0242 (11)	0.0336 (12)	−0.0026 (9)	−0.0065 (10)	0.0123 (10)
C26	0.0212 (11)	0.0189 (10)	0.0175 (10)	0.0001 (8)	−0.0016 (8)	0.0001 (8)
C45	0.0177 (11)	0.0323 (12)	0.0240 (11)	−0.0015 (9)	−0.0016 (9)	−0.0092 (9)
C13	0.0225 (11)	0.0242 (11)	0.0245 (11)	−0.0006 (9)	0.0061 (9)	−0.0028 (9)
C55	0.0318 (13)	0.0272 (12)	0.0248 (11)	−0.0075 (10)	0.0088 (10)	−0.0033 (9)
C35	0.0210 (11)	0.0281 (12)	0.0239 (11)	−0.0019 (9)	−0.0052 (9)	0.0003 (9)
C65	0.0275 (12)	0.0219 (11)	0.0251 (11)	0.0022 (9)	0.0079 (9)	−0.0006 (9)

C23	0.0315 (13)	0.0227 (11)	0.0316 (12)	0.0061 (9)	0.0120 (10)	0.0023 (10)
C53	0.0238 (12)	0.0457 (15)	0.0403 (14)	0.0127 (11)	0.0048 (10)	−0.0025 (12)

Geometric parameters (Å, °)

Se1—P1	2.1149 (5)	C15—C16	1.383 (3)
Se2—P2	2.1113 (6)	C15—H15	0.95
P1—C21	1.8116 (19)	C42—C43	1.384 (3)
P1—C31	1.8143 (19)	C42—H42	0.95
P1—C11	1.8161 (19)	C11—C12	1.394 (3)
P2—C61	1.8111 (19)	C11—C16	1.395 (3)
P2—C51	1.811 (2)	C33—C34	1.369 (3)
P2—C41	1.8161 (19)	C33—C32	1.384 (3)
F6—C64	1.361 (2)	C33—H33	0.95
F3—C34	1.362 (2)	C24—C23	1.367 (3)
F2—C24	1.359 (2)	C24—C25	1.373 (3)
F4—C44	1.363 (2)	C54—C53	1.364 (3)
F1—C14	1.365 (2)	C54—C55	1.371 (3)
F5—C54	1.362 (2)	C12—C13	1.389 (3)
C41—C46	1.393 (3)	C12—H12	0.95
C41—C42	1.398 (3)	C25—C26	1.385 (3)
C44—C43	1.369 (3)	C25—H25	0.95
C44—C45	1.376 (3)	C64—C65	1.367 (3)
C14—C13	1.367 (3)	C64—C63	1.371 (3)
C14—C15	1.372 (3)	C63—H63	0.95
C62—C63	1.392 (3)	C31—C32	1.387 (3)
C62—C61	1.392 (3)	C43—H43	0.95
C62—H62	0.95	C16—H16	0.95
C52—C53	1.384 (3)	C22—C23	1.385 (3)
C52—C51	1.392 (3)	C22—C21	1.389 (3)
C52—H52	0.95	C22—H22	0.95
C51—C56	1.397 (3)	C34—C35	1.365 (3)
C66—C65	1.383 (3)	C21—C26	1.398 (3)
C66—C61	1.402 (3)	C32—H32	0.95
C66—H66	0.95	C26—H26	0.95
C56—C55	1.381 (3)	C45—H45	0.95
C56—H56	0.95	C13—H13	0.95
C46—C45	1.387 (3)	C55—H55	0.95
C46—H46	0.95	C35—H35	0.95
C36—C31	1.388 (3)	C65—H65	0.95
C36—C35	1.390 (3)	C23—H23	0.95
C36—H36	0.95	C53—H53	0.95
C21—P1—C31	107.33 (9)	C13—C12—C11	120.04 (18)
C21—P1—C11	104.00 (8)	C13—C12—H12	120
C31—P1—C11	105.43 (8)	C11—C12—H12	120
C21—P1—Se1	112.67 (6)	C24—C25—C26	118.00 (18)
C31—P1—Se1	113.79 (6)	C24—C25—H25	121
C11—P1—Se1	112.87 (6)	C26—C25—H25	121
C61—P2—C51	104.82 (9)	F6—C64—C65	118.44 (18)

C61—P2—C41	103.70 (9)	F6—C64—C63	118.33 (18)
C51—P2—C41	108.21 (9)	C65—C64—C63	123.23 (19)
C61—P2—Se2	111.96 (6)	C64—C63—C62	118.02 (19)
C51—P2—Se2	113.46 (7)	C64—C63—H63	121
C41—P2—Se2	113.86 (6)	C62—C63—H63	121
C46—C41—C42	119.59 (18)	C32—C31—C36	119.05 (18)
C46—C41—P2	120.01 (15)	C32—C31—P1	121.01 (15)
C42—C41—P2	120.39 (15)	C36—C31—P1	119.91 (15)
F4—C44—C43	118.09 (19)	C44—C43—C42	118.10 (19)
F4—C44—C45	118.21 (19)	C44—C43—H43	121
C43—C44—C45	123.68 (19)	C42—C43—H43	121
F1—C14—C13	118.01 (18)	C15—C16—C11	120.53 (18)
F1—C14—C15	118.40 (18)	C15—C16—H16	119.7
C13—C14—C15	123.59 (18)	C11—C16—H16	119.7
C63—C62—C61	120.67 (18)	C23—C22—C21	120.66 (19)
C63—C62—H62	119.7	C23—C22—H22	119.7
C61—C62—H62	119.7	C21—C22—H22	119.7
C53—C52—C51	120.9 (2)	F3—C34—C35	118.53 (18)
C53—C52—H52	119.6	F3—C34—C33	118.48 (18)
C51—C52—H52	119.6	C35—C34—C33	122.99 (18)
C52—C51—C56	118.69 (19)	C22—C21—C26	119.27 (18)
C52—C51—P2	118.29 (15)	C22—C21—P1	119.77 (14)
C56—C51—P2	122.88 (15)	C26—C21—P1	120.96 (14)
C65—C66—C61	120.25 (18)	C62—C61—C66	119.08 (18)
C65—C66—H66	119.9	C62—C61—P2	122.53 (15)
C61—C66—H66	119.9	C66—C61—P2	118.27 (14)
C55—C56—C51	120.6 (2)	C33—C32—C31	121.06 (19)
C55—C56—H56	119.7	C33—C32—H32	119.5
C51—C56—H56	119.7	C31—C32—H32	119.5
C45—C46—C41	120.38 (19)	C25—C26—C21	120.44 (18)
C45—C46—H46	119.8	C25—C26—H26	119.8
C41—C46—H46	119.8	C21—C26—H26	119.8
C31—C36—C35	120.34 (19)	C44—C45—C46	117.90 (19)
C31—C36—H36	119.8	C44—C45—H45	121
C35—C36—H36	119.8	C46—C45—H45	121
C14—C15—C16	117.95 (18)	C14—C13—C12	118.32 (19)
C14—C15—H15	121	C14—C13—H13	120.8
C16—C15—H15	121	C12—C13—H13	120.8
C43—C42—C41	120.33 (19)	C54—C55—C56	118.4 (2)
C43—C42—H42	119.8	C54—C55—H55	120.8
C41—C42—H42	119.8	C56—C55—H55	120.8
C12—C11—C16	119.56 (17)	C34—C35—C36	118.50 (19)
C12—C11—P1	121.81 (14)	C34—C35—H35	120.8
C16—C11—P1	118.59 (14)	C36—C35—H35	120.8
C34—C33—C32	118.03 (19)	C64—C65—C66	118.73 (19)
C34—C33—H33	121	C64—C65—H65	120.6
C32—C33—H33	121	C66—C65—H65	120.6
F2—C24—C23	118.01 (19)	C24—C23—C22	118.15 (19)
F2—C24—C25	118.54 (19)	C24—C23—H23	120.9

C23—C24—C25	123.45 (19)	C22—C23—H23	120.9
F5—C54—C53	118.5 (2)	C54—C53—C52	118.3 (2)
F5—C54—C55	118.4 (2)	C54—C53—H53	120.9
C53—C54—C55	123.1 (2)	C52—C53—H53	120.9
C61—P2—C41—C46	136.08 (15)	P1—C11—C16—C15	−177.74 (15)
C51—P2—C41—C46	−112.98 (16)	C32—C33—C34—F3	179.50 (19)
Se2—P2—C41—C46	14.17 (17)	C32—C33—C34—C35	0.1 (3)
C61—P2—C41—C42	−42.60 (17)	C23—C22—C21—C26	0.4 (3)
C51—P2—C41—C42	68.34 (17)	C23—C22—C21—P1	−178.87 (16)
Se2—P2—C41—C42	−164.52 (13)	C31—P1—C21—C22	−103.15 (16)
C53—C52—C51—C56	−1.9 (3)	C11—P1—C21—C22	145.44 (16)
C53—C52—C51—P2	174.03 (18)	Se1—P1—C21—C22	22.88 (17)
C61—P2—C51—C52	−96.43 (17)	C31—P1—C21—C26	77.59 (17)
C41—P2—C51—C52	153.38 (16)	C11—P1—C21—C26	−33.82 (18)
Se2—P2—C51—C52	26.01 (18)	Se1—P1—C21—C26	−156.38 (14)
C61—P2—C51—C56	79.32 (18)	C63—C62—C61—C66	−0.7 (3)
C41—P2—C51—C56	−30.86 (19)	C63—C62—C61—P2	175.17 (15)
Se2—P2—C51—C56	−158.23 (14)	C65—C66—C61—C62	−0.1 (3)
C52—C51—C56—C55	1.6 (3)	C65—C66—C61—P2	−176.15 (15)
P2—C51—C56—C55	−174.11 (15)	C51—P2—C61—C62	15.23 (18)
C42—C41—C46—C45	−0.2 (3)	C41—P2—C61—C62	128.63 (16)
P2—C41—C46—C45	−178.91 (14)	Se2—P2—C61—C62	−108.19 (15)
F1—C14—C15—C16	−179.93 (17)	C51—P2—C61—C66	−168.88 (15)
C13—C14—C15—C16	0.2 (3)	C41—P2—C61—C66	−55.48 (16)
C46—C41—C42—C43	1.3 (3)	Se2—P2—C61—C66	67.70 (16)
P2—C41—C42—C43	179.97 (15)	C34—C33—C32—C31	1.0 (3)
C21—P1—C11—C12	131.31 (16)	C36—C31—C32—C33	−0.9 (3)
C31—P1—C11—C12	18.53 (18)	P1—C31—C32—C33	−178.87 (17)
Se1—P1—C11—C12	−106.26 (15)	C24—C25—C26—C21	−0.2 (3)
C21—P1—C11—C16	−51.11 (17)	C22—C21—C26—C25	−0.8 (3)
C31—P1—C11—C16	−163.89 (15)	P1—C21—C26—C25	178.45 (15)
Se1—P1—C11—C16	71.32 (16)	F4—C44—C45—C46	178.24 (16)
C16—C11—C12—C13	0.0 (3)	C43—C44—C45—C46	−0.1 (3)
P1—C11—C12—C13	177.56 (15)	C41—C46—C45—C44	−0.4 (3)
F2—C24—C25—C26	−177.91 (18)	F1—C14—C13—C12	179.82 (17)
C23—C24—C25—C26	1.8 (3)	C15—C14—C13—C12	−0.3 (3)
F6—C64—C63—C62	−179.67 (17)	C11—C12—C13—C14	0.2 (3)
C65—C64—C63—C62	0.6 (3)	F5—C54—C55—C56	−179.98 (18)
C61—C62—C63—C64	0.4 (3)	C53—C54—C55—C56	−0.9 (3)
C35—C36—C31—C32	−0.5 (3)	C51—C56—C55—C54	−0.3 (3)
C35—C36—C31—P1	177.54 (15)	F3—C34—C35—C36	179.19 (17)
C21—P1—C31—C32	−35.25 (19)	C33—C34—C35—C36	−1.4 (3)
C11—P1—C31—C32	75.17 (18)	C31—C36—C35—C34	1.6 (3)
Se1—P1—C31—C32	−160.61 (15)	F6—C64—C65—C66	178.87 (17)
C21—P1—C31—C36	146.77 (15)	C63—C64—C65—C66	−1.4 (3)
C11—P1—C31—C36	−102.81 (16)	C61—C66—C65—C64	1.1 (3)
Se1—P1—C31—C36	21.41 (17)	F2—C24—C23—C22	177.51 (19)
F4—C44—C43—C42	−177.21 (17)	C25—C24—C23—C22	−2.2 (3)
C45—C44—C43—C42	1.2 (3)	C21—C22—C23—C24	1.1 (3)

C41—C42—C43—C44	−1.7 (3)	F5—C54—C53—C52	179.7 (2)
C14—C15—C16—C11	0.0 (3)	C55—C54—C53—C52	0.6 (4)
C12—C11—C16—C15	−0.1 (3)	C51—C52—C53—C54	0.8 (3)

Fig. 1

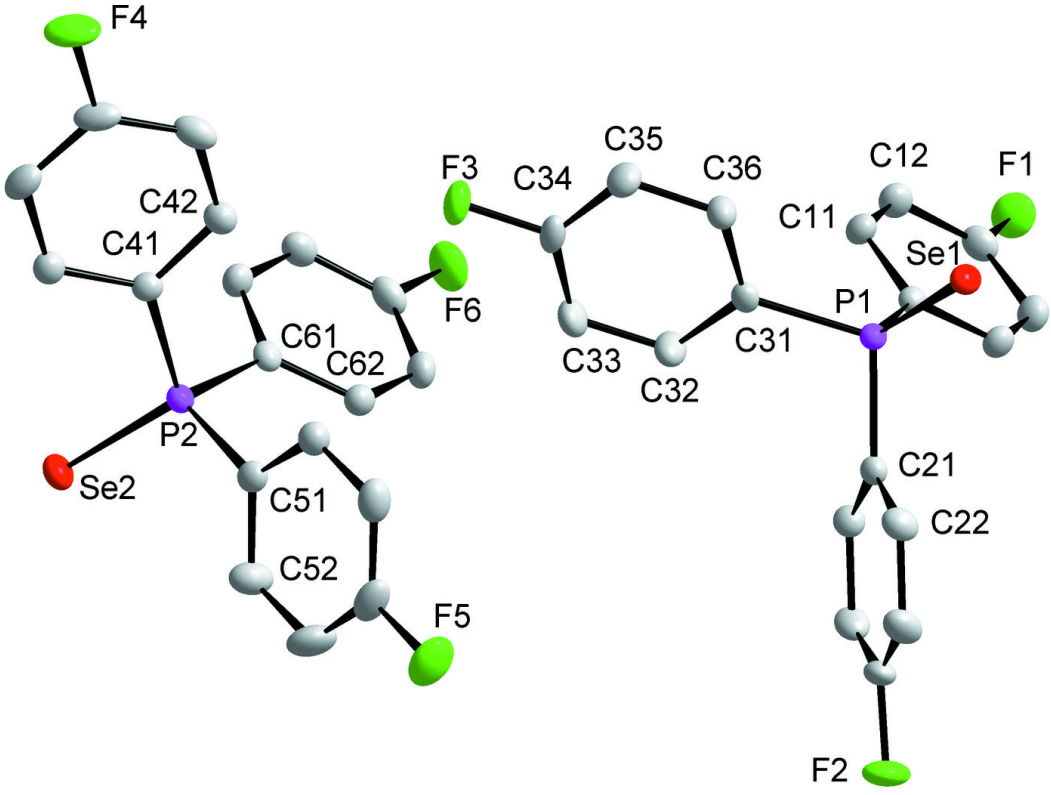

F4
C42
C41
C61
C62
F6
F3
C34
C35
C36
C12
F1
C11
Se1
P1
C31
C33
C32
P2
Se2
C51
C52
F5
C21
C22
F2

Fig. 2