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1-Bromo-8-(phenylselenyl)naphthalene

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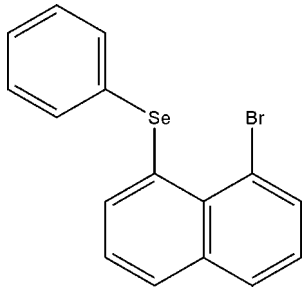
Key indicators: single-crystal X-ray study; T = 125 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.067; data-to-parameter ratio = 14.2.

We are investigating the structures of 1,8-disubstituted naphthalenes as part of a wider study into steric crowding and hyperconjugation. In the title compound, $C_{16}H_{11}BrSe$, the Se···Br distance is 3.1136 (5) Å. The Br and Se atoms lie 0.400 (1) and −0.421 (1) Å, respectively, from the mean plane of the naphthalene backbone. The heavy atoms are further accommodated by in-plane distortions in the C—C—C group between the Br and Se atoms. As expected from the heavy atom displacement, the phenylselenyl group lies on one side of the naphthalene plane, the phenyl ring being inclined at 88° to the naphthalene plane.

Related literature

For examples of sterically crowded 1,8 naphthalenes, see: Nakanishi & Hayashi (2002); Aucott *et al.* (2004).



Experimental

Crystal data

$C_{16}H_{11}BrSe$
M_r = 362.13
Monoclinic, $P2_1/c$
a = 12.2378 (6) Å
b = 7.8921 (4) Å
c = 14.7367 (8) Å
β = 110.980 (1)°
V = 1328.94 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.82 mm^{-1}
T = 125.1 K
0.40 × 0.16 × 0.13 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.220, T_{max} = 0.469
10966 measured reflections
2337 independent reflections
2043 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.067
S = 1.08
2337 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.919 (3)	C1—C10	1.434 (4)
Se9—C9	1.949 (3)	C9—C10	1.430 (5)
Se9—C11	1.933 (3)		
C9—Se9—C11	99.77 (14)	Se9—C9—C8	117.7 (2)
Br1—C1—C2	113.9 (2)	Se9—C9—C10	122.8 (2)
Br1—C1—C10	122.1 (3)	C1—C10—C9	128.3 (3)

Data collection: *SCXmini Benchtop Crystallography System Software* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2006); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2482).

References

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supplementary materials

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1-Bromo-8-(phenylselenyl)naphthalene

A. L. Fuller, F. R. Knight, A. M. Z. Slawin and J. D. Woollins

Experimental

1 was prepared as described previously (Nakanishi & Hayashi, 2002) and crystallized from dichloromethane/hexane.

Refinement

All H atoms were included in calculated positions (C—H = 0.95 Å) and were refined as riding atoms with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

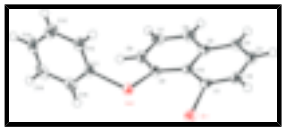

Fig. 1. The structure of (**1**) with displacement ellipsoids drawn at the 50% probability level, hydrogen atoms omitted for clarity.

1-Bromo-8-(phenylselenyl)naphthalene

Crystal data

$C_{16}H_{11}BrSe$	F_{000} = 704.00
M_r = 362.13	D_x = 1.810 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71075 Å
Hall symbol: -P 2ybc	Cell parameters from 12100 reflections
a = 12.2378 (6) Å	θ = 3.1–27.6º
b = 7.8921 (4) Å	μ = 5.82 mm^{-1}
c = 14.7367 (8) Å	T = 125.1 K
β = 110.980 (1)º	Platelet, colourless
V = 1328.94 (12) Å^3	0.40 × 0.16 × 0.13 mm
Z = 4	

Data collection

Rigaku SCXmini diffractometer	2043 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 6.85 pixels mm^{-1}	R_{int} = 0.052
ω scans	θ_{max} = 25.0º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −14→14

T_{min} = 0.220, T_{max} = 0.469
10966 measured reflections
2337 independent reflections

k = −9→9
l = −17→17

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)]$ = 0.033

$wR(F^2)$ = 0.067

S = 1.08

2337 reflections

164 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.7022P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.47 e Å^{-3}

$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Extinction correction: none

Special details

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (S) are based on F^2. *R*-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.80907 (3)	1.30949 (5)	1.08664 (3)	0.02935 (13)
Se9	0.84102 (3)	1.01534 (4)	0.95754 (3)	0.02578 (12)
C1	0.6476 (3)	1.2463 (4)	1.0269 (2)	0.0221 (7)
C2	0.5766 (3)	1.3160 (4)	1.0701 (2)	0.0275 (8)
C3	0.4554 (3)	1.2950 (4)	1.0284 (2)	0.0295 (9)
C4	0.4080 (3)	1.2124 (4)	0.9428 (2)	0.0266 (8)
C5	0.4810 (3)	1.1365 (4)	0.8965 (2)	0.0232 (8)
C6	0.4278 (3)	1.0509 (4)	0.8072 (2)	0.0264 (8)
C7	0.4950 (3)	0.9717 (4)	0.7629 (2)	0.0244 (8)
C8	0.6160 (3)	0.9719 (4)	0.8073 (2)	0.0242 (8)
C9	0.6731 (2)	1.0525 (4)	0.8952 (2)	0.0222 (7)
C10	0.6061 (2)	1.1454 (3)	0.9404 (2)	0.0197 (7)
C11	0.8593 (3)	0.8208 (4)	0.8845 (2)	0.0229 (7)
C12	0.8590 (3)	0.6595 (4)	0.9222 (2)	0.0278 (8)
C13	0.8799 (3)	0.5192 (4)	0.8747 (3)	0.0359 (9)
C14	0.9009 (3)	0.5404 (5)	0.7892 (3)	0.0374 (10)
C15	0.9007 (3)	0.7004 (5)	0.7512 (2)	0.0351 (10)
C16	0.8812 (3)	0.8409 (4)	0.7994 (2)	0.0302 (8)
H2	0.6095	1.3789	1.1285	0.033*
H3	0.4063	1.3388	1.0602	0.035*
H4	0.3253	1.2044	0.9130	0.032*
H6	0.3449	1.0483	0.7777	0.032*
H7	0.4590	0.9170	0.7020	0.029*
H8	0.6614	0.9145	0.7764	0.029*
H12	0.8443	0.6455	0.9809	0.033*

H13	0.8800	0.4090	0.9006	0.043*
H14	0.9154	0.4442	0.7564	0.045*
H15	0.9139	0.7139	0.6919	0.042*
H16	0.8829	0.9512	0.7740	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0282 (2)	0.0288 (2)	0.0277 (2)	−0.00345 (16)	0.00590 (17)	−0.00670 (15)
Se9	0.0200 (2)	0.0255 (2)	0.0294 (2)	0.00067 (15)	0.00594 (17)	−0.00458 (16)
C1	0.027 (2)	0.0157 (17)	0.0219 (19)	−0.0002 (14)	0.0065 (16)	0.0055 (14)
C2	0.041 (2)	0.0201 (19)	0.026 (2)	−0.0010 (16)	0.0177 (18)	0.0012 (15)
C3	0.037 (2)	0.024 (2)	0.034 (2)	0.0054 (17)	0.0190 (19)	0.0050 (16)
C4	0.023 (2)	0.026 (2)	0.033 (2)	0.0014 (15)	0.0124 (17)	0.0076 (16)
C5	0.028 (2)	0.0168 (17)	0.0260 (19)	0.0022 (15)	0.0108 (16)	0.0066 (14)
C6	0.0206 (19)	0.027 (2)	0.028 (2)	−0.0006 (15)	0.0048 (17)	0.0045 (16)
C7	0.026 (2)	0.0259 (19)	0.0174 (18)	−0.0074 (16)	0.0034 (16)	−0.0030 (15)
C8	0.027 (2)	0.0256 (19)	0.0231 (19)	0.0044 (15)	0.0124 (17)	0.0009 (15)
C9	0.0188 (18)	0.0223 (18)	0.0248 (19)	0.0014 (14)	0.0070 (16)	0.0043 (15)
C10	0.0243 (19)	0.0151 (17)	0.0205 (18)	−0.0001 (14)	0.0091 (15)	0.0058 (14)
C11	0.0191 (19)	0.0242 (19)	0.0230 (19)	0.0028 (14)	0.0047 (15)	−0.0028 (14)
C12	0.025 (2)	0.029 (2)	0.028 (2)	0.0032 (16)	0.0069 (17)	−0.0017 (16)
C13	0.027 (2)	0.028 (2)	0.045 (2)	0.0028 (17)	0.0039 (19)	−0.0043 (18)
C14	0.017 (2)	0.042 (2)	0.050 (2)	0.0001 (17)	0.0076 (19)	−0.024 (2)
C15	0.021 (2)	0.060 (2)	0.026 (2)	−0.0035 (19)	0.0098 (17)	−0.0071 (19)
C16	0.023 (2)	0.036 (2)	0.033 (2)	−0.0002 (17)	0.0127 (18)	0.0042 (17)

Geometric parameters (Å, °)

Br1—C1	1.919 (3)	C12—C13	1.381 (5)
Se9—C9	1.949 (3)	C13—C14	1.383 (6)
Se9—C11	1.933 (3)	C14—C15	1.381 (6)
C1—C2	1.362 (6)	C15—C16	1.383 (5)
C1—C10	1.434 (4)	C2—H2	0.950
C2—C3	1.397 (5)	C3—H3	0.950
C3—C4	1.352 (4)	C4—H4	0.950
C4—C5	1.435 (6)	C6—H6	0.950
C5—C6	1.414 (4)	C7—H7	0.950
C5—C10	1.434 (4)	C8—H8	0.950
C6—C7	1.371 (5)	C12—H12	0.950
C7—C8	1.388 (4)	C13—H13	0.950
C8—C9	1.387 (4)	C14—H14	0.950
C9—C10	1.430 (5)	C15—H15	0.950
C11—C12	1.390 (5)	C16—H16	0.950
C11—C16	1.383 (5)		
Br1···C14^{i}	3.564 (3)	H2···H16^{vi}	3.528
Br1···C15^{i}	3.501 (3)	H3···C1^{ii}	3.493
C2···C3^{ii}	3.358 (4)	H3···C2^{ii}	3.383

C2···C6^{iii}	3.425 (5)	H3···C7^{iii}	3.465
C3···C2^{ii}	3.358 (4)	H3···C7^{vi}	3.164
C3···C5^{iii}	3.579 (4)	H3···C8^{iii}	3.206
C3···C6^{iii}	3.590 (4)	H3···C9^{iii}	3.372
C3···C7^{iii}	3.595 (5)	H3···C12^{iii}	3.348
C3···C8^{iii}	3.546 (5)	H3···H2^{ii}	3.515
C3···C9^{iii}	3.540 (5)	H3···H7^{vi}	2.744
C4···C5^{iii}	3.568 (4)	H3···H8^{iii}	3.451
C4···C9^{iii}	3.571 (5)	H3···H12^{iii}	2.909
C4···C10^{iii}	3.343 (4)	H4···C9^{iii}	3.474
C5···C3^{iii}	3.579 (4)	H4···C10^{iii}	3.420
C5···C4^{iii}	3.568 (4)	H4···C14^{vii}	3.508
C6···C2^{iii}	3.425 (5)	H4···C15^{vii}	2.951
C6···C3^{iii}	3.590 (4)	H4···C16^{vii}	3.417
C7···C3^{iii}	3.595 (5)	H4···H2^{ii}	3.489
C8···C3^{iii}	3.546 (5)	H4···H8^{vii}	3.299
C9···C3^{iii}	3.540 (5)	H4···H12^{iii}	3.238
C9···C4^{iii}	3.571 (5)	H4···H15^{vii}	2.779
C10···C4^{iii}	3.343 (4)	H4···H16^{vii}	3.584
C14···Br1^{i}	3.564 (3)	H6···C2^{iii}	3.560
C15···Br1^{i}	3.501 (3)	H6···C11^{vii}	3.508
Br1···H12^{iv}	3.183	H6···C12^{vii}	3.227
Br1···H13^{iv}	3.254	H6···C13^{vii}	2.871
Br1···H14^{v}	3.104	H6···C14^{vii}	2.810
Br1···H16^{vi}	3.197	H6···C15^{vii}	3.120
Se9···H13^{iv}	3.297	H6···C16^{vii}	3.468
C1···H3^{ii}	3.493	H6···H8^{vii}	2.992
C1···H7^{vii}	3.427	H6···H13^{vii}	3.242
C2···H3^{ii}	3.383	H6···H14^{vii}	3.151
C2···H6^{iii}	3.560	H6···H15^{vii}	3.599
C2···H7^{vi}	3.507	H7···C1^{ix}	3.427
C2···H8^{vi}	3.547	H7···C2^{viii}	3.507
C3···H2^{ii}	3.360	H7···C3^{viii}	3.411
C3···H7^{vi}	3.411	H7···C4^{ix}	3.507
C4···H2^{ii}	3.376	H7···C5^{ix}	2.883
C4···H7^{vii}	3.507	H7···C6^{ix}	3.228
C4···H8^{vii}	3.426	H7···C7^{ix}	3.567
C5···H7^{vii}	2.883	H7···C9^{ix}	3.359
C5···H8^{vii}	3.341	H7···C10^{ix}	2.904
C6···H2^{iii}	3.595	H7···H2^{viii}	2.931
C6···H7^{vii}	3.228	H7···H3^{viii}	2.744

C6···H8^{vii}	3.159	H8···C2^{viii}	3.547
C7···H2^{viii}	3.043	H8···C4^{ix}	3.426
C7···H3^{iii}	3.465	H8···C5^{ix}	3.341
C7···H3^{viii}	3.164	H8···C6^{ix}	3.159
C7···H7^{vii}	3.567	H8···H2^{viii}	2.611
C8···H2^{viii}	2.861	H8···H3^{iii}	3.451
C8···H3^{iii}	3.206	H8···H4^{ix}	3.299
C9···H3^{iii}	3.372	H8···H6^{ix}	2.992
C9···H4^{iii}	3.474	H12···Br1^{xiii}	3.183
C9···H7^{vii}	3.359	H12···C13^{x}	3.530
C10···H4^{iii}	3.420	H12···H3^{iii}	2.909
C10···H7^{vii}	2.904	H12···H4^{iii}	3.238
C11···H6^{ix}	3.508	H12···H13^{x}	3.225
C12···H3^{iii}	3.348	H12···H15^{v}	3.119
C12···H6^{ix}	3.227	H13···Br1^{xiii}	3.254
C12···H13^{x}	3.367	H13···Se9^{xiii}	3.297
C13···H6^{ix}	2.871	H13···C12^{x}	3.367
C13···H12^{x}	3.530	H13···C13^{x}	3.598
C13···H13^{x}	3.598	H13···H6^{ix}	3.242
C14···H4^{ix}	3.508	H13···H12^{x}	3.225
C14···H6^{ix}	2.810	H14···Br1^{xiv}	3.104
C14···H15^{xi}	3.377	H14···C15^{xi}	2.994
C14···H16^{xi}	3.183	H14···C16^{xi}	3.000
C15···H4^{ix}	2.951	H14···H6^{ix}	3.151
C15···H6^{ix}	3.120	H14···H15^{xi}	2.666
C15···H14^{xii}	2.994	H14···H16^{xi}	2.662
C15···H16^{xi}	3.424	H15···C14^{xii}	3.377
C16···H4^{ix}	3.417	H15···H4^{ix}	2.779
C16···H6^{ix}	3.468	H15···H6^{ix}	3.599
C16···H14^{xii}	3.000	H15···H12^{xiv}	3.119
H2···C3^{ii}	3.360	H15···H14^{xii}	2.666
H2···C4^{ii}	3.376	H15···H16^{xi}	3.137
H2···C6^{iii}	3.595	H16···Br1^{viii}	3.197
H2···C7^{vi}	3.043	H16···C14^{xii}	3.183
H2···C8^{vi}	2.861	H16···C15^{xii}	3.424
H2···H3^{ii}	3.515	H16···H2^{viii}	3.528
H2···H4^{ii}	3.489	H16···H4^{ix}	3.584
H2···H7^{vi}	2.931	H16···H14^{xii}	2.662
H2···H8^{vi}	2.611	H16···H15^{xii}	3.137
C9—Se9—C11	99.77 (14)	C14—C15—C16	120.0 (4)
Br1—C1—C2	113.9 (2)	C11—C16—C15	119.9 (3)

Br1—C1—C10	122.1 (3)	C1—C2—H2	120.0
C2—C1—C10	123.9 (3)	C3—C2—H2	120.0
C1—C2—C3	120.1 (3)	C2—C3—H3	120.0
C2—C3—C4	120.1 (4)	C4—C3—H3	120.0
C3—C4—C5	120.8 (3)	C3—C4—H4	119.6
C4—C5—C6	118.9 (3)	C5—C4—H4	119.6
C4—C5—C10	120.8 (2)	C5—C6—H6	119.8
C6—C5—C10	120.3 (3)	C7—C6—H6	119.8
C5—C6—C7	120.4 (3)	C6—C7—H7	120.1
C6—C7—C8	119.7 (3)	C8—C7—H7	120.1
C7—C8—C9	122.5 (3)	C7—C8—H8	118.8
Se9—C9—C8	117.7 (2)	C9—C8—H8	118.8
Se9—C9—C10	122.8 (2)	C11—C12—H12	119.9
C8—C9—C10	119.2 (2)	C13—C12—H12	119.9
C1—C10—C5	114.1 (3)	C12—C13—H13	120.2
C1—C10—C9	128.3 (3)	C14—C13—H13	120.2
C5—C10—C9	117.6 (2)	C13—C14—H14	119.8
Se9—C11—C12	119.2 (3)	C15—C14—H14	119.8
Se9—C11—C16	120.8 (2)	C14—C15—H15	120.0
C12—C11—C16	119.8 (3)	C16—C15—H15	120.0
C11—C12—C13	120.3 (4)	C11—C16—H16	120.0
C12—C13—C14	119.6 (3)	C15—C16—H16	120.0
C13—C14—C15	120.4 (4)		
C9—Se9—C11—C12	−96.0 (2)	C6—C5—C10—C9	−5.5 (4)
C9—Se9—C11—C16	88.8 (2)	C10—C5—C6—C7	1.7 (5)
C11—Se9—C9—C8	−14.9 (3)	C5—C6—C7—C8	1.7 (5)
C11—Se9—C9—C10	159.1 (2)	C6—C7—C8—C9	−1.2 (5)
Br1—C1—C2—C3	173.5 (2)	C7—C8—C9—Se9	171.6 (2)
Br1—C1—C10—C5	−169.3 (2)	C7—C8—C9—C10	−2.7 (5)
Br1—C1—C10—C9	12.1 (5)	Se9—C9—C10—C1	10.6 (5)
C2—C1—C10—C5	5.8 (4)	Se9—C9—C10—C5	−168.0 (2)
C2—C1—C10—C9	−172.9 (3)	C8—C9—C10—C1	−175.5 (3)
C10—C1—C2—C3	−1.9 (5)	C8—C9—C10—C5	5.9 (4)
C1—C2—C3—C4	−3.1 (5)	Se9—C11—C12—C13	−175.5 (2)
C2—C3—C4—C5	3.8 (5)	Se9—C11—C16—C15	176.3 (2)
C3—C4—C5—C6	179.8 (3)	C12—C11—C16—C15	1.1 (4)
C3—C4—C5—C10	0.5 (5)	C16—C11—C12—C13	−0.3 (4)
C4—C5—C6—C7	−177.6 (3)	C11—C12—C13—C14	−0.2 (4)
C4—C5—C10—C1	−5.0 (4)	C12—C13—C14—C15	−0.1 (3)
C4—C5—C10—C9	173.8 (3)	C13—C14—C15—C16	1.0 (5)
C6—C5—C10—C1	175.7 (3)	C14—C15—C16—C11	−1.5 (5)

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+2; (ii) −*x*+1, −*y*+3, −*z*+2; (iii) −*x*+1, −*y*+2, −*z*+2; (iv) *x*, *y*+1, *z*; (v) *x*, −*y*+3/2, *z*+1/2; (vi) *x*, −*y*+5/2, *z*+1/2; (vii) −*x*+1, *y*+1/2, −*z*+3/2; (viii) *x*, −*y*+5/2, *z*−1/2; (ix) −*x*+1, *y*−1/2, −*z*+3/2; (x) −*x*+2, −*y*+1, −*z*+2; (xi) −*x*+2, *y*−1/2, −*z*+3/2; (xii) −*x*+2, *y*+1/2, −*z*+3/2; (xiii) *x*, *y*−1, *z*; (xiv) *x*, −*y*+3/2, *z*−1/2.

Fig. 1