Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of 4-phenyl-1-{2-[(2,4,6-trimethylphenyl)selanyl]phenyl}-1*H*-1,2,3-triazole

Leandro R. S. Camargo,[a] Julio Zukerman-Schpector,[a]* Anna M. Deobald,[b]‡ Antonio L. Braga[c] and Edward R. T. Tiekink[d]

[a]Departmento de Química, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil, [b]Departmento de Química, Universidade Federal de Santa Maria, 97105-900 Santa Maria, RS, Brazil, [c]Departmento de Química, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, SC, Brazil, and [d]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia. *Correspondence e-mail: julio@power.ufscar.br

Received 12 February 2015; accepted 16 February 2015

Edited by P. C. Healy, Griffith University, Australia

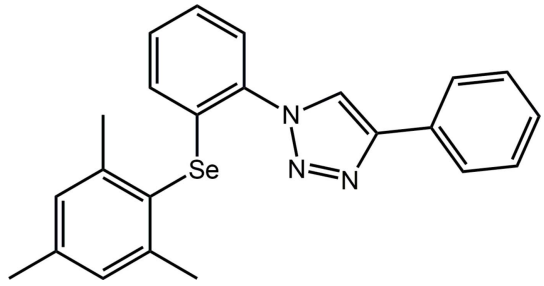
In the title compound, $C_{23}H_{21}N_3Se$, the C-bound phenyl ring is almost coplanar with the central five-membered ring [dihedral angle = 2.84 (10)°], but the N-bound benzene ring is inclined [dihedral angle = 47.52 (10)°]. The dihedral angle between the Se-bound rings is 69.24 (9)°. An intramolecular Se···N interaction of 3.0248 (15) Å is noted. In the crystal, C—H···π interactions connect molecules into double layers that stack along the *a* axis with no directional interactions between them.

Keywords: crystal structure; organoselenium; hydrogen bonding; Se···N halogen bonding; C—H···π interactions.

CCDC reference: 1049547

1. Related literature

For background and synthesis of arylseleno-1,2,3-triazoles, including of the title compound, see: Deobald *et al.* (2011). For Se···N interactions, see: Pati & Zade (2014). For a related organoselenium compound with a 1,2,3-triazole residue, see: Camargo *et al.* (2015).



2. Experimental

2.1. Crystal data

$C_{23}H_{21}N_3Se$
M_r = 418.39
Monoclinic, $P2_1/c$
a = 21.3924 (4) Å
b = 6.9332 (1) Å
c = 12.9204 (2) Å
β = 92.231 (2)°
V = 1914.87 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.97 mm^{-1}
T = 100 K
0.20 × 0.15 × 0.10 mm

2.2. Data collection

Agilent SuperNova CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.809, T_{max} = 1.000
9275 measured reflections
4252 independent reflections
3740 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.063
S = 1.03
4252 reflections
247 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C10–C15 and C18–C23 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···*Cg*1^{i}	0.95	2.68	3.481 (2)	143
C7—H7a···*Cg*2^{ii}	0.98	2.61	3.492 (2)	150
C16—H16···*Cg*3^{iii}	0.95	2.66	3.399 (2)	135

Symmetry codes: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, y-1, z$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MarvinSketch* (ChemAxon, 2010) and *publCIF* (Westrip, 2010).

‡ Present address: Instituto Federal de Educação, Ciência e Tecnologia Farroupilha Rua Erechim, 860 - Bairro Planalto, 98280-000 Panambi, RS, Brazil.

Acknowledgements

The Brazilian agencies CNPq (305626/2013–2 to JZ-S), CAPES, FAPESC and FAPESP (2010/10855-5 to LRSC) are acknowledged for financial support.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5433).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Burla, M. C., Caliandro, R., Carrozzini, B., Cascarano, G. L., Cuocci, C., Giacovazzo, C., Mallamo, M., Mazzone, A. & Polidori, G. (2015). *J. Appl. Cryst.* **48**, 306–309.
Camargo, L. R. S., Zukerman-Schpector, J., Deobald, A. M., Braga, A. L. & Tiekink, E. R. T. (2015). *Acta Cryst.* E**71**, o200–o201.
ChemAxon (2010). *Marvinsketch.* http://www.chemAxon.com
Deobald, A. M., Camargo, L. R. S., Hörner, M., Rodrigues, O. E. D., Alves, D. & Braga, A. L. (2011). Synthesis, pp. 2397–2406.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Pati, P. B. & Zade, S. S. (2014). *Cryst. Growth Des.* **14**, 1695–1700.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2015). E**71**, o204–o205 [doi:10.1107/S2056989015003229]

Crystal structure of 4-phenyl-1-{2-[(2,4,6-trimethylphenyl)-selanyl]phenyl}-1*H*-1,2,3-triazole

Leandro R. S. Camargo, Julio Zukerman-Schpector, Anna M. Deobald, Antonio L. Braga and Edward R. T. Tiekink

S1. Experimental

The compound was prepared in accord with the literature (Deobald *et al.*, 2011). Crystals were obtained by taking 200 mg of sample into a sample vial containing methanol (5 ml) and ethyl acetate (5 ml) and letting it stand at room temperature.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

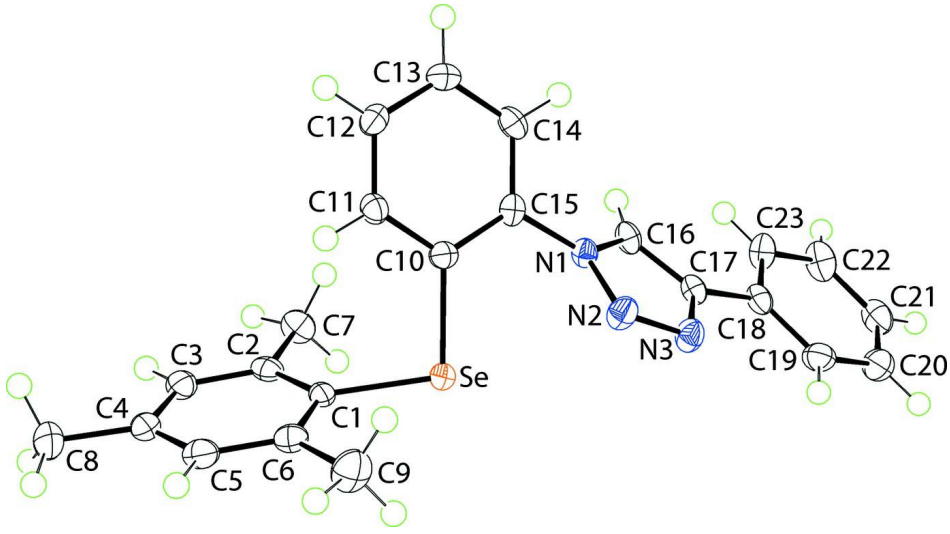


Figure 1

The molecular structure of the title compound showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

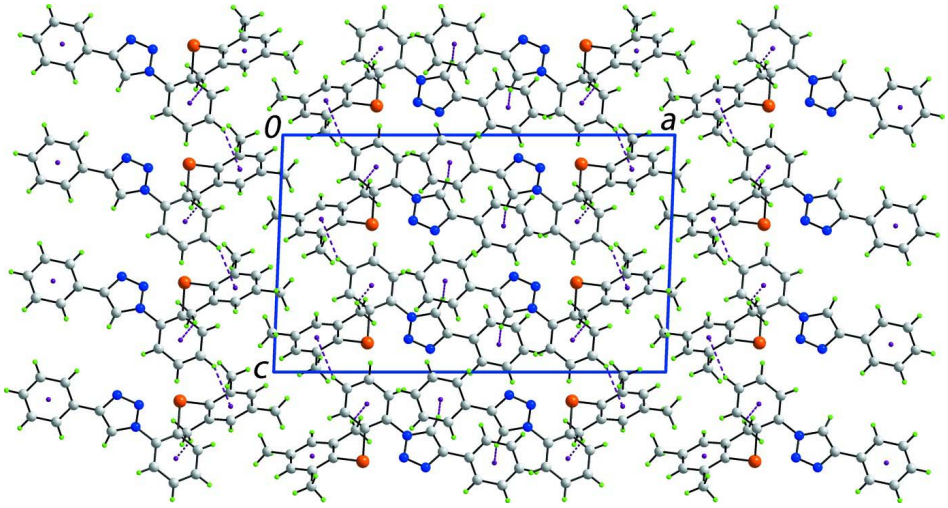


Figure 2

A view in projection down the *b* axis of the unit-cell contents. The C—H···π interactions are shown as purple dashed lines.

4-Phenyl-1-{2-[(2,4,6-trimethylphenyl)selanyl]phenyl}-1*H*-1,2,3-triazole

Crystal data

$C_{23}H_{21}N_3Se$
$M_r = 418.39$
Monoclinic, $P2_1/c$
$a = 21.3924$ (4) Å
$b = 6.9332$ (1) Å
$c = 12.9204$ (2) Å
$\beta = 92.231$ (2)°
$V = 1914.87$ (5) Å^3
$Z = 4$
$F(000) = 856$
$D_x = 1.451$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4584 reflections
$\theta = 2.4$–29.3°
$\mu = 1.97$ mm^{-1}
$T = 100$ K
Prism, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Agilent SuperNova CCD diffractometer
Radiation source: SuperNova (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.809$, $T_{max} = 1.000$
9275 measured reflections
4252 independent reflections
3740 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
$h = -25\rightarrow27$
$k = -8\rightarrow7$
$l = -16\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.063$
$S = 1.03$
4252 reflections
247 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 1.1744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Se	0.76393 (2)	0.40426 (3)	0.12277 (2)	0.01683 (7)
N1	0.65328 (7)	0.6076 (2)	0.23160 (12)	0.0130 (3)
N2	0.65949 (7)	0.6956 (2)	0.13866 (12)	0.0175 (4)
N3	0.60302 (7)	0.7185 (2)	0.09728 (12)	0.0171 (3)
C1	0.83935 (8)	0.2521 (3)	0.13795 (14)	0.0132 (4)
C2	0.84041 (9)	0.0834 (3)	0.19790 (14)	0.0143 (4)
C3	0.89540 (9)	−0.0249 (3)	0.20417 (15)	0.0168 (4)
H3	0.8966	−0.1393	0.2447	0.020*
C4	0.94859 (9)	0.0300 (3)	0.15272 (15)	0.0181 (4)
C5	0.94552 (9)	0.1966 (3)	0.09317 (15)	0.0182 (4)
H5	0.9814	0.2347	0.0571	0.022*
C6	0.89188 (9)	0.3100 (3)	0.08433 (14)	0.0157 (4)
C7	0.78440 (9)	0.0169 (3)	0.25528 (16)	0.0192 (4)
H7A	0.7944	−0.1043	0.2912	0.029*
H7B	0.7490	−0.0033	0.2060	0.029*
H7C	0.7734	0.1152	0.3060	0.029*
C8	1.00802 (10)	−0.0852 (4)	0.16441 (17)	0.0291 (5)
H8A	0.9984	−0.2228	0.1570	0.044*
H8B	1.0277	−0.0615	0.2330	0.044*
H8C	1.0367	−0.0464	0.1109	0.044*
C9	0.89247 (10)	0.4894 (3)	0.01805 (17)	0.0250 (5)
H9A	0.8830	0.6021	0.0605	0.038*
H9B	0.8609	0.4775	−0.0386	0.038*
H9C	0.9339	0.5050	−0.0107	0.038*
C10	0.76174 (8)	0.4997 (3)	0.26208 (14)	0.0130 (4)
C11	0.81423 (9)	0.4896 (3)	0.32961 (14)	0.0146 (4)
H11	0.8524	0.4401	0.3055	0.017*
C12	0.81130 (9)	0.5511 (3)	0.43132 (15)	0.0153 (4)
H12	0.8473	0.5421	0.4764	0.018*
C13	0.75617 (9)	0.6257 (3)	0.46787 (15)	0.0163 (4)
H13	0.7541	0.6652	0.5381	0.020*
C14	0.70405 (9)	0.6421 (3)	0.40097 (15)	0.0160 (4)
H14	0.6663	0.6954	0.4248	0.019*
C15	0.70724 (8)	0.5805 (3)	0.29941 (14)	0.0123 (4)
C16	0.59254 (8)	0.5762 (3)	0.24976 (15)	0.0145 (4)
H16	0.5756	0.5184	0.3091	0.017*
C17	0.56039 (8)	0.6464 (3)	0.16345 (15)	0.0135 (4)
C18	0.49267 (9)	0.6540 (3)	0.13925 (15)	0.0151 (4)
C19	0.46969 (9)	0.7268 (3)	0.04465 (15)	0.0198 (4)

H19	0.4980	0.7722	−0.0047	0.024*
C20	0.40557 (9)	0.7336 (3)	0.02211 (16)	0.0240 (5)
H20	0.3902	0.7846	−0.0422	0.029*
C21	0.36407 (9)	0.6660 (3)	0.09340 (17)	0.0221 (5)
H21	0.3203	0.6688	0.0775	0.026*
C22	0.38639 (9)	0.5945 (3)	0.18778 (17)	0.0223 (4)
H22	0.3579	0.5493	0.2369	0.027*
C23	0.45047 (9)	0.5887 (3)	0.21079 (16)	0.0186 (4)
H23	0.4655	0.5399	0.2758	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se	0.01516 (10)	0.02217 (11)	0.01296 (10)	0.00690 (8)	−0.00215 (7)	−0.00303 (8)
N1	0.0107 (7)	0.0140 (8)	0.0142 (8)	0.0002 (6)	0.0017 (6)	0.0018 (7)
N2	0.0137 (8)	0.0231 (9)	0.0157 (8)	0.0002 (7)	0.0015 (6)	0.0047 (7)
N3	0.0119 (8)	0.0213 (9)	0.0182 (8)	0.0012 (7)	0.0001 (6)	0.0031 (7)
C1	0.0109 (9)	0.0163 (9)	0.0121 (9)	0.0018 (7)	−0.0019 (7)	−0.0050 (8)
C2	0.0144 (9)	0.0154 (9)	0.0131 (9)	−0.0029 (8)	0.0009 (7)	−0.0050 (8)
C3	0.0212 (10)	0.0146 (9)	0.0145 (9)	0.0024 (8)	−0.0002 (8)	−0.0005 (8)
C4	0.0155 (10)	0.0244 (11)	0.0141 (9)	0.0035 (8)	−0.0022 (7)	−0.0044 (8)
C5	0.0133 (9)	0.0272 (11)	0.0142 (9)	−0.0034 (8)	0.0013 (7)	−0.0026 (9)
C6	0.0168 (9)	0.0168 (10)	0.0134 (9)	−0.0023 (8)	−0.0002 (7)	−0.0020 (8)
C7	0.0183 (10)	0.0189 (10)	0.0208 (10)	−0.0021 (8)	0.0042 (8)	0.0006 (9)
C8	0.0208 (11)	0.0446 (14)	0.0218 (11)	0.0143 (10)	0.0007 (9)	0.0016 (11)
C9	0.0254 (11)	0.0257 (11)	0.0241 (11)	−0.0018 (9)	0.0027 (9)	0.0078 (10)
C10	0.0162 (9)	0.0105 (9)	0.0124 (9)	−0.0008 (7)	0.0006 (7)	0.0003 (8)
C11	0.0122 (9)	0.0147 (9)	0.0167 (9)	0.0008 (7)	0.0006 (7)	−0.0013 (8)
C12	0.0164 (9)	0.0138 (9)	0.0154 (9)	−0.0005 (8)	−0.0034 (7)	0.0011 (8)
C13	0.0199 (10)	0.0167 (10)	0.0125 (9)	−0.0016 (8)	0.0021 (7)	−0.0013 (8)
C14	0.0134 (9)	0.0154 (9)	0.0196 (10)	0.0012 (7)	0.0052 (8)	−0.0007 (8)
C15	0.0109 (9)	0.0096 (9)	0.0165 (9)	−0.0020 (7)	0.0005 (7)	0.0032 (8)
C16	0.0111 (9)	0.0124 (9)	0.0201 (10)	0.0004 (7)	0.0033 (7)	0.0009 (8)
C17	0.0122 (9)	0.0107 (9)	0.0178 (9)	0.0007 (7)	0.0015 (7)	−0.0014 (8)
C18	0.0137 (9)	0.0116 (9)	0.0199 (10)	0.0010 (7)	0.0005 (8)	−0.0027 (8)
C19	0.0174 (10)	0.0259 (11)	0.0162 (10)	0.0017 (8)	0.0016 (8)	−0.0032 (9)
C20	0.0196 (10)	0.0305 (12)	0.0215 (10)	0.0059 (9)	−0.0055 (8)	−0.0053 (10)
C21	0.0124 (9)	0.0234 (11)	0.0300 (12)	0.0015 (8)	−0.0042 (8)	−0.0089 (10)
C22	0.0145 (10)	0.0182 (10)	0.0344 (12)	−0.0018 (8)	0.0030 (9)	0.0016 (10)
C23	0.0151 (9)	0.0160 (10)	0.0245 (10)	0.0005 (8)	−0.0004 (8)	0.0048 (9)

Geometric parameters (Å, º)

Se—C10	1.9199 (18)	C9—H9C	0.9800
Se—C1	1.9311 (18)	C10—C15	1.396 (3)
N1—C16	1.347 (2)	C10—C11	1.397 (2)
N1—N2	1.358 (2)	C11—C12	1.385 (3)
N1—C15	1.434 (2)	C11—H11	0.9500

N2—N3	1.311 (2)	C12—C13	1.387 (3)
N3—C17	1.369 (2)	C12—H12	0.9500
C1—C6	1.402 (3)	C13—C14	1.389 (3)
C1—C2	1.403 (3)	C13—H13	0.9500
C2—C3	1.395 (3)	C14—C15	1.384 (3)
C2—C7	1.506 (3)	C14—H14	0.9500
C3—C4	1.393 (3)	C16—C17	1.376 (3)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.388 (3)	C17—C18	1.471 (3)
C4—C8	1.504 (3)	C18—C23	1.393 (3)
C5—C6	1.392 (3)	C18—C19	1.394 (3)
C5—H5	0.9500	C19—C20	1.392 (3)
C6—C9	1.510 (3)	C19—H19	0.9500
C7—H7A	0.9800	C20—C21	1.385 (3)
C7—H7B	0.9800	C20—H20	0.9500
C7—H7C	0.9800	C21—C22	1.384 (3)
C8—H8A	0.9800	C21—H21	0.9500
C8—H8B	0.9800	C22—C23	1.392 (3)
C8—H8C	0.9800	C22—H22	0.9500
C9—H9A	0.9800	C23—H23	0.9500
C9—H9B	0.9800		

C10—Se—C1	98.26 (8)	C15—C10—C11	117.77 (17)
C16—N1—N2	110.77 (15)	C15—C10—Se	120.88 (13)
C16—N1—C15	129.16 (16)	C11—C10—Se	121.34 (14)
N2—N1—C15	119.66 (14)	C12—C11—C10	120.82 (17)
N3—N2—N1	107.14 (14)	C12—C11—H11	119.6
N2—N3—C17	109.07 (15)	C10—C11—H11	119.6
C6—C1—C2	121.05 (16)	C11—C12—C13	120.54 (17)
C6—C1—Se	118.43 (14)	C11—C12—H12	119.7
C2—C1—Se	120.48 (14)	C13—C12—H12	119.7
C3—C2—C1	118.44 (17)	C12—C13—C14	119.42 (18)
C3—C2—C7	119.49 (17)	C12—C13—H13	120.3
C1—C2—C7	122.06 (17)	C14—C13—H13	120.3
C4—C3—C2	121.86 (18)	C15—C14—C13	119.79 (17)
C4—C3—H3	119.1	C15—C14—H14	120.1
C2—C3—H3	119.1	C13—C14—H14	120.1
C5—C4—C3	118.04 (17)	C14—C15—C10	121.60 (17)
C5—C4—C8	121.29 (19)	C14—C15—N1	118.08 (16)
C3—C4—C8	120.65 (19)	C10—C15—N1	120.30 (16)
C4—C5—C6	122.45 (18)	N1—C16—C17	104.89 (16)
C4—C5—H5	118.8	N1—C16—H16	127.6
C6—C5—H5	118.8	C17—C16—H16	127.6
C5—C6—C1	118.15 (18)	N3—C17—C16	108.13 (16)
C5—C6—C9	119.12 (18)	N3—C17—C18	121.92 (17)
C1—C6—C9	122.73 (17)	C16—C17—C18	129.94 (18)
C2—C7—H7A	109.5	C23—C18—C19	118.95 (17)
C2—C7—H7B	109.5	C23—C18—C17	120.39 (17)

H7A—C7—H7B	109.5	C19—C18—C17	120.66 (18)
C2—C7—H7C	109.5	C20—C19—C18	120.43 (19)
H7A—C7—H7C	109.5	C20—C19—H19	119.8
H7B—C7—H7C	109.5	C18—C19—H19	119.8
C4—C8—H8A	109.5	C21—C20—C19	120.09 (19)
C4—C8—H8B	109.5	C21—C20—H20	120.0
H8A—C8—H8B	109.5	C19—C20—H20	120.0
C4—C8—H8C	109.5	C22—C21—C20	119.93 (18)
H8A—C8—H8C	109.5	C22—C21—H21	120.0
H8B—C8—H8C	109.5	C20—C21—H21	120.0
C6—C9—H9A	109.5	C21—C22—C23	120.1 (2)
C6—C9—H9B	109.5	C21—C22—H22	119.9
H9A—C9—H9B	109.5	C23—C22—H22	120.0
C6—C9—H9C	109.5	C22—C23—C18	120.50 (19)
H9A—C9—H9C	109.5	C22—C23—H23	119.8
H9B—C9—H9C	109.5	C18—C23—H23	119.8

C16—N1—N2—N3	−0.6 (2)	C11—C10—C15—C14	−2.5 (3)
C15—N1—N2—N3	−173.99 (15)	Se—C10—C15—C14	177.07 (14)
N1—N2—N3—C17	0.3 (2)	C11—C10—C15—N1	175.45 (16)
C6—C1—C2—C3	0.8 (3)	Se—C10—C15—N1	−4.9 (2)
Se—C1—C2—C3	178.16 (13)	C16—N1—C15—C14	−43.5 (3)
C6—C1—C2—C7	−179.33 (17)	N2—N1—C15—C14	128.46 (18)
Se—C1—C2—C7	−2.0 (2)	C16—N1—C15—C10	138.4 (2)
C1—C2—C3—C4	−0.1 (3)	N2—N1—C15—C10	−49.6 (2)
C7—C2—C3—C4	−179.96 (18)	N2—N1—C16—C17	0.7 (2)
C2—C3—C4—C5	−0.6 (3)	C15—N1—C16—C17	173.24 (17)
C2—C3—C4—C8	177.51 (18)	N2—N3—C17—C16	0.1 (2)
C3—C4—C5—C6	0.7 (3)	N2—N3—C17—C18	179.00 (17)
C8—C4—C5—C6	−177.43 (18)	N1—C16—C17—N3	−0.5 (2)
C4—C5—C6—C1	0.0 (3)	N1—C16—C17—C18	−179.26 (18)
C4—C5—C6—C9	179.89 (18)	N3—C17—C18—C23	−176.52 (18)
C2—C1—C6—C5	−0.8 (3)	C16—C17—C18—C23	2.1 (3)
Se—C1—C6—C5	−178.15 (14)	N3—C17—C18—C19	3.3 (3)
C2—C1—C6—C9	179.32 (18)	C16—C17—C18—C19	−178.05 (19)
Se—C1—C6—C9	1.9 (2)	C23—C18—C19—C20	−0.2 (3)
C15—C10—C11—C12	2.5 (3)	C17—C18—C19—C20	179.96 (18)
Se—C10—C11—C12	−177.11 (14)	C18—C19—C20—C21	−0.6 (3)
C10—C11—C12—C13	−0.6 (3)	C19—C20—C21—C22	1.0 (3)
C11—C12—C13—C14	−1.3 (3)	C20—C21—C22—C23	−0.6 (3)
C12—C13—C14—C15	1.3 (3)	C21—C22—C23—C18	−0.2 (3)
C13—C14—C15—C10	0.7 (3)	C19—C18—C23—C22	0.6 (3)
C13—C14—C15—N1	−177.35 (16)	C17—C18—C23—C22	−179.55 (18)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the C1–C6, C10–C15 and C18–C23 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···*Cg*1^{i}	0.95	2.68	3.481 (2)	143
C7—H7a···*Cg*2^{ii}	0.98	2.61	3.492 (2)	150
C16—H16···*Cg*3^{iii}	0.95	2.66	3.399 (2)	135

Symmetry codes: (i) *x*, −*y*−1/2, *z*−1/2; (ii) *x*, *y*−1, *z*; (iii) −*x*+1, *y*−1/2, −*z*+1/2.