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5-[2-Methyl-1-(4-methylphenyl)-2-nitropropyl]-4-phenyl-1,2,3-selenadiazole

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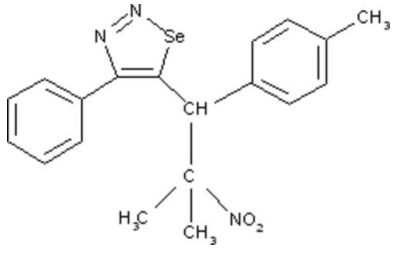
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.119; data-to-parameter ratio = 19.0.

In the title compound, $C_{19}H_{19}N_3O_2Se$, the heterocyclic ring makes dihedral angles of 40.74 (12) and 70.38 (15)° with the phenyl and methylphenyl rings, respectively. The molecular structure is stabilized by weak intramolecular C—H···Se interactions, and the crystal packing is stabilized by weak C—H···π interactions.

Related literature

For related literature see: Mellini & Merlino (1976*a*,*b*); Bertini *et al.* (1984); El-Kashef *et al.* (1986); El-Bahaie *et al.* (1990); Kuroda *et al.* (2001); Padmavathi *et al.* (2002); Saravanan *et al.* (2006). A similar compound with a chlorophenyl ring has been reported recently (Gunasekaran *et al.*, 2007).



Experimental

Crystal data

$C_{19}H_{19}N_3O_2Se$
M_r = 400.34
Monoclinic, $P2_1/c$
a = 10.184 (3) Å
b = 10.592 (3) Å
c = 17.408 (4) Å
β = 101.637 (4)°
V = 1839.1 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.06 mm^{-1}
T = 290 (2) K
0.38 × 0.32 × 0.26 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.512, T_{max} = 0.621
15748 measured reflections
4343 independent reflections
2586 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.119
S = 0.99
4343 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

Cg is the centroid of the selenadiazole ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3*B*···Se1	0.96	2.63	3.371 (4)	134
C10—H10···Se1	0.93	2.96	3.659 (4)	133
C16—H16···*Cg*^{i}	0.93	2.88	3.712	150

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2516).

References

Bertini, V., Dapporto, P., Lucchesini, F., Sega, A. & De Munno, A. (1984). *Acta Cryst.* C**40**, 653–655.
Bruker (2004). *APEX2* (Version 1.0-27) and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
El-Bahaie, S., Assy, M. G. & Hassanien, M. M. (1990). *Pharmazie*, **45**, 791–793.
El-Kashef, H. S., E-Bayoumy, B. & Aly, T. I. (1986). *Egypt. J. Pharm. Sci.* **27**, 27–30.
Gunasekaran, B., Manivannan, V., Saravanan, S., Muthusubramanian, S. & Nethaji, M. (2007). *Acta Cryst.* E**63**, o4024.
Kuroda, K., Uchikurohane, T., Tajima, S. & Tsubata, K. (2001). US Patent No. 6 166 054.
Mellini, M. & Merlino, S. (1976*a*). *Acta Cryst.* B**32**, 1074–1078.
Mellini, M. & Merlino, S. (1976*b*). *Acta Cryst.* B**32**, 1079–1082.
Padmavathi, V., Sumathi, R. P. & Padmaja, A. (2002). *J. Ecobiol.* **14**, 9–12.
Saravanan, S., Nithya, A. & Muthusubramanian, S. (2006). *J. Heterocycl. Chem.* **43**, 149–151.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

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5-[2-Methyl-1-(4-methylphenyl)-2-nitropropyl]-4-phenyl-1,2,3-selenadiazole

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Comment

Selenium containing compounds like 1,2,3-selenadiazole possess various beneficial activities like antifungal (Kuroda *et al.*, 2001), antibacterial (El-Kashef *et al.*, 1986), antimicrobial (El-Bahaie *et al.*, 1990) and insecticidal (Padmavathi *et al.*, 2002) activities. As naturally occurring nitro compounds exhibit broad antibiotic activity and certain alkyl nitro compounds exhibit antitumor activity, it was decided to synthesize and structurally characterize a set of 1,2,3- selenadiazoles with a nitro group in the side chain (Saravanan *et al.*, 2006).

The geometric parameters in the compound agree with the values of similar structures (Mellini & Merlino, 1976*a*; Mellini & Merlino, 1976*b*; Bertini *et al.*, 1984; Gunasekaran *et al.*, 2007). The phenyl ring makes a dihedral angle of 40.74 (12) ° with the heterocyclic ring. The methylphenyl ring makes a dihedral angle of 70.38 (15)° with the heterocyclic ring (Fig 1.). The heterocyclic ring is planar. The molecular structure is stabilized by weak intramolecular C—H···Se interactions and the crystal packing is stabilized by weak C—H···π interactions (Table 1; *Cg* is the centre of gravity of the heterocyclic ring).

Experimental

A solution of 0.005 mol of 2-[(*E*)-4-methyl-3-(4-methylphenyl)-4-nitro-1- phenylpentylidene]-1-hydrazine carboxamide and 0.05 mol of powdered selenium dioxide in dry THF was gently heated on a water bath for two hours. The selenium deposited on cooling was removed by filtration, and the filtrate was poured onto crushed ice, extracted with chloroform, and purified by column chromatography using silica gel (60–120 mesh) with 97:3 petroleum ether: ethyl acetate as eluent to give the title compound, which were recrystallized from ethyl alcohol.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.96Å and U_{iso}(H) = 1.5Ueq(C) for methyl groups, C—H = 0.98° A and U_{iso}(H) = 1.2Ueq(C) for tertiary CH.

Figures

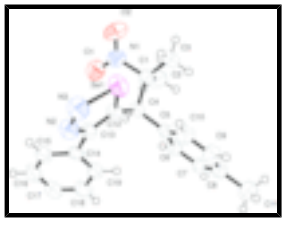
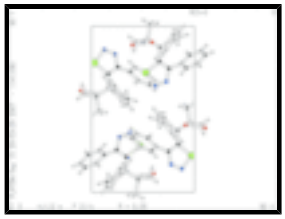


Fig. 1. The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids for non-H atoms.



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Crystal data

$C_{19}H_{19}N_3O_2Se$	F_{000} = 816
M_r = 400.34	D_x = 1.442 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 96 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.184 (3) Å	θ = 2.5–26.5º
b = 10.592 (3) Å	μ = 2.06 mm^{-1}
c = 17.408 (4) Å	T = 290 (2) K
β = 101.637 (4)º	Rectangular, colourless
V = 1839.1 (9) Å^3	0.38 × 0.32 × 0.26 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	4343 independent reflections
Radiation source: fine focus sealed tube	2586 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 290(2) K	θ_{max} = 28.1º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.512, T_{max} = 0.621	k = −14→13
15748 measured reflections	l = −21→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.119	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.2894P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001
4343 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
229 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Primary atom site location: structure-invariant direct methods

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.

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}
Se1	0.62856 (4)	0.97210 (4)	0.21983 (2)	0.06318 (17)
C12	0.6830 (3)	0.8384 (3)	0.28730 (17)	0.0411 (7)
C6	0.5378 (3)	0.7007 (3)	0.44772 (17)	0.0431 (7)
H6	0.6177	0.6715	0.4781	0.052*
C14	0.7937 (3)	0.6240 (3)	0.27483 (17)	0.0400 (7)
C7	0.4183 (3)	0.6583 (3)	0.46331 (19)	0.0482 (8)
H7	0.4191	0.6017	0.5043	0.058*
N2	0.7293 (3)	0.7725 (3)	0.16744 (16)	0.0554 (7)
C13	0.7322 (3)	0.7463 (3)	0.24593 (17)	0.0409 (7)
C4	0.6769 (3)	0.8331 (3)	0.37373 (17)	0.0410 (7)
H4	0.7424	0.7688	0.3965	0.049*
C5	0.5421 (3)	0.7858 (3)	0.38795 (17)	0.0390 (7)
C19	0.7418 (4)	0.5485 (3)	0.3259 (2)	0.0508 (8)
H19	0.6659	0.5744	0.3436	0.061*
N1	0.8566 (4)	0.9935 (3)	0.40256 (18)	0.0628 (9)
C8	0.2964 (3)	0.6981 (3)	0.41917 (19)	0.0487 (8)
C16	0.9658 (4)	0.4693 (3)	0.2746 (2)	0.0617 (10)
H16	1.0416	0.4427	0.2570	0.074*
C9	0.3006 (4)	0.7811 (3)	0.3593 (2)	0.0562 (9)
H9	0.2204	0.8092	0.3286	0.067*
N3	0.6823 (3)	0.8769 (3)	0.14081 (16)	0.0649 (8)
C15	0.9056 (4)	0.5814 (3)	0.2484 (2)	0.0524 (8)
H15	0.9402	0.6295	0.2125	0.063*
C1	0.7206 (4)	0.9554 (3)	0.4213 (2)	0.0513 (9)
C10	0.4205 (4)	0.8243 (3)	0.3432 (2)	0.0536 (9)
H10	0.4193	0.8800	0.3017	0.064*
C17	0.9146 (4)	0.3968 (3)	0.3265 (2)	0.0658 (11)
H17	0.9566	0.3217	0.3450	0.079*
O1	0.9395 (3)	0.9132 (3)	0.40488 (18)	0.0858 (9)
O2	0.8748 (4)	1.1026 (3)	0.3878 (2)	0.1088 (11)
C2	0.7536 (4)	0.9262 (4)	0.5097 (2)	0.0724 (11)

H2A	0.7923	0.9995	0.5380	0.109*
H2B	0.8162	0.8574	0.5195	0.109*
H2C	0.6729	0.9033	0.5269	0.109*
C11	0.1656 (4)	0.6533 (4)	0.4359 (2)	0.0720 (11)
H11A	0.1432	0.7026	0.4778	0.108*
H11B	0.1731	0.5661	0.4510	0.108*
H11C	0.0967	0.6627	0.3897	0.108*
C3	0.6242 (4)	1.0648 (4)	0.4045 (3)	0.0777 (12)
H3A	0.5382	1.0395	0.4137	0.117*
H3B	0.6156	1.0904	0.3509	0.117*
H3C	0.6576	1.1341	0.4384	0.117*
C18	0.8018 (4)	0.4346 (3)	0.3511 (2)	0.0628 (10)
H18	0.7653	0.3837	0.3850	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0819 (3)	0.0553 (2)	0.0553 (3)	0.0203 (2)	0.0209 (2)	0.01726 (18)
C12	0.0446 (18)	0.0381 (16)	0.0396 (17)	0.0023 (14)	0.0059 (14)	0.0001 (13)
C6	0.049 (2)	0.0409 (16)	0.0386 (17)	0.0052 (15)	0.0060 (15)	−0.0009 (14)
C14	0.0472 (19)	0.0373 (16)	0.0348 (16)	−0.0038 (14)	0.0067 (14)	−0.0086 (13)
C7	0.061 (2)	0.0426 (18)	0.0430 (19)	−0.0002 (16)	0.0157 (17)	−0.0007 (15)
N2	0.071 (2)	0.0576 (18)	0.0373 (16)	0.0006 (15)	0.0096 (14)	0.0016 (13)
C13	0.0470 (19)	0.0411 (16)	0.0330 (17)	−0.0029 (14)	0.0042 (14)	−0.0020 (13)
C4	0.052 (2)	0.0338 (15)	0.0379 (17)	0.0035 (14)	0.0098 (15)	−0.0023 (13)
C5	0.0476 (19)	0.0370 (16)	0.0328 (16)	0.0038 (14)	0.0088 (14)	−0.0037 (13)
C19	0.059 (2)	0.044 (2)	0.052 (2)	0.0020 (16)	0.0180 (17)	−0.0061 (15)
N1	0.071 (2)	0.066 (2)	0.0539 (19)	−0.0185 (18)	0.0177 (17)	−0.0116 (16)
C8	0.051 (2)	0.0513 (19)	0.044 (2)	−0.0050 (16)	0.0109 (17)	−0.0120 (16)
C16	0.062 (2)	0.059 (2)	0.067 (2)	0.0095 (19)	0.020 (2)	−0.009 (2)
C9	0.050 (2)	0.065 (2)	0.049 (2)	0.0069 (18)	−0.0016 (17)	−0.0024 (18)
N3	0.082 (2)	0.070 (2)	0.0415 (17)	0.0073 (18)	0.0117 (16)	0.0077 (15)
C15	0.060 (2)	0.0431 (18)	0.057 (2)	−0.0012 (17)	0.0196 (18)	−0.0035 (17)
C1	0.060 (2)	0.050 (2)	0.048 (2)	−0.0101 (16)	0.0203 (17)	−0.0112 (15)
C10	0.058 (2)	0.0506 (19)	0.049 (2)	0.0029 (17)	0.0047 (17)	0.0088 (16)
C17	0.088 (3)	0.044 (2)	0.062 (2)	0.016 (2)	0.009 (2)	−0.0048 (18)
O1	0.0616 (18)	0.092 (2)	0.107 (2)	−0.0078 (17)	0.0265 (17)	−0.015 (2)
O2	0.121 (3)	0.072 (2)	0.148 (3)	−0.0319 (19)	0.062 (2)	0.009 (2)
C2	0.092 (3)	0.082 (3)	0.049 (2)	−0.026 (2)	0.025 (2)	−0.022 (2)
C11	0.062 (2)	0.088 (3)	0.067 (3)	−0.011 (2)	0.017 (2)	−0.009 (2)
C3	0.094 (3)	0.047 (2)	0.099 (3)	0.003 (2)	0.035 (3)	−0.023 (2)
C18	0.094 (3)	0.0431 (19)	0.057 (2)	0.000 (2)	0.027 (2)	0.0017 (17)

Geometric parameters (Å, °)

Se1—C12	1.852 (3)	C8—C9	1.370 (5)
Se1—N3	1.874 (3)	C8—C11	1.497 (5)
C12—C13	1.366 (4)	C16—C17	1.367 (5)
C12—C4	1.519 (4)	C16—C15	1.371 (5)

C6—C7	1.375 (4)	C16—H16	0.9300
C6—C5	1.384 (4)	C9—C10	1.385 (5)
C6—H6	0.9300	C9—H9	0.9300
C14—C19	1.378 (4)	C15—H15	0.9300
C14—C15	1.387 (4)	C1—C3	1.508 (5)
C14—C13	1.482 (4)	C1—C2	1.540 (5)
C7—C8	1.387 (5)	C10—H10	0.9300
C7—H7	0.9300	C17—C18	1.364 (5)
N2—N3	1.256 (4)	C17—H17	0.9300
N2—C13	1.389 (4)	C2—H2A	0.9600
C4—C5	1.528 (4)	C2—H2B	0.9600
C4—C1	1.553 (4)	C2—H2C	0.9600
C4—H4	0.9800	C11—H11A	0.9600
C5—C10	1.385 (4)	C11—H11B	0.9600
C19—C18	1.383 (5)	C11—H11C	0.9600
C19—H19	0.9300	C3—H3A	0.9600
N1—O1	1.193 (4)	C3—H3B	0.9600
N1—O2	1.207 (4)	C3—H3C	0.9600
N1—C1	1.540 (5)	C18—H18	0.9300
C12—Se1—N3	87.69 (13)	C8—C9—H9	119.0
C13—C12—C4	126.0 (3)	C10—C9—H9	119.0
C13—C12—Se1	107.9 (2)	N2—N3—Se1	110.4 (2)
C4—C12—Se1	126.1 (2)	C16—C15—C14	121.0 (3)
C7—C6—C5	121.7 (3)	C16—C15—H15	119.5
C7—C6—H6	119.2	C14—C15—H15	119.5
C5—C6—H6	119.2	C3—C1—N1	109.6 (3)
C19—C14—C15	118.2 (3)	C3—C1—C2	110.5 (3)
C19—C14—C13	122.4 (3)	N1—C1—C2	103.9 (3)
C15—C14—C13	119.5 (3)	C3—C1—C4	115.6 (3)
C6—C7—C8	121.3 (3)	N1—C1—C4	106.2 (2)
C6—C7—H7	119.3	C2—C1—C4	110.3 (3)
C8—C7—H7	119.3	C5—C10—C9	120.9 (3)
N3—N2—C13	118.1 (3)	C5—C10—H10	119.6
C12—C13—N2	116.0 (3)	C9—C10—H10	119.6
C12—C13—C14	128.3 (3)	C18—C17—C16	120.0 (3)
N2—C13—C14	115.6 (3)	C18—C17—H17	120.0
C12—C4—C5	113.0 (2)	C16—C17—H17	120.0
C12—C4—C1	115.6 (2)	C1—C2—H2A	109.5
C5—C4—C1	110.9 (2)	C1—C2—H2B	109.5
C12—C4—H4	105.4	H2A—C2—H2B	109.5
C5—C4—H4	105.4	C1—C2—H2C	109.5
C1—C4—H4	105.4	H2A—C2—H2C	109.5
C6—C5—C10	117.0 (3)	H2B—C2—H2C	109.5
C6—C5—C4	120.1 (3)	C8—C11—H11A	109.5
C10—C5—C4	122.9 (3)	C8—C11—H11B	109.5
C14—C19—C18	120.6 (3)	H11A—C11—H11B	109.5
C14—C19—H19	119.7	C8—C11—H11C	109.5
C18—C19—H19	119.7	H11A—C11—H11C	109.5
O1—N1—O2	123.6 (4)	H11B—C11—H11C	109.5

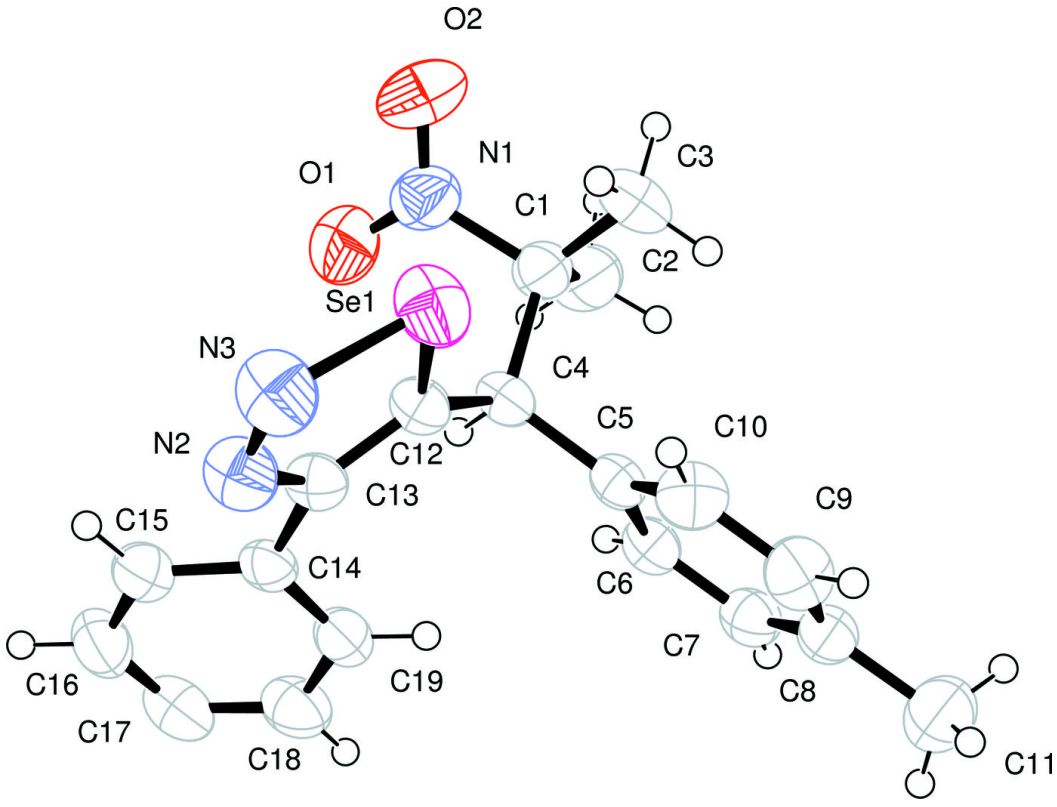
O1—N1—C1	117.8 (3)	C1—C3—H3A	109.5
O2—N1—C1	118.6 (4)	C1—C3—H3B	109.5
C9—C8—C7	117.1 (3)	H3A—C3—H3B	109.5
C9—C8—C11	121.1 (3)	C1—C3—H3C	109.5
C7—C8—C11	121.9 (3)	H3A—C3—H3C	109.5
C17—C16—C15	120.1 (3)	H3B—C3—H3C	109.5
C17—C16—H16	120.0	C17—C18—C19	120.1 (3)
C15—C16—H16	120.0	C17—C18—H18	119.9
C8—C9—C10	122.0 (3)	C19—C18—H18	119.9
N3—Se1—C12—C13	0.5 (2)	C6—C7—C8—C11	−179.5 (3)
N3—Se1—C12—C4	179.3 (3)	C7—C8—C9—C10	−0.2 (5)
C5—C6—C7—C8	0.6 (5)	C11—C8—C9—C10	179.5 (3)
C4—C12—C13—N2	−179.2 (3)	C13—N2—N3—Se1	0.6 (4)
Se1—C12—C13—N2	−0.3 (4)	C12—Se1—N3—N2	−0.6 (3)
C4—C12—C13—C14	−2.1 (5)	C17—C16—C15—C14	1.1 (5)
Se1—C12—C13—C14	176.7 (3)	C19—C14—C15—C16	−2.3 (5)
N3—N2—C13—C12	−0.2 (5)	C13—C14—C15—C16	179.3 (3)
N3—N2—C13—C14	−177.6 (3)	O1—N1—C1—C3	−172.3 (3)
C19—C14—C13—C12	42.8 (5)	O2—N1—C1—C3	9.0 (5)
C15—C14—C13—C12	−138.9 (3)	O1—N1—C1—C2	69.6 (4)
C19—C14—C13—N2	−140.2 (3)	O2—N1—C1—C2	−109.1 (4)
C15—C14—C13—N2	38.1 (4)	O1—N1—C1—C4	−46.7 (4)
C13—C12—C4—C5	−94.5 (4)	O2—N1—C1—C4	134.6 (3)
Se1—C12—C4—C5	86.9 (3)	C12—C4—C1—C3	72.0 (4)
C13—C12—C4—C1	136.2 (3)	C5—C4—C1—C3	−58.3 (4)
Se1—C12—C4—C1	−42.4 (4)	C12—C4—C1—N1	−49.9 (4)
C7—C6—C5—C10	−1.5 (4)	C5—C4—C1—N1	179.8 (3)
C7—C6—C5—C4	178.5 (3)	C12—C4—C1—C2	−161.8 (3)
C12—C4—C5—C6	137.4 (3)	C5—C4—C1—C2	67.9 (3)
C1—C4—C5—C6	−90.9 (3)	C6—C5—C10—C9	1.5 (5)
C12—C4—C5—C10	−42.6 (4)	C4—C5—C10—C9	−178.5 (3)
C1—C4—C5—C10	89.1 (3)	C8—C9—C10—C5	−0.7 (5)
C15—C14—C19—C18	1.2 (5)	C15—C16—C17—C18	1.3 (6)
C13—C14—C19—C18	179.6 (3)	C16—C17—C18—C19	−2.3 (6)
C6—C7—C8—C9	0.2 (5)	C14—C19—C18—C17	1.0 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3B···Se1	0.96	2.63	3.371 (4)	134
C10—H10···Se1	0.93	2.96	3.659 (4)	133
C16—H16···Cg^{i}	0.93	2.88	3.712	150

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

Fig. 1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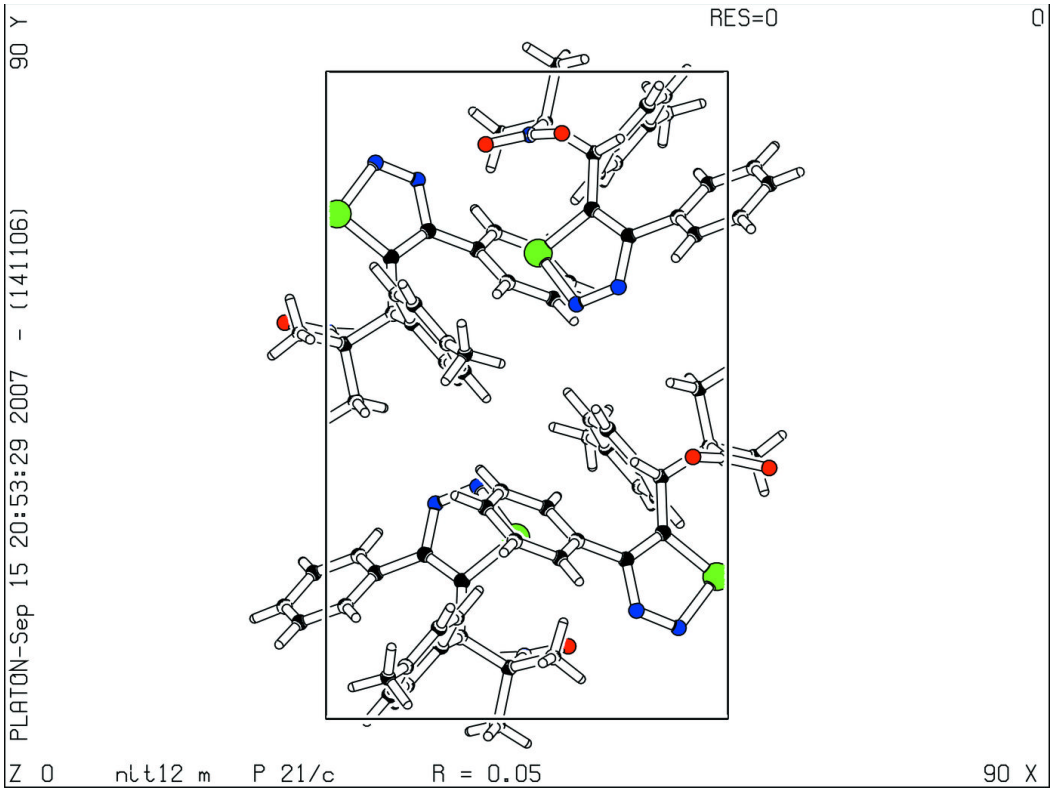
C1
C3
C2
Se1
N3
C4
C5
C10
N2
C12
C13
C9
C15
C14
C6
C7
C16
C19
C8
C17
C18
C11

Fig. 2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nlt12 m
P 21/c
R = 0.05
90 X