

## 4-(4-Chlorophenyl)-5-[2-methyl-1-(4-methylphenyl)-2-nitropropyl]-1,2,3-selenadiazole

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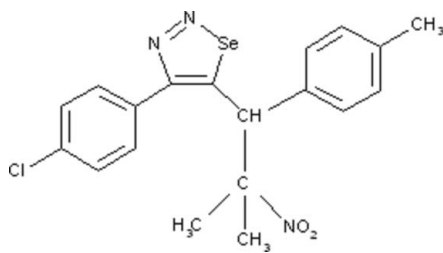
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Key indicators: single-crystal X-ray study;  $T = 290$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.102; data-to-parameter ratio = 16.4.

In the title compound,  $\text{C}_{19}\text{H}_{18}\text{ClN}_3\text{O}_2\text{Se}$ , the heterocyclic ring makes dihedral angles of  $40.74$  (12) and  $51.76$  (11)° with the chlorophenyl and methylphenyl rings, respectively. The molecular structure is stabilized by weak intramolecular  $\text{C}-\text{H}\cdots\text{Se}$  and  $\text{C}-\text{H}\cdots\text{O}$  interactions, and the crystal packing is stabilized by weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions.

### Related literature

For related literature, see: Mellini & Merlino (1976*a,b*); Bertini *et al.* (1984); El-Bahaie *et al.* (1990); El-Kashef *et al.* (1986); Kuroda *et al.* (2001); Padmavathi *et al.* (2002); Saravanan *et al.* (2006).



### Experimental

#### Crystal data

$\text{C}_{19}\text{H}_{18}\text{ClN}_3\text{O}_2\text{Se}$   
 $M_r = 434.77$   
Monoclinic,  $P2_1/n$   
 $a = 13.346$  (3) Å

$b = 9.636$  (2) Å  
 $c = 14.887$  (3) Å  
 $\beta = 95.668$  (4)°  
 $V = 1905.1$  (7) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 2.13$  mm<sup>-1</sup>

$T = 290$  (2) K  
 $0.35 \times 0.25 \times 0.22$  mm

#### Data collection

Bruker SMART APEX CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.527$ ,  $T_{\max} = 0.651$

14877 measured reflections  
3884 independent reflections  
2618 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.102$   
 $S = 1.01$   
3884 reflections

237 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.54$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.23$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3}\cdots\text{O2}$	0.98	2.53	2.887 (4)	102
$\text{C5}-\text{H5A}\cdots\text{Se1}$	0.96	2.71	3.387 (4)	128
$\text{C12}-\text{H12}\cdots\text{Se1}$	0.93	2.85	3.546 (3)	132
$\text{C18}-\text{H18}\cdots\text{O1}^{\dagger}$	0.93	2.46	3.393 (4)	177

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

Data collection: SMART (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: BT2479).

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**supplementary materials**

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## 4-(4-Chlorophenyl)-5-[2-methyl-1-(4-methylphenyl)-2-nitropropyl]-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 nitro group in the side chain (Saravanan *et al.*, 2006).

The geometric parameters in the compound agree with the reported values of similar structures (Mellini & Merlino, 1976*a*; Mellini & Merlino, 1976*b*; Bertini *et al.*, 1984). The Chlorophenyl ring makes a dihedral angle of 40.74 (12) ° with the heterocyclic ring. The methylphenyl ring makes a dihedral angle of 51.76 (11) ° with the heterocyclic ring (Fig 1.).

The molecular structure is stabilized by weak intramolecular C—H...Se and C—H...O interactions and the crystal packing (Fig. 2) is stabilized by weak intermolecular C—H...O interactions.

### Experimental

A solution of 0.005 mole of 2-[(*E*)-1-(4-chlorophenyl)-4-methyl-3-(4-methylphenyl)-4-nitropentylidene]-1-hydrazinecarboxamide and 0.05 mole 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 into 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 = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic C—H, C—H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub> and C—H = 0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for tertiary CH.

### Figures

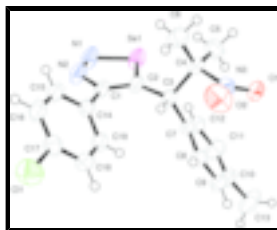


Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

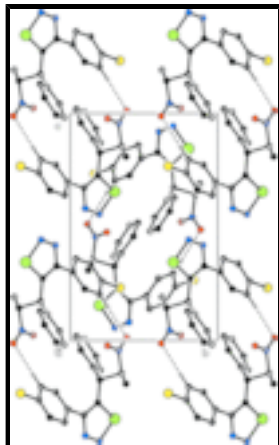


Fig. 2. The packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

**4-(4-Chlorophenyl)-5-[2-methyl-1-(4-methylphenyl)-2-nitropropyl]-1,2,3- selenadiazole**

*Crystal data*

$C_{19}H_{18}ClN_3O_2Se$

$M_r = 434.77$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 13.346 (3) \text{ \AA}$

$b = 9.636 (2) \text{ \AA}$

$c = 14.887 (3) \text{ \AA}$

$\beta = 95.668 (4)^\circ$

$V = 1905.1 (7) \text{ \AA}^3$

$Z = 4$

$F_{000} = 880$

$D_x = 1.516 \text{ Mg m}^{-3}$

Melting point: 134 K

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

$\theta = 2.5\text{--}26.5^\circ$

$\mu = 2.13 \text{ mm}^{-1}$

$T = 290 (2) \text{ K}$

Rectangular, colourless

$0.35 \times 0.25 \times 0.22 \text{ mm}$

*Data collection*

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 290(2) \text{ K}$

$\omega$  scan

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.527$ ,  $T_{\max} = 0.651$

14877 measured reflections

3884 independent reflections

2618 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 26.4^\circ$

$\theta_{\min} = 2.0^\circ$

$h = -16 \rightarrow 16$

$k = -12 \rightarrow 11$

$l = -17 \rightarrow 18$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.044$$

$$wR(F^2) = 0.102$$

$$S = 1.01$$

3884 reflections

237 parameters

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.4482P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

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.

**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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.28743 (3)	0.19923 (4)	0.15518 (2)	0.05775 (16)
C3	0.4001 (2)	0.2992 (3)	0.32749 (19)	0.0354 (7)
H3	0.4552	0.3649	0.3427	0.042*
Cl1	0.73325 (7)	0.83606 (10)	0.26746 (7)	0.0688 (3)
C2	0.3746 (2)	0.3123 (3)	0.2263 (2)	0.0391 (7)
N3	0.4788 (2)	0.1728 (3)	0.45710 (19)	0.0487 (7)
N1	0.3193 (2)	0.3034 (4)	0.05636 (18)	0.0636 (9)
C7	0.3166 (2)	0.3435 (3)	0.38403 (19)	0.0345 (7)
O1	0.4309 (2)	0.1161 (3)	0.51175 (16)	0.0681 (8)
C17	0.6391 (2)	0.7137 (3)	0.2389 (2)	0.0451 (8)
C8	0.3411 (2)	0.4283 (3)	0.4583 (2)	0.0431 (8)
H8	0.4056	0.4655	0.4679	0.052*
C12	0.2184 (2)	0.2959 (4)	0.3705 (2)	0.0469 (8)
H12	0.1986	0.2429	0.3197	0.056*
C14	0.4913 (2)	0.5163 (3)	0.1966 (2)	0.0377 (7)
C1	0.4149 (2)	0.4079 (3)	0.17203 (19)	0.0406 (8)
C15	0.5673 (2)	0.5389 (3)	0.1404 (2)	0.0439 (8)
H15	0.5684	0.4867	0.0880	0.053*
C18	0.5641 (3)	0.6962 (3)	0.2950 (2)	0.0463 (8)
H18	0.5632	0.7495	0.3471	0.056*
N2	0.3820 (2)	0.3981 (3)	0.08075 (18)	0.0549 (8)
C9	0.2712 (3)	0.4583 (4)	0.5183 (2)	0.0519 (9)
H9	0.2897	0.5155	0.5675	0.062*
C16	0.6408 (2)	0.6376 (4)	0.1614 (2)	0.0480 (8)

## supplementary materials

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H16	0.6910	0.6524	0.1233	0.058*
O2	0.5502 (2)	0.2477 (3)	0.4770 (2)	0.0834 (9)
C19	0.4901 (2)	0.5986 (3)	0.2731 (2)	0.0431 (8)
H19	0.4385	0.5876	0.3101	0.052*
C4	0.4443 (2)	0.1525 (3)	0.3560 (2)	0.0400 (8)
C10	0.1748 (3)	0.4054 (4)	0.5069 (2)	0.0542 (9)
C5	0.3720 (3)	0.0321 (3)	0.3480 (2)	0.0589 (10)
H5A	0.3516	0.0142	0.2854	0.088*
H5B	0.3140	0.0541	0.3785	0.088*
H5C	0.4045	-0.0488	0.3750	0.088*
C6	0.5383 (3)	0.1222 (5)	0.3094 (3)	0.0729 (12)
H6A	0.5718	0.0422	0.3365	0.109*
H6B	0.5827	0.2007	0.3157	0.109*
H6C	0.5196	0.1046	0.2465	0.109*
C11	0.1494 (3)	0.3253 (4)	0.4309 (3)	0.0581 (10)
H11	0.0843	0.2906	0.4203	0.070*
C13	0.1020 (3)	0.4306 (5)	0.5764 (3)	0.0898 (15)
H13A	0.1286	0.3914	0.6331	0.135*
H13B	0.0386	0.3878	0.5571	0.135*
H13C	0.0925	0.5286	0.5834	0.135*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Se1	0.0682 (3)	0.0690 (3)	0.0356 (2)	-0.0224 (2)	0.00294 (16)	-0.00654 (18)
C3	0.0380 (17)	0.0384 (17)	0.0303 (16)	-0.0051 (14)	0.0064 (13)	0.0013 (14)
C11	0.0588 (6)	0.0648 (7)	0.0821 (7)	-0.0143 (5)	0.0038 (5)	-0.0075 (5)
C2	0.0413 (17)	0.0449 (19)	0.0322 (17)	-0.0011 (15)	0.0095 (13)	-0.0007 (14)
N3	0.064 (2)	0.0423 (18)	0.0390 (17)	0.0131 (15)	0.0004 (15)	0.0019 (13)
N1	0.076 (2)	0.084 (2)	0.0303 (16)	-0.0160 (19)	0.0026 (15)	-0.0032 (16)
C7	0.0420 (18)	0.0334 (17)	0.0283 (16)	0.0032 (13)	0.0040 (13)	0.0000 (12)
O1	0.106 (2)	0.0651 (18)	0.0368 (14)	0.0214 (16)	0.0236 (14)	0.0095 (13)
C17	0.0432 (19)	0.045 (2)	0.046 (2)	0.0017 (15)	0.0030 (16)	0.0058 (16)
C8	0.0483 (19)	0.045 (2)	0.0351 (18)	0.0027 (16)	0.0013 (15)	-0.0020 (15)
C12	0.049 (2)	0.054 (2)	0.0390 (18)	-0.0033 (17)	0.0091 (16)	-0.0097 (16)
C14	0.0444 (18)	0.0392 (18)	0.0300 (17)	0.0035 (14)	0.0057 (14)	0.0055 (14)
C1	0.0456 (18)	0.051 (2)	0.0261 (17)	0.0020 (16)	0.0077 (14)	0.0015 (14)
C15	0.0494 (19)	0.052 (2)	0.0313 (18)	0.0017 (16)	0.0100 (15)	-0.0002 (15)
C18	0.060 (2)	0.043 (2)	0.0371 (18)	0.0053 (17)	0.0086 (16)	-0.0015 (15)
N2	0.0635 (19)	0.070 (2)	0.0320 (16)	-0.0083 (17)	0.0073 (14)	-0.0013 (14)
C9	0.067 (2)	0.058 (2)	0.0300 (18)	0.0177 (19)	0.0003 (17)	-0.0061 (16)
C16	0.047 (2)	0.059 (2)	0.041 (2)	0.0017 (17)	0.0147 (16)	0.0068 (17)
O2	0.081 (2)	0.077 (2)	0.084 (2)	-0.0086 (17)	-0.0328 (17)	-0.0016 (17)
C19	0.050 (2)	0.044 (2)	0.0379 (19)	0.0038 (16)	0.0158 (15)	0.0049 (15)
C4	0.0491 (19)	0.0430 (19)	0.0292 (17)	0.0025 (15)	0.0104 (14)	-0.0019 (13)
C10	0.058 (2)	0.069 (3)	0.037 (2)	0.019 (2)	0.0139 (17)	0.0045 (18)
C5	0.078 (3)	0.042 (2)	0.055 (2)	-0.0044 (19)	0.000 (2)	-0.0013 (17)
C6	0.075 (3)	0.080 (3)	0.070 (3)	0.029 (2)	0.037 (2)	0.011 (2)

C11	0.044 (2)	0.074 (3)	0.058 (2)	0.0010 (18)	0.0143 (18)	-0.004 (2)
C13	0.082 (3)	0.139 (4)	0.053 (3)	0.039 (3)	0.030 (2)	0.001 (3)

*Geometric parameters (Å, °)*

Se1—C2	1.849 (3)	C1—N2	1.389 (4)
Se1—N1	1.865 (3)	C15—C16	1.381 (4)
C3—C2	1.517 (4)	C15—H15	0.9300
C3—C7	1.522 (4)	C18—C19	1.379 (4)
C3—C4	1.573 (4)	C18—H18	0.9300
C3—H3	0.9800	C9—C10	1.378 (5)
C11—C17	1.745 (3)	C9—H9	0.9300
C2—C1	1.370 (4)	C16—H16	0.9300
N3—O2	1.209 (4)	C19—H19	0.9300
N3—O1	1.213 (4)	C4—C5	1.507 (4)
N3—C4	1.543 (4)	C4—C6	1.520 (4)
N1—N2	1.266 (4)	C10—C11	1.383 (5)
C7—C12	1.384 (4)	C10—C13	1.508 (5)
C7—C8	1.387 (4)	C5—H5A	0.9600
C17—C16	1.369 (5)	C5—H5B	0.9600
C17—C18	1.376 (4)	C5—H5C	0.9600
C8—C9	1.386 (4)	C6—H6A	0.9600
C8—H8	0.9300	C6—H6B	0.9600
C12—C11	1.379 (4)	C6—H6C	0.9600
C12—H12	0.9300	C11—H11	0.9300
C14—C19	1.388 (4)	C13—H13A	0.9600
C14—C15	1.393 (4)	C13—H13B	0.9600
C14—C1	1.481 (4)	C13—H13C	0.9600
C2—Se1—N1	87.39 (13)	C10—C9—C8	121.5 (3)
C2—C3—C7	114.9 (2)	C10—C9—H9	119.2
C2—C3—C4	112.6 (2)	C8—C9—H9	119.2
C7—C3—C4	112.3 (2)	C17—C16—C15	119.3 (3)
C2—C3—H3	105.4	C17—C16—H16	120.4
C7—C3—H3	105.4	C15—C16—H16	120.4
C4—C3—H3	105.4	C18—C19—C14	121.2 (3)
C1—C2—C3	125.4 (3)	C18—C19—H19	119.4
C1—C2—Se1	108.7 (2)	C14—C19—H19	119.4
C3—C2—Se1	125.9 (2)	C5—C4—C6	111.5 (3)
O2—N3—O1	124.0 (3)	C5—C4—N3	107.5 (3)
O2—N3—C4	117.8 (3)	C6—C4—N3	106.8 (3)
O1—N3—C4	118.1 (3)	C5—C4—C3	116.7 (3)
N2—N1—Se1	110.9 (2)	C6—C4—C3	110.8 (3)
C12—C7—C8	117.2 (3)	N3—C4—C3	102.5 (2)
C12—C7—C3	124.1 (3)	C9—C10—C11	117.3 (3)
C8—C7—C3	118.5 (3)	C9—C10—C13	120.8 (4)
C16—C17—C18	121.3 (3)	C11—C10—C13	121.9 (4)
C16—C17—C11	119.7 (3)	C4—C5—H5A	109.5
C18—C17—C11	119.0 (3)	C4—C5—H5B	109.5
C9—C8—C7	121.1 (3)	H5A—C5—H5B	109.5

## supplementary materials

C9—C8—H8	119.5	C4—C5—H5C	109.5
C7—C8—H8	119.5	H5A—C5—H5C	109.5
C11—C12—C7	121.4 (3)	H5B—C5—H5C	109.5
C11—C12—H12	119.3	C4—C6—H6A	109.5
C7—C12—H12	119.3	C4—C6—H6B	109.5
C19—C14—C15	118.1 (3)	H6A—C6—H6B	109.5
C19—C14—C1	122.8 (3)	C4—C6—H6C	109.5
C15—C14—C1	119.1 (3)	H6A—C6—H6C	109.5
C2—C1—N2	115.2 (3)	H6B—C6—H6C	109.5
C2—C1—C14	129.1 (3)	C12—C11—C10	121.5 (3)
N2—C1—C14	115.7 (3)	C12—C11—H11	119.3
C16—C15—C14	121.0 (3)	C10—C11—H11	119.3
C16—C15—H15	119.5	C10—C13—H13A	109.5
C14—C15—H15	119.5	C10—C13—H13B	109.5
C17—C18—C19	119.1 (3)	H13A—C13—H13B	109.5
C17—C18—H18	120.5	C10—C13—H13C	109.5
C19—C18—H18	120.5	H13A—C13—H13C	109.5
N1—N2—C1	117.8 (3)	H13B—C13—H13C	109.5
C7—C3—C2—C1	109.3 (3)	Se1—N1—N2—C1	0.1 (4)
C4—C3—C2—C1	-120.5 (3)	C2—C1—N2—N1	-0.2 (5)
C7—C3—C2—Se1	-72.7 (3)	C14—C1—N2—N1	177.5 (3)
C4—C3—C2—Se1	57.5 (3)	C7—C8—C9—C10	0.0 (5)
N1—Se1—C2—C1	-0.1 (2)	C18—C17—C16—C15	-1.7 (5)
N1—Se1—C2—C3	-178.4 (3)	C11—C17—C16—C15	178.6 (2)
C2—Se1—N1—N2	0.0 (3)	C14—C15—C16—C17	0.4 (5)
C2—C3—C7—C12	51.4 (4)	C17—C18—C19—C14	1.2 (5)
C4—C3—C7—C12	-79.0 (4)	C15—C14—C19—C18	-2.5 (5)
C2—C3—C7—C8	-134.0 (3)	C1—C14—C19—C18	178.3 (3)
C4—C3—C7—C8	95.7 (3)	O2—N3—C4—C5	167.1 (3)
C12—C7—C8—C9	2.9 (5)	O1—N3—C4—C5	-15.1 (4)
C3—C7—C8—C9	-172.2 (3)	O2—N3—C4—C6	47.3 (4)
C8—C7—C12—C11	-3.3 (5)	O1—N3—C4—C6	-134.9 (3)
C3—C7—C12—C11	171.4 (3)	O2—N3—C4—C3	-69.2 (3)
C3—C2—C1—N2	178.5 (3)	O1—N3—C4—C3	108.5 (3)
Se1—C2—C1—N2	0.2 (3)	C2—C3—C4—C5	-71.2 (3)
C3—C2—C1—C14	1.1 (5)	C7—C3—C4—C5	60.3 (3)
Se1—C2—C1—C14	-177.2 (3)	C2—C3—C4—C6	57.9 (4)
C19—C14—C1—C2	-42.9 (5)	C7—C3—C4—C6	-170.6 (3)
C15—C14—C1—C2	138.0 (3)	C2—C3—C4—N3	171.6 (2)
C19—C14—C1—N2	139.7 (3)	C7—C3—C4—N3	-56.9 (3)
C15—C14—C1—N2	-39.4 (4)	C8—C9—C10—C11	-2.5 (5)
C19—C14—C15—C16	1.7 (5)	C8—C9—C10—C13	175.5 (3)
C1—C14—C15—C16	-179.1 (3)	C7—C12—C11—C10	0.9 (6)
C16—C17—C18—C19	0.9 (5)	C9—C10—C11—C12	2.0 (5)
C11—C17—C18—C19	-179.4 (2)	C13—C10—C11—C12	-175.9 (4)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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C3—H3···O2	0.98	2.53	2.887 (4)	102
C5—H5A···Se1	0.96	2.71	3.387 (4)	128
C12—H12···Se1	0.93	2.85	3.546 (3)	132
C18—H18···O1 <sup>i</sup>	0.93	2.46	3.393 (4)	177

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ .

Fig. 1

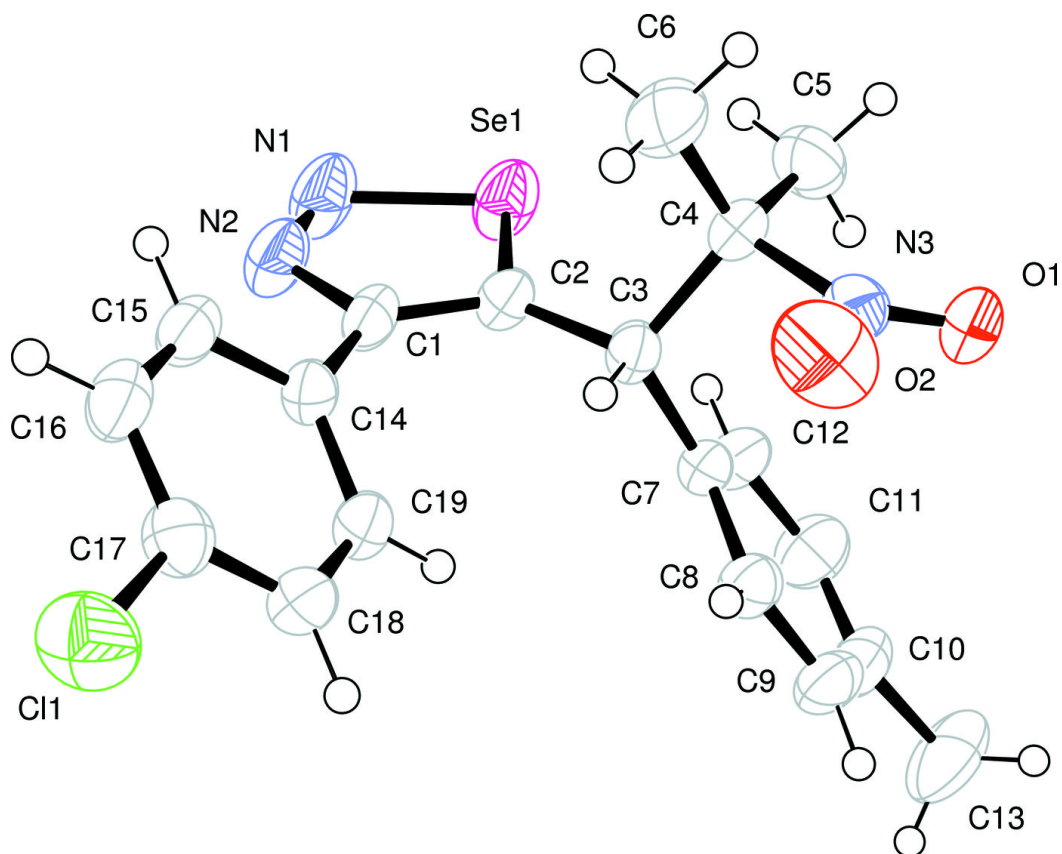


Fig. 2

