Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diethyl 2-[(4-nitrophenyl)(4-phenyl-1,2,3-selenadiazol-5-yl)methyl]-malonate

A. Marx,[a] S. Saravanan,[b] S. Muthusubramanian,[b] V. Manivannan[a]* and Nigam P. Rath[c]

[a]Department of Physics, Presidency College, Chennai 600 005, India, [b]Department of Organic Chemistry, School of Chemistry, Madurai Kamarajar University, Madurai 625 021, India, and [c]Department of Chemistry and Biochemistry, University of Missouri–St Louis, 8001 Natural Bridge Road, St Louis, MO 63121, USA
Correspondence e-mail: manivan_1999@yahoo.com

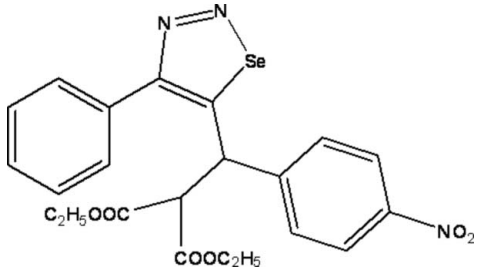
Received 29 February 2008; accepted 13 March 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.054; wR factor = 0.162; data-to-parameter ratio = 14.3.

In the title compound, $C_{22}H_{21}N_3O_6Se$, the heterocyclic ring makes dihedral angles of 50.03 (11) and 67.75 (11)°, respectively, with the benzene and phenyl rings. The terminal C atoms of the ester groups are disordered over two positions: the site occupancies for the C atoms are 0.62 (3)/0.38 (3) and 0.48 (3)/0.52 (3). In the crystal structure, weak intra- and intermolecular C—H···O interactions are observed.

Related literature

For biological activities, see: El-Kashef *et al.* (1986); El-Bahaie *et al.* (1990). For closely related compounds, see: Bertini *et al.* (1984); Gunasekaran *et al.* (2007).



Experimental

Crystal data

$C_{22}H_{21}N_3O_6Se$
M_r = 502.38
Triclinic, $P\overline{1}$
a = 9.9530 (6) Å
b = 10.5220 (6) Å
c = 12.2305 (7) Å
α = 79.350 (3)°
β = 74.632 (3)°
γ = 67.632 (3)°
V = 1137.05 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 295 (2) K
0.23 × 0.17 × 0.16 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.697, T_{max} = 0.773
30194 measured reflections
4477 independent reflections
3053 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.161
S = 1.04
4477 reflections
313 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C22A—H22D···O2^{i}	0.96	2.47	3.38 (4)	159
C11—H11···O6^{ii}	0.93	2.56	3.410 (6)	152
C18—H18A···O4	0.97	2.29	2.686 (7)	103
C21—H21C···O6	0.97	2.17	2.627 (6)	107

Symmetry codes: (i) $x-1, y+1, z$; (ii) $-x+2, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2278).

References

Bertini, V., Dapporto, P., Lucchesini, F., Sega, A. & De Munno, A. (1984). *Acta Cryst.* C**40**, 653–655.
Bruker (2004). *APEX2*. 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.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2008). E**64**, o729 [**doi:10.1107/S160053680800706X**]

Diethyl 2-[(4-nitrophenyl)(4-phenyl-1,2,3-selenadiazol-5-yl)methyl]malonate

A. Marx, S. Saravanan, S. Muthusubramanian, V. Manivannan and N. P. Rath

Comment

Selenium containing compounds like 1,2,3-selenadiazole possess various beneficial activities like antibacterial (El-Kashef *et al.*, 1986), antimicrobial (El-Bahaie *et al.*, 1990) activities. The geometric parameters in the compound, (I) (Fig. 1), agree with the reported values of similar structures (Bertini *et al.*, 1984; Gunasekaran *et al.*, 2007).

The heterocyclic ring makes the dihedral angles of 50.03 (11) and 67.75 (11)° with the benzene and phenyl rings. The terminal C atoms of the ester groups are disordered over two positions; the site occupancies for the C atoms are 0.62/0.38 and 0.48/0.52. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing of (I) is stabilized by weak intermolecular C—H···O contacts (Table 1 and Fig. 2).

Experimental

2.22 g (0.02 mol) of powdered selenium dioxide was dissolved in glacial acetic acid by gentle warming. To this warm solution, 0.002 mol of diethyl 2-{3-[2-(aminocarbonyl)hydrazono]-1-(4-nitrophenyl)-3-phenylpropyl} malonate was added at once and the mixture was gently heated on a water bath until gas evolution ceased. The selenium deposited on cooling was removed by filtration and the filtrate poured into crushed ice, extracted with chloroform and purified by column chromatography, using silica gel (60–120 mesh) to yield diethyl 2-[(4-nitrophenyl) (4-phenyl-1,2,3-selenadiazol-5-yl)methyl]malonate. Solvent used for crystallization is ethanol.

Refinement

The site occupancy factors were refined as C19 = 0.62 (3), C19A = 0.38 (3), C22 = 0.48 (3) and C22A = 0.52 (3) during anisotropic refinement. The C21—C22A, C21—C22, C18—C19 and C18—C19A bond distances were restrained to be 1.5 (1) Å. H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

Figures

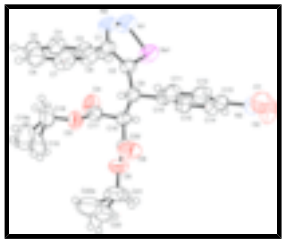


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

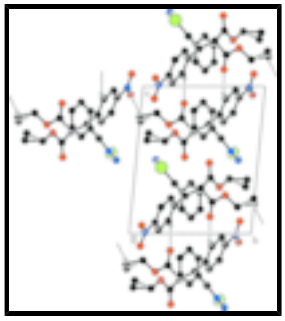


Fig. 2. The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

Diethyl 2-[(4-nitrophenyl)(4-phenyl-1,2,3-selenadiazol-5-yl)methyl]malonate

Crystal data

$C_{22}H_{21}N_3O_6Se$	$Z = 2$
$M_r = 502.38$	$F_{000} = 512$
Triclinic, $P\overline{1}$	$D_x = 1.467$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.9530$ (6) Å	Cell parameters from 8446 reflections
$b = 10.5220$ (6) Å	$\theta = 1.7$–26º
$c = 12.2305$ (7) Å	$\mu = 1.69$ mm^{-1}
$\alpha = 79.350$ (3)º	$T = 295$ (2) K
$\beta = 74.632$ (3)º	Block, colourless
$\gamma = 67.632$ (3)º	0.23 × 0.17 × 0.16 mm
$V = 1137.05$ (11) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	4477 independent reflections
Radiation source: fine-focus sealed tube	3053 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 295$(2) K	$\theta_{max} = 26.1$º
ω and φ scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.697$, $T_{max} = 0.773$	$k = -12 \rightarrow 12$
30194 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.9842P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
4477 reflections	$\Delta\rho_{max} = 0.93$ e Å^{-3}
313 parameters	$\Delta\rho_{min} = -0.80$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Se1	1.00900 (5)	0.21345 (6)	0.44996 (4)	0.0888 (3)	
O1	1.5749 (5)	0.1019 (4)	−0.0847 (4)	0.1160 (15)	
O2	1.6666 (5)	0.0959 (5)	0.0564 (5)	0.1327 (17)	
O4	0.7916 (3)	0.6035 (4)	0.4808 (2)	0.0859 (10)	
O6	1.0425 (4)	0.6499 (3)	0.1149 (2)	0.0859 (10)	
N1	0.8397 (5)	0.1628 (5)	0.5006 (4)	0.0939 (13)	
N2	0.7447 (4)	0.2286 (4)	0.4410 (3)	0.0753 (10)	
N3	1.5628 (6)	0.1283 (4)	0.0109 (5)	0.0929 (14)	
C1	0.7808 (4)	0.3215 (4)	0.3527 (3)	0.0558 (9)	
C2	0.9155 (4)	0.3332 (4)	0.3410 (3)	0.0521 (8)	
C3	0.6670 (4)	0.4007 (4)	0.2854 (3)	0.0542 (9)	
C4	0.5213 (5)	0.4674 (5)	0.3410 (4)	0.0686 (11)	
H4	0.4952	0.4563	0.4201	0.082*	
C5	0.4156 (5)	0.5494 (5)	0.2804 (5)	0.0807 (13)	
H5	0.3193	0.5953	0.3187	0.097*	
C6	0.4514 (6)	0.5637 (5)	0.1641 (5)	0.0837 (14)	
H6	0.3801	0.6198	0.1231	0.100*	
C7	0.5930 (6)	0.4949 (5)	0.1085 (4)	0.0796 (13)	
H7	0.6168	0.5031	0.0293	0.095*	
C8	0.7013 (5)	0.4133 (5)	0.1679 (3)	0.0640 (10)	
H8	0.7970	0.3671	0.1288	0.077*	
C9	0.9818 (4)	0.4288 (4)	0.2556 (3)	0.0495 (8)	
H9	0.9199	0.4661	0.1987	0.059*	
C10	1.1371 (4)	0.3504 (4)	0.1923 (3)	0.0509 (8)	
C11	1.1559 (5)	0.3109 (4)	0.0853 (3)	0.0627 (10)	
H11	1.0739	0.3346	0.0529	0.075*	
C12	1.2940 (5)	0.2375 (5)	0.0274 (4)	0.0738 (12)	
H12	1.3063	0.2109	−0.0441	0.089*	
C13	1.4136 (5)	0.2034 (4)	0.0754 (4)	0.0696 (12)	
C14	1.4005 (5)	0.2414 (4)	0.1802 (4)	0.0677 (11)	
H14	1.4837	0.2182	0.2110	0.081*	
C15	1.2595 (4)	0.3154 (4)	0.2393 (3)	0.0592 (9)	
H15	1.2477	0.3413	0.3109	0.071*	
C16	0.9754 (4)	0.5531 (4)	0.3084 (3)	0.0529 (9)	
H16	1.0474	0.5205	0.3577	0.064*	
C17	0.8230 (4)	0.6224 (4)	0.3794 (3)	0.0574 (9)	
O3	0.7304 (3)	0.7037 (3)	0.3154 (3)	0.0766 (8)	

C18	0.5803 (5)	0.7789 (5)	0.3722 (6)	0.110 (2)	
H18A	0.5602	0.7413	0.4510	0.132*	0.62 (3)
H18B	0.5088	0.7732	0.3345	0.132*	0.62 (3)
H18C	0.5834	0.7912	0.4481	0.132*	0.38 (3)
H18D	0.5213	0.7210	0.3811	0.132*	0.38 (3)
C19	0.571 (2)	0.9256 (10)	0.366 (2)	0.150 (8)	0.62 (3)
H19A	0.6297	0.9317	0.4139	0.226*	0.62 (3)
H19B	0.4690	0.9830	0.3907	0.226*	0.62 (3)
H19C	0.6074	0.9561	0.2886	0.226*	0.62 (3)
C19A	0.500 (3)	0.917 (2)	0.318 (2)	0.140 (12)	0.38 (3)
H19D	0.5704	0.9573	0.2711	0.209*	0.38 (3)
H19E	0.4360	0.9769	0.3760	0.209*	0.38 (3)
H19F	0.4407	0.9071	0.2717	0.209*	0.38 (3)
C20	1.0180 (4)	0.6576 (4)	0.2149 (3)	0.0580 (10)	
O5	1.0258 (4)	0.7581 (3)	0.2602 (3)	0.0796 (9)	
C21	1.0583 (9)	0.8667 (6)	0.1809 (6)	0.131 (3)	
H21A	1.0011	0.8895	0.1224	0.157*	0.48 (3)
H21B	1.1629	0.8346	0.1442	0.157*	0.48 (3)
H21C	1.0677	0.8480	0.1040	0.157*	0.52 (3)
H21D	1.1521	0.8705	0.1864	0.157*	0.52 (3)
C22	1.022 (4)	0.9937 (15)	0.2377 (14)	0.109 (8)	0.48 (3)
H22A	0.9262	1.0138	0.2880	0.164*	0.48 (3)
H22B	1.0221	1.0702	0.1810	0.164*	0.48 (3)
H22C	1.0961	0.9786	0.2806	0.164*	0.48 (3)
C22A	0.937 (2)	1.0027 (12)	0.205 (2)	0.152 (8)	0.52 (3)
H22D	0.8533	1.0101	0.1765	0.228*	0.52 (3)
H22E	0.9727	1.0763	0.1694	0.228*	0.52 (3)
H22F	0.9072	1.0087	0.2862	0.228*	0.52 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0812 (4)	0.1012 (4)	0.0863 (4)	−0.0446 (3)	−0.0377 (3)	0.0424 (3)
O1	0.116 (3)	0.095 (3)	0.110 (3)	−0.042 (2)	0.047 (3)	−0.035 (2)
O2	0.067 (2)	0.126 (4)	0.170 (5)	−0.014 (2)	0.018 (3)	−0.035 (3)
O4	0.0721 (19)	0.109 (2)	0.0520 (17)	−0.0186 (18)	0.0079 (14)	−0.0072 (16)
O6	0.125 (3)	0.082 (2)	0.0519 (18)	−0.051 (2)	−0.0073 (17)	0.0087 (14)
N1	0.091 (3)	0.103 (3)	0.085 (3)	−0.051 (2)	−0.023 (2)	0.041 (2)
N2	0.070 (2)	0.082 (2)	0.070 (2)	−0.039 (2)	−0.0106 (18)	0.0203 (19)
N3	0.076 (3)	0.067 (3)	0.115 (4)	−0.029 (2)	0.025 (3)	−0.014 (3)
C1	0.059 (2)	0.060 (2)	0.049 (2)	−0.0287 (18)	−0.0026 (16)	−0.0018 (16)
C2	0.056 (2)	0.054 (2)	0.0456 (19)	−0.0232 (17)	−0.0087 (16)	0.0014 (15)
C3	0.054 (2)	0.058 (2)	0.055 (2)	−0.0286 (18)	−0.0118 (17)	0.0014 (17)
C4	0.061 (3)	0.082 (3)	0.066 (3)	−0.033 (2)	−0.004 (2)	−0.011 (2)
C5	0.055 (3)	0.082 (3)	0.109 (4)	−0.022 (2)	−0.021 (3)	−0.018 (3)
C6	0.080 (3)	0.076 (3)	0.108 (4)	−0.035 (3)	−0.047 (3)	0.015 (3)
C7	0.087 (3)	0.100 (3)	0.068 (3)	−0.052 (3)	−0.032 (2)	0.017 (2)
C8	0.060 (2)	0.080 (3)	0.059 (2)	−0.037 (2)	−0.0125 (19)	0.002 (2)

C9	0.0473 (19)	0.054 (2)	0.0480 (19)	−0.0215 (16)	−0.0091 (15)	0.0014 (15)
C10	0.052 (2)	0.0492 (19)	0.049 (2)	−0.0221 (17)	−0.0031 (16)	−0.0016 (15)
C11	0.065 (2)	0.071 (3)	0.053 (2)	−0.030 (2)	−0.0024 (19)	−0.0099 (19)
C12	0.083 (3)	0.077 (3)	0.061 (2)	−0.038 (3)	0.010 (2)	−0.018 (2)
C13	0.064 (3)	0.051 (2)	0.080 (3)	−0.025 (2)	0.020 (2)	−0.016 (2)
C14	0.053 (2)	0.057 (2)	0.087 (3)	−0.0197 (19)	−0.009 (2)	0.000 (2)
C15	0.054 (2)	0.057 (2)	0.061 (2)	−0.0173 (18)	−0.0054 (18)	−0.0079 (18)
C16	0.052 (2)	0.051 (2)	0.051 (2)	−0.0203 (17)	−0.0052 (16)	0.0026 (16)
C17	0.054 (2)	0.052 (2)	0.061 (2)	−0.0203 (18)	−0.0008 (18)	−0.0071 (18)
O3	0.0510 (16)	0.0754 (19)	0.0778 (19)	−0.0092 (14)	−0.0015 (14)	0.0076 (15)
C18	0.054 (3)	0.088 (4)	0.148 (5)	−0.004 (3)	0.004 (3)	0.003 (4)
C19	0.089 (11)	0.096 (9)	0.207 (18)	0.014 (7)	0.010 (11)	−0.036 (9)
C19A	0.083 (14)	0.159 (19)	0.119 (16)	−0.017 (14)	−0.001 (11)	0.041 (13)
C20	0.050 (2)	0.053 (2)	0.060 (2)	−0.0169 (17)	−0.0017 (17)	0.0025 (18)
O5	0.096 (2)	0.0653 (18)	0.0764 (19)	−0.0450 (17)	0.0138 (16)	−0.0137 (15)
C21	0.165 (6)	0.074 (4)	0.132 (5)	−0.070 (4)	0.049 (5)	−0.015 (3)
C22	0.134 (18)	0.069 (8)	0.116 (11)	−0.042 (9)	−0.006 (10)	0.000 (7)
C22A	0.168 (17)	0.117 (12)	0.181 (18)	−0.080 (13)	−0.056 (15)	0.053 (11)

Geometric parameters (Å, °)

Se1—C2	1.836 (4)	C14—H14	0.9300
Se1—N1	1.875 (4)	C15—H15	0.9300
O1—N3	1.216 (6)	C16—C17	1.510 (5)
O2—N3	1.208 (7)	C16—C20	1.525 (5)
O4—C17	1.195 (5)	C16—H16	0.9800
O6—C20	1.195 (5)	C17—O3	1.315 (5)
N1—N2	1.260 (5)	O3—C18	1.447 (5)
N2—C1	1.386 (5)	C18—C19	1.4991 (10)
N3—C13	1.472 (6)	C18—C19A	1.4992 (10)
C1—C2	1.361 (5)	C18—H18A	0.9700
C1—C3	1.476 (5)	C18—H18B	0.9700
C2—C9	1.514 (5)	C18—H18C	0.9700
C3—C8	1.379 (5)	C18—H18D	0.9700
C3—C4	1.392 (5)	C19—H19A	0.9600
C4—C5	1.374 (6)	C19—H19B	0.9600
C4—H4	0.9300	C19—H19C	0.9600
C5—C6	1.366 (7)	C19A—H19D	0.9600
C5—H5	0.9300	C19A—H19E	0.9600
C6—C7	1.368 (7)	C19A—H19F	0.9600
C6—H6	0.9300	C20—O5	1.316 (5)
C7—C8	1.380 (6)	O5—C21	1.434 (6)
C7—H7	0.9300	C21—C22	1.4989 (10)
C8—H8	0.9300	C21—C22A	1.4990 (10)
C9—C10	1.517 (5)	C21—H21A	0.9700
C9—C16	1.535 (5)	C21—H21B	0.9700
C9—H9	0.9800	C21—H21C	0.9700
C10—C15	1.378 (5)	C21—H21D	0.9700
C10—C11	1.391 (5)	C22—H22A	0.9600

C11—C12	1.366 (6)	C22—H22B	0.9600
C11—H11	0.9300	C22—H22C	0.9600
C12—C13	1.363 (7)	C22A—H22D	0.9600
C12—H12	0.9300	C22A—H22E	0.9600
C13—C14	1.371 (6)	C22A—H22F	0.9600
C14—C15	1.392 (5)		
C2—Se1—N1	87.20 (17)	C17—C16—C9	111.8 (3)
N2—N1—Se1	110.9 (3)	C20—C16—C9	110.1 (3)
N1—N2—C1	117.2 (4)	C17—C16—H16	108.4
O2—N3—O1	123.6 (5)	C20—C16—H16	108.4
O2—N3—C13	117.9 (6)	C9—C16—H16	108.4
O1—N3—C13	118.5 (6)	O4—C17—O3	124.9 (4)
C2—C1—N2	115.9 (4)	O4—C17—C16	123.6 (4)
C2—C1—C3	127.3 (3)	O3—C17—C16	111.5 (3)
N2—C1—C3	116.7 (3)	C17—O3—C18	117.6 (4)
C1—C2—C9	127.6 (3)	O3—C18—C19	106.1 (6)
C1—C2—Se1	108.8 (3)	O3—C18—C19A	118.2 (9)
C9—C2—Se1	123.7 (3)	O3—C18—H18A	110.5
C8—C3—C4	118.5 (4)	C19—C18—H18A	110.5
C8—C3—C1	121.9 (3)	O3—C18—H18B	110.5
C4—C3—C1	119.6 (3)	C19—C18—H18B	110.5
C5—C4—C3	120.7 (4)	H18A—C18—H18B	108.7
C5—C4—H4	119.6	O3—C18—H18C	107.7
C3—C4—H4	119.6	C19A—C18—H18C	107.7
C6—C5—C4	120.2 (4)	O3—C18—H18D	107.7
C6—C5—H5	119.9	C19A—C18—H18D	107.7
C4—C5—H5	119.9	H18C—C18—H18D	107.1
C5—C6—C7	119.5 (5)	C18—C19—H19A	109.5
C5—C6—H6	120.3	C18—C19—H19B	109.5
C7—C6—H6	120.3	C18—C19—H19C	109.5
C6—C7—C8	121.1 (4)	C18—C19A—H19D	109.5
C6—C7—H7	119.4	C18—C19A—H19E	109.5
C8—C7—H7	119.4	H19D—C19A—H19E	109.5
C3—C8—C7	119.8 (4)	C18—C19A—H19F	109.5
C3—C8—H8	120.1	H19D—C19A—H19F	109.5
C7—C8—H8	120.1	H19E—C19A—H19F	109.5
C2—C9—C10	111.3 (3)	O6—C20—O5	124.2 (4)
C2—C9—C16	112.8 (3)	O6—C20—C16	125.6 (4)
C10—C9—C16	112.6 (3)	O5—C20—C16	110.2 (3)
C2—C9—H9	106.5	C20—O5—C21	115.6 (4)
C10—C9—H9	106.5	O5—C21—C22	112.0 (7)
C16—C9—H9	106.5	O5—C21—C22A	110.3 (8)
C15—C10—C11	119.3 (3)	O5—C21—H21A	109.2
C15—C10—C9	121.5 (3)	C22—C21—H21A	109.2
C11—C10—C9	119.1 (3)	O5—C21—H21B	109.2
C12—C11—C10	120.4 (4)	C22—C21—H21B	109.2
C12—C11—H11	119.8	H21A—C21—H21B	107.9
C10—C11—H11	119.8	O5—C21—H21C	109.6
C13—C12—C11	119.4 (4)	C22A—C21—H21C	109.6

C13—C12—H12	120.3	O5—C21—H21D	109.6
C11—C12—H12	120.3	C22A—C21—H21D	109.6
C12—C13—C14	122.2 (4)	H21C—C21—H21D	108.1
C12—C13—N3	119.1 (5)	C21—C22—H22A	109.5
C14—C13—N3	118.7 (5)	C21—C22—H22B	109.5
C13—C14—C15	118.3 (4)	C21—C22—H22C	109.5
C13—C14—H14	120.9	C21—C22A—H22D	109.5
C15—C14—H14	120.9	C21—C22A—H22E	109.5
C10—C15—C14	120.4 (4)	H22D—C22A—H22E	109.5
C10—C15—H15	119.8	C21—C22A—H22F	109.5
C14—C15—H15	119.8	H22D—C22A—H22F	109.5
C17—C16—C20	109.6 (3)	H22E—C22A—H22F	109.5
C2—Se1—N1—N2	0.3 (4)	C10—C11—C12—C13	−0.2 (6)
Se1—N1—N2—C1	0.3 (6)	C11—C12—C13—C14	−0.5 (6)
N1—N2—C1—C2	−1.0 (6)	C11—C12—C13—N3	−178.0 (4)
N1—N2—C1—C3	−178.4 (4)	O2—N3—C13—C12	−178.0 (5)
N2—C1—C2—C9	−177.9 (4)	O1—N3—C13—C12	1.8 (6)
C3—C1—C2—C9	−0.8 (6)	O2—N3—C13—C14	4.4 (6)
N2—C1—C2—Se1	1.1 (4)	O1—N3—C13—C14	−175.8 (4)
C3—C1—C2—Se1	178.2 (3)	C12—C13—C14—C15	0.9 (6)
N1—Se1—C2—C1	−0.8 (3)	N3—C13—C14—C15	178.4 (4)
N1—Se1—C2—C9	178.3 (3)	C11—C10—C15—C14	0.1 (5)
C2—C1—C3—C8	50.7 (6)	C9—C10—C15—C14	178.9 (3)
N2—C1—C3—C8	−132.2 (4)	C13—C14—C15—C10	−0.7 (6)
C2—C1—C3—C4	−127.9 (4)	C2—C9—C16—C17	−48.0 (4)
N2—C1—C3—C4	49.2 (5)	C10—C9—C16—C17	−175.1 (3)
C8—C3—C4—C5	−3.1 (6)	C2—C9—C16—C20	−170.0 (3)
C1—C3—C4—C5	175.6 (4)	C10—C9—C16—C20	62.9 (4)
C3—C4—C5—C6	1.7 (7)	C20—C16—C17—O4	−138.2 (4)
C4—C5—C6—C7	0.5 (7)	C9—C16—C17—O4	99.5 (5)
C5—C6—C7—C8	−1.3 (7)	C20—C16—C17—O3	42.6 (4)
C4—C3—C8—C7	2.3 (6)	C9—C16—C17—O3	−79.7 (4)
C1—C3—C8—C7	−176.4 (4)	O4—C17—O3—C18	1.7 (6)
C6—C7—C8—C3	−0.1 (7)	C16—C17—O3—C18	−179.0 (4)
C1—C2—C9—C10	−128.4 (4)	C17—O3—C18—C19	105.5 (15)
Se1—C2—C9—C10	52.8 (4)	C17—O3—C18—C19A	149 (2)
C1—C2—C9—C16	103.8 (4)	C17—C16—C20—O6	−118.3 (4)
Se1—C2—C9—C16	−75.0 (4)	C9—C16—C20—O6	5.1 (6)
C2—C9—C10—C15	−81.3 (4)	C17—C16—C20—O5	62.4 (4)
C16—C9—C10—C15	46.6 (4)	C9—C16—C20—O5	−174.3 (3)
C2—C9—C10—C11	97.5 (4)	O6—C20—O5—C21	3.5 (7)
C16—C9—C10—C11	−134.6 (3)	C16—C20—O5—C21	−177.2 (5)
C15—C10—C11—C12	0.3 (6)	C20—O5—C21—C22	163.5 (15)
C9—C10—C11—C12	−178.5 (4)	C20—O5—C21—C22A	121.8 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22A—H22D···O2^{i}	0.96	2.47	3.38 (4)	159

C11—H11···O6^{ii}	0.93	2.56	3.410 (6)	152
C18—H18A···O4	0.97	2.29	2.686 (7)	103
C21—H21C···O6	0.97	2.17	2.627 (6)	107

Symmetry codes: (i) $x-1, y+1, z$; (ii) $-x+2, -y+1, -z$.

Fig. 1

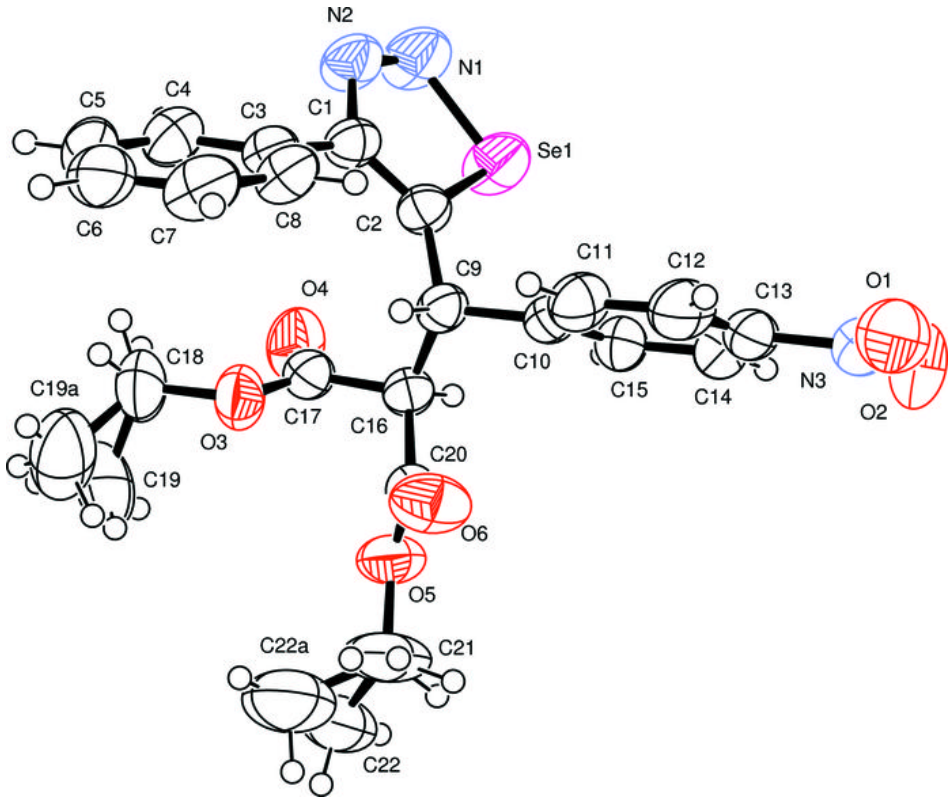

N2
N1
C5
C4
C3
C1
Se1
C6
C7
C8
C2
C9
C11
C12
C13
O1
O4
C18
C10
C15
C14
N3
O2
C19a
C17
C16
O3
C20
C19
O6
O5
C22a
C21
C22

Fig. 2