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o-Methylselenobenzoyl cyanide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.041
wR factor = 0.111
Data-to-parameter ratio = 11.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, C_9H_7NOSe, a potential anti-oxidizing agent, the whole molecule lies in the $(0,y,z)$ plane except for two methyl H atoms, whose positions are symmetry-related across that plane. A close Se···Se contact [3.359 (2) Å] is observed. There are no hydrogen bonds.

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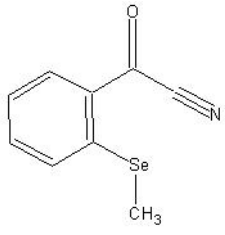
Comment

Some modifications of the molecular structure of Ebselen (Natterman/RP, 1981; Dupont *et al.*, 1990), an anti-inflammatory compound, have been attempted in order to obtain a more soluble derivative which retains the pharmacological properties. The crystal structure of the title compound, (I), was determined in order to identify, without ambiguity, a potential anti-oxidant derivative. The crystal packing is governed by van der Waals interactions. There is an Se···Se^{i} close contact [symmetry code: (i) $x, -y, 1-z$) of 3.359 (2) Å, rather less than the sum of Se atom radii (3.8 Å; Bondi, 1964). The distance is, nevertheless, larger than that of a covalent Se—Se bond [2.3229 (6) Å; Kumar & Nangia, 2000].



(I)

Experimental

The synthesis of the title compound was carried out in two steps. *o*-Methylselenobenzoic acid was treated with α,α-dichloromethyl ether and then with KCN (Messali, 2001). A yellow single crystal was obtained by slow evaporation of a toluene solution.

Crystal data

C_9H_7NOSe
M_r = 224.12
Orthorhombic, *Cmca*
a = 6.8433 (19) Å
b = 15.585 (9) Å
c = 16.6460 (12) Å
V = 1775.4 (12) Å^3
Z = 8
D_x = 1.677 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 32 reflections
θ = 31.5–36.3°
μ = 5.31 mm^{-1}
T = 293 (2) K
Prism, yellow
0.61 × 0.38 × 0.23 mm

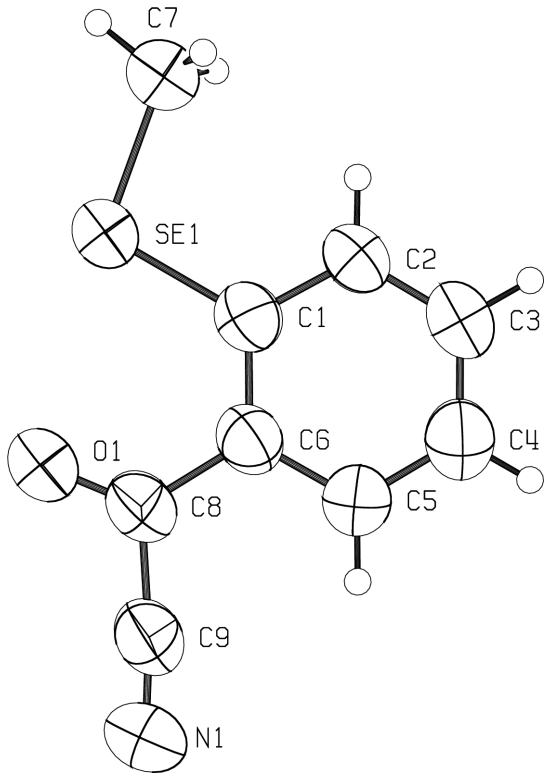


Figure 1
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are shown at the 50% probability level.

Data collection

Stoe–Siemens AED four-circle diffractometer
ω scans
Absorption correction: ψ scan (*EMPIR*; Stoe & Cie, 1987)
T_{min} = 0.140, T_{max} = 0.375
848 measured reflections
848 independent reflections
624 reflections with $I > 2\sigma(I)$
θ_{max} = 67.9°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 20$
2 standard reflections
frequency: 60 min
intensity decay: 5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.111
S = 1.01
848 reflections
74 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2 + 0.7549P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0078 (6)

Table 1
Selected geometric parameters (Å, °).

Se1—C1	1.887 (5)	N1—C9	1.135 (7)
Se1—C7	1.932 (5)	C6—C8	1.454 (5)
O1—C8	1.210 (7)		
C1—Se1—C7	100.2 (2)	C6—C8—C9	117.6 (5)
O1—C8—C6	125.9 (5)	N1—C9—C8	174.4 (6)
O1—C8—C9	116.5 (4)		

H atoms were placed at standard calculated positions and included in the refinement in the riding-model approximation, with isotropic displacement parameters fixed at 1.2U_{eq} of the parent atom (1.5 U_{eq} for methyl H atoms).

Data collection: *DIF*4 (Stoe & Cie, 1987); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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