Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2,2′-Diselenobis(4,4-diphenylcyclohexa-2,5-dienone)

V. S. Senthil Kumar and Ashwini Nangia*

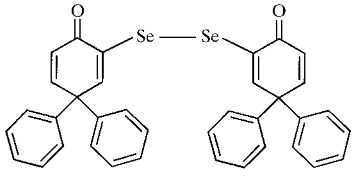
School of Chemistry, University of Hyderabad, Hyderabad 500 046, India
Correspondence e-mail: ansc@uohyd.ernet.in

Received 6 July 1999
Accepted 7 October 1999

The title compound, $C_{36}H_{26}O_2Se_2$, displays crystallographic twofold symmetry. The packing involves corrugated linear ribbons mediated through C—H···O and C—H···Se interactions. The ribbons are connected through C—H···π interactions.

Comment

The role of weak hydrogen bonds such as C—H···O, C—H···π, or in general C—H···X (X = heteroatom or metal) and X···X interactions in the stabilization of crystal structures is a theme of current interest (Desiraju & Steiner, 1999). In this context, the crystal structure of the title compound, (I), is pertinent because it has phenyl C—H donor groups, carbonyl acceptor atoms and an Se—Se bond.



(I)

The molecular structure of (I) is shown in Fig. 1 (Johnson, 1976). The molecule lies on a twofold axis that bisects the Se1—Se1′ bond [symmetry code: (′) $\frac{3}{2} - x, \frac{1}{2} - y, z$]; the asymmetric unit contains half a molecule of (I). The cyclohexa-2,5-dienone ring forms dihedral angles of 58.1 (1) and 89.85 (1)° with the two phenyl rings (C7—C12 and C13—C18). The diselenide geometry in (I) is normal, with an Se1—Se1′ bond length of 2.3229 (6) Å and a C2—Se1—Se1′—C2′ torsion angle of 79.35 (8)°. These values are comparable with those found in the crystal structure of dimesityl diselenide reported recently by Jeske *et al.* (1998) [Se—Se 2.3341 (6) Å and C—Se—Se—C 83.96 (12)°].

In the crystal structure of (I), space group *Pccn*, inversion related molecules are connected through C—H···O and C—H···Se interactions (Iwaoka & Tomoda, 1994; Narayanan *et al.*, 1998) to produce a corrugated ribbon-like structure in (101) [C16—H16*A*···O1 2.82 Å, 125°; C17—H17*A*···Se1 3.10 Å, 141°] (Fig. 2). Such ribbons are connected by chains of C—H···O and C—H···π interactions along [001] through the C5 and C6 H atoms of the cyclohexa-2,5-dienone as donors and the carbonyl group and phenyl ring as acceptors [C5—H5*A*···O1 2.93 Å, 157°; C6—H6*A*···$\pi_{\rm centroid}$ 2.57 Å, 153°]. The hydrogen bonds in this study have been considered with liberal distance and angle cut-off criteria of 2.0 < H···O < 3.0 Å and 120 < C—H···O < 180°, as advocated by Desiraju & Steiner (1999).

The approach of electrophilic and nucleophilic groups (X) to divalent Se (Y—Se—Z) has been discussed by Ramasubbu & Parthasarathy (1987) and categorized as type I or type II depending on whether the approaching atom is normal to the selenide plane and along the Se lone pair orbital ($\langle\theta\rangle$ = 23°)

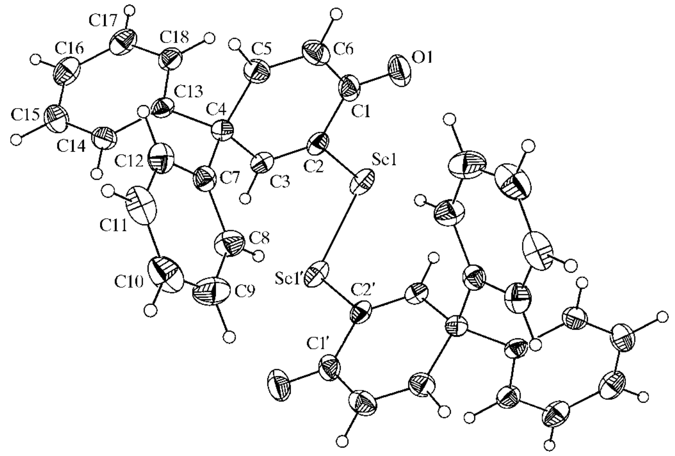


Figure 1
*ORTEP*II (Johnson, 1976) plot and atom-numbering scheme [symmetry code: (′) $\frac{3}{2} - x, \frac{1}{2} - y, z$] for (I). Displacement ellipsoids are drawn at the 50% probability level.

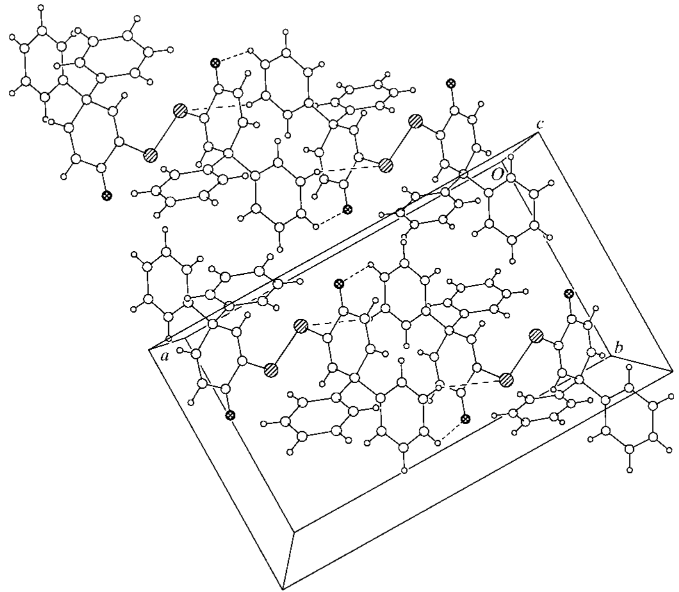


Figure 2
A view of (I) showing the corrugated ribbons connected by C—H···O and C—H···Se hydrogen bonds along [100]. Se atoms are shown as large hatched circles and O atoms as small crossed circles. The C—H···O and C—H···π interactions along [001] are omitted for clarity.

or in the plane and along the C—Se σ^* antibonding orbital ($<\theta>$ = 79°). In the spherical coordinate system, θ is the polar angle between the direction $X\cdots$Se and the normal to the Y—Se—Z selenide plane. There are two interactions in (I) involving the Se atom that deserve a mention. In the C17—H17$A\cdots$Se1 interaction, the C—H group approaches the Se acceptor along the direction for electrophilic donors with θ = 18.5°. Interestingly, the structure also has a C—Se$\cdots\pi_{\rm centroid}$ contact of 3.59 Å (166.4°), which is shorter than the sum of the van der Waals radii (Se 2.0 and C 1.7 Å). The approach of the phenyl ring is in the C—Se—Se plane and from behind the C—Se bond, *i.e.* it is a type II contact with θ = 83.9°. Based on this approach geometry, the interaction could be viewed as electrophile–nucleophile pairing, *i.e.* Se(δ+)$\cdots\pi$(δ−). Thus, the stereochemical distribution of charge density at Se and its behaviour both as a donor and as an acceptor in the crystal structure of (I) are rationalized.

Experimental

Compound (I) was obtained as an unexpected product in 60% yield during the SeO_2 oxidation of 4,4-diphenyl-2-cyclohexenone (Zimmerman & Schuster, 1962). Yellow crystals of (I) were obtained upon crystallization from ethyl acetate and hexane (m.p. 483 K).

Crystal data

$C_{36}H_{26}O_2Se_2$
M_r = 648.49
Orthorhombic, *Pccn*
a = 17.4144 (16) Å
b = 10.6767 (10) Å
c = 15.2187 (14) Å
V = 2829.6 (5) Å^3
Z = 4
D_x = 1.522 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1650 reflections
θ = 2.19–26.43°
μ = 2.646 mm^{-1}
T = 168 (2) K
Plate, yellow
0.8 × 0.5 × 0.14 mm

Data collection

Siemens CCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\rm min}$ = 0.218, $T_{\rm max}$ = 0.690
29 316 measured reflections
2839 independent reflections
2412 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.026
$\theta_{\rm max}$ = 26.43°
$h = -21 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.086$
S = 1.060
2839 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.9536P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = -0.002$
$\Delta\rho_{\rm max}$ = 0.55 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.73 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$A\cdots$O1$^{\rm i}$	0.95	2.93	3.82 (3)	157
C16—H16$A\cdots$O1$^{\rm ii}$	0.95	2.82	3.463 (3)	125
C17—H17$A\cdots$Se1$^{\rm ii}$	0.95	3.10	3.886 (2)	141

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

All the H atoms have been generated at idealized geometries and refined isotropically using a riding model.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLUTON* (Spek, 1992); software used to prepare material for publication: *SHELXL*97.

We thank Professor W. T. Robinson and Dr R. Kadirvelraj (University of Canterbury, New Zealand) for X-ray data collection. VSSK thanks the CSIR (1/1431/96/EMR-II) for fellowship support. We thank Professor G. R. Desiraju for discussions.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1370). Services for accessing these data are described at the back of the journal.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*, pp. 40–68. Oxford University Press.
Iwaoka, M. & Tomoda, S. (1994). *J. Am. Chem. Soc.* **116**, 4463–4464.
Jeske, J., Martens-von Salzen, A., du Mont, W.-W. & Jones, P. G. (1998). *Acta Cryst.* C**54**, 1873–1875.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Narayanan, S. J., Sridevi, B., Chandrashekar, T. K., Vij, A. & Roy, R. (1998). *Angew. Chem. Int. Ed. Engl.* **37**, 3394–3397.
Ramasubbu, N. & Parthasarathy, R. (1987). *Phosphorus Sulfur*, **31**, 221–229.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97. Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.
Siemens (1994). *SHELXTL*. Release 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1995). *SMART. Software Reference Manual.* Version 4.050. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (1992). *PLUTON. Molecular Graphics Program.* University of Utrecht, The Netherlands.
Zimmerman, H. E. & Schuster, D. I. (1962). *J. Am. Chem. Soc.* **84**, 4527–4540.