



Crystal structure and Hirshfeld surface analysis of (2*E*,2'*E*)-1,1'-[selenobis(4,1-phenylene)]bis[3-(4-chlorophenyl)prop-2-en-1-one]

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Received 9 September 2019

Accepted 15 October 2019

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; organoselenium; selenium; Hirshfeld surface analysis.

CCDC reference: 1959404

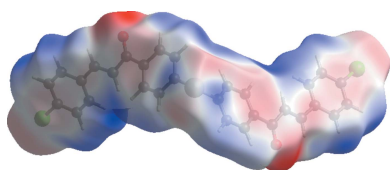
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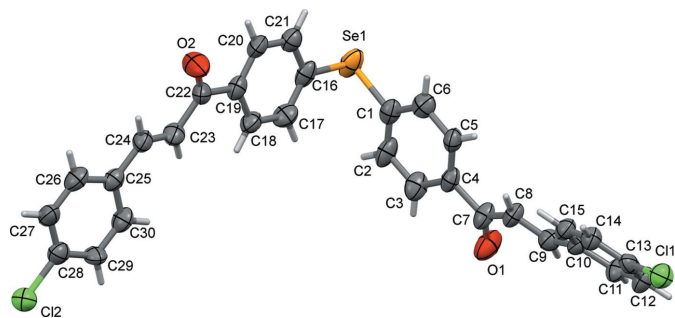
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In the title compound, C₃₀H₂₀Cl₂O₂Se, the C—Se—C angle is 99.0 (2)°, with the dihedral angle between the planes of the attached benzene rings being 79.1 (3)°. The average endocyclic angles (Se—C—C) facing the Se atom are 122.1 (5) and 122.2 (5)°. The Se atom is essentially coplanar with the attached benzene rings, deviating by 0.075 (1) and 0.091 (1) Å. In the two phenylene(4-chlorophenyl)-prop-2-en-1-one units, the benzene rings are inclined to each other by 44.6 (3) and 7.8 (3)°. In the crystal, the molecules stack up the *a* axis, forming layers parallel to the *ac* plane. There are no significant classical intermolecular interactions present. Hirshfeld surface analysis, two-dimensional fingerprint plots and the molecular electrostatic potential surface were used to analyse the crystal packing. The Hirshfeld surface analysis suggests that the most significant contributions to the crystal packing are by C···H/H···C contacts (17.7%).

1. Chemical context

During the last few years, organoselenium chemistry (Procter, 2001) has been the subject of constant scientific interest and organoselenium compounds have been used intensively as important reagents and intermediates in organic synthesis (Zade *et al.*, 2005). Recently, various organoselenium compounds have attracted growing attention in medicine. Selenoproteins are very important for neuronal survival and function. It has been found that selenoprotein P may influence Alzheimer pathology (Bellinger *et al.*, 2008). Furthermore, the potential of selenoproteins to protect against oxidative stress led to the expectation that selenium would be protective against type 2 diabetes, and indeed in the 1990s, selenium was shown to have antidiabetic and insulin mimetic effects (Steinbrenner *et al.*, 2011). However, more recently, findings from observational epidemiological studies and randomized clinical trials have raised concern that high selenium exposure may lead to type 2 diabetes or insulin resistance at least in well-nourished populations (Stranges *et al.*, 2010). In addition, molecules involving selenium are still efficient and encouraged in medicinal chemistry (Zhao *et al.*, 2012). Moreover, organoselenium compounds are of considerable interest in academia, as anticancer (Zhu & Jiang, 2008), anti-oxidant (Anderson *et al.*, 1996), anti-inflammatory and antiallergic




Figure 1

The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

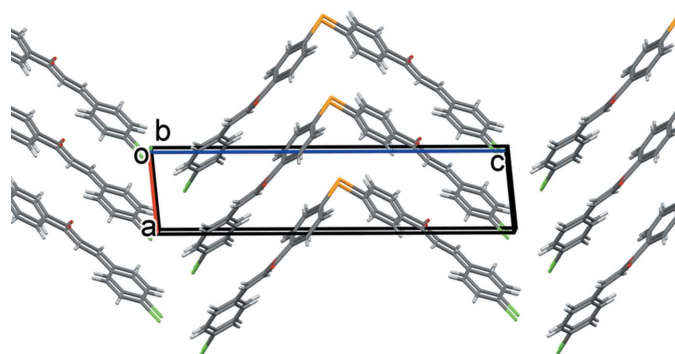
Table 1

Short contacts (Å) in the crystal of the title compound.

Atom 1	Atom 2	Length (Å)	vdW length (Å)
H3	H10 ⁱ	2.498	0.098
O2	H19 ⁱⁱ	2.632	−0.088
H12	O2 ⁱⁱⁱ	2.759	0.039
O1	H3 ⁱⁱⁱ	2.770	0.050
O2	H20 ⁱⁱ	2.818	0.098
H2	C6 ⁱⁱⁱ	2.922	0.022
C3	H4 ⁱⁱ	2.943	0.043
H3	C15 ⁱ	2.964	0.064
O2	C29 ⁱⁱ	3.217	−0.003
O2	C30 ⁱⁱ	3.314	0.094
C5	C8 ⁱ	3.461	0.061
Se1	C17 ⁱ	3.475	−0.125
C20	C23 ⁱ	3.480	0.080
Cl2	Cl1 ^{iv}	3.549	0.049

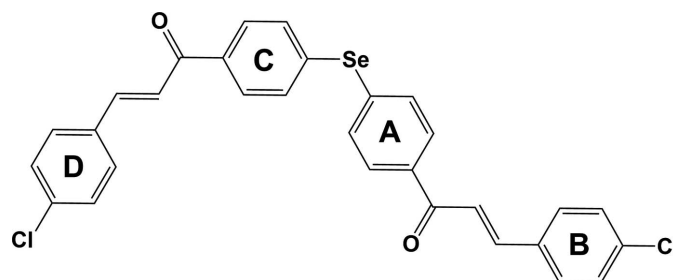
Symmetry codes: (i) $x - 1, y, z$; (ii) $x - 1, y + 1, z$; (iii) $x, y - 1, z$; (iv) $x - 1, y - 1, z + 1$.

agents (Abdel-Hafez, 2008), and in industry because of their involvement as key intermediates in the synthesis of pharmaceuticals (Woods *et al.*, 1993), fine chemicals and polymers (Hellberg *et al.*, 1997). Moreover, chalcone derivatives are notable for their excellent blue-light transmittance and good crystallizability; they also show considerable promise as organic nonlinear optical materials (Uchida *et al.*, 1998). In continuation of our work on chalcone organoselenium derivatives, we report herein on the crystal structure of (*2E,2'E*-


Figure 2

A view along the *b* axis of the crystal packing of the title compound, showing the layer-like structure.

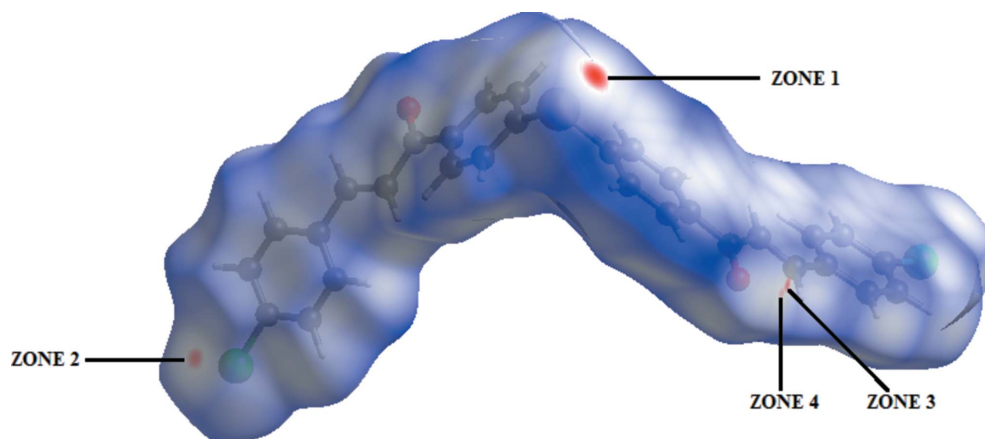
1,1'-[selenobis(4,1-phenylene)]bis[3-(4-chlorophenyl)prop-2-en-1-one].



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The C1—Se1—C16 angle is $99.0(2)^\circ$, which is close to the value observed in three very similar compounds, *viz.* $99.47(10)^\circ$ in bis(4-nitrophenyl) selenide, where the Se atom lies on a twofold rotation axis (Zuo, 2013), $99.59(14)^\circ$ in bis(4-acetylphenyl) selenide (Bouraoui *et al.*, 2011) and $100.03(15)^\circ$ in bis(2-chloroethan-1-one-phenyl) selenide (Bouraoui *et al.*, 2015).

In the title compound, inner benzene rings *A* (atoms C1–C6) and *C* (C16–C21) (see Scheme) are inclined to each other by $79.1(3)^\circ$. This is similar to the same angle observed for the acetylphenyl derivative, *viz.* $87.08(15)^\circ$, but considerably


Figure 3

A view of the Hirshfeld surface mapped over d_{norm} in the colour range -0.0711 to 1.3645 a.u.

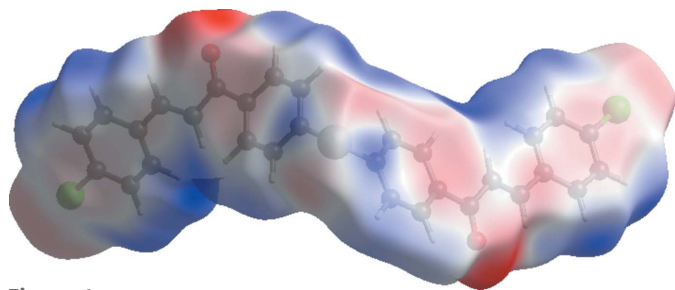


Figure 4
A view of the Hirshfeld surface plotted over the calculated electrostatic potential energy in the range -0.0489 to 0.0448 a.u.

different to that observed for the 4-nitrophenyl derivative, *viz.* 63.76 (10) $^\circ$.

In each phenylene-(4-chlorophenyl)prop-2-en-1-one unit, the C=C has an *E* configuration. The C=C bond lengths

C8=C9 and C23=C24 are 1.317 (8) and 1.325 (8) \AA , respectively, which confirms their double-bond character. Benzene rings *A* and *B* (C10–C15) of one unit are inclined to one another by 44.6 (3) $^\circ$, while rings *C* and *D* (C25–C30) of the other unit are almost coplanar, with a dihedral angle of 7.8 (3) $^\circ$. The outer benzene rings, *B* and *D*, are almost normal to one another, with a dihedral angle of 84.4 (3) $^\circ$.

3. Supramolecular features

In the crystal, molecules stack up the *a* axis, forming layers parallel to the *ac* plane (Fig. 2). There are no significant classical intermolecular interactions present (*PLATON*; Spek, 2009). The shortest atom–atom contacts in the crystal (Figs. 3 and 4) are given in Table 1 and are discussed in §4 (*Hirshfeld surface analysis*).

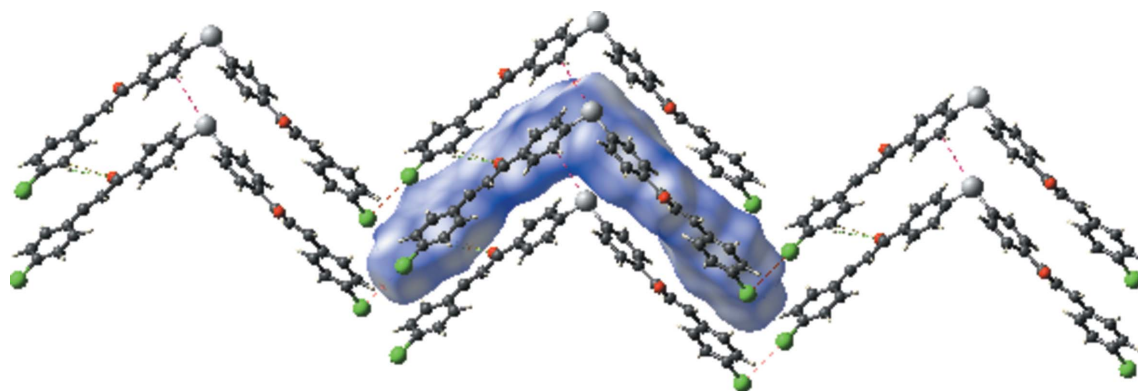


Figure 5
Hirshfeld surface mapped over d_{norm} to visualize some of the short intermolecular contacts in the crystal (see Table 1).

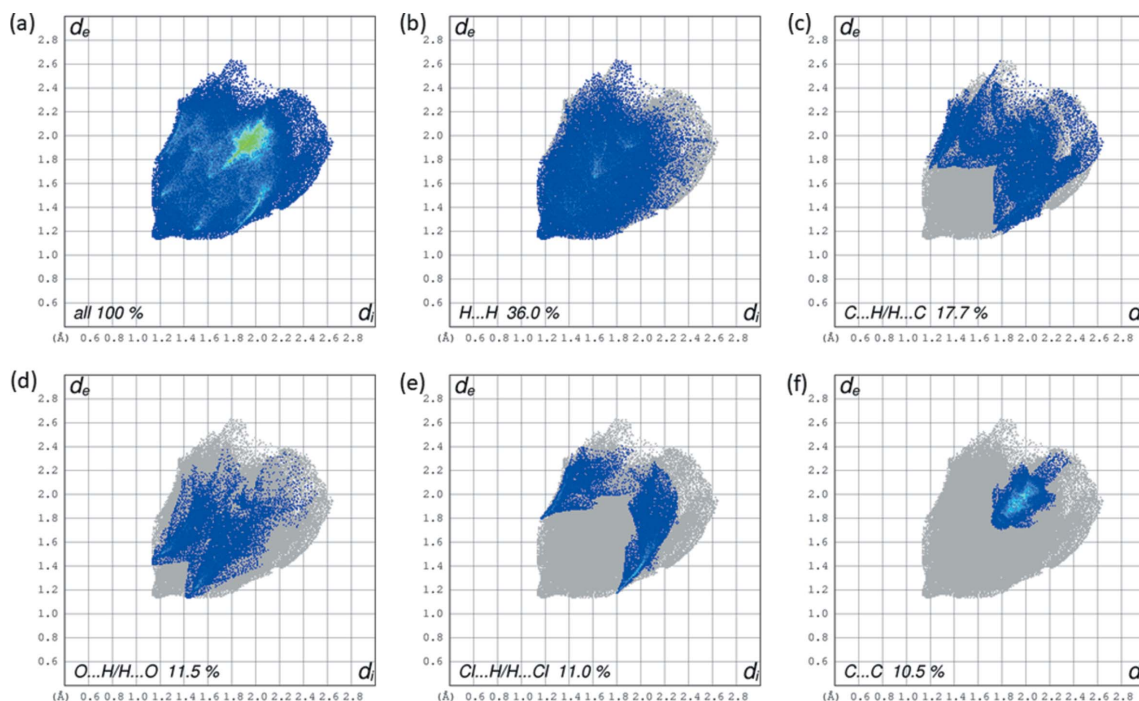


Figure 6
(*a*) The full two-dimensional fingerprint plot for the title compound and those delineated into (*b*) H...H, (*c*) C...H/H...C, (*d*) O...H/H...O, (*e*) Cl...H/H...Cl and (*f*) C...C contacts.

4. Hirshfeld surface analysis

Insight into the intermolecular interactions in the crystal were obtained from an analysis of the Hirshfeld surface (Spackman & Jayatilaka, 2009) and the two-dimensional fingerprint plots (McKinnon *et al.*, 2007). The program *CrystalExplorer* (Turner *et al.*, 2017) was used to generate both the Hirshfeld surfaces, mapped over d_{norm} , and the electrostatic potential for the title compound. The function d_{norm} is a ratio enclosing the distances of any surface point to the nearest interior (d_i) and exterior (d_e) atom and the van der Waals (vdW) radii of the atoms. The function d_{norm} will be equal to zero when intermolecular distances are close to the van der Waals contacts. They are indicated by a white colour on the Hirshfeld surface, while contacts longer than the sum of the vdW radii with positive d_{norm} values are coloured blue.

The analysis of the Hirshfeld surface (HS) mapped over d_{norm} is shown in Fig. 4. The H...O contacts between the corresponding donor and acceptor atoms are visualized as bright-red spots on the side (zone 4) of the Hirshfeld surface (Fig. 4). Three other red spots exist, corresponding to the C...Se, Cl...Cl and C...O contacts, *viz.* zones 1, 2 and 3, respectively (Fig. 4). These contacts are considered to be the strongest when comparing them to the sum of the vdW radii [Table 1; calculated using *Mercury* (Macrae *et al.*, 2008)].

A view of the molecular electrostatic potential using the 6-31G(d) basis set with the density functional theory (DFT) method for the title compound is shown in Fig. 5. The H...O donors and acceptors are shown as blue and red areas around the atoms related with positive (hydrogen-bond donors) and negative (hydrogen-bond acceptors) electrostatic potentials, respectively.

The full two-dimensional fingerprint plot for the title compound is given in Fig. 6(a). Those for the most significant contacts contributing to the HS are given in Fig. 6(b) for H...H, Fig. 6(c) for C...H/H...C, Fig. 6(d) for O...H/H...O, Fig. 6(e) for Cl...H/H...Cl and Fig. 6(f) for C...C. A full list of the relative percentage contributions of the close contacts to the HS of the title compound are given in Table 2.

A contribution of 36.0% was found for the H...H contacts (Fig. 6b), representing the largest contribution, and is displayed on the fingerprint plots by a pair of very short spikes at $d_e + d_i = 2.3 \text{ \AA}$; the vdW radius for this interaction is 2.18 Å, which means it is a weak interaction.

The C...H/H...C (17.7%, Fig. 6c) and Cl...H/H...Cl (Fig. 6e) contacts are seen as pairs of spikes at $d_e + d_i = 2.9$ and 2.9 Å, respectively.

The plot of O...H/H...O contacts between H atoms located inside the Hirshfeld surface and oxygen from outside and *vice versa* is shown in Fig. 6(d). These contacts account for 11.5% and are characterized by two symmetrical peaks with $d_e + d_i = 2.5 \text{ \AA}$; this reveals the presence of strong O...H contacts.

The C...C contacts (Fig. 6f) give a contribution of 10.5%, while the C...Cl, C...Se, Se...H/H...Se and Cl...Cl contacts in the structure give weak contributions of 4.3, 3.5, 2.8 and 2.4%, respectively, to the Hirshfeld surface.

Table 2

Relative percentage contributions of the close contacts to the Hirshfeld surface of the title compound.

Contact	Percentage contribution
H...H	36.0
C...H/H...C	17.7
O...H/H...O	11.5
Cl...H/H...Cl	11.0
C...C	10.5
C...Cl	4.3
C...Se	3.5
Se...H/H...Se	2.8
Cl...Cl	2.4
C...O	0.3

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, last update May 2019; Groom *et al.*, 2016) for 4,4'-substituted bis(phenyl) selenides yielded six relevant hits. These are bis(2-chloroethan-1-one-phenyl) selenide (CSD refcode HUYRUC; Bouraoui *et al.*, 2015), bis(4-nitrophenyl) selenide (IDIOG; Zuo, 2013), bis(4-methoxyphenyl) selenide (LAFNAK; Verma *et al.*, 2016), bis(4-acetylphenyl) selenide (UPAGAU; Bouraoui *et al.*, 2011), bis(phenyl) selenide itself (YEWYUX; Bhandary *et al.*, 2018) and bis(*p*-tolyl) selenide (TOLYSE; Blackmore & Abrahams, 1955). In IDIOG, the Se atom lies on a twofold rotation axis, and only YEWYUX and TOLYSE crystallize in chiral space groups, *i.e.* $P2_1$ and $P2_12_12_1$, respectively.

In the title compound (Fig. 1), the C—Se—C angle is 99.0 (2)°, similar to the value observed in five of the compounds mentioned above, *viz.* 100.03 (15), 99.47 (10), 102.25 (19), 99.59 (14) and 98.31 (16)° for HUYRUQ, IDITOG, LAFNAK, UPAGAU and YEWYUX, respectively. In the sixth compound, TOLYSE, the dihedral angle is 105.65 (19)°. The two inner benzene rings, A and C, in the title compound are inclined to each other by 79.1 (3)°. This value is quite different to that observed in the five compounds mentioned above, *i.e.* 69.92 (17), 63.76 (10), 69.6 (2), 87.08 (15), 68.46 (18) and *ca* 56.99° for HUYRUQ, IDITOG, LAFNAK, UPAGAU, YEWYUX and TOLYSE, respectively.

6. Synthesis and crystallization

The title compound was prepared according to a method proposed by Mechehoud *et al.* (2010). 2-Chloro-1-(4-chlorophenyl)ethan-1-one ($\text{ClC}_8\text{H}_6\text{COCl}$; 36.5 mmol) and anhydrous aluminium chloride (5 g, 37.5 mmol, 3 equiv.) were taken up in dry methylene chloride (100 ml). The reaction mixture was cooled to 273–278 K, protected from atmospheric moisture and stirred continuously for 15 min. A solution of diphenyl selenide (3 g, 1.87 mmol) in CH_2Cl_2 was added dropwise over a period of 5 min. The reaction mixture was allowed to reach room temperature gradually and then stirred at this temperature overnight. The solution was then washed with ice water–HCl (80 ml) and extracted with CH_2Cl_2 . The organic layer was separated and dried (Na_2SO_4). Removal of

the solvent under reduced pressure afforded the crude product, which was recrystallized from petroleum ether to yield 4.2 g of the title compound. Yellow single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from CH₂Cl₂.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms could all be located in a difference Fourier map. During refinement, they were included in calculated positions and refined as riding on the parent C atom, with C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

This work was supported by the Laboratoire de Cristallographie, Departement de Physique, Universite Constantine 1, Algeria. We also thank Mr F. Saidi, Engineer at the Laboratory of Crystallography, University Constantine 1, for assistance in collecting data on the Xcalibur X-ray diffractometer.

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Table 3

Experimental details.

Crystal data	
Chemical formula	C ₃₀ H ₂₀ Cl ₂ O ₂ Se
M_r	562.32
Crystal system, space group	Triclinic, <i>P1</i>
Temperature (K)	293
a, b, c (Å)	4.9468 (3), 5.8712 (6), 21.3530 (18)
α, β, γ (°)	85.019 (8), 84.094 (6), 86.465 (7)
V (Å ³)	613.68 (9)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.77
Crystal size (mm)	0.03 × 0.02 × 0.01
Data collection	
Diffractometer	Agilent Technologies Xcalibur Eos
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5341, 3672, 2465
R_{int}	0.030
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.038, 0.074, 0.81
No. of reflections	3672
No. of parameters	317
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.41, -0.32
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.002 (11)

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae et al., 2008), *SHELXL2018* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2019). E75, 1724-1728 [https://doi.org/10.1107/S2056989019014038]

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

(2*E*,2'*E*)-1,1'-[Selenobis(4,1-phenylene)]bis[3-(4-chlorophenyl)prop-2-en-1-one]

Crystal data

C₃₀H₂₀Cl₂O₂Se

M_r = 562.32

Triclinic, *P*1

a = 4.9468 (3) Å

b = 5.8712 (6) Å

c = 21.3530 (18) Å

α = 85.019 (8)°

β = 84.094 (6)°

γ = 86.465 (7)°

V = 613.68 (9) Å³

Z = 1

F(000) = 284

D_x = 1.522 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 1538 reflections

θ = 3.9–28.9°

μ = 1.77 mm⁻¹

T = 293 K

Prism, yellow

0.03 × 0.02 × 0.01 mm

Data collection

Agilent Technologies Xcalibur Eos
diffractometer

Graphite monochromator

ω scans

5341 measured reflections

3672 independent reflections

2465 reflections with *I* > 2 σ (*I*)

*R*_{int} = 0.030

θ_{\max} = 28.0°, θ_{\min} = 2.9°

h = -6→6

k = -7→5

l = -28→28

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2 σ (*F*²)] = 0.038

wR(*F*²) = 0.074

S = 0.81

3672 reflections

317 parameters

3 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[$\sigma^2(F_o^2) + (0.0181P)^2$]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

$\Delta\rho_{\max}$ = 0.41 e Å⁻³

$\Delta\rho_{\min}$ = -0.32 e Å⁻³

Absolute structure: Refined as an inversion twin

Absolute structure parameter: 0.002 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.41094 (7)	0.32993 (9)	0.51703 (4)	0.0688 (2)
C11	2.5172 (3)	0.7697 (3)	0.08312 (8)	0.0590 (4)
C12	2.0618 (3)	-0.0037 (3)	0.97993 (8)	0.0649 (5)
O1	1.4087 (9)	-0.1409 (9)	0.3126 (3)	0.0780 (15)
O2	0.9496 (10)	0.8409 (8)	0.7498 (2)	0.0823 (16)
C1	0.7186 (10)	0.2486 (11)	0.4597 (3)	0.0479 (15)
C2	0.8352 (11)	0.0295 (12)	0.4605 (3)	0.0615 (18)
H1	0.768523	-0.081384	0.490939	0.074*
C3	1.0483 (12)	-0.0293 (12)	0.4171 (3)	0.0593 (17)
H2	1.122475	-0.178850	0.418221	0.071*
C4	1.1520 (10)	0.1346 (11)	0.3718 (3)	0.0444 (14)
C5	1.0451 (11)	0.3551 (11)	0.3723 (3)	0.0503 (16)
H3	1.120388	0.468932	0.343979	0.060*
C6	0.8227 (12)	0.4092 (12)	0.4153 (3)	0.0553 (18)
H4	0.744240	0.557370	0.413526	0.066*
C7	1.3680 (11)	0.0604 (11)	0.3220 (3)	0.0507 (15)
C8	1.5292 (10)	0.2372 (11)	0.2840 (3)	0.0461 (15)
H5	1.522998	0.383771	0.297588	0.055*
C9	1.6809 (10)	0.1939 (11)	0.2315 (3)	0.0457 (15)
H6	1.666213	0.051207	0.216721	0.055*
C10	1.8698 (9)	0.3462 (10)	0.1941 (3)	0.0439 (14)
C11	2.0024 (10)	0.2799 (11)	0.1368 (3)	0.0499 (15)
H7	1.958306	0.143756	0.122056	0.060*
C12	2.1960 (11)	0.4092 (11)	0.1015 (3)	0.0534 (16)
H8	2.277520	0.364813	0.062900	0.064*
C13	2.2653 (10)	0.6084 (11)	0.1255 (3)	0.0464 (15)
C14	2.1353 (11)	0.6771 (12)	0.1810 (3)	0.0479 (15)
H9	2.180794	0.813002	0.195644	0.057*
C15	1.9411 (10)	0.5512 (11)	0.2153 (3)	0.0484 (15)
H10	1.855730	0.601551	0.252860	0.058*
C16	0.5992 (10)	0.4225 (11)	0.5837 (3)	0.0498 (16)
C17	0.7975 (12)	0.2824 (11)	0.6111 (3)	0.0577 (18)
H11	0.848615	0.141757	0.595285	0.069*
C18	0.9211 (12)	0.3470 (11)	0.6615 (3)	0.0542 (16)
H12	1.051962	0.248547	0.679406	0.065*
C19	0.8519 (11)	0.5582 (11)	0.6859 (3)	0.0457 (14)

C20	0.6508 (12)	0.6967 (12)	0.6588 (3)	0.0580 (17)
H13	0.596947	0.836179	0.675061	0.070*
C21	0.5295 (10)	0.6326 (11)	0.6087 (3)	0.0509 (15)
H14	0.398311	0.731000	0.590920	0.061*
C22	0.9847 (12)	0.6393 (11)	0.7381 (3)	0.0540 (16)
C23	1.1622 (12)	0.4833 (11)	0.7744 (3)	0.0510 (16)
H15	1.186238	0.331934	0.764354	0.061*
C24	1.2909 (10)	0.5463 (11)	0.8210 (3)	0.0499 (15)
H16	1.258745	0.697969	0.830360	0.060*
C25	1.4776 (10)	0.4073 (10)	0.8597 (3)	0.0453 (14)
C26	1.5525 (11)	0.4873 (11)	0.9142 (3)	0.0574 (17)
H17	1.481261	0.629389	0.925872	0.069*
C27	1.7295 (11)	0.3629 (12)	0.9516 (3)	0.0553 (16)
H18	1.775600	0.419691	0.988224	0.066*
C28	1.8357 (10)	0.1557 (11)	0.9342 (3)	0.0505 (16)
C29	1.7647 (11)	0.0694 (11)	0.8801 (3)	0.0529 (17)
H19	1.836285	-0.073216	0.868869	0.063*
C30	1.5893 (10)	0.1942 (10)	0.8431 (3)	0.0522 (16)
H20	1.544135	0.136366	0.806609	0.063*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0439 (3)	0.1060 (6)	0.0592 (4)	-0.0158 (3)	0.0067 (3)	-0.0279 (4)
Cl1	0.0504 (8)	0.0624 (11)	0.0618 (11)	-0.0106 (7)	0.0025 (7)	0.0047 (9)
Cl2	0.0606 (9)	0.0696 (12)	0.0622 (11)	0.0083 (9)	-0.0051 (8)	-0.0008 (10)
O1	0.101 (4)	0.052 (3)	0.075 (4)	-0.015 (3)	0.031 (3)	-0.013 (3)
O2	0.130 (4)	0.054 (3)	0.068 (3)	0.025 (3)	-0.035 (3)	-0.024 (3)
C1	0.038 (3)	0.067 (5)	0.042 (4)	-0.014 (3)	-0.004 (2)	-0.013 (3)
C2	0.061 (4)	0.075 (5)	0.047 (4)	-0.024 (4)	0.017 (3)	-0.010 (4)
C3	0.066 (4)	0.053 (4)	0.057 (5)	-0.020 (3)	0.011 (3)	-0.004 (4)
C4	0.040 (3)	0.060 (4)	0.036 (3)	-0.012 (3)	-0.003 (2)	-0.014 (3)
C5	0.057 (4)	0.059 (4)	0.033 (4)	-0.009 (3)	0.004 (3)	-0.002 (3)
C6	0.051 (4)	0.061 (5)	0.057 (5)	-0.010 (3)	-0.004 (3)	-0.019 (4)
C7	0.056 (3)	0.054 (4)	0.043 (4)	-0.016 (3)	0.007 (3)	-0.013 (3)
C8	0.046 (3)	0.053 (4)	0.039 (4)	-0.007 (3)	0.006 (3)	-0.016 (3)
C9	0.041 (3)	0.050 (4)	0.046 (4)	0.002 (3)	-0.004 (3)	-0.002 (3)
C10	0.039 (3)	0.048 (4)	0.045 (3)	0.003 (3)	0.000 (2)	-0.010 (3)
C11	0.060 (4)	0.046 (4)	0.045 (4)	-0.002 (3)	0.002 (3)	-0.017 (3)
C12	0.056 (4)	0.063 (5)	0.040 (4)	-0.012 (3)	0.012 (3)	-0.011 (3)
C13	0.037 (3)	0.056 (4)	0.042 (3)	0.007 (3)	-0.003 (2)	0.012 (3)
C14	0.053 (3)	0.050 (4)	0.040 (4)	-0.003 (3)	-0.001 (3)	-0.004 (3)
C15	0.048 (3)	0.059 (4)	0.038 (3)	0.002 (3)	0.002 (3)	-0.013 (3)
C16	0.036 (3)	0.062 (4)	0.050 (4)	-0.019 (3)	0.013 (3)	-0.010 (3)
C17	0.061 (4)	0.047 (4)	0.065 (5)	-0.003 (3)	0.007 (3)	-0.016 (4)
C18	0.064 (4)	0.053 (4)	0.045 (4)	-0.008 (3)	0.006 (3)	-0.012 (3)
C19	0.049 (3)	0.050 (4)	0.036 (3)	-0.003 (3)	0.006 (3)	-0.005 (3)
C20	0.064 (4)	0.059 (4)	0.049 (4)	0.002 (3)	0.009 (3)	-0.014 (3)

C21	0.045 (3)	0.060 (4)	0.047 (4)	0.000 (3)	0.003 (3)	-0.009 (3)
C22	0.066 (4)	0.054 (4)	0.037 (3)	0.016 (3)	0.004 (3)	-0.003 (3)
C23	0.075 (4)	0.038 (4)	0.039 (4)	-0.003 (3)	0.004 (3)	-0.002 (3)
C24	0.056 (3)	0.049 (4)	0.042 (3)	0.002 (3)	0.006 (3)	-0.004 (3)
C25	0.045 (3)	0.046 (4)	0.044 (4)	-0.005 (3)	0.006 (3)	-0.009 (3)
C26	0.059 (4)	0.052 (4)	0.061 (5)	0.000 (3)	0.006 (3)	-0.015 (4)
C27	0.050 (3)	0.069 (5)	0.047 (4)	0.008 (3)	-0.002 (3)	-0.019 (3)
C28	0.040 (3)	0.059 (4)	0.049 (4)	-0.002 (3)	0.006 (3)	0.001 (3)
C29	0.060 (4)	0.042 (4)	0.057 (4)	0.016 (3)	-0.012 (3)	-0.012 (3)
C30	0.056 (3)	0.052 (4)	0.050 (4)	-0.004 (3)	-0.002 (3)	-0.020 (3)

Geometric parameters (Å, °)

Se1—C1	1.916 (5)	C14—C15	1.362 (8)
Se1—C16	1.913 (6)	C14—H9	0.9300
C11—C13	1.741 (6)	C15—H10	0.9300
C12—C28	1.737 (6)	C16—C17	1.385 (8)
O1—C7	1.217 (7)	C16—C21	1.396 (8)
O2—C22	1.229 (7)	C17—C18	1.383 (9)
C1—C2	1.376 (8)	C17—H11	0.9300
C1—C6	1.364 (8)	C18—C19	1.396 (8)
C2—C3	1.377 (8)	C18—H12	0.9300
C2—H1	0.9300	C19—C20	1.387 (7)
C3—C4	1.386 (8)	C19—C22	1.477 (8)
C3—H2	0.9300	C20—C21	1.371 (8)
C4—C5	1.368 (8)	C20—H13	0.9300
C4—C7	1.500 (7)	C21—H14	0.9300
C5—C6	1.398 (8)	C22—C23	1.459 (7)
C5—H3	0.9300	C23—C24	1.325 (8)
C6—H4	0.9300	C23—H15	0.9300
C7—C8	1.482 (8)	C24—C25	1.466 (7)
C8—C9	1.317 (8)	C24—H16	0.9300
C8—H5	0.9300	C25—C26	1.383 (8)
C9—C10	1.462 (8)	C25—C30	1.395 (7)
C9—H6	0.9300	C26—C27	1.380 (8)
C10—C11	1.401 (7)	C26—H17	0.9300
C10—C15	1.400 (8)	C27—C28	1.361 (8)
C11—C12	1.380 (7)	C27—H18	0.9300
C11—H7	0.9300	C28—C29	1.387 (8)
C12—C13	1.392 (8)	C29—C30	1.369 (7)
C12—H8	0.9300	C29—H19	0.9300
C13—C14	1.369 (8)	C30—H20	0.9300
C1—Se1—C16	99.0 (2)	C17—C16—C21	117.4 (6)
C2—C1—C6	118.2 (5)	C17—C16—Se1	122.2 (5)
C2—C1—Se1	122.1 (5)	C21—C16—Se1	120.3 (5)
C6—C1—Se1	119.7 (5)	C18—C17—C16	121.4 (6)
C1—C2—C3	121.5 (6)	C18—C17—H11	119.3

C1—C2—H1	119.2	C16—C17—H11	119.3
C3—C2—H1	119.2	C17—C18—C19	120.8 (6)
C2—C3—C4	120.0 (6)	C17—C18—H12	119.6
C2—C3—H2	120.0	C19—C18—H12	119.6
C4—C3—H2	120.0	C20—C19—C18	117.6 (6)
C5—C4—C3	119.0 (5)	C20—C19—C22	119.4 (6)
C5—C4—C7	122.4 (5)	C18—C19—C22	123.0 (6)
C3—C4—C7	118.5 (6)	C21—C20—C19	121.5 (6)
C4—C5—C6	120.0 (6)	C21—C20—H13	119.3
C4—C5—H3	120.0	C19—C20—H13	119.3
C6—C5—H3	120.0	C20—C21—C16	121.3 (6)
C1—C6—C5	121.2 (6)	C20—C21—H14	119.4
C1—C6—H4	119.4	C16—C21—H14	119.4
C5—C6—H4	119.4	O2—C22—C19	119.4 (6)
O1—C7—C8	120.5 (6)	O2—C22—C23	120.2 (6)
O1—C7—C4	120.7 (6)	C19—C22—C23	120.4 (6)
C8—C7—C4	118.7 (6)	C24—C23—C22	123.3 (6)
C9—C8—C7	122.3 (6)	C24—C23—H15	118.3
C9—C8—H5	118.9	C22—C23—H15	118.3
C7—C8—H5	118.9	C23—C24—C25	128.2 (6)
C8—C9—C10	127.0 (6)	C23—C24—H16	115.9
C8—C9—H6	116.5	C25—C24—H16	115.9
C10—C9—H6	116.5	C26—C25—C30	117.6 (5)
C11—C10—C15	117.6 (6)	C26—C25—C24	120.2 (6)
C11—C10—C9	119.8 (6)	C30—C25—C24	122.2 (6)
C15—C10—C9	122.5 (6)	C27—C26—C25	122.1 (6)
C12—C11—C10	122.4 (6)	C27—C26—H17	118.9
C12—C11—H7	118.8	C25—C26—H17	118.9
C10—C11—H7	118.8	C28—C27—C26	119.0 (6)
C13—C12—C11	117.8 (6)	C28—C27—H18	120.5
C13—C12—H8	121.1	C26—C27—H18	120.5
C11—C12—H8	121.1	C27—C28—C29	120.6 (5)
C12—C13—C14	120.5 (6)	C27—C28—C12	120.1 (5)
C12—C13—C11	118.7 (5)	C29—C28—C12	119.3 (5)
C14—C13—C11	120.8 (6)	C30—C29—C28	120.0 (6)
C15—C14—C13	121.6 (7)	C30—C29—H19	120.0
C15—C14—H9	119.2	C28—C29—H19	120.0
C13—C14—H9	119.2	C29—C30—C25	120.7 (6)
C14—C15—C10	120.1 (6)	C29—C30—H20	119.7
C14—C15—H10	120.0	C25—C30—H20	119.7
C10—C15—H10	120.0		
C6—C1—C2—C3	-1.1 (9)	C21—C16—C17—C18	0.4 (9)
Se1—C1—C2—C3	176.9 (5)	Se1—C16—C17—C18	-176.5 (5)
C1—C2—C3—C4	0.7 (10)	C16—C17—C18—C19	-0.9 (10)
C2—C3—C4—C5	2.0 (9)	C17—C18—C19—C20	1.6 (9)
C2—C3—C4—C7	-174.9 (6)	C17—C18—C19—C22	-177.7 (6)
C3—C4—C5—C6	-4.2 (9)	C18—C19—C20—C21	-2.0 (9)

C7—C4—C5—C6	172.5 (6)	C22—C19—C20—C21	177.4 (5)
C2—C1—C6—C5	-1.3 (9)	C19—C20—C21—C16	1.5 (9)
Se1—C1—C6—C5	-179.3 (5)	C17—C16—C21—C20	-0.7 (8)
C4—C5—C6—C1	4.0 (10)	Se1—C16—C21—C20	176.2 (4)
C5—C4—C7—O1	-160.6 (6)	C20—C19—C22—O2	-12.2 (9)
C3—C4—C7—O1	16.1 (9)	C18—C19—C22—O2	167.1 (6)
C5—C4—C7—C8	18.7 (8)	C20—C19—C22—C23	169.6 (6)
C3—C4—C7—C8	-164.5 (5)	C18—C19—C22—C23	-11.1 (9)
O1—C7—C8—C9	13.7 (10)	O2—C22—C23—C24	0.5 (10)
C4—C7—C8—C9	-165.7 (5)	C19—C22—C23—C24	178.8 (5)
C7—C8—C9—C10	-172.9 (5)	C22—C23—C24—C25	-178.6 (5)
C8—C9—C10—C11	-175.5 (6)	C23—C24—C25—C26	-167.4 (6)
C8—C9—C10—C15	9.4 (8)	C23—C24—C25—C30	13.7 (9)
C15—C10—C11—C12	-0.3 (8)	C30—C25—C26—C27	-0.5 (9)
C9—C10—C11—C12	-175.6 (5)	C24—C25—C26—C27	-179.4 (5)
C10—C11—C12—C13	2.1 (8)	C25—C26—C27—C28	0.6 (10)
C11—C12—C13—C14	-2.9 (8)	C26—C27—C28—C29	-0.8 (9)
C11—C12—C13—C11	177.9 (4)	C26—C27—C28—C12	179.3 (5)
C12—C13—C14—C15	1.9 (9)	C27—C28—C29—C30	0.9 (9)
C11—C13—C14—C15	-178.9 (4)	C12—C28—C29—C30	-179.2 (5)
C13—C14—C15—C10	0.0 (8)	C28—C29—C30—C25	-0.8 (9)
C11—C10—C15—C14	-0.8 (8)	C26—C25—C30—C29	0.6 (9)
C9—C10—C15—C14	174.4 (5)	C24—C25—C30—C29	179.5 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C29—H19...O2 ⁱ	0.93	2.63	3.218 (8)	122

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