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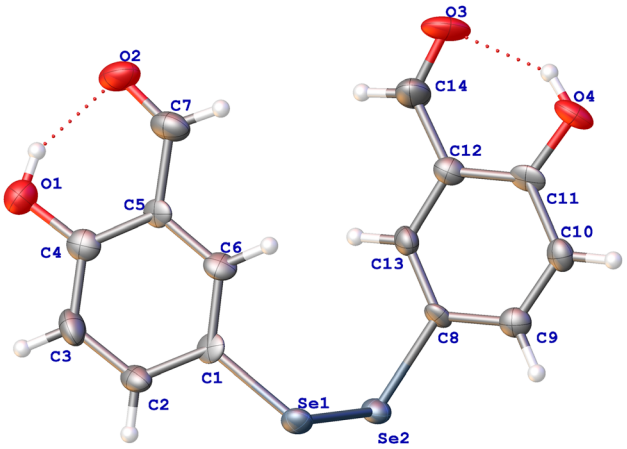
The crystal structure of 5,5′-diselanediyl-bis(2-hydroxybenzaldehyde), $C_{14}H_{10}O_4Se_2$



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Abstract

$C_{14}H_{10}O_4Se_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.6836(11) Å, b = 8.9933(11) Å, c = 11.5062(19) Å, α = 77.128(12)°, β = 87.684(14)°, γ = 89.975(12)°, V = 673.65(18) Å^3, Z = 2, $R_{gt}(F)$ = 0.0564, w$R_{ref}(F^2)$ = 0.1512, T = 293 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The chemical reagents used in the reaction were all purchased from commercial companies and without further purification. The synthesis of the title molecule is similar to the procedure reported in the literature [4], and a yellow needle crystal is used for the single crystal X-ray analysis.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.12 × 0.10 × 0.09 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	5.50 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4100, 2365, 0.042
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 1886
$N(param)_{refined}$:	183
Programs:	Bruker [1], SHELX [2, 3]

Experimental details

The C-bound H atoms were geometrically placed (C—H = 0.95–0.98 Å) and refined as riding with U_{iso}(H) = 1.2–1.5 U_{eq}(C).

Comment

Organoselenium compounds have attracted great interest because of their unique properties and applications in various fields, especially for public health and disease therapy. For example, organoselenium derivatives exhibit antioxidant, antiviral, anti-microbial and antitumour effects [5–8]. Diselenides are important reagents or precursors for the synthesis of organoselenium compounds [9]. Therein, a new molecule was prepared and characterized by single-crystal X-ray diffraction.

In this title crystal structure, two salicylaldehyde units are linked by two selenium atoms. Meanwhile, the carbon and oxygen atoms in salicylaldehyde unit is almost coplanar with the linked selenium. It can be seen that the torsion angle of C(1)–Se(1)–Se(2)–C(8) is 82.98°. The bond angle of C1–Se1–Se2 and C8–Se2–Se1 are 101.45(19)° and 101.6(2)°, respectively. The Se1–Se2 single bond length is 2.3465(11) Å, the value which is shorter than those reported in publications [10, 11]. The bond length of Se1–C1 and Se2–C8 are 1.924(7) and 1.930(5) Å, respectively. The title molecule contains two hydrogen bonds,

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.26529 (9)	−0.03005 (7)	0.17022 (7)	0.0258 (3)
Se2	0.31435 (9)	0.18881 (7)	0.01671 (6)	0.0245 (3)
O1	−0.3861 (7)	0.1874 (6)	0.4771 (5)	0.0388 (13)
H1	−0.346618	0.259561	0.502958	0.058*
O2	−0.0945 (8)	0.3329 (6)	0.5609 (6)	0.0457 (15)
O3	0.5943 (8)	0.6358 (6)	0.3519 (6)	0.0494 (16)
O4	0.9131 (7)	0.5407 (5)	0.2369 (5)	0.0373 (14)
H4	0.858510	0.588143	0.282323	0.056*
C1	0.0646 (9)	0.0383 (7)	0.2706 (6)	0.0220 (14)
C2	−0.1353 (9)	−0.0061 (7)	0.2675 (6)	0.0265 (16)
H2	−0.170181	−0.066900	0.215676	0.032*
C3	−0.2827 (9)	0.0396 (8)	0.3408 (7)	0.0334 (18)
H3	−0.413024	0.002696	0.342388	0.040*
C4	−0.2356 (10)	0.1398 (7)	0.4113 (7)	0.0274 (16)
C5	−0.0349 (9)	0.1839 (7)	0.4171 (6)	0.0214 (14)
C6	0.1125 (9)	0.1315 (7)	0.3458 (6)	0.0245 (15)
H6	0.245314	0.160291	0.349381	0.029*
C7	0.0211 (12)	0.2844 (8)	0.4949 (7)	0.0358 (18)
H7	0.155057	0.312979	0.493387	0.043*
C8	0.5005 (8)	0.3046 (7)	0.0863 (6)	0.0195 (14)
C9	0.7045 (9)	0.2985 (7)	0.0590 (6)	0.0256 (16)
H9	0.750299	0.237933	0.007834	0.031*
C10	0.8396 (9)	0.3814 (7)	0.1071 (7)	0.0261 (16)
H10	0.975028	0.380615	0.085306	0.031*
C11	0.7726 (9)	0.4669 (6)	0.1890 (6)	0.0244 (16)
C12	0.5656 (9)	0.4742 (7)	0.2164 (6)	0.0238 (15)
C13	0.4331 (9)	0.3931 (7)	0.1625 (6)	0.0242 (15)
H13	0.296210	0.399059	0.178592	0.029*
C14	0.4887 (11)	0.5630 (8)	0.2986 (8)	0.039 (2)
H14	0.350731	0.565165	0.312097	0.047*

each consisting of the OH group and the adjacent carbonyl oxygen in the salicylaldehyde unit.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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