

1771
MW

C₄H₈Se

Tetrahydroselenophene

C₂

α D₄-¹²C₄H₄⁸⁰Se

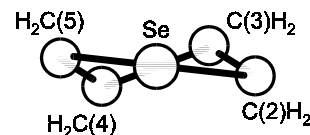
r_s	Å ^{a)}	θ_s	deg ^{a)}
C–Se	1.9630(15)	C–Se–C	90.33(9)
C(2)–C(3)	1.5346(30)	Se–C–C	105.51(15)
C(3)–C(4)	1.5240(24)	C–C–C	107.64(21)
		ϕ ^{b)}	28.19(42)



Atom	a_s [Å]	b_s [Å]	c_s [Å]
Se	0.8642	0.0	0.0
C(2)	–0.5199	1.3877	0.1095
C(3)	–1.8262	0.6979	–0.3060
C(4)	–1.8262	–0.6979	0.3060
C(5)	–0.5199	–1.3877	–0.1095
D(6)	–0.5663	1.7459	1.1406
D(7)	–0.2183	2.2122	–0.5468
D(12)	–0.2183	–2.2122	0.5468
D(13)	–0.5663	–1.7459	–1.1406

^{a)} Three times the uncertainties of the original data.

^{b)} Dihedral angle of the ring twist between the C(2)SeC(5) and C(3)...Se...C(4) planes.



Galeev, R.V., Gunderova, L.N., Mamleev, A.Kh., Magdesieva, N.N., Pozdeev, N.M.: Zh. Strukt. Khim. **33** No.2 (1992) 48; Russ. J. Struct. Chem. (Engl. Transl.) **33** (1992) 196.

ED

r_a	Å ^{a)}	θ_a	deg ^{a)}
Se–C	1.975(3)	C–Se–C	89.1(5)
C–C	1.538(4)	Se–C–C	105.8(3)
C–H	1.116(12)	C–C–C	106.0(7)
		τ_1 ^{b)}	15.4(5)
		τ_2 ^{c)}	–42.7(14)
		τ_3 ^{d)}	56.9(17)

The nozzle temperature was ≈ 65 °C.

^{a)} Estimated standard errors.

^{b)} Torsional angle C(5)–Se–C(2)–C(3).

^{c)} Torsional angle Se–C(2)–C(3)–C(4).

^{d)} Torsional angle C(2)–C(3)–C(4)–C(5).

Náhlovská, Z., Náhlovský, B., Seip, H.M.: Acta Chem. Scand. **24** (1970) 1903.