

1226
MW

C₃H₅NSe

Ethyl selenocyanate

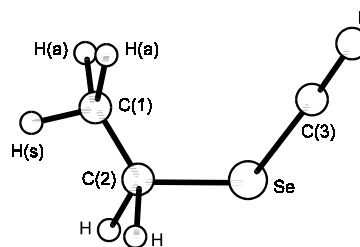
C_s (*gauche*)
H₃C–CH₂–Se–C≡N

r_0	Å	θ_0	deg ^{a)}
C(1)–H(s)	1.079 ^{a)}	H–C(2)–Se	109.3 ^{a)}
C(1)–H(a)	1.091 ^{a)}	H(a)–C(1)–C(2)	110.47 ^{a)}
C(1)–C(2)	1.537 ^{a)}	H(s)–C(1)–C(2)	111.08 ^{a)}
C(3)≡N	1.162 ^{a)}	H–C(2)–H	111.4 ^{a)}
C(2)–H	1.094 ^{a)}	H(a)–C(1)–H(a)	107.85 ^{a)}
C(2)–Se	1.954(10)	Se–C(3)≡N	180 ^{a)}
Se–C(3)	1.836(10)	C(2)–Se–C(3)	97.0(20)
		C(1)–C(2)–Se	113.1(20)
		ϕ ^{b)}	58.95(150)

Only one conformer (*gauche*) was identified.

^{a)} Assumed.

^{b)} Dihedral angle C–C–Se–C from *syn*.



Sakaizumi, T., Itakura, T.: J. Mol. Spectrosc. **163** (1994) 1.