

1656
ED

C₄H₆OS

Divinyl sulfoxide
1,1-Sulfinylbisethene

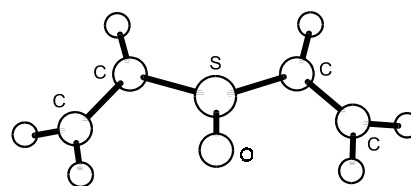
C_s (main conformer)
H₂C=CH–S(O)–CH=CH₂

| r_g | Å ^{a)} | θ_a | deg ^{a)} |
|-------|-----------------|------------------------|-------------------|
| S=O | 1.477(3) | C–S–C | 99.2(18) |
| C=C | 1.330(3) | S–C=C | 118.5(8) |
| C–H | 1.091(5) | C–S=O | 107.5(14) |
| S–C | 1.785(4) | C=C–H | 124.2(10) |
| | | τ_1 ^{b)} | 121(4) |
| | | τ_2 ^{b)} | –121(4) |

The molecule exists as a mixture of conformers with different torsional angles (τ_1 , τ_2). The main conformer (78(17)%) has C_s symmetry and τ_1 , τ_2 listed above; i.e., the C=C bonds are eclipsed with respect to the S=O bond. Other conformers in the mixture could have the torsional angles (0°, –120°) and/or (120°, 120°), also the C=C bonds eclipsing a bond or the lone electron pair of sulfur. The presence of further forms is also possible.
The nozzle temperature was 82 °C.

^{a)} Estimated total errors.

^{b)} Torsional angle C=C–S–C; $\tau_1 = \tau_2 = 0^\circ$ for the *syn-syn* C=C–S–C=C chain.



Rozsondai, B., Horváth, Z.E.: J. Chem. Soc. Perkin Trans. II (1993) 1175.