

1280
MW

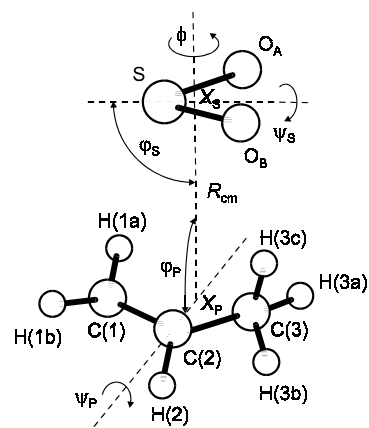
C₃H₆O₂S

Propylene – sulfur dioxide (1/1)
(weakly bound complex)

C₁
H₂C=CH–CH₃ · SO₂

r_0	\AA	θ_0	deg
R_{cm} ^{a)}	3.26(5)	φ_{S} ^{b)}	93.1(7)
		φ_{P} ^{b)}	96.3(3)
		ψ_{S} ^{c)}	89.9(2)
		ψ_{P} ^{d)}	82.1(1)
		ϕ ^{e)}	–60.1(1)

	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
O _A	1.284	–0.688	1.079
O _B	1.247	1.216	–0.494
S	1.323	–0.194	–0.264
X _S	1.294	0.035	0.014
X _P	–1.969	–0.053	–0.022
C(1)	–1.763	–1.211	–0.522
C(2)	–2.020	0.109	–0.460
C(3)	–2.116	0.884	0.821
H(1a)	–1.610	–1.790	0.374
H(1b)	–1.704	–1.725	–1.471
H(2)	–2.162	0.620	–1.400
H(3a)	–1.952	0.239	1.686
H(3b)	–3.098	1.338	0.941
H(3c)	–1.373	1.667	0.865



Complex has a stacked, near parallel planes configuration. The sulfur atom is approximately above the propene double bond. The C₂ axis of SO₂ is nearly eclipsed with respect to the C–C single bond with the O atoms towards the methyl group.

^{a)} Distance between X_S and X_P; X_S and X_P are cm of SO₂ and propene, respectively.

^{b)} φ_{S} is the tilt angle of the C₂ axis of SO₂ with respect to R_{cm} and φ_{P} is formed between R_{cm} and X_P...C(2) of propylene.

^{c)} The twist of the SO₂ plane with respect to R_{cm} , O_B–S–X_S–X_P.

^{d)} The twist of the propene plane with respect to R_{cm} , C(1)–C(2)–X_P–X_S.

^{e)} Dihedral angle S–X_S–X_P–C(2).

Xu, L.-W., Kuczkowski, R.L.: J. Chem. Phys. **100** (1994) 15.