

1668
MW

C₄H₆O₂S

1,3-Butadiene – sulfur dioxide (1/1)
(weakly bound complex)

C₁
H₂C=CH–CH=CH₂ · SO₂

r_0	Å	θ_0	deg
R_{cm}	3.3192(2)	$\Theta_S (X_B \dots X_S \dots S)^a$	96.5(7)
		$\Theta_B (X_S \dots X_B - C(2))$	81.1(6)
		$\Psi_S (X_B \dots X_S \dots S - O_B)^b$	90.6(4)
		$\Psi_B (C(1) - C(2) - X_B \dots X_S)^c$	109.8(5)
		$\Phi (S \dots X_S \dots X_B - C(3))^d$	-44.2(3)

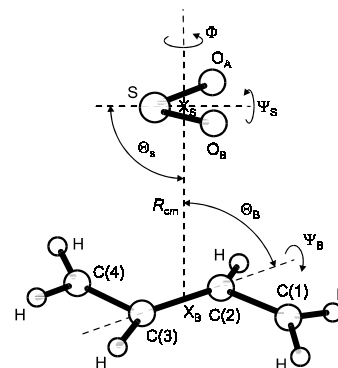
The two molecular planes are close to parallel.

^a) A value of θ_S greater than 90° implies that the sulfur end is tipped away from butadiene.

^b) A value of Ψ_S larger than 90° implies that O_A is tipped toward butadiene and O_B is away.

^c) A value of Ψ_B greater than 90° implies that C(4) is tipped toward SO₂ and C(1) is tipped away.

^d) The torsional angle Φ is viewed along R_{cm} from SO₂ to butadiene. It is 0° when the C₂ axis of SO₂ and the C(2)–C(3) bond axis are eclipsed and S is over C(3). The negative sign implies that C(3)–X_B is rotated counter-clockwise from S...X_S.



X_S and X_B are the centers of mass of SO₂ and butadiene, respectively

Xu, L.-W., Taleb-Bendiab, A., Nemes, L., Kuczkowski, R.L.: J. Am. Chem. Soc. **115** (1993) 5723.