

1168
MW

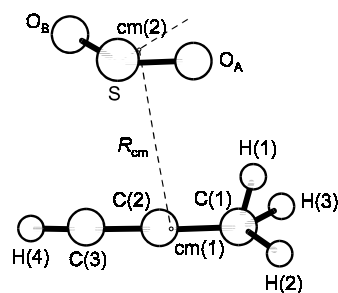
C₃H₄O₂S

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

C₁
H₃C–C≡CH · SO₂

r_0	Å	θ_0	deg
R_{cm}	3.382(10)	C(3)...cm(1)...cm(2)	77.81(27)
		S...cm(2)...cm(1)	86.48(99)
		S...cm(2)...cm(1)...C(3)	58.36(43)
		O _A ...S...cm(2)...cm(1)	73.53(25)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)	2.483	−0.956	0.284
C(2)	2.014	0.393	−0.014
C(3)	1.627	1.508	−0.261
H(1)	1.624	−1.643	0.399
H(2)	3.126	−1.327	−0.535
H(3)	3.067	−0.959	1.222
H(4)	1.288	2.484	−0.477
S	−1.282	−0.031	−0.351
O _A	−0.818	−1.353	−0.048
O _B	−1.788	0.797	0.705



SO₂ sits above the carbon-carbon triple bond, with one of the S–O bonds roughly parallel to the symmetry axis of methylacetylene.

Tan, X.-Q., Xu, L.-W., Tubergen, M.J., Kuczkowski, R.L.: J. Chem. Phys. **101** (1994) 6512.