

1407
MW

C₃H₉NO₂S

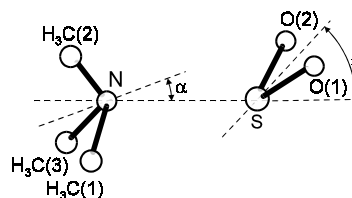
Trimethylamine – sulfur dioxide (1/1)
(weakly bound complex)

C_s
(effective symmetry class)
(CH₃)₃N · SO₂

r_0	Å ^{a)}	θ_0	deg ^{a)}
N–S	2.285(30)	S–N–C(2)	104.3(20)
S–O	1.435(20)	S–N–C(1,3)	107.6(20)
N–C(1,3)	1.468(20)	O–S–O	117.9(20)
N–C(2)	1.455(20)	O–S–N	95.6(20)
		C(2)–N–C(1,3)	112.6(15)
		C(1)–N–C(3)	111.7(15)
		α^b	0.8(20)
		β^b	79.0(30)

r_s	Å ^{a)}	θ_s	deg ^{a)}
N–S	2.260(30)	S–N–C(2)	104.3(20)
S–O	1.444(10)	S–N–C(1,3)	107.9(20)
N–C(1,3)	1.461(15)	O–S–O	116.9(20)
N–C(2)	1.468(10)	O–S–N	95.9(20)
		C(2)–N–C(1,3)	111.8(10)
		C(1)–N–C(3)	112.6(10)
		α^b	0.8(10)
		β^b	78.5(20)

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
S	1.147	0.0	0.428
O	1.434	1.230	0.271
N	1.072	0.0	0.0
C(2)	1.157	0.0	1.466
C(1,3)	1.641	1.216	0.577



The structure of this complex is consistent with the nitrogen lone pair pointing toward the sulfur atom, with the SO₂ plane tilted by $\approx 75^\circ$ from the C₃ axis of the trimethylamine. The methyl groups are staggered with respect to the oxygen atoms.

^{a)} Uncertainties were not given in the original paper.

^{b)} See figure for definition.

Oh, J.J., LaBarge, M.S., Matos, J., Kampf, J.W., Hillig, K.W., Kuczkowski, R.L.: J. Am. Chem. Soc. **113** (1991) 4732.