

64 MW	BF₃O₂S	Sulfur dioxide – trifluoroborane (1/1) (weakly bound complex)	C_s (<i>anti-syn</i>)
			(effective symmetry class) (large-amplitude motion) SO ₂ · BF ₃

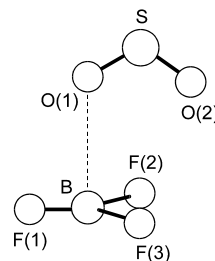
r_0	Å ^{a)}	θ_0	deg ^{a)}
B...O(1)	2.600(5)	B...O(1)=S	135.0(5)
		B...O(1)=S=O(2)	0.0 ^{b)}
		F(1)–B...O(1)=S	180.0 ^{b)}
		F(2)–B...O(1)=S	–60.0 ^{b)}
		F(3)–B...O(1)=S	60.0 ^{b)}

The complex is an asymmetric top with the SO₂ located above the BF₃ plane. The oxygen end of the SO₂ triangle is directed towards the BF₃ with non-equivalent oxygen atoms. One oxygen atom sits on or nearly on the C₃ axis of the BF₃ about 2.6 Å from the boron atom, while the second oxygen lies above the fluorine perimeter of the BF₃. Two low-lying states are observed in the spectrum suggesting that a tunneling process occurs between equivalent nuclear frameworks.

The same rotational constants are obtained if the three F–B...O(1)=S dihedral angles are rotated ±60° or 180° to give a *syn-syn* conformer.

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

^{b)} Assumed.



Peebles, S.A., Sun, L., Kuczkowski, R.L., Nxumalo, L.M., Ford, T.A.: J. Mol. Struct. **471** (1998) 235.