

1569
MW

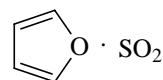
C₄H₄O₃S

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

C₁
(effective symmetry class)

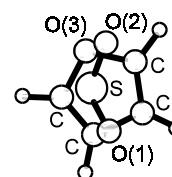
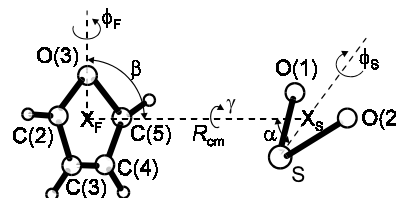
r_0	Å
R_{cm}	3.433(10) ^{a)}

θ_0	deg
$\alpha(\text{S}-\text{X}_\text{S}-\text{X}_\text{F})$ ^{b)}	52.5(24)
$\beta(\text{X}_\text{S}-\text{X}_\text{F}-\text{O}(3))$ ^{b)}	101.0(20) ^{a)}
$\phi_\text{S}(\text{O}(2)-\text{S}-\text{X}_\text{S}-\text{X}_\text{F})$ ^{c)}	-93.5(10)
$\phi_\text{F}(\text{C}(2)-\text{O}(3)-\text{X}_\text{F}-\text{X}_\text{S})$ ^{d)}	-98.2(11)
$\gamma(\text{S}-\text{X}_\text{S}-\text{X}_\text{F}-\text{O}(3))$ ^{e)}	65.6(42)



Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
O(1) ^{f)}	1.965	1.276	0.125
O(2) ^{f)}	2.055	1.191	0.202

The two C₂ axes of the monomer units are skewed by ≈65° and the plane of the SO₂ is tipped considerably from parallel to the furan plane, with the sulfur atom closest to the furan. While one oxygen in SO₂ lies approximately above the oxygen of the furan, the other is located closer to a β-carbon of the furan. A tunneling motion between two equivalent forms of the complex is suggested.



Projection in the
bc principal axis
plane.

- ^{a)} Uncertainty is larger than that of the original paper.
^{b)} X_F and X_S are the centers-of-mass of furan and SO₂, respectively.
^{c)} Dihedral angle of SO₂. See figure.
^{d)} Dihedral angle of furan. See figure.
^{e)} Torsional angle. See figure.
^{f)} For definition see figure.

Oh, J.J., Xu, L.W., Taleb-Bendiab, A., Hillig, K.W., Kuczkowski, R.L.: J. Mol. Spectrosc. **153** (1992) 497.