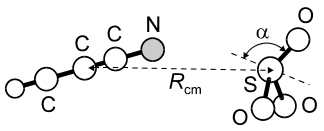
341 **C_3HNO_3S** **Cyanoacetylene – sulfur trioxide (1/1)** **C_{3v}**
MW 2-Propynenitrile – sulfur trioxide (1/1) (effective symmetry class)
(weakly bound complex) (large-amplitude motion)
$HC{\equiv}C{-}C{\equiv}N \cdot SO_3$

r_0	Å	θ_0	deg
N...S	2.567(13)	α [a])	91.7(4)



The vibrationally averaged structure of the complex is that of a symmetric top, with the HCCCN axis along the C_3 axis of the SO_3, and the nitrogen end near the sulfur atom. The observed N...S=O angle indicates a small but distinct distortion of the SO_3 group from the planarity.

[a]) See figure for the definition.

Hunt, S.W., Fiacco, D.L., Craddock, M., Leopold, K.R.: J. Mol. Spectrosc. **212** (2002) 213.