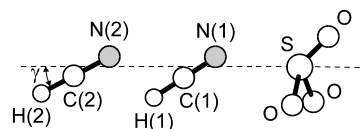


<b>223</b> MW	<b>C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S</b>	<b>Hydrogen cyanide – sulfur trioxide (2/1)</b> (weakly bound complex)	<b>C<sub>3v</sub></b> (effective symmetry class) (large-amplitude motion) 2(HC≡N) · SO <sub>3</sub>
------------------	--	---	--

$r_0$	Å	$\theta_0$	deg
N(1)...S	2.470(20)	N(1)...S=O	92.2(6)
N(2)...H(1)	2.213(29)	$\gamma^a$	9.4(10) <sup>b</sup>

The results indicate significant changes in the HCN · SO<sub>3</sub> subunit upon interaction with a single HCN “solvent” molecule, with relatively little change in the HCN...HCN interaction.



<sup>a</sup>) Deviation of HCN(2) from the equilibrium C<sub>3</sub> axis of the complex. See figure for the definition.

<sup>b</sup>) Uncertainty was not estimated in the original paper.

Fiacco, D.L., Hunt, S.W., Leopold, K.R.: J. Phys. Chem. A **104** (2000) 8323.