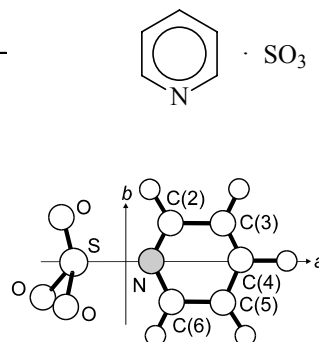


632  
MW $\text{C}_5\text{H}_5\text{NO}_3\text{S}$ **Pyridine – sulfur trioxide (1/1)**  
(weakly bound complex)**G<sub>12</sub>**  
(effective symmetry class)  
(large-amplitude motion)

$r_0$	Å	$\theta_0$	deg
N...S	1.915(1)	N...S=O	98.91(2)
N–C(2)	1.3409(6)	C(2)–N–C(6)	122.0(1)
C(2)–C(3)	1.3863(3)	N–C(2)–C(3)	120.55(6)
C(3)–C(4)	1.402(6)	C(2)–C(3)–C(4)	118.6(1)
N...C(4)	2.740		
S...C(4)	4.656		



The  $\text{SO}_3$  undergoes free or nearly free internal motion within the complex. The N...S bond length and the N...S=O angle, which were derived, indicate that the formation of the dative bond is nearly, but not entirely, complete. Small but significant changes in the heavy-atom ring structure of the pyridine upon complexation are also measured by a series of  $^{13}\text{C}$  substitution experiments.

Hunt, S.W., Leopold, K.R.: J. Phys. Chem. A **105** (2001) 5498.