

547
MW

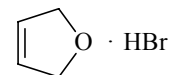
 $\text{C}_4\text{H}_7\text{BrO}$
2,5-Dihydrofuran – hydrogen bromide (1/1)

(weakly bound complex)

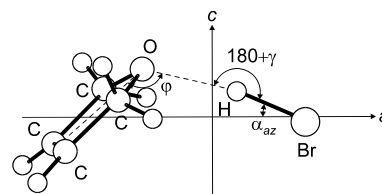
 C_s

 (effective symmetry class)
(large-amplitude motion)

r_0	Å	θ_0	deg	
			$\text{C}_4\text{H}_6\text{O} \cdot \text{H}^{79}\text{Br}$	$\text{C}_4\text{H}_6\text{O} \cdot \text{H}^{81}\text{Br}$
O...H	1.799(5)	α_{az} ^{a)}	23.674(4)	23.635(4)
		β ^{b)}	24.85(1)	24.87(1)
		φ ^{a)}	122.5(3)	
		γ ^{a)}	10.2(1)	



A detailed interpretation of the spectroscopic constants establishes that the complex has C_s symmetry, with the HBr subunit lying in the molecular symmetry plane and forming a hydrogen bond to the oxygen atom of 2,5-dihydrofuran.



^{a)} See figure for the definition.

^{b)} Average angle between the R_{cm} axis and the HBr molecular axis.

Cooke, S.A., Corlett, G.K., Evans, C.M., Legon, A.C.: J. Chem. Soc., Faraday Trans. **93** (1997) 2973.