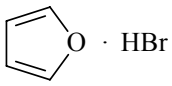
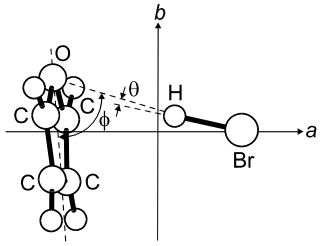
**518** **$C_4H_5BrO$** **Furan – hydrogen bromide (1/1)** **$C_s$**
MW (weakly bound complex) (large-amplitude motion)
(effective symmetry class)




| $r_0$ | Å |
|---|---|
| O...H | 2.599(3) |

| $\theta_0$ | deg |
|---|---|
| $\phi$ [a]) | 112.90(14) |
| $\theta$ [b]) | 6.05(4) |




The observed complex does not have $C_{2v}$ symmetry, with HBr lying along the $C_2$ axis of furan. Instead, the geometry is of the face-on type, with the Br atom of HBr lying close to the perpendicular drawn through the center of the mass of the furan ring. The H atom of HBr lies between the Br atom and the face of the furan ring. The angles made by the HBr internuclear axis *z* with the *a*-inertial axis has the two possible values, ±11.929°. The preferred structure is that generated when the positive value of the angle is chosen and has the HBr subunit pointing in the direction of the O atom of furan.

[a]) Angle made by the O…H internuclear line with the local $C_2$ axis of furan.
[b]) Angular deviation of the O…H–Br nuclei from collinearity.

Cole, G.C., Legon, A.C., Ottaviani, P.: J. Chem. Phys. **117** (2002) 2790.