

531  
MW

 $\text{C}_4\text{H}_6\text{KrO}$ 
**2,5-Dihydrofuran – krypton (1/1)**  
(weakly bound complex)

 $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$$\frac{r_0}{R_{\text{cm}}} \quad \frac{\text{\AA}}{3.635(8)}$$

$$\frac{\theta_0}{\varphi^{\text{a}}} \quad \frac{\text{deg}}{10.5(4)}$$

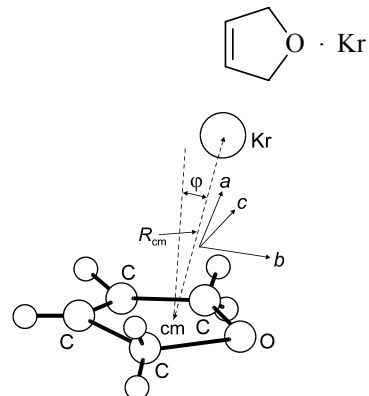
$$\frac{r_{\text{s}}}{R_{\text{cm}}} \quad \frac{\text{\AA}^{\text{b)}}{3.635(8)}$$

$$\frac{\theta_{\text{s}}}{\varphi^{\text{a}}} \quad \frac{\text{deg}^{\text{b)}}{8.4(4)}$$

$$\frac{r_{\text{e}}^{\text{c)}}}{R_{\text{cm}}} \quad \frac{\text{\AA}^{\text{b)}}{3.606(10)}$$

$$\frac{\theta_{\text{e}}^{\text{c)}}}{\varphi^{\text{a}}} \quad \frac{\text{deg}^{\text{b)}}{12.8(5)}$$

The intermolecular stretching force constant is  $3.260 \text{ N m}^{-1}$  and the dissociation energy is estimated to be *ca.*  $3.5 \text{ kJ mol}^{-1}$ .



<sup>a)</sup> Angle between the line connecting the Kr atom to cm and the normal to the ring plane, see figure for the definition.

<sup>b)</sup> Uncertainties were not estimated in the original paper.

<sup>c)</sup> Estimated by taking into account contributions of van der Waals modes, but not corrected for those of other vibrational modes.

Velino, B., Melandri, S., Maris, A., Favero, P.G., Caminati, W.: Mol. Phys. **98** (2000) 1919.