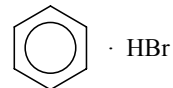


724  
MW**C<sub>6</sub>H<sub>7</sub>Br****Benzene – hydrogen bromide (1/1)**  
(weakly bound complex)**C<sub>6v</sub>**  
(effective symmetry class)  
(large-amplitude motion)

Isotopic species	$r_0(R_{\text{cm}})^{\text{a) b)}}$ [Å]	$r_0(\text{X} \cdots \text{Br})^{\text{a) b) c)}}$ [Å]	$\theta_0(\beta_{\text{av}})^{\text{d)}}$ [deg]
C <sub>6</sub> H <sub>6</sub> · H <sup>79</sup> Br	3.7624(30)	3.7803(30)	22.559(1)
C <sub>6</sub> H <sub>6</sub> · H <sup>81</sup> Br	3.7627(30)	3.7802(30)	22.556(1)
C <sub>6</sub> H <sub>6</sub> · D <sup>79</sup> Br	3.7539(30)	3.7893(30)	20.500(5)
C <sub>6</sub> H <sub>6</sub> · D <sup>81</sup> Br	3.7547(30)	3.7891(30)	20.505(11)
C <sub>6</sub> D <sub>6</sub> · H <sup>79</sup> Br	3.7595(30)	3.7775(30)	25.547(3)
C <sub>6</sub> D <sub>6</sub> · H <sup>81</sup> Br	3.7598(30)	3.7774(30)	22.547(4)



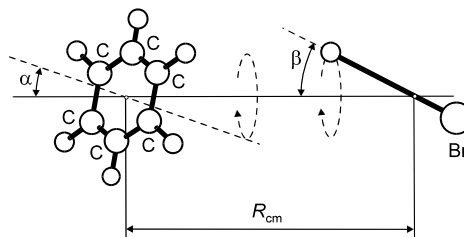
It is concluded that in the zero-point state the complex has effective C<sub>6v</sub> symmetry, with HBr oriented so that H lies closest to the benzene ring and undergoes a circular motion which allows it to sample the  $\pi$ -electron density of the ring. The intermolecular stretching force constant is 7.65 N m<sup>-1</sup>.

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

<sup>b)</sup>  $\alpha_{\text{av}} = 0^\circ$  was assumed. When  $\alpha_{\text{av}} = 30^\circ$ , the distance is reduced by 0.0376, 0.0371, 0.0374, 0.0370, 0.0438, 0.0432 Å for the six isotopomers, respectively.

<sup>c)</sup> X denotes the center of the benzene ring.

<sup>d)</sup> See figure for the definition.



Cooke, S.A., Corlett, G.K., Evans, C.M., Legon, A.C.: Chem. Phys. Lett. **272** (1997) 61.