

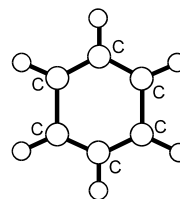
715 **C₆H₆**ED, *ab initio*
calculations**Benzene****D_{6h}** assumed

$r_e^a)$	$\text{\AA}^b)$
C–C	1.393(3)
C–H	1.086(4)

The equilibrium bond lengths were estimated using the ED data reported in [1,2], taken at room temperature. The structural analysis was based on the Morse-like potential function with $a_3(\text{C–C})$ and $a_3(\text{C–H})$ parameters assumed at 2.131 \AA^{-1} and 1.980 \AA^{-1} , respectively, being taken from the literature. The force constants were constrained to the values from MP2/6-31G(d) calculations.

^{a)} Anharmonic approximation.

^{b)} Uncertainties were not estimated in the original paper. The listed uncertainties were roughly estimated from the reported dependence on the three models on the effect of anharmonic potential field, in addition to those in the original experimental data.



Kochikov, I.V., Tarasov, Yu.I., Kuramshina, G.M., Spiridonov, V.P., Yagola, A.G., Strand, T.G.: J. Mol. Struct. **445** (1998) 243.

[1] Bastiansen, O., Graber, R., Wegmann, L.: Balzers High Vac. Rep. **25** (1969) 1.

[2] Gundersen, G., Strand, T.G., Volden, H.V.: J. Mol. Struct. **445** (1998) 35.

[II/25D \(3, 2227\)](#)