# Frequencies and Normal Modes of Vibration of Benz[*a*]anthracene Radical Ions

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MINDO/3-FORCES calculations were carried out for the radical ions of benz[*a*]anthracene. Both ions exhibit $C_s$ symmetry with C-C bond alternation in all four rings. The obtained equilibrium geometry was applied for the calculation of all $3N-6$ vibration frequencies of each ion, and for the analysis of their normal coordinates. The so calculated frequencies of the radical cation were close to the experimental frequencies and those of the ab initio calculations. They fall in the ranges

$\nu$CHstr. (3034 – 3087 cm$^{-1}$), $\nu$CCstr. (1237 – 1609 cm$^{-1}$), $\delta$CH (1142 – 1216 cm$^{-1}$).

Interesting correlations could be obtained for the frequencies of similar vibrations, e. g.

$\nu_{sym}$CHstr. > $\nu_{asym}$CHstr.

Exception is the frequency of vibration of $CH_\alpha$ in ring A for the radical cation and the same bond in ring D for the radical anion. The vibration frequencies for the CH bonds depend on the $\sigma$-electron densities of the corresponding carbon atoms, i. e.

$\nu$CH$^{\cdot+}$str. > $\nu$CHstr. > $\nu$CH$^{\cdot-}$str., where $\sigma-\rho_C^{\cdot+} > \sigma-\rho_C > \sigma-\rho_C^{\cdot-}$.

For the C-C stretching vibrations the relation

$\nu$(C-C)*str.* > $\nu$(C-C)$^{\cdot-}$str. > $\nu$(C-C)$^{\cdot+}$str.

holds, with the exception of the $C_\beta$-$C_\beta$ bond, for which the relation

$\nu$(C-C)str. > $\nu$(C-C)$^{\cdot+}$str. > $\nu$(C-C)$^{\cdot-}$str.

is found. As for the in-plane and out of-plane deformations, the following general correlations

$\delta(\mathrm{CH}) > \delta(\mathrm{CH})^{\cdot-} > \delta(\mathrm{CH})^{\cdot+}$ and $\gamma(\mathrm{CC}) > \gamma(\mathrm{CC})^{\cdot-} > \gamma(\mathrm{CC})^{\cdot+}$.

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