

# Carbon $\sigma$ -Electron Densities and C-H Stretching Vibration Frequencies of Phenanthrene

Rehab M. Kubba, Raghida I. Al-ani, and Muthana Shanshal

Department of Chemistry, College of Science, University of Baghdad, Jadiriya, Baghdad, Iraq

Reprint requests to Prof. M. S.; E-mail: mshanshal2003@yahoo.com

Z. Naturforsch. **60a**, 165 – 170 (2005); received September 7, 2004

MINDO/3-FORCES calculations were carried out for the vibration frequencies and IR absorption intensities of phenanthrene radical ions. The obtained frequencies were compared with the experimental values possible. It was found that the C-H stretching frequencies are directly related to the carbon  $\sigma$ -electron densities of the relevant atoms.

*Key words:* Phenanthrene; Vibration;  $\sigma$ -Electrons.