SIMULATION OF THE INFRARED SPECTRA OF LARGE CARBONACEOUS MOLECULES : INFLUENCE OF THE CHARGE STATE AND OF TEMPERATURE

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The family of Polycyclic Aromatic Hydrocarbons (PAHs) and their derivatives are deeply involved in the interpretation of the aromatic infrared bands (AIBs) observed in emission from many regions of interstellar space. Among the critical points which have to be considered to account for the observed spectra, and their local variations as observed by ISO, are the size distribution, the charge state, and the temperature of the species. The last two aspects in particular are not easy to access by experiment. This has motivated the development of a theoretical approach devoted to the a priori simulation of the infrared spectra of PAHs in relevant astrophysical conditions.
The results of these "tight-binding molecular dynamics" simulations will be presented, and compared with :

- 1) data obtained by ab-initio methods
- 2) available experimental data.

Spectra have been obtained for the series of small PAHs (naphthalene, azulene, fluorene, phenantrene, anthracene, pyrene, tetracene, pentacene), as well as some large PAHs : coronene, ovalene, up to circumcoronene $C_{54}H_{18}$. Emphasis will be put on the influence of ionization and vibrational temperature on the spectral patterns (relative intensities, band positions and bandwidths).