PROTONATED PAH'S

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The kinetics of formation of carbon structures fron elemtal carbon in high temperature environments or in an interstellar medium can derive in the formation of polycyclic structures or fullerenes. Conditions in which such two structures can be presentare distinguished. In low density vapors in the presence of hydrogen atoms, carbon polycyclic structures can form very stable curved poycyclic aromatic hydrocarbons.

This work analizes the particular properties of polyciclic structures C48, C48H12 and C48H18. The first one is an arm chair carbon polyciclic, the second one is a curved PAH and the third one is a protonated PAH. Ion potentials, electron affinities, infrared spectra and catalytical properties of these molecules are shown with the aid of theoretical calculations.