

# Infrared Spectroscopy of Matrix-Isolated Polycyclic Aromatic Hydrocarbons and Associated Ions. PAHs Incorporating Pyrene and Peropyrene Structures

A.L. Mattioda, D.M. Hudgins, C.W. Bauschlicher, Jr., and L.J. Allamandola  
*Space Science Division, NASA Ames Research Center*

The matrix-isolation technique has been employed to measure the mid- and near infrared spectra of a wide variety of polycyclic aromatic hydrocarbons and their associated ions which contain pyrene and peropyrene structures. These include 3,4;5,6;7,8;12,13 tetrabenzoperopyrene ( $C_{36}H_{16}$ ); 3,4;5,6;10,11;12,13 tetrabenzoperopyrene ( $C_{36}H_{16}$ ); dipyreno-(1',3';2,10) (1'',3'';5,7)-pyrene ( $C_{40}H_{18}$ ); 1,2;3,4;5,6;7,8;9,10; 12,13 hexabenzoperopyrene ( $C_{44}H_{20}$ ); 1,18;3,5;9,10;13,14 tetrabenzoheptacene ( $C_{42}H_{22}$ ); dianthraceno-(2,3;3,4),(2''3'';9,10)-pyrene ( $C_{40}H_{22}$ ); and 2,3;12,13;15,16-tribenoterrylene ( $C_{42}H_{22}$ ). The experimental data are compared to theoretically calculated values obtained using density functional theory (DFT) at the B3LYP/4-31G level. Generally there is good overall agreement between the experimental and theoretical data, the positional agreement being somewhat better than the agreement between intensities. With the exception of dianthraceno-(2,3;3,4),(2''3'';9,10)-pyrene, the results are consistent with previous experimental studies of polycyclic aromatic compounds and their ions. Specifically, in both the cationic and anionic species the strongest bands typically appear in the 1450 to 1300  $cm^{-1}$  range (the CC stretching and CH in-plane bending modes) whereas the neutral molecules tend to exhibit their strongest features between 700 and 900  $cm^{-1}$  (the aromatic CH out-of-plane bending modes). Ionized dianthraceno-(2,3;3,4),(2''3'';9,10)-pyrene strongly deviates from this trend with intense features, attributed to its anion observed in the 500 to 800  $cm^{-1}$  region. This is the first time PAH anion features of this magnitude have been observed in this region. The astrophysical implications of the data derived from these large PAHs will be discussed.