SPECTRA OF JET-COOLED ALL-BENZENOID PAHS - TRIPHENYLENE (C_{14}H_{12}) AND HEXA-PERI-HEXABENZOCORONENE (C_{42}H_{38})

DAMIAN L. KOKKIN, TYLER P. TROY, NEIL J. REILLY, MASAKAZU NAKAJIMA, KLAAS NAUTA, NIGEL LUCAS and TIMOTHY W. SCHMIDT, School of Chemistry, University of Sydney, NSW 2006, Australia; THOMAS D. VARBERG, Department of Chemistry, Macalester College, St. Paul, MN 55105 USA; GREGORY F. METHA, School of Chemistry & Physics, The University of Adelaide, SA 5005 Australia.

- The jet-cooled laser-induced fluorescence and dispersed fluorescence spectra of the S_{1} (A_1' \leftrightarrow S_0(A_1')) transition of triphenylene are reported. The spectra exhibit false origins of e' symmetry which are modelled by performing calculations of Herzberg-Teller coupling using time-dependent density functional theory. It is found that this level of theory reproduces the main features of the observed spectra. The oscillator strength of the strongest band is calculated to be f \approx 7 \times 10^{-4}.
- The resonant 2-color 2-photon ionization spectrum of the all benzenoid polycyclic aromatic hydrocarbon hexa-peri-hexabenzocoronene is reported. Vibronic bands of the S_{1} \leftrightarrow S_0 transition were observed in the 4080 – 4530 Å range. The strongest feature at 4261 Å is estimated to have an oscillator strength of f = 1.4 \times 10^{-3}, placing an upper limit on the interstellar abundance of this polycyclic aromatic hydrocarbon at 4 \times 10^{12} cm^{-2}, accounting for a maximum of \sim 0.02% of interstellar carbon.