INTERROGATING HYDROCARBON RADICALS

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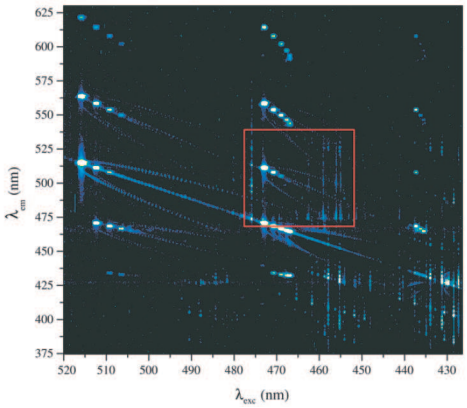
Motivated by astrophysical problems (and a sense of fun) for some years my research group has been obtaining new spectra of hitherto unobserved hydrocarbon radicals. We employ the complementary techniques of resonant ionization and laser induced fluorescence to rigorously identify radicals by matching their ground state vibrational frequencies to those obtained using density functional theory (DFT).

While some radicals were made to order in our pulsed electrical discharge source, others of particular chemical importance have been found lurking in the congested forest of dicarbon and tricarbon fluorescence. Using a 2-dimensional fluorescence (2df) map, we have extracted pure spectra, unpolluted by C_2 and C_3, from a benzene discharge. One spectrum was first presented at this symposium in 2006, but at that stage was not identified. Subsequent measurement of a matching resonant ionization spectrum revealed a mass of 115, much higher than the benzene precursor. With the aid of DFT calculations, the species was positively identified, giving clues to hydrocarbon-building chemistry of relevance to combustion; planetary atmospheres; and the interstellar and circumstellar space. Further experiments revealed other surprising additions to the radical zoo, also identified with the help of 2df.



Along the way we have also identified two new band systems of C_2, the first involving the hidden $c^3\Sigma_u^+$ state, and have ventured into the world of larger molecules, such as hexabenzocoronene, $C_{42}H_{18}$.