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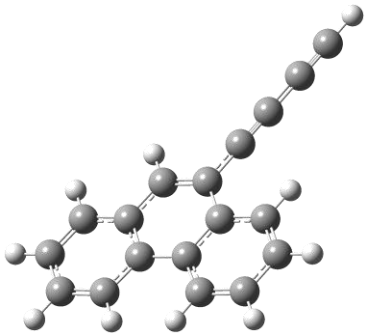

seit 1558
Friedrich-Schiller-Universität Jena

Spectroscopy of PAHs with carbon side chains

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Acknowledgments

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Motivations

Polycyclic aromatic hydrocarbon (PAH) molecules in space

- IR emission bands have been attributed to PAHs ("aromatic IR bands")
- PAHs are candidates for the carriers of the diffuse interstellar bands (DIBs)
- PAHs may contribute to the UV bump of the interstellar extinction curve at 2175 Å (Steglich et al. 2010)

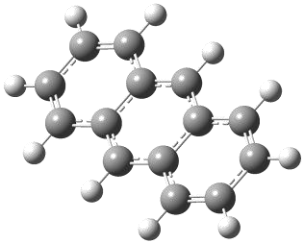
Aromatic-aliphatic structures in analogues of cosmic carbonaceous grains

- Interconnected aromatic and aliphatic structures (e.g. Jäger et al. 2008)
- Duley & Hu (2009): "[...] we suggest that a component of PAHs in interstellar sources have attached sp-bonded chains."

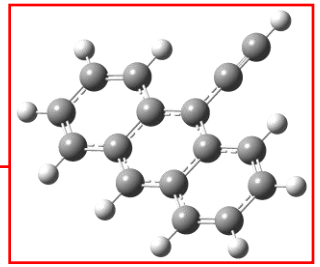
Species

TU Dresden

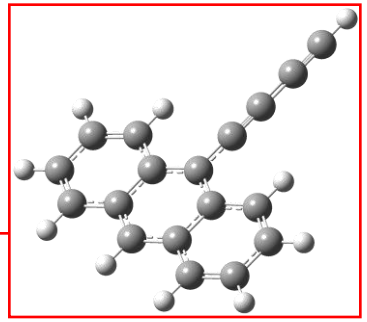
Anthracene



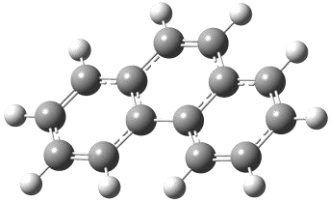
9-ethynylanthracene



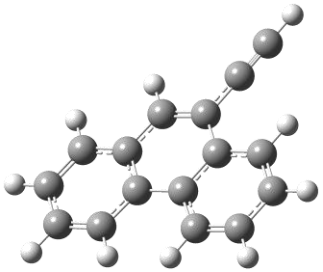
9-butadiynylanthracene



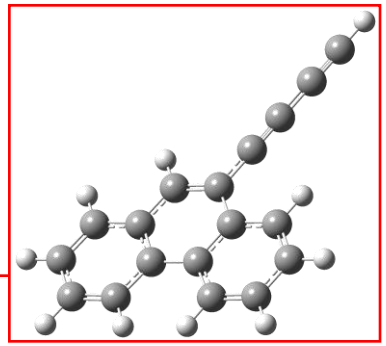
Phenanthrene



9-ethynylphenanthrene



9-butadiynylphenanthrene



Expectations in comparison with parent PAHs

IR region

Emission at typical vibrational wavelengths (not molecule specific), for instance:

- C≡C stretching at 4.7 μm
- ≡C−H stretching at 3.0 μm

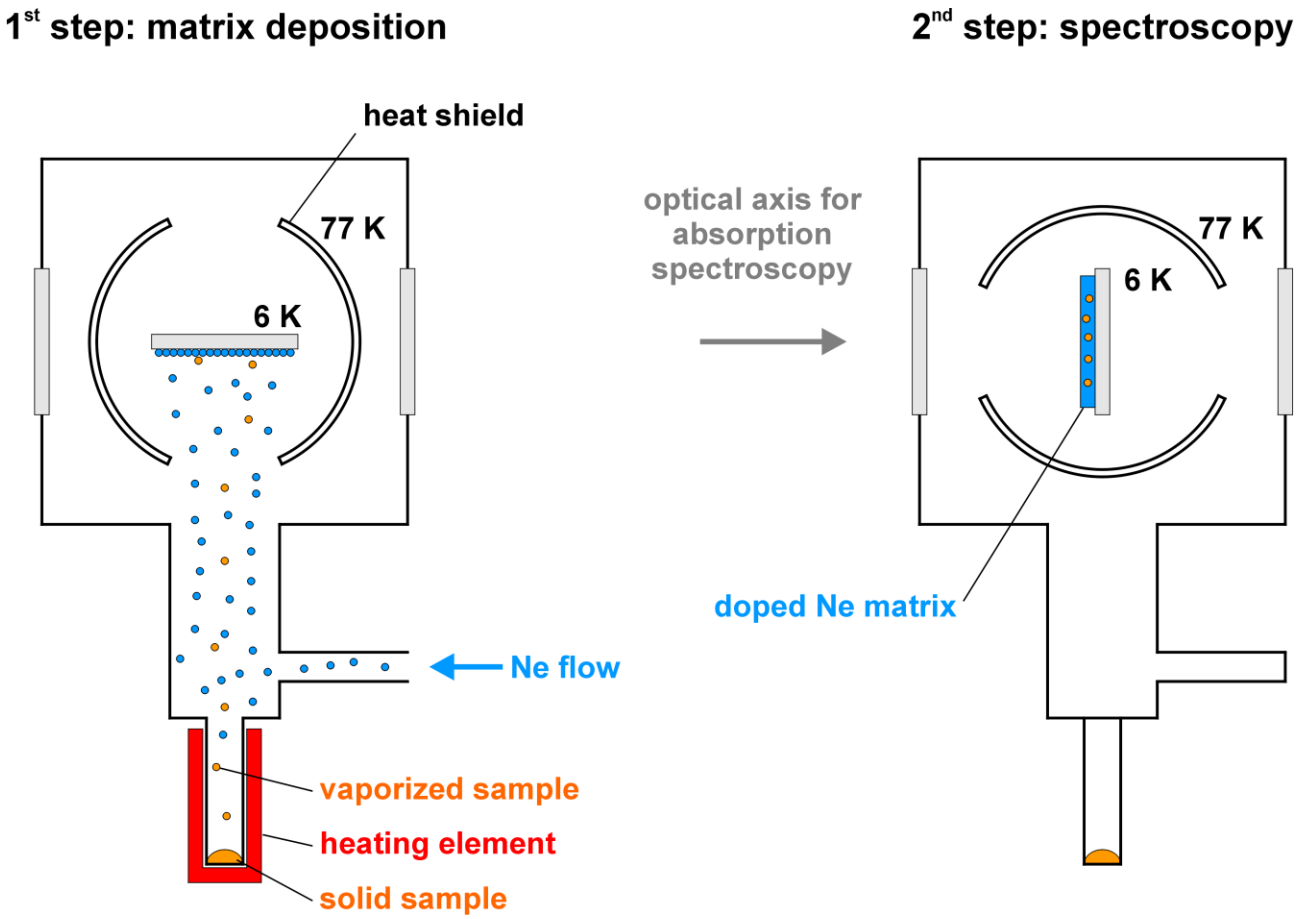
Radio domain

Emission of rotational lines due to the permanent electric dipole moment

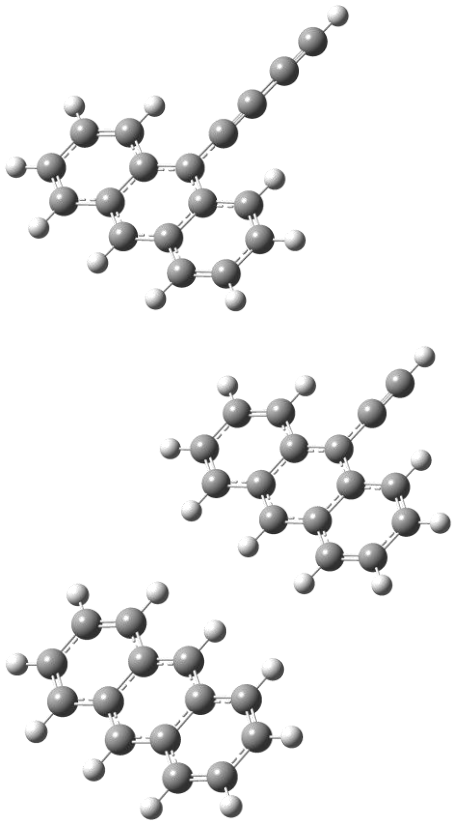
UV/vis region

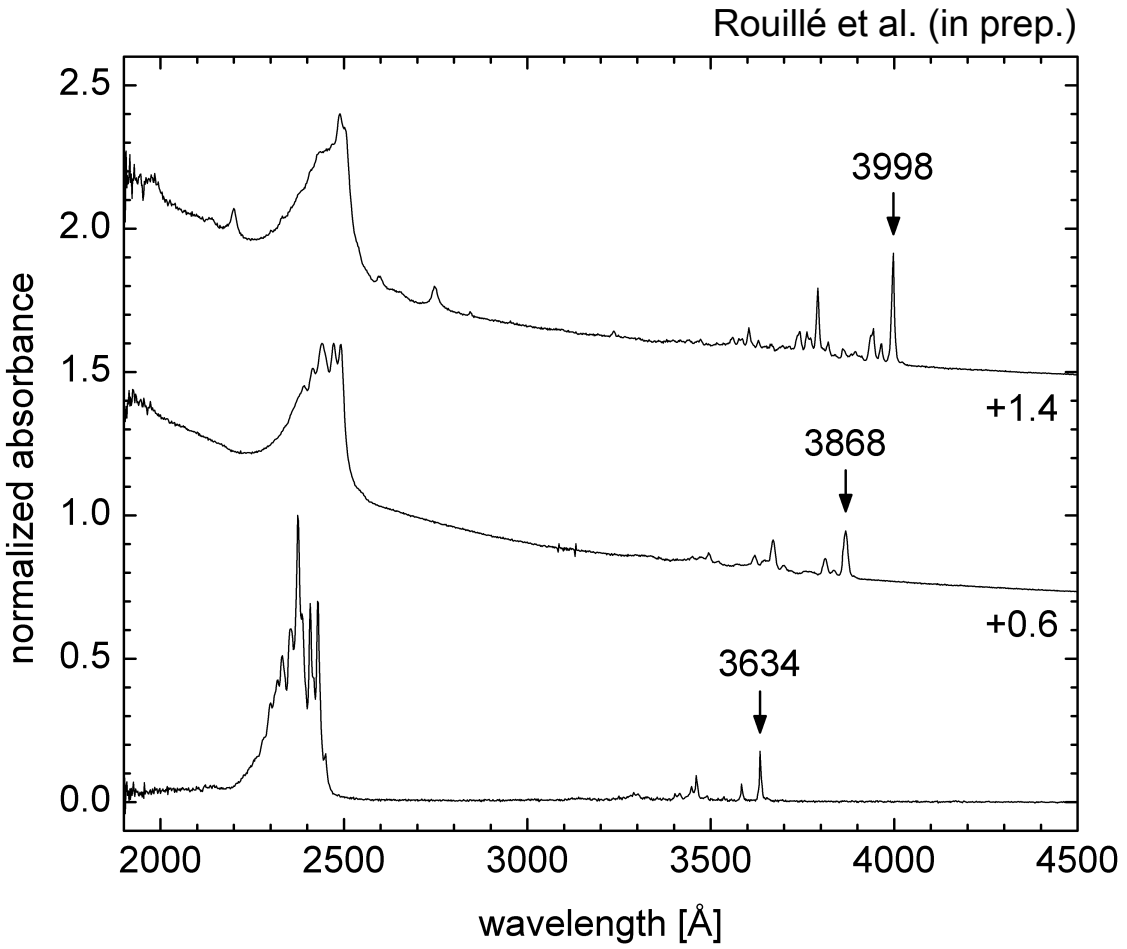
Redshifted electronic transitions: Marsh & Wornat (2000) on the absorption spectra of ethynyl-PAHs in solution at room temperature

Matrix isolation spectroscopy

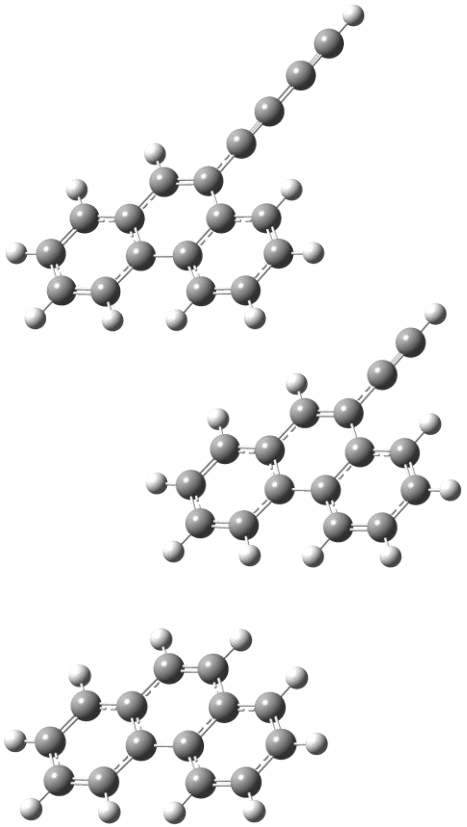


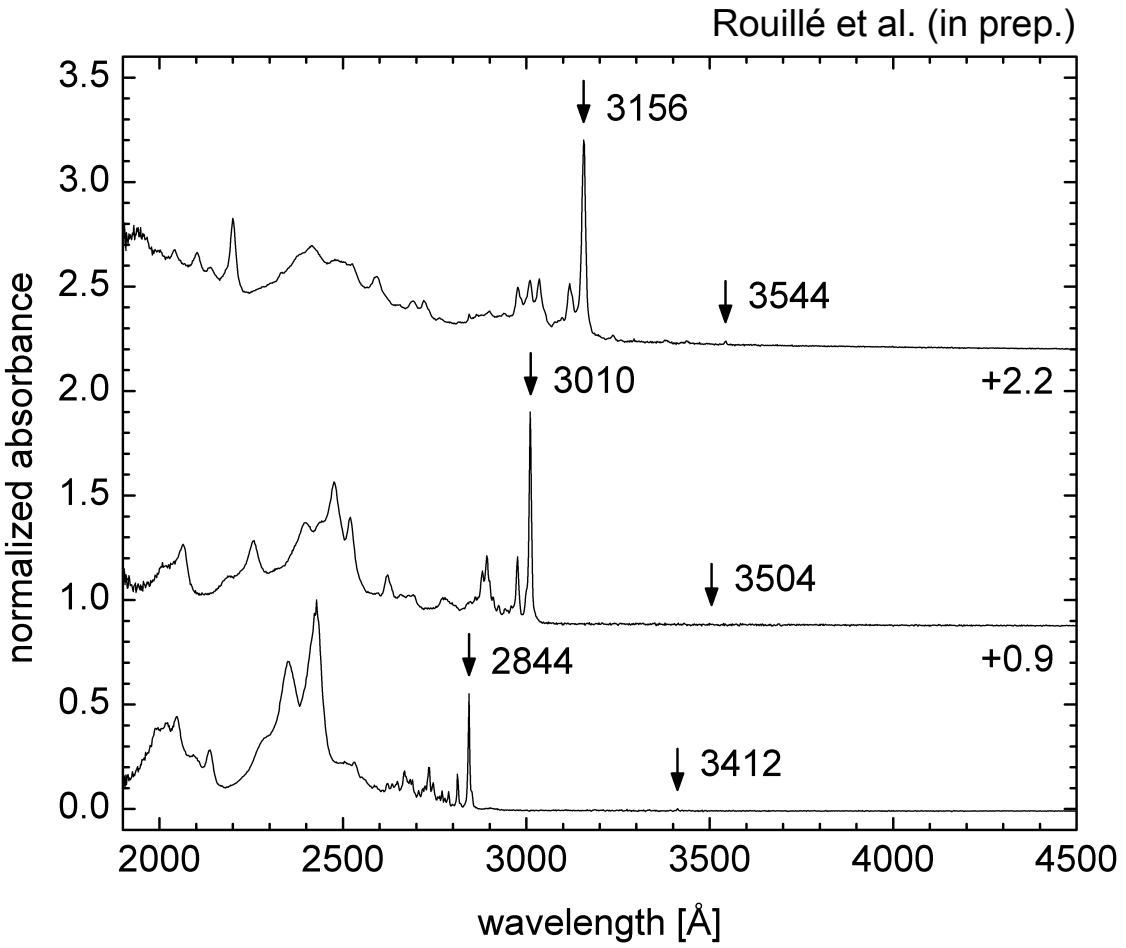
Anthracene and derivatives – in Ne matrix at 6 K





Phenanthrene and derivatives – in Ne matrix at 6 K





Laboratory data for searches in space

UV/vis region jet-cooled absorption spectra – column densities of interstellar PAHs (Gredel et al. 2011, Salama et al. 2011)

IR region rare gas matrix-isolated absorption spectra

Radio domain jet-cooled rotational spectra

DFT-B3LYP/6-311+G(d,p) level of theory:

Permanent electric dipole moment (D)	−H	−CCH	−CCCCH
9-*R*-anthracene	0	0.63	1.35
9-*R*-phenanthrene	0.015	0.87	1.46
1-*R*-pyrene	0	0.95	1.80

Summary and outlook

- New: low temperature matrix-isolated UV absorption spectra of ethynyl- and butadiynyl-substituted PAHs
- Longer chain → greater redshift of the electronic transitions
  → broader transitions at short wavelengths
  → stronger transitions at long wavelengths
  → greater permanent electric dipole moment (theory)
- Jet-cooled spectra (challenging): band positions and widths
- Theoretical studies of the electronic states
- Measurements with other side groups of relevance: with N, O, …; with larger PAH moities
- Searches in observational spectra