Contribution ID: **42** Type: **Contributed talk**

Ligand exchange in a supersonic expansion

Wednesday 17 September 2025 12:10 (20 minutes)

The smallest possible molecule that involves hydrogen atoms forming a van der Waals complex is dihydrogen itself. Complexes of dihydrogen with other binding partners are complicated by the fact that H_2 can exist in two different nuclear spin isomeric forms, one of which must retain its rotation in the complex (*ortho*-H_2, I = 1) whereas the other does not (*para*-H_2, I = 0). This results in different physical behaviour and can even impact their reactivity in the gas phase.[1] Hence, seemingly simple complexes are not necessarily easy to understand and it is commonly observed that *ortho*-H_2 complexes are more stable than *para*-H_2.

Inspired by a rotational study on the OCS-H_2 complex[2], we investigated the formation of the *ortho*-H_2, *para*-H_2 and He complex with benzonitrile dependent on the H_2 content in the expansion using cavity-resonator rotational jet spectroscopy. Similar to OCS-H_2, an enhancement of the signal intensity of the *ortho*-complex with increasing H_2 content was observed, whereas an inverse behaviour was found for the *para* and He-complex. To understand this behaviour we kinetically modelled their intensity on the basis of an often proposed ligand exchange mechanism. These results may have implications for the *ortho/para*-H_2 ratio observed in the interstellar medium (ISM) for which polycyclic aromatic hydrocarbons (PAHs) have been found to be important.[3,4] Benzonitrile can serve as a small model system for PAHs and has itself been detected in the ISM.[5]

[1] Yang, T. et al. Nat. Chem. 2019 11, 744–749.
[2] Z. Yu et al. J. Chem. Phys. 2007 127, 054305.
[3] E. Bron et al. A&A 2016 588, A27.
[4] B. Fleming et al. Astrophys. J. 2010 725, 159–172.
[5] B. A. McGuire et al. Science 2018 359, 202–205.

Keywords

Hydrogen bond: weak; State of system: gas

This abstract is submitted for....

HBond 2025 conference

Primary authors: Dr HARTWIG, Beppo (Georg-August-Universität Göttingen); HASSELHORN, Jannes Niels (Georg-August-Universität Göttingen)

Co-authors: TOVTIK, Radek (Georg-August-Universität Göttingen); Prof. SIMETH, Nadja A. (Georg-August-Universität Göttingen); Prof. OBENCHAIN, Daniel (Georg-August-Universität Göttingen)

Presenter: Dr HARTWIG, Beppo (Georg-August-Universität Göttingen)