

ITFE – A More Complicated Halogen Bond Donor

Feßner, Malte,^{1*} Prof. Merten, Christian¹

*presenter

¹malte.fessner@rub.de, Ruhr Universität Bochum, Fakultät für Chemie und Biochemie, Organische Chemie II, Universitätsstraße 150, 44801 Bochum, Germany

The technique of matrix isolation (MI) spectroscopy is already established as an ideal tool to investigate weak intermolecular interactions, like halogen bonding (XB).¹

Iodo trifluoroethylene (C₂F₃I; ITFE), because of its small size and large σ -hole on the iodine, has already been shown to be a useful molecule to obtain information on halogen bonding and other interactions, like C-I $\cdots\pi$ and $\pi\cdots\pi$ interactions.²

ITFE only has a few, but very intense, bands in the MIR region. Especially the C=C stretching vibration, which is located at around 1760 cm⁻¹ also is very isolated, and therefore ideal for the analysis of changes induced when forming different kinds of complexes. We were interested in the interaction of ITFE with different phenylethylamine (PEA) derivatives. Not only the C-I \cdots N halogen bond complex, which induces a red shift of about 10 cm⁻¹, could be seen for all investigated derivatives, additionally, reasonable assumptions about the formation of C-I $\cdots\pi$ and $\pi\cdots\pi$ interactions can also be made.

The characterization of these interactions is rather challenging, since ITFE was also found to form complexes with itself. When changing different parameters for a measurement of purely ITFE like the ITFE concentration, the flow rate of the premixed sample, or the deposition temperature, later showed to have a significant influence on the kind of the formed complexes. Depending on the deposition temperature, ranging from 4 K up to 25 K, not only the ITFE monomer structure, but also different C-I $\cdots\pi$ and $\pi\cdots\pi$ interactions were already formed. Upon annealing these depositions to 35 K, changes could also be observed.

¹ a) D. Pal, S. K. Agrawal, A. Chakraborty and S. Chakraborty, *Phys. Chem. Chem. Phys.*, 2020, **22**, 22465; b) P. Wang, N. Zhao and Y. Tang, *J. Phys. Chem. A*, 2017, **121**, 5045.

² N. M. Kreienborg, F. Otte, C. Strohmam and C. Merten, *Phys. Chem. Chem. Phys.*, 2023, **25**, 15110 —15114.