Stereochemical configuration and selective excitation of the chiral molecule halothane

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Synopsis The molecular configuration of the chiral ethane derivative halothane ($CHBrClCF_3$) was investigated via Coulomb Explosion Imaging using a COLTRIMS (Cold Target Recoil Ion Momentum Spectroscopy) setup. Several four-particle fragmentation pathways were found that yield information on the absolute stereoconfiguration. In addition, the effect of selective excitation on two-body break-ups was studied.

Coulomb Explosion Imaging can provide structural information of molecules or van-der-Waals-bound systems. In this approach, the system under investigation is multiply ionized within a timescale that is short compared to structural changes. The positively charged ion cores subsequently repel each other due to Coulombic forces so that their momentum vectors carry information on the initial structure. These momentum vectors can be measured for single molecules in coincidence, e.g. with a COLTRIMS setup (Cold Target Recoil Ion Momentum Spectroscopy)[1].

In recent years, Coulomb explosion imaging has been more and more extended to study structural properties of polyatomic molecules by collecting four or more charged fragments. In particular, it has been demonstrated as a way to determine the absolute stereochemical configuration of chiral molecules [2, 3].

This contribution presents Coulomb Explosion results of the chiral ethane derivative halothane ($CF_3CHClBr$), a substance that can be used as an anaesthetic drug. Single X-ray photons with energies corresponding to the carbon K-edge (286 - 305 eV) were used to induce multiple ionization and fragmentation.

A clear separation of enantiomers has been found using the fragmentation into CF_3^+, Cl^+, Br^+ and CH^+ (Figure 1). Additional fragmentation pathways with incomplete detection of fragments show a less pronounced enantiomer signal. For some of these break-ups, a slight increase in the yield was observed when the photon energy was high enough to ionize from either of the carbon 1*s* shells.

Additional information about the selective excitation can be drawn from the photoelectron spectra measured in coincidence. In this case, a clear correlation between the primary excitation site and the fragmentation pathway could be established.

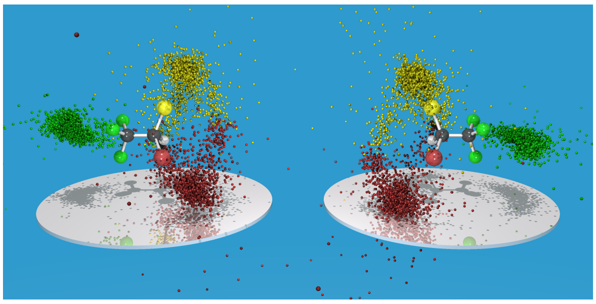

Figure 1. Momenta of the fragments CF_3^+ (green), Cl^+ (yellow), Br^+ (red) and CH^+ (black) in the molecular frame, overlaid with a structural model of the parent molecule halothane. Modified from [4]

References

[1] Dörner R *et al* 2000 *Phys. Rep.* **330** 95

[2] Pitzer M *et al* 2013 *Science* **341** 1096

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