

Finding the Absolute Configuration of Chiral Molecules with Coulomb Explosion Imaging

Martin Pitzer¹, Markus S. Schöffler¹, Maksim Kunitski¹, Allan S. Johnson², Till Jahnke¹, Lothar Ph. H. Schmidt¹, Horst Schmidt-Böcking¹ and Reinhard Dörner¹

¹Institut für Kernphysik, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany

²University of Ottawa, Ottawa, ON, Canada K1N 6N5

pitzer@atom.uni-frankfurt.de

A deeper understanding of molecular chirality is of great interest in many domains: in pharmaceutical diagnostics, concerning the origin of biological homochirality and even for fundamental physics, as molecular properties may be linked to parity violation [1]. So far, experimental methods on the microscopic scale are restricted either to the investigation of electronic properties (Photoelectron circular dichroism, [2]) or to the analysis of fragment ion yields [3]. In both cases, however, quantities are typically averaged over all different orientations of the molecule in space.

Multi-fragment coincident imaging via the COLTRIMS technique (Cold Target Recoil Ion Momentum Spectroscopy, [4]) opens a new way to explore the properties of chiral molecules. Fully three-dimensional momenta of electrons and ionic fragments are recorded for each molecule individually. Here, we report for the first time the complete fragmentation of chiral molecules, namely CHFCIBr and the isotopically chiral analogue CHCl_2Br . While the former is of interest in the search for dichroism effects, the latter poses a challenge for the distinction of enantiomers because its structural chirality is only due to the mass difference of the chlorine isotopes ^{35}Cl and ^{37}Cl .

In our study, femto-second laser pulses were used to multiply ionize molecules from a gas jet, resulting in a Coulomb explosion of the ionic cores. These positive charges were guided by an electric field onto a position sensitive delay-line detector. We can show that fragmentation into all five constituent atoms occurred, and derive the 3D momentum for each fragment. Figure 1 illustrates the distinct separation between the left- and right-handed enantiomers of CHCl_2Br in momentum space. In addition, these momentum vectors permit to define a molecular frame in which directional properties can be investigated.

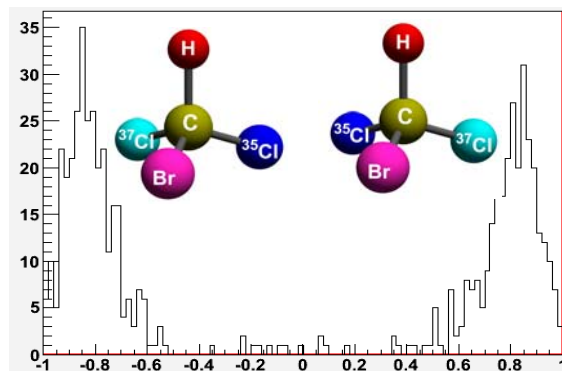


Figure 1: Histogram for the angle $\cos(\theta) = (\vec{p}_{\text{bromine}} \times \vec{p}_{\text{hydrogen}}) \cdot \vec{p}_{\text{chlorine}^{35}}$, showing clear separation between the enantiomers.

This result is an important proof-of-principle for the distinction of enantiomers, allowing a range of questions to be addressed: Do the fragment ions show circular dichroism in their angular distribution? Is there an effect of the molecule's orientation with respect to the direction of light propagation? Can vector quantities be derived that carry a hint for parity violation?

References

- [1] Martin Quack, *Angew.Chemie.Int.Ed.*, **41**, 4618-4630 (2002)
- [2] Ivan Powis, *Adv.Chem.Phys.*, **138**, 267-329 (2008)
- [3] H. Georg Breunig, et al, *Chem.Phys.Chem.*, **10(8)**, 1199-1202 (2009)
- [4] Reinhard Dörner, et al, *Phys.Rep.*, **330**, 95-192 (2000)