Three-dimensional momentum imaging of core-excited molecules or molecular clusters

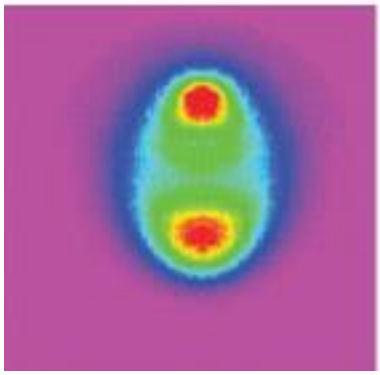

Figure 1 Ion image of Cl+ from HCl showing alignment of molecule

Imaging of molecules is a powerful technique for understanding how molecules respond to photoionization or photoexcitation. We are particularly interested in understanding how the geometry of a molecule changes: one example is isomerization or proton transfer that is driven by vibrational excitation. We image ionic fragments in a multicoincidence time-of-flight spectrometer. Our method allows us to extract a detailed picture of changes in molecular geometry on both rapid and slow time scales. The project involves analysis of data obtained at MAX-Lab and includes interpretation of the alignment of core-excited molecules based upon the quantum mechanical dipole operator, as well as analysis of the three-dimensional momentum of fragments from single dissociation events in order to extract information about the geometry and the final dissociative states. The analysis is based upon correlations between the energies of particles as well as angular correlations.

Examples of recent studies

Acetylene is linear in the ground state. Our study finds that proton migration to the vinylidene configuration takes place very rapidly, and we find a bridge transition state leads to a complete collapse of the molecule during the 100 fs life time of the core-excited state.

J. Laksman, D. Céolin, M. Gisselbrecht, S. E. Canton, and S. L. Sorensen
Dynamics of proton migration and dissociation in core-excited ethyne probed by multiple ion momentum imaging
J. Chem. Phys. 131 244305 (2009)

In carbonyl sulfide nuclear motion is imaged after excitation of the C1s and O1s electrons. The discovery of a two-body fragmentation channel SO+/C+ with a well defined angular anisotropy indicates the rapid formation of the CSO isomeric species.

J. Laksman, D. Céolin, M. Gisselbrecht, and S. L. Sorensen
Nuclear motion in carbonyl sulfide induced by resonant core electron excitation
133, 144314, J. Chem. Phys. (2010)

For more information contact Professor Stacey Sorensen (Stacey.sorensen@sljus.lu.se)

Previous diploma projects within this theme:

Zeynep Erudhan, Three-dimensional ion imaging of diatomic molecules, 2008

Christian Stråhlman**, Dissociation of C 1s excited states of OCS** , 2009
http://www.lu.se/o.o.i.s?id=19464&postid=1528045

Christian Stråhlman, **Electronic state dependence in dissociation of core-excited water**, 2011 http://www.lu.se/o.o.i.s?id=19464&postid=1988390