

Chris MAYHEW
School of Physics and Astronomy
University of Birmingham
Edgbaston
Birmingham
UK
B15 2TT

Reference: Short Term Scientific Mission COST CM601
Beneficiary: Dr. Chris A. Mayhew, University of Birmingham
Host: Dr. Paul Scheier, Institut für Ionenphysik
Period: from 10/09/08 to 20/09/08 Place: Innsbruck (AU)
Reference Code: COST-STSM-CM0601-03907

Purpose of Visit

The proposed visit to Innsbruck was to use apparatus to investigate electron attachment to chlorinated molecules in order to investigate the effects of changes in molecular structure on the process.

Description of the Work Carried Out

The initial proposal was to understand the effect of increasing the number of chlorine substituents on the electron attachment process to chloroethenes. Anion yields as a function of electron energy with the positions and intensities of the electron attachment resonances were to be determined. However, soon after arrival at Innsbruck it came to our attention that a preprint of a paper had just appeared in International Journal of Mass Spectrometry which detailed experiments on two of the three molecules we planned to investigate, namely trichloroethene (C_2HCl_3) and tetrachloroethene (C_2Cl_4).¹ Therefore, we decided that the target molecules had to be revised. We could still continue investigating analysis to the third proposed molecule, monochloroethene (C_2H_3Cl), but to that we would investigate electron attachment to chlorinated acetones. By investigating these molecules the key objective of the study would be maintained. During my visit we investigated 1,3-Dichloroacetone ($ClCH_2COCH_2Cl$, Formula Weight: 126.97 amu), 1-Dichloro-2-propanone ($CH_3COCHCl_2$, Formula Weight: 126.97), and Chloroacetone ($ClCH_2COCH_3$, Formula Weight: 92.52). The plan was to use two instruments. One is a double focusing sector field mass spectrometer (VG-ZAB-2SEQ), which is useful for measurements requiring high sensitivity and for obtaining accurate relative anion yields. The other is trochoidal electron monochromator coupled to a quadrupole mass filter with a pulse counting system, which provides a much higher energy resolution than the VG-

¹ Yury V. Vasil'ev, Valery G. Voinov, Douglas F. Barofsky, Max L. Deinzer, Absolute dissociative electron attachment cross-sections of chloro- and bromo-ethylenes International Journal of Mass Spectrometry xxx (2008) xxx-xxx

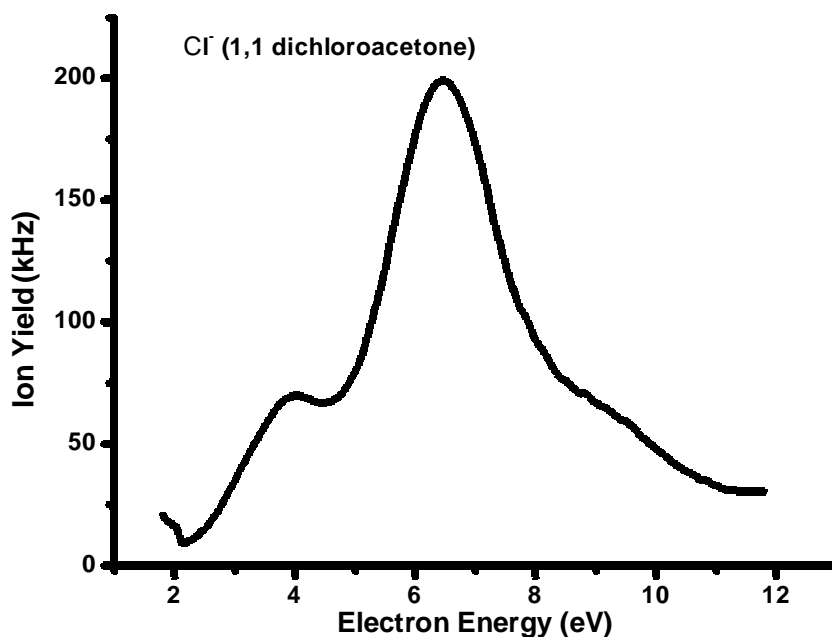
ZAB, and is a better instrument to investigate narrow energy resonances close to 0 eV. The trochoidal instrument was not available. Therefore all of the data presented below were taken on the VG-ZAB. The resolution is no better than about 500 meV.

Preliminary Report of Results

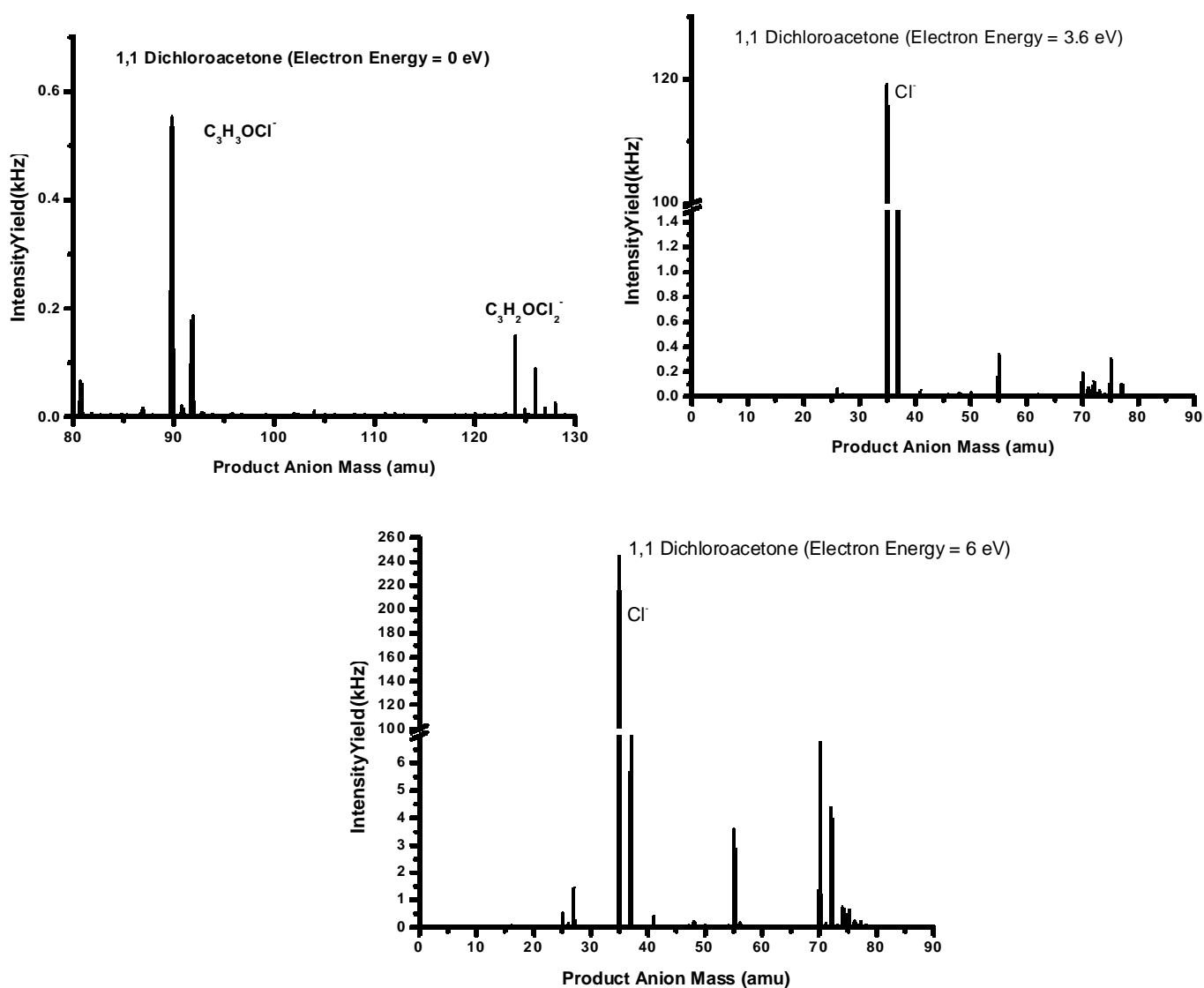
A selection of the results (mass spectra at fixed electron energies and electron energy scans at fixed molecular mass) are presented below. There is a significant amount of new data which should result in the publication of one paper once the high resolution electron attachment details are obtained near to 0 eV electron attachment energies.

1,1 Dichloroacetone

By far the most dominant channel results in the product of Cl^- over all electron energies. The zero energy peak is not shown in the figure below, but as measured on the VG-ZAB the zero energy peak intensity is approximately 200 times that of the peak observed at 6 eV.

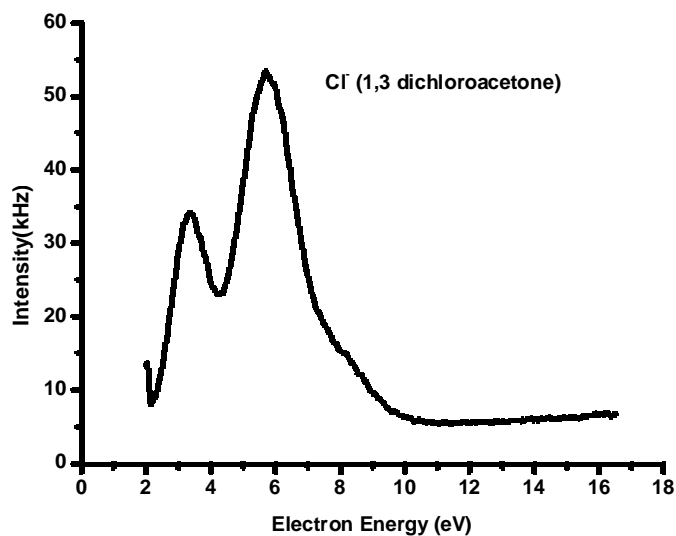


Mass spectra recorded at the electron energies corresponding to the peaks in the electron attachment resonances are provided below. These illustrate the various anion channels available. Owing to the intensity of the Cl^- signal at zero eV we are unable to provide a mass scan over than mass.

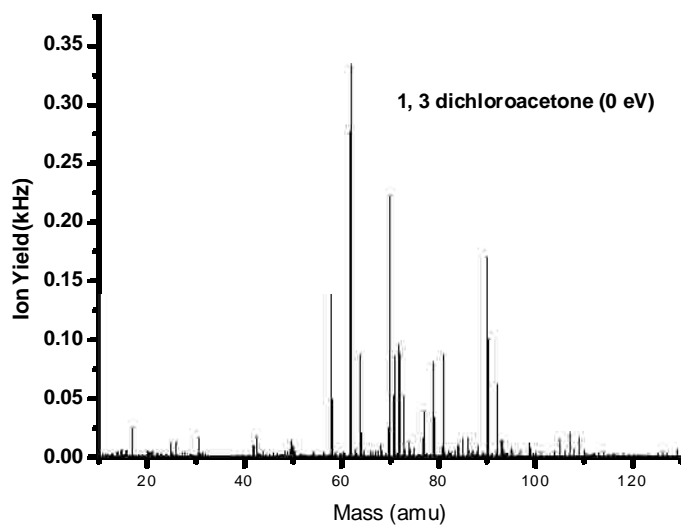


1,3 Dichloroacetone

As found for the 1,1 dichloroacetone, the dominant anion channel is Cl^- for all electron energies. However, various other channels have also been detected, although at much less intensities than that found for Cl^- . The electron energy scan for Cl^- is shown below. Again the zero energy peak is not shown, but its intensity is approximately 200 times that of the peak at 6 eV.



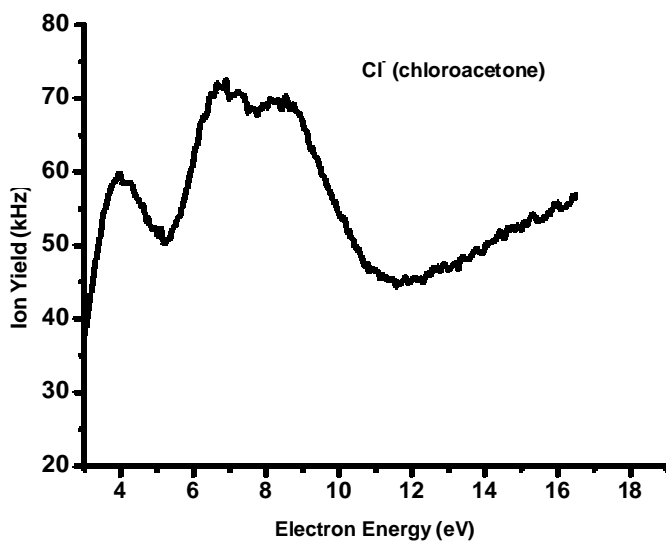
A mass spectrum taken at 0 eV over the mass ranges 10 – 33 amu and 38 – 130 amu is shown below. There are noticeable differences between this spectrum and that obtained for the 1,1 isomer.



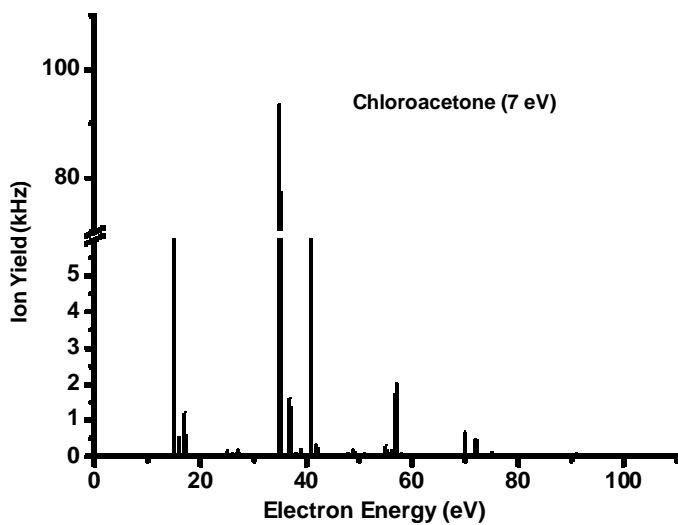
The main anion channels observed are $[M-H_2]^-$, $[M-HCl]^-$, $[M-Cl]^-$, HCl_2^- and Cl_2^- . The intensity of the zero energy Cl⁻ peak at 0 eV is 240 times greater than that observed at 6.5 eV.

Chloroacetone

Cl⁻ is the dominant anion with the zero energy resonance peak being by far the most intense of any of the resonances (approximately 420 times larger than that observed at 7 eV). The figure below provides a scan for the Cl⁻ channel as a function of electron energy from about 3eV to 18 eV.



A mass spectrum obtained at an electron energy of approximately 7 eV is provided below.



Future Collaboration

We plan to continue this study. In the short amount of time we had access to the VG-ZAB a number of interesting and encouraging results were obtained on the partially chlorinated acetones. We need to obtain high resolution data, and in addition expand on this study to include other halogenated acetones. These provide an interesting series of molecules for investigating isomeric effects and substitutions on electron attachment processes.