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Beneficiary: Dr. Chris A. Mayhew, University of Birmingham
Host: Dr. Paul Scheier, Institut für Ionenphysik
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Period: 06/05/2009 to 16/05/2009

Purpose of Visit

The main purpose of the visit to Innsbruck was to continue and complete our investigations of electron attachment to halogenated acetones in order to provide enough results for unique comparisons between various species in order to investigate the effects of substitution on the electron attachment process to acetone, i.e. the effects of multiple fluorine/chlorine substitution on the dissociative electron attachment pathways.

Description of the Work Carried Out

During my previous visit (September 2008) we investigated 1,3-Dichloroacetone ($\text{ClCH}_2\text{COCH}_2\text{Cl}$, Formula Weight: 126.97 amu), 1-Dichloro-2-propanone ($\text{CH}_3\text{COCHCl}_2$, Formula Weight: 126.97), and Chloroacetone ($\text{ClCH}_2\text{COCH}_3$, Formula Weight: 92.52). For this final visit to investigate halogenated acetones we have studied the effects of electron attachment on the following species: 1,1,1 Trichloroacetone ($\text{CCl}_3\text{COCH}_3$), 1,1,1 Trifluoroacetone (CF_3COCH_3) and Fluoroacetone ($\text{FCH}_2\text{COCH}_3$). We also repeated the study for 1,3-Dichloroacetone, because the earlier results were not consistent. Given that at room temperature 1,3-Dichloroacetone is a solid, we believe that complications arose in the earlier experiments owing to cluster formation. Therefore for the repeat measurements we heated the sample and inlet lines to 70 °C. In addition to the above halogenated compounds, we decided during the visit to investigate electron attachment to acetone in order to complete the series and to provide comparisons with the halogenated species. Remarkably no detailed study of electron attachment to this very basic molecule has been reported in any detail in the literature. Taken together we have significantly extended the series of molecular systems studied and have enough data to write an interesting joint paper. I should mention that the work was carried out with the help of three students. Achim Wilhelm Edtbauer (PhD student), who was responsible for the running of the machine, Christian Mitterdofer (Diploma Student – May 2009 visit) and Elahe Alizadeh (PhD student – September 2008 visit). Thus the paper(s), which we

are currently writing will include the following authors: A. W. Edtbauer, C. Mitterdofer, E. Alizadeh, T. Märk, P. Scheier, and C. A. Mayhew.

Acknowledgments

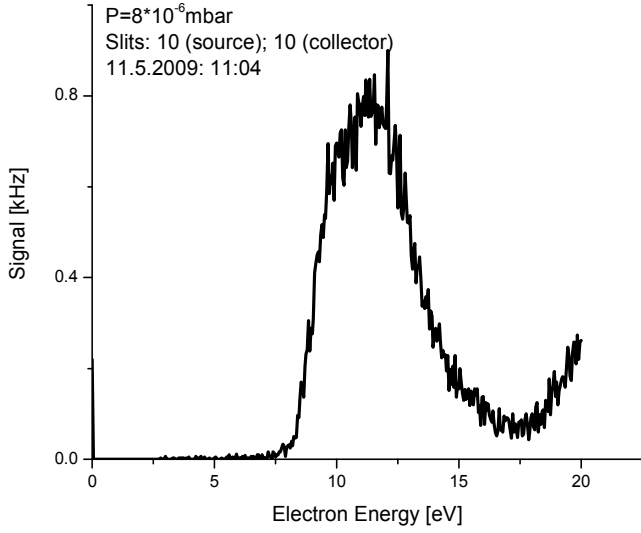
I am indebted to Paul Scheier for the invitation and for providing me with unlimited access to the equipment during the visit. I especially wish to thank Achim Edtbauer who spent many long evenings (including one weekend!) with me in order to keep the instrument running and in order get as much data as possible during my short visit.

Preliminary Presentation of Results

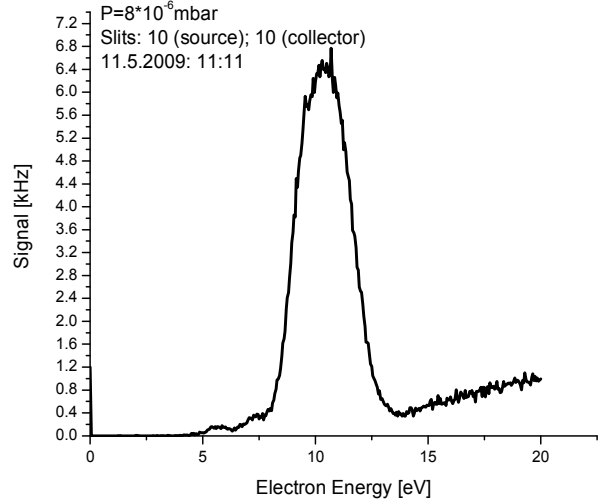
Given the large amount of data produced, it is not possible to provide all the results in this report. Certainly the analysis and preparation of the results will take some time. For the purposes of this report we present below a selection of the measurements taken during the visit. These include mass spectra at fixed electron energies corresponding to the peak intensities found in electron energy scans and (mainly as yet uncalibrated) electron energy scans at fixed molecular mass.

Acetone

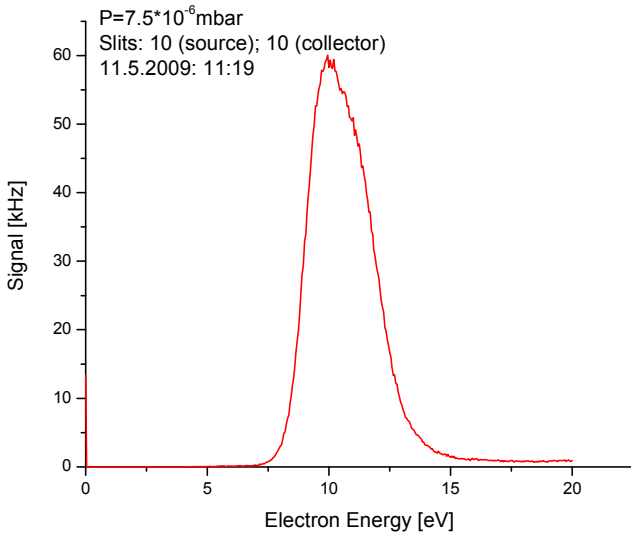
Energy scan for m14 (15.231) uncalibrated
Acetone



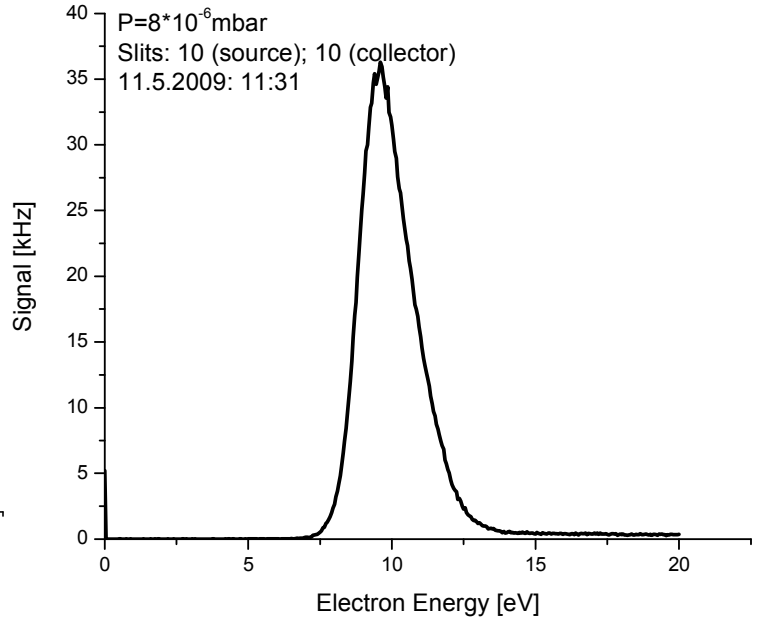
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Acetone



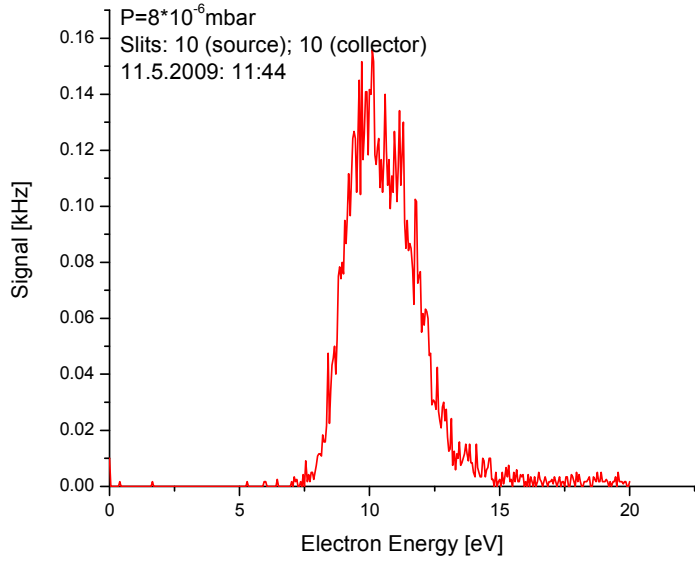
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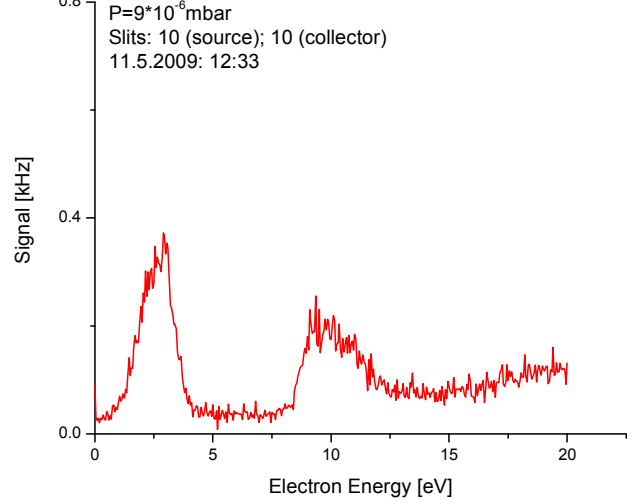
Energy scan for m17 (18.231) uncalibrated
Acetone



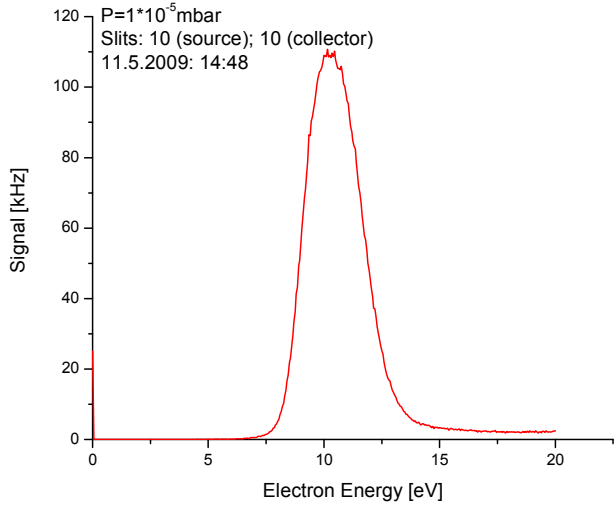
Energy scan for m18 (19.231) uncalibrated
Acetone



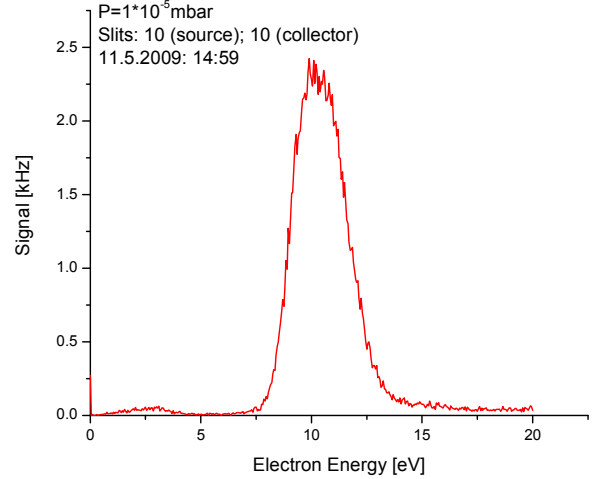
Energy scan for m26 (27.352) uncalibrated
Acetone



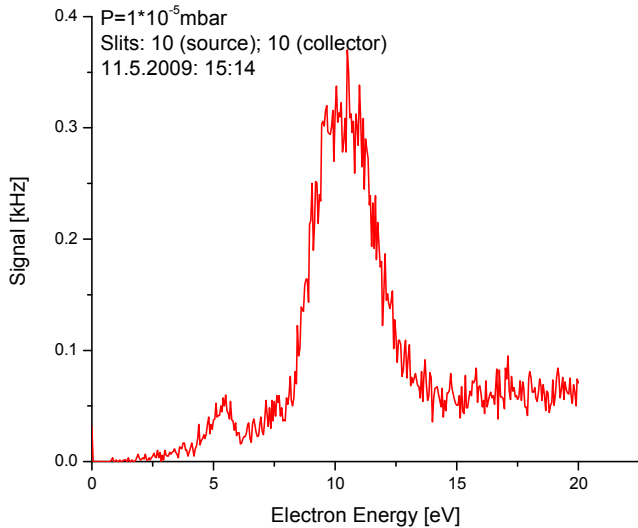
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Acetone



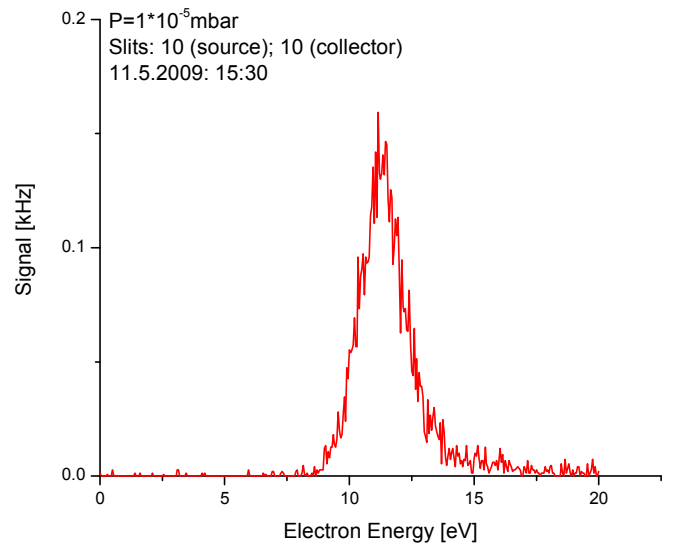
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Acetone

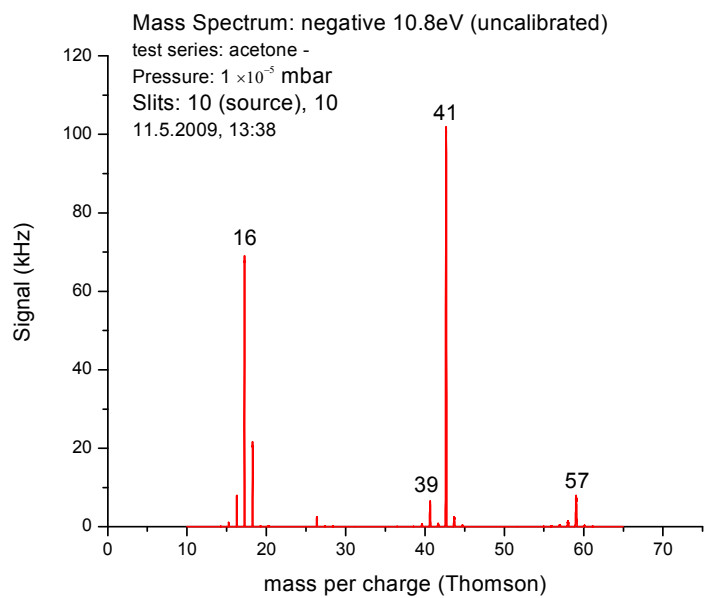
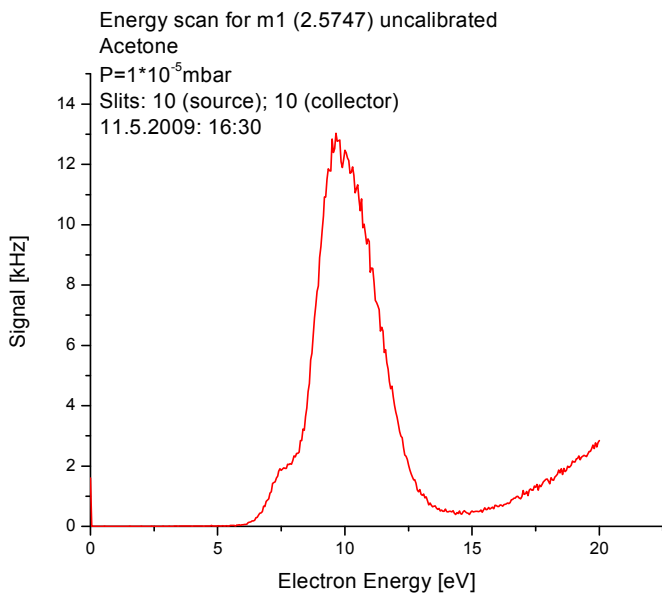
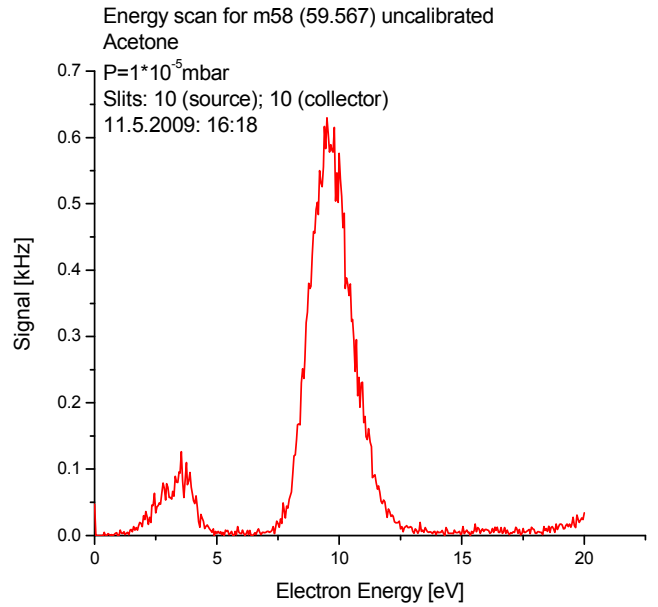
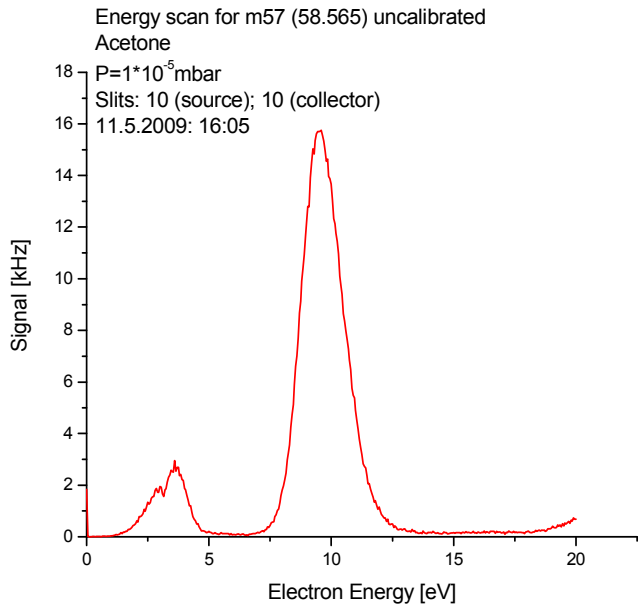
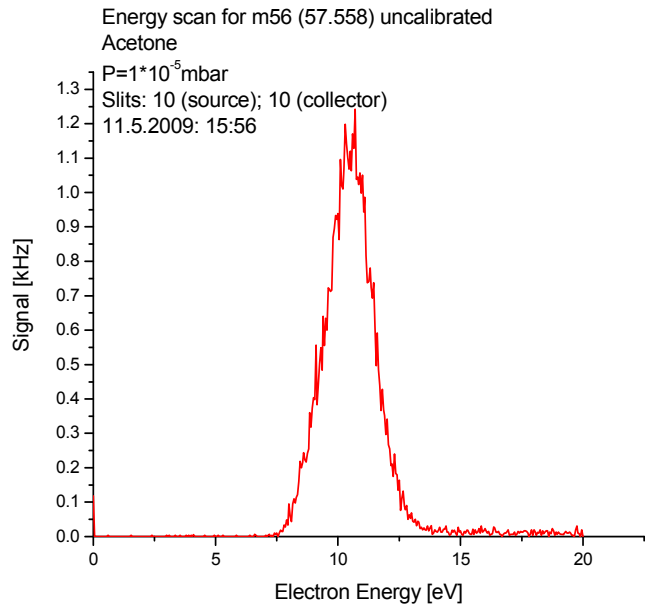
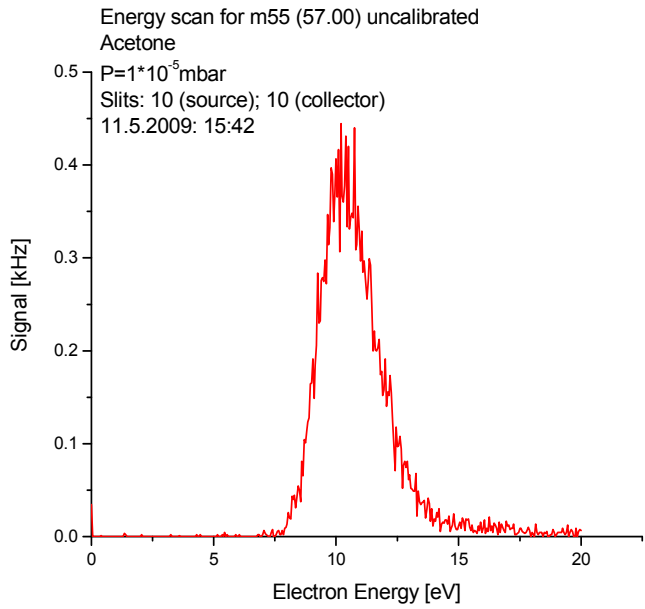


Energy scan for m43 (44.749) uncalibrated
Acetone

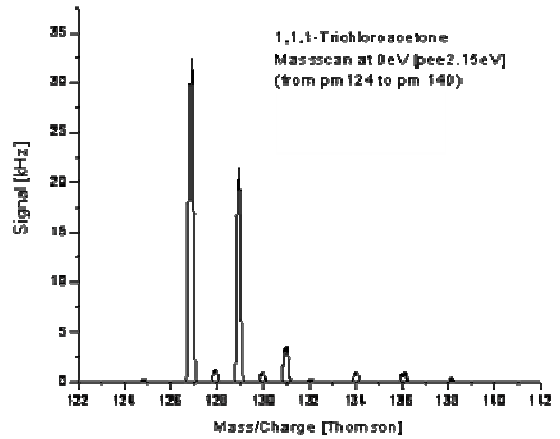
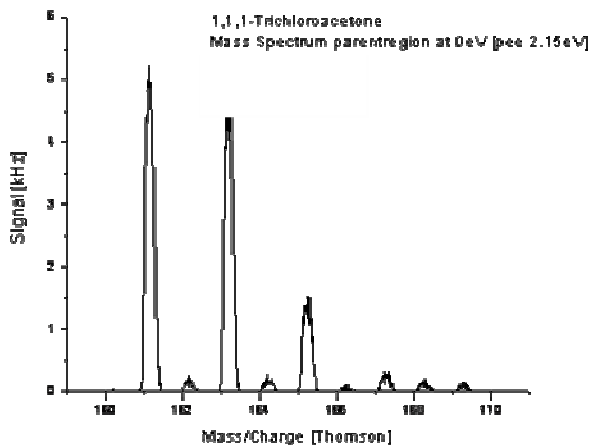
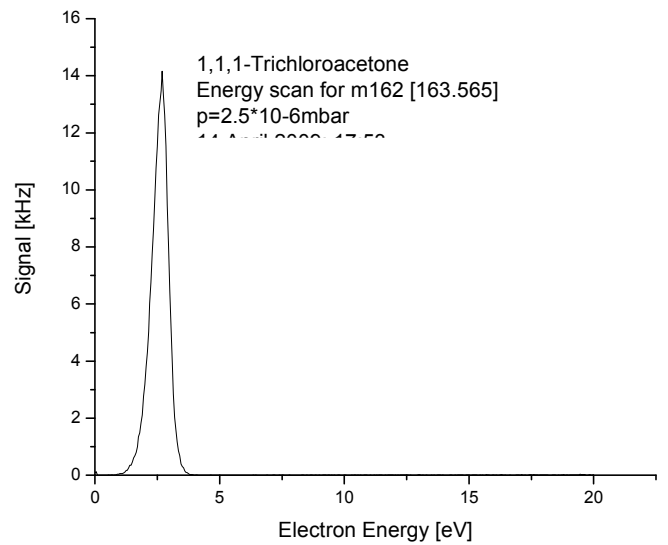
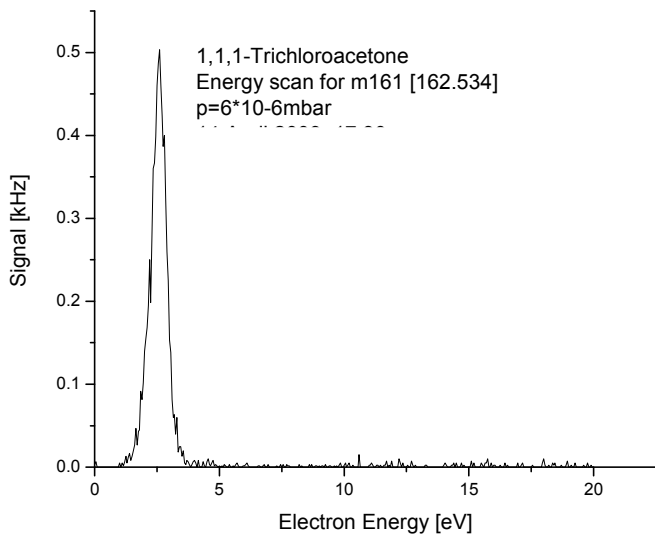
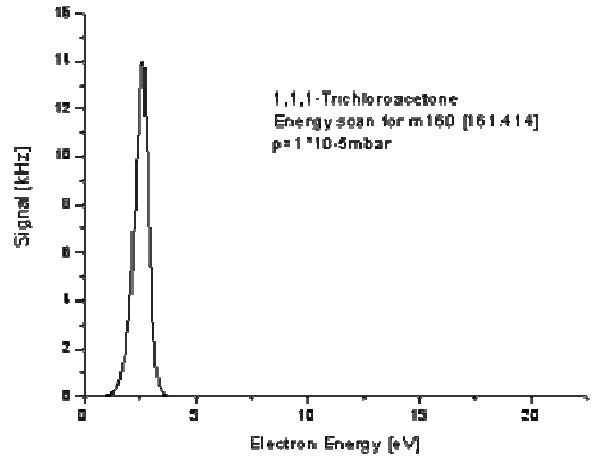
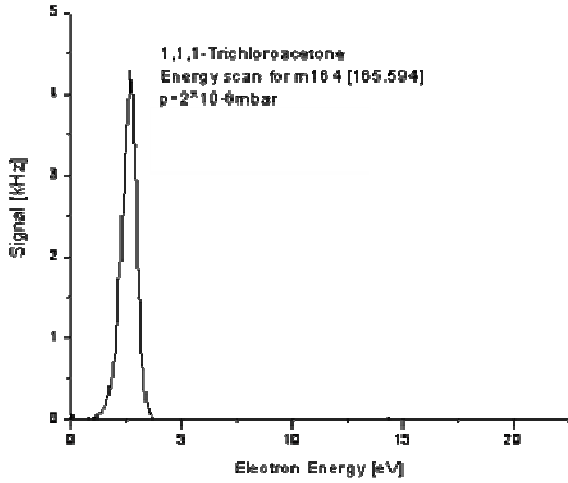


Energy scan for m54 (55.9909) uncalibrated
Acetone





1,1,1 Trichloroacetone



1,1,1 Trifluoroacetone

