CFEL SCIENCE

SEMINAR

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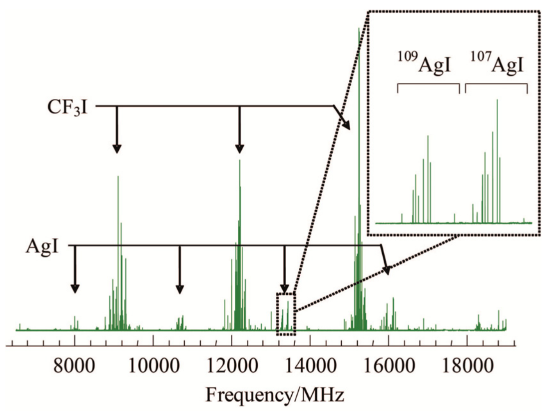
Chirped-pulse Fourier transform microwave spectroscopy of halogen-bonded and metal-containing complexes

Chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy allows the simultaneous measurement of pure rotational transitions across a bandwidth of more than one gigahertz. Advantages of the new technique include the possibility of rapid data acquisition and the opportunity to compare transition intensities across a broad frequency interval. The design of a CP-FTMW spectrometer recently constructed at the University of Bristol will be described. The spectra of $Kr\cdots ICF_3$, $OC\cdots ICF_3$, $H_3N\cdots ICF_3$ and $(CH_3)_3N\cdots ICF_3$ have been assigned to determine the length of the halogen bond in each complex and observe internal rotation in $H_3N\cdots ICF_3$ and $(CH_3)_3N\cdots ICF_3$.

The spectra of $H_2O\cdots ICF_3$ and $H_2S\cdots ICF_3$ display interesting features that cannot be modelled using simple Hamiltonians. A laser ablation source has recently been added to the CP-FTMW spectrometer allowing the study of metal-containing complexes. The molecular geometries of $OC\cdots AgI$ and $H_2S\cdots AgI$ have been determined from their broadband rotational spectra. These results will be placed in context of other recent work to characterise the molecular geometries of $H_2O\cdots MCl$, $H_2S\cdots MCl$, $H_3N\cdots MCl$ and $C_2H_4\cdots MCl$ by microwave spectroscopy, where M=Cu or Ag.



Host: Melanie Schnell - CFEL Molecular Physics seminar