

ERG Mid Term Report
Grant agreement number: 203885

MetOxAd Project Summary by Dr. Martin A. Collier

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Stage 1: Production of Ca/RG solids

Stage 1 of the MetOxAd project, the production and characterisation of rare gas solids doped with 'isolated' calcium atoms, has been accomplished. High quality Ca/RG films of have been deposited at 10 K. Absorption spectra recorded following sample production have allowed the assignment of atomic transitions to the ¹P and ¹D excited states of atomic Calcium.

Deviations:

- Initially it was proposed to deposit at 12 K. However a lower deposition temperature of 10.5 K was achieved following the re-design and installation of a pre-existing radiation shield on the cryostat. The lower temperature has allows easier identification of Ca absorption bands.
- It was proposed to produce Calcium vapour by laser ablation of the bulk metal from a rotating rod. Due to financial constraints a Knudsen Cell, high temperature oven was employed instead. See note regarding project finances below.

Installation of the Knudsen Cell allowed an investigation of the luminescence spectroscopy of atomic Sodium. The results of which were published by the Maynooth Group in collaboration with Patrick de Pujo Laboratoire Francis Perrin, CNRS URA 2453, CEA Saclay, France, and Claudine Crepin, Laboratoire de PhotoPhysique Moleculaire, CNRS UPR 3361, Universite Paris-Sud 11, Orsay, France.

Stage 2: Luminescence of solvated Ca atoms

Stage 2, characterisation of rare gas solids doped with 'isolated' calcium atoms, has for the most part been accomplished. The luminescence spectroscopy recorded has allowed the effect of inert rare-gas (RG) solvation on the metal atom to be determined.

The ¹D luminescence has been shown to depend on the rare gas host (solvent) and the site/cavity size available to the metal atom within the solid. Recent high-resolution ¹D measurements have indicated the presence of weak crystal field effects.

The extension of the luminescence measurement to Calcium atoms in reactive halo-carbon and hydrocarbon matrices are still ongoing. Early results indicate novel thermal Ca + CH₃F reactivity occurring at 10 K.

The observation of weak crystal field splitting of Ca atoms prompted a more detailed analysis of the existing manganese data leading to two recent publications.

Deviations:

- The novel thermal reaction $\text{Ca} + \text{CH}_3\text{F}$ observed at 10 K has hampered subsequent spectroscopic investigations.

Stage 3: Step-Scan FTIR Ca + Molecule Reactions

Rare gas matrices containing Calcium and the molecule of interest have been produced for investigation using IR spectroscopy. However no evidence of the $\text{Ca} (^1\text{S}) + \text{CH}_3\text{F}$ van der Waals reaction precursor ($\text{Ca-CH}_3\text{F}$) has been observed to date.

Deviations:

- Low concentrations of the precursor complex were anticipated in the initial project outline. It was proposed to increase the concentration of precursor substantially a pulsed ablation source. The projected ablation source would have allowed direct injection of the *pre-formed* gas phase cluster into the rare gas solvent. Financial constraints (see note below regarding project finances) have not allowed the design and construction of the ablation source.

Researcher Training/Integration Activities

The researcher, Dr. Martin Collier has also been engaged in contract / part-time teaching and supervision of first to final year undergraduate and postgraduate students within the Department of Chemistry, National University of Ireland - Maynooth.

Deviations:

- The proposed application by the researcher and the Host (Department of Chemistry) for a tenure track position under the Stokes Professorship & Lectureship Programme, Science Foundation Ireland (SFI), 2007 did not proceed. The researchers application was turned down within the host department.

Project Finances

No salary contribution was sought on application for the ERG Grant. Following receipt of funding under the MetOxAd project no additional source of financial support for the researchers salary could be found within the host institution. Discussions with the EU allowed the use of the MetOxAd budget to pay the researchers salary for the 2008 calendar year.

Since 31/12/2008, the researcher has not been in full time employment at the host institution. The researcher has spent 15 months of the 30 available to-date actively working on the MetOxAd project. Contract dates: 01/01/2008 – 31/12/2008 and 01/09/2009 – present.