Journal of Physics: Conference Series **635** (2015) 072037 doi:10.1088/1742-6596/635/7/072037

Electron driven water formation from oxyhydrogen clusters in superfluid helium nanodroplets

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Synopsis Helium nanodroplets provide an enviroment that allow studies of chemical reactions at ultracold temperatures. We use these droplets as a matrix to study the formation of water upon electron bombardment of oxyhydrogen clusters

The production of water from the combution of oxyhydrogen is one of the most well known chemical reactions. It is highly exorthermic with an energy release of 572 $\frac{\text{kJ}}{\text{mol}}$ and in order to be ignited the oxyhydrogen mixture needs to be heated up to about 600 °C (at ambient pressure). In our study we employ a radically different method to observe a oxyhydrogen reaction. Superfluid helium nanodroplets (HND) offer an unique environment to study chemical reactions at ultracold temperatures and have been employed by our group to study a variety of different systems [1], [2].

HNDs were produced by supersonic expansion of helium (purity: 99.9999%) through a 5 µm1 nozzle at a temperature of 9.4 K and a stagnation pressure of 20 bar into vacuum, they are superfluid and have a temperature of 0.37 K. Under these conditions their size can be estimated to be $5 \cdot 10^5$ helium atoms per droplet. The HND then traversed through two differentially pumped pick-up cells where we introduced first O_2 and afterwards H_2. The dopants were able to move frictionless to the centre of the droplet were they formed oxyhydrogen clusters. Afterwards the doped HNDs were exposed to electron bombardment at various energies in a Nier-type ion source in order to form cations and anions respectively. The resulting ions were then mass-analyzed by a commercial time-of-flight instrument (Tofwerk AG, model HTOF) with a mass resolution of up to $R \approx 5000$.

The recorded mass spectra show series of O_n clusters with various hydrogen atoms attached to them. From the raw data we can extract cluster series of the different species to look for magic numbers with a specially developed software [3]. These magic numbers indicate ions with a higher binding energy compared to those of lower yield. Several findings can be gained from these cluster series:

1. There is a distinct odd-even oscillation in the ion yield of the oxygen clusters. When looking at the attachment of hydrogen to the oxygen clusters one has to differentiate between the cationic and the anionic case.

2. Even numbered oxygen cluster anions show a strong ion yield for the attachment of one hydrogen atom, whereas the signal drops considerably for the attachment of subsequent hydrogen atoms showing a distinct odd-even oscillation.

3. Odd numbered oxygen cluster anions on the other hand show a magic number for the attachment of H_2, thus indicating the formation of $O_{2n}H_2O^-$ complexes.

4. Even and odd numbered oxygen clustercations show magic numbers for the attachment of three hydrogen atoms, thus indicating the formation of $O_nH_3O^+$ complexes

As already mentioned magic numbers correspond to ions with an enhanced binding energy thus our findings indicate water formation on these oxygen clusters.

Acknowledgements: This work has been supported by the FWF Austrian Science Fund (FWF, P26635), Wien.

References

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