

Cluster analysis emitted from condensed Argon ices irradiated by heavy ions

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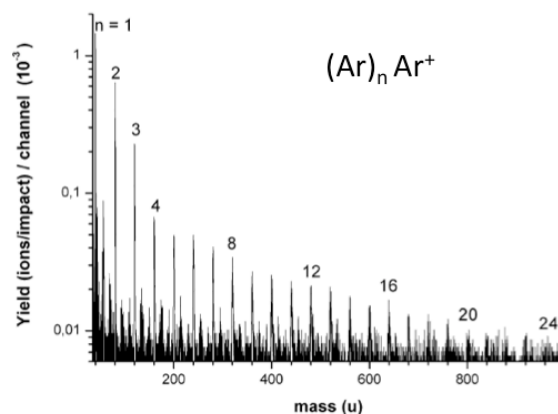
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Synopses. Argon ice is present in our Solar System mainly on grains and on comets, inside and beyond the region of giant planets. In this sense it is exposed to solar wind and cosmic ray radiation. The aim of this work is to study in laboratory the molecular species produced due to those interactions.

Ices are very important among the materials occurring in the Solar System. H₂O, CO, CO₂ and NH₃ are ices commonly found in many cosmic objects. Argon is less common but is present mainly inside and beyond the region of giant planets. The local low temperatures (< 30 K) cause its condensation on grains and on comets. Solid argon is exposed to solar wind and cosmic rays, which induce its sputtering, that is, emission of argon atoms, ions and clusters. As a laboratory approach, Ar condensed gas was deposited onto an Au substrate at ~ 30 K and bombarded by ~ 65 MeV multiply charged heavy ions (fission fragments of ²⁵²Cf). The emitted positive secondary ions were analyzed by time-of-flight mass spectrometry (PDMS-TOF). Typically, the secondary ions are emitted as clusters [1] with the structure (Ar)_nAr⁺, where Ar⁺ is a positive charged central core and Ar_n symbolizes n neutral ice Ar molecules surrounding the core.

Cluster ion desorption distributions based on Ar is very similar to that of other frozen gases, whose yields decrease exponentially in the n = 1 to 24 range. Actually the mass distribution shows an exponential fast decrease up to n ~ 6 and keeps decreasing exponentially – but slowly – for n > 6. In addition theoretical calculations were performed using the Density Functional Theory (DFT) in order to investigate the structure of neutral and charged argon clusters. DFT is generally used as a successful research tool due to the inclusion of electron correlation effects. Cluster geometries were optimized at the B3LYP level, with the 6-311G* basis set. Vibrational frequencies were analyzed to identify

minimum energy structures without negative frequencies. Preliminary calculations show well defined (Ar)_n like-icosahedra structures up to n = 60. Also “magic numbers” were identified indicating shell formations. Further analysis is being performed to verify this magic numbers and to corre-



late theoretical and experimental results.

Figure 1: TOF mass spectra from Argon ice irradiated by multiply charged heavy ion beams at ~ 65 MeV.

References

- [1] L. S. Farenzena, P. Iza, R. Martinez, F. A. Fernandez-Lima, E. Seperuelo Duarte, G. S. Faraudo, C. R. Ponciano, E. F. da Silveira, M. G. P. Homem, A. Naves De Brito, K. Wien, *Earth, Moon. and Planets*, 2005, 97, 311-329.

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