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Where do noble gases hide in space?

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Abstract.

Observations showing anomalous amounts of noble gas, especially in planetary atmospheres, are at the origin of a series of controversial interpretations from 1990 to nowadays (Hersant *et al.* (2004)). If, in a first step, we adopt a chemical point of view, we have to consider the possibility of associations of such elements (though usually considered as non reactive), with other molecules or atoms. Such complexes could trap the noble gases in some astrophysical objects at one time of their evolution, for example, in the early step of formation of protoplanetary disks. But two questions have to be answered to assert this type of hypothesis: which stable compounds could exist taking into account the environnement and which reactions could lead to such compounds?

Hydrogen being by far the most abundant element in space, and neutral systems whose cohesion is driven by weak Van der Waals forces being unable to resist turbulence in space, the first and simplest association to consider is the one between the noble gas and the H_3^+ ion. Thus, DFT in the B3LYP, PW91 and BHandHLYP formalisms together with ab-initio methods of Coupled Cluster type have been employed to determine the equilibrium geometries, the spectroscopic constants and the bonding energies of the possible complexes between noble gases and hydrogen.

We have first performed an extensive study of the associations $Ar_nH_3^+$ possible with Argon (the first noble gas which rose questions in the area of Jupiter's poles). We have found that several Argon atoms can be stabilized around the H_3^+ ion, the first complexation being in the plane of the ion. The spectroscopic data (rotational constants, dipole moments and IR signatures) were calculated (Pauzat & Ellinger (2005)) so that the laboratory experiments and spatial observations of these species could then be carried out. From our results and previous observations on this complex (Bogey *et al.* (1987)) we can say that the ArH_3^+ ion is certainly a good candidate for observation and, if observed, a good test of the hypothesis.

In a second step, we have extended the study of the association of one atom of noble gas X with the H_3^+ ion, to all noble gas from Helium to Xenon. All XH_3^+ are found stable with respect to dissociation but the stability of the complexes increases with the size and polarizability of the X atom. Unfortunately, the more stable complexes are also those with the less abundant noble gas.

Particular attention has been given to Helium. The association HeH^+ between the two most abundant elements has been looked for in most areas of space and nowhere detected. The problem is worth being addressed. State of the art calculations can be performed for these small size molecules. We found that the HeH_3^+ ion is stable by only 0.1Kcal/mol with respect to its components (He and H_3^+). By contrast, HeH_2^+ is found stable by a much larger binding energy (6Kcal/mol). However, from all our investigations, there is no way to form it. As an efficient way to form the simplest association, HeH^+, has also not been found, it seems that Helium is to be observed only as an isolated species and does not participate into any chemistry in spite of its large abundance in space.

Keywords. astrochemistry, molecular data, ISM: molecules

References

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