Pick-Up of Organic Molecules by Mixed Ar Clusters: A Function of Gas Properties and Composition

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Clusters present an intriguing field of research, with their properties bridging the gap between isolated atoms/molecules and bulk matter. They also exhibit strong surface-related phenomena. Formation of clusters is relatively straightforward, requiring the expansion of pressurized gas into a vacuum, combined with cooling for some gases. Clusters can be studied as such, serve for sputtering of the surfaces, and act as substrates for dopant molecules located on or inside the cluster. The properties of dopants in such highly specific environments can be studied with their concentration and localization on/in the cluster, influenced by many factors, one of which is the composition of the cluster. [1] Doping of clusters can be performed during their formation via pre-mixing, whereas for solid compounds, the pick-up of the heated compound's vapors by already formed clusters is more common.

Our research on Ar clusters reveals that gas pressure and composition are crucial parameters that determine the pickup probability of evaporated adenine, uracil, glycine, and ascorbic acid molecules. Clusters were formed with a pulsed Even-Lavie valve, and the cluster beam was made to traverse a heated cell containing the target biomolecule. Analysis of clusters doped in this way was performed with a quadrupole mass spectrometer. For pure Ar expansion, the most intense molecular signals were observed at stagnation pressures between 10 and 30 bar. Adding up to 33 mol% of He or O_2 at fixed total pressure caused no change in the intensity of dopant and Ar oligomer signals. [2] The addition of N_2O or CO_2 resulted in a significant decrease in intensity. Signals from the molecule and Ar oligomers even disappeared above 3 mol% of N_2O or CO_2. [2] The opposite effect was observed with the Ar-H_2 mixture at 25 bar. Optimal results were obtained for H_2 concentrations between 40 and 50 mol% versus D_2 concentrations between 20 and 35 mol%. Substitution of Ar with an Ar-H_2 mixture caused signal intensities of dopants and Ar oligomers to increase by more than threefold. [2] A compound-specific minimal temperature was also required to provide molecular vapors of sufficient density for the H_2 effects to become apparent.

[1] Dvorak, M.; Müller, M.; Bünermann, O.; Stienkemeier, F. Size dependent transition to solid hydrogen and argon clusters probed via spectroscopy of PTCDA embedded in helium nanodroplets. *J. Chem. Phys.* **2014**, *140*, 144301.
[2] Ekar, J.; Plekan, O. Pick-Up of Organic Molecules by Mixed Ar Clusters: A Function of Gas Properties and Composition. *Molecules* **2026**, *31*, 553.