Structure of mixed molecular clusters and its effect on laser induced intracluster dynamics

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Dynamics of intracluster processes were measured in the pump-probe experiments for $(CF_3I)_nXe_m$ and $[Fe(CO)_5]_nXe_m$ mixed molecular clusters. These mixed clusters, which were produced by expansion of a mixture with Xe carrier gas from pulsed nozzle, tend to have a shell structure: strongly bonded molecules in the core of the cluster are surrounded by weakly bonded atomic shells.

Photochemical reactions induced in such clusters by femtosecond UV laser pulses proved to be sensitive to laser intensity. XeI^+ ions are formed much more effectively with stretched from 150 fs to 2.2 ps UV laser pulses during the multiphoton ionization (MPI) process of $(CF_3I)_nXe_m$ mixed clusters. Real-time kinetics for XeI^+ and I_2^+ ions formed from these mixed clusters allow us to conclude that the presence of atomic shells in the mixed cluster prevent ultrafast (in 100 fs time domain) formation of products that require particles from the core of the cluster. In contrast to I_2^+ ions, formed in 1 ps from pure $(CF_3I)_n$ clusters [1], a rate for XeI^+ and I_2^+ ions in the case of mixed cluster is ~ 50 ps [2]. We believe the latter time constant is a good estimate on dissociation rate of the shell of the mixed cluster.

Dissociative ionization has a significant impact on the process of probing weakly bonded cluster beams by means of MPI. It could lead to high kinetic energy of produced ion products and, therefore, mark the mechanism of ion formation process as well as the origin of produced ions. Kinetic energy of Xe^+ ions, formed during MPI of dissociated shells of the mixed cluster, was measured and equals to several electronvolts in the experiment with $[Fe(CO)_5]_nXe_m$ mixed clusters. The mechanism of dissociation of Xe shells was revealed: these atoms are dissociated from the surface of the mixed cluster as a small Xe_n clusters.

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[2] D.G. Poydashev, O.S. Ablyasova, E.A. Ryabov, *JETP Letters* **2022**, *115 (9)*, accepted for publication.