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Noble gas cluster ions

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In recent decades, quantum chemistry calculations have been used for various chemical fields such as reaction pathway analysis and spectroscopic assignments due to the theoretical developments, especially accuracy improvement of functionals in density functional theory (DFT), and high-speed parallel computers.

The kinetic studies of formation Xe+Xe cluster in Xe, Ar+Ar cluster in Ar, and Ne+Ne cluster in Ne have not been found as experimentally or theoretically in literature. Therefore, in this study, we report the DFT-based mechanistic studies and spectroscopic analyses on formations of these clusters. In addition, we will calculate the rate constants all cluster formations.

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