Molecular Dynamics Simulation of Sympathetic Crystallization of Molecular Ions
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abstract It is shown that the translational degrees of freedom of a large variety of molecules, from light diatomic to heavy organic ones, can be cooled sympathetically and brought to rest (crystallized) in a linear Paul trap. The method relies on endowing the molecules with an appropriate positive charge, storage in a linear radiofrequency trap, and sympathetic cooling. Two well–known atomic coolant species, \(^{9}\text{Be}^+\) and \(^{137}\text{Ba}^+\), are sufficient for cooling the molecular mass range from 2 to 20,000 amu. The large molecular charge required for simultaneous trapping of heavy molecules and of the coolant ions can easily be produced using electrospray ionization. Crystallized molecular ions offer vast opportunities for novel studies.