Collisional dynamics of ultracold diatomic molecules

A.V.Avdeenkov and J.L.Bohn
JILA and Department of Physics, University of Colorado, Boulder, CO

Two new experimental techniques now exist for producing cold ground state molecules: buffer-gas cooling for paramagnetic molecules like $O_2$ [1] and Stark slowing for polar molecules like OH [2]. We have investigated ultracold collisions of these two types of molecules to understand the effectiveness of evaporative cooling. Collision cross sections and rate constants between two ground-state molecules have been investigated theoretically at translational energies below $\sim 1K$ for weak-seeking field states.

We present calculations for elastic and spin-changing inelastic collision rates for different isotopic combinations of oxygen atoms to understand their collisional stability in ultracold magnetic traps. Specifically, $^{17}O_2$ looks like a good candidate for ultracold studies, while $^{16}O_2$ is unlikely to survive evaporative cooling. Since $^{17}O_2$ is representative of a wide class of molecules that are paramagnetic in their ground state we conclude that many molecules can be successfully magnetically trapped at ultralow temperatures [3].

Analogously, we have considered the stability of polar OH molecules in an electrostatic trap [4]. The main feature of this gas is that molecules interact primarily via long-range dipole-dipole forces, and the interplay of this interaction with the Stark interaction defines the properties of their collisional dynamics. We have analyzed the dominant role of long-range potentials in determining the basic features of rate constants. At an electrostatic field up to several tens of thousands of $V/cm$ the inelastic rate constant is large and comparable with the elastic one, which implies that evaporative cooling is unlikely to succeed. However at high enough electrostatic fields (several hundreds of thousands $V/cm$), there may exist cases where elastic collisions greatly outnumber loss collisions.

The strong dipole-dipole couplings between channels with different partial waves restrict the interaction to their long-range contribution only, which an implies extremely weak dependence on the short-range potential for weak-seeking field states. This circumstance will greatly simplify the theoretical analysis of cold collision data.