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Cold collisions of an open-shell S-state atom with a ^2Pi molecule: N (^4S) colliding with OH in a magnetic field

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We present quantum-theoretical studies of collisions between an open-shell S-state atom and a ^2Pi-state molecule in the presence of a magnetic field. We analyze the collisional Hamiltonian and discuss possible mechanisms for inelastic collisions in such systems. The theory is applied to the collisions of the nitrogen atom (^4S) with the OH molecule, with both collision partners initially in fully spin-stretched (magnetically trappable) states, assuming that the interaction takes place exclusively on the two high-spin (quintet) potential energy surfaces. The surfaces for the quintet states are obtained from spin-unrestricted coupled-cluster calculations with single, double, and noniterative triple excitations. We find substantial inelasticity, arising from strong couplings due to the anisotropy of the interaction potential and the anisotropic spin-spin dipolar interaction. The mechanism involving the dipolar interaction dominates for small magnetic field strengths and ultralow collision energies, while the mechanism involving the potential anisotropy prevails when the field strength is larger (above 100 G) or the collision energy is higher (above 1 mK). The numerical results suggest that sympathetic cooling of magnetically trapped OH by collisions with ultracold N atoms will not be successful at higher temperatures.

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