

Abstract Submitted
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Intermolecular interactions involving ultracold linear polyatomic molecules JONATHAN SMUCKER, JOHN MONTGOMERY, ROBIN CÔTÉ, University of Connecticut — Recent advances in cooling molecules are making it possible to reach ultracold temperatures for simple polyatomic molecules. In this work, we investigate the interactions between such molecules. In particular, we consider linear polyatomic molecules such as CaOH, SrOH, CaOCH₃ or SrOCH₃ that are being pursued experimentally. We report their dipole, quadrupole, and octupole moments appearing in the multipole expansion of the long-range interaction between molecules. The multipole moments are calculated using coupled cluster theory with single and double excitations (CCSD) and the correlation consistent basis sets. We also show results from *ab initio* calculations of the interaction energy curves for specific molecular orientations, also calculated using couple cluster methods. We also consider mixed molecular species.

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