STRUCTURE, DIPOLE MOMENTS, POLARIZABILITIES, AND MOLECULAR SPIN ORBIT OF STRONG DIPOLAR ALKALI DIATOMICS

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The obtention of ultracold samples of dipolar molecules is a current challenge which requires a accurate knowlege of their electronic properties to guide ongoing experiments. [a, b, c, d,e] Such heteronuclear molecules, if deeply bound, have a significant permanent electric dipole moment leading to strong, long-range, and alignment dependent intermolecular forces, which offer control by external electromagnetic fields.
We have calculated potential curves, R-dependent permanent and transition dipole moments, and static polarizabilities for all heteronuclear dimers using quantum chemistry methods [f]. We also follow a new approach to include spin-orbit coupling in calculations of molecular potentials: a full-CI calculation with effective core potentials and a diabatization procedure is used to determine potential curves with fine structure. These new insights will be used to find efficient routes to produce and stabilize polar molecules, to model the dynamics of a dipolar gas in an optical dipole trap and to explore external field dependent scattering properties.

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