Abstract Submitted
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LiYb molecule in traps: potential energies, long-range energies, dipole moments, ...[1] H.R. SADEGHPOUR, P. ZHANG, A. DALGARNO, ITAMP, Harvard-Smithsonian CFA, ITAMP COLLABORATION — We employ multireference configurations interaction and coupled cluster techniques to determine the potential energy curves of the ground and low-lying excited states of the LiYb molecule. The scalar relativistic effects have been included by means of the Douglas-Kroll Hamiltonian and effective core potentials, and the spin-orbit couplings have been evaluated by the full microscopic Breit-Pauli operator. The dipole moment, static dipole polarizability, transition dipole moments, van der Waals coefficients, and Franck-Condon spectroscopy of the LiYb molecule have been determined. Perturbations to the vibrational spectrum due to the non-adiabatic interactions are included. Implications for double-MOT trapping of LiYb are discussed and we find that dimer of these molecules should easily form.

[1]NSF

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