

Abstract Submitted
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Calculations of long-range three-body interactions for Li(2S)-Li(2S)-Li⁺(1S)¹ PEI-GEN YAN, U. New Brunswick, LI-YAN TANG, WIPM, CAS, ZONG-CHAO YAN, U. New Brunswick & WIPM, CAS, JAMES F BABB, ITAMP, Harvard-Smithsonian CfA, — We theoretically investigate long-range interactions between a ground state Li⁺ ion and two ground state neutral Li atoms with highly accurate variationally-generated wave functions in Hylleraas coordinates. Using perturbation theory for the energies up to third-order, we evaluate the coefficients C_4 , C_6 and C_8 of the second order dispersion interactions and the coefficients C_7 and C_9 of the third-order additive and nonadditive interactions. The nonadditive interactions coefficients depend on the geometrical configurations of this three-body system and on the different positions of the ion for each configuration. Our calculations may be of interest for the study of three-body recombination and for constructing potential energy surfaces.

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