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Long-Range Three-Body Dispersion Interactions LI-YAN TANG, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, P. R. China, ZONG-CHAO YAN, Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3, TING-YUN SHI, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, P. R. China, JAMES F. BABB, ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA — There is an increasing interest in producing alkali-metal homonuclear or heteronuclear trimers using the photoassociation or magnetic-association techniques. Such trimers are formed near the zero-energy threshold and the constituent atoms typically have large internuclear separations where the dominant interactions are the long-range dispersion interactions. A general theoretical and computational framework is developed for the evaluation of long-range non-additive three-body dispersion interactions. The formalism allows for the possibility of one of the atoms to exist in an excited state. In the case of a homonuclear system such as Li(2s)Li(2s)Li(2p), the long-range interaction will have a lower order R-dependence due to the possibility of particle interchange. The lowest order three-body dispersion coefficients are presented for systems involving the H, He, Li atoms and the Li⁺, Be⁺ and H⁺₂ ions. The results of our calculations can be used as reference data for the long-range part of three-body potential energy curves for these systems.

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