IMPROVED ANALYTICAL POTENTIALS FOR THE $a\,^3\Sigma_u^+$ and $X\,^1\Sigma_g^+$ STATES OF Cs_2

JESSE BALDWIN, ROBERT J. LE ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.*

Recent studies of the collisional properties of ultracold Cs atoms have led to a renewed interest in the singlet and triplet ground-state potential energy functions of Cs_2. Coxon and Hajigeorgiou recently determined an analytic potential function for the $X\,^1\Sigma_g^+$ state that accurately reproduces a large body of spectroscopic data that spanned 99.45% of the potential well.[a] However, their potential explicitly incorporates only the three leading inverse-power terms in the long-range potential, and does not distinguish between the three asymptotes associated with the different Cs atom spin states. Similarly, Xie *et al.* have reported two versions of an analytic potential energy function for the $a\,^3\Sigma_u^+$ state that they determined from direct potential fits to emission data that spanned 93 % of its potential energy well.[b,c] However, the tail of their potential function model was not constrained to have the inverse-power-sum form required by theory. Moreover, a physically correct description of cold atom collision phenomena requires the long-range inverse-power tails of these two potentials to be identical, and they are not. Thus, these functions cannot be expected to describe cold atom collision properties correctly. The present paper describes our efforts to determine improved analytic potential energy functions for these states that have identical long-range tails, and fully represent all of the spectroscopic data used in the earlier work[a,b,c] as well as photoassociation data that was not considered there[d] and experimental values of the collisional scattering lengths for the two states.[e]

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[d] J. G. Danzl *et al.*, Science, **321**, 1062 (2008).
[e] C. Chin, *et al.*, Phys. Rev. Lett. **85**, 2717 (2000); P. J. Leo, C. J. Williams, and P. S. Julienne, Phys. Rev. Lett. **85**, 2721 (2000).