AN ACCURATE NEW POTENTIAL FUNCTION FOR GROUND-STATE Xe_2 FROM UV AND VIRIAL COEFFICIENT DATA

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Determining accurate analytic pair potentials for rare gas dimers has been a longstanding goal in molecular physics. However, most potential energy functions reported to date fail to optimally represent the available spectroscopic data, in spite of the fact that such data provide constraints of unparalleled precision on the attractive potential energy wells of these species. A recent study of ArXe showed that it is a straightforward matter to combine multi-isotopologue spectroscopic data (in that case, microwave, and high resolution UV measurements) and virial coefficients in a direct fit to obtain a flexible analytic potential function that incorporates the theoretically predicted damped inverse-power long-range behaviour.[a] The present work reports the application of this approach to Xe_2, with a direct fit to high resolution rotationally resolved UV emission data for $v''=0$ and 1,[b] band head data for $v''=0-9$,[c] and virial coefficient data for $T=165-950\,\mathrm{K}$[d] being used to obtain an accurate new potential energy function for the ground state of this Van der Waals molecule. Analogous results for other rare-gas pairs will also be presented, as time permits.

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