

AN EMPIRICAL DIPOLE POLARIZABILITY FOR He FROM A FIT TO SPECTROSCOPIC DATA YIELDING ANALYTIC EMPIRICAL POTENTIALS FOR ALL ISOTOPOLOGUES OF HeH<sup>+</sup>

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All available spectroscopic data for all stable isotopologues of HeH<sup>+</sup> are analyzed with a direct-potential-fit (DPF) procedure that uses least-squares fits to experimental data in order to optimize the parameters defining an analytic potential. Since the coefficient of the leading ( $1/r^4$ ) inverse-power term is  $C_4 = \alpha^{\text{He}}/2$ , when treated as a free parameter in the fit, it provides an independent empirical estimate of the polarizability of the He atom. The fact that the present model for the long-range behaviour includes accurate theoretical  $C_6$ ,  $C_7$  and  $C_8$  coefficients (which are held fixed in the fits) should make it possible to obtain a good estimate of this quantity.

The Boltzmann constant  $k_B$ , a fundamental constant that can define temperature, is directly related to the dipole polarizability  $\alpha$  of a gas by the expression  $k_B = \frac{\alpha}{3\epsilon_0} \left( \frac{\epsilon_r + 2}{\epsilon_r - 1} \right) \frac{p}{T}$ , in which  $\epsilon_0$  is the permittivity of free space, and  $\epsilon_r$  is the relative dielectric permittivity at pressure  $p$  and temperature  $T$ . If  $k_B$  can be determined with greater precision, it can be used to define temperature based on a fundamental constant, rather than based on the rather arbitrary triple point of water, which is only known to 5 digits of precision.  $\alpha$  for He is known theoretically to 8 digits of precision, but an empirical value lags behind. This work, examines the question of how precisely  $\alpha^{\text{He}}$  can be determined from a DPF to spectroscopic HeH<sup>+</sup> data, where the limiting long-range tail of the analytic potential has the correct form implied by Rydberg theory:  $\alpha^{\text{He}}/2r^4$ . Although the highest observed vibrational level is bound by over  $1000 \text{ cm}^{-1}$ , our current fits determine an empirical  $C_4 = \alpha^{\text{He}}/2$  with an uncertainty of only 0.6%. It has been shown that with more precise spectroscopic data near the dissociation,  $\alpha^{\text{He}}$  can be determined with high enough precision to determine a more precise  $k_B$  and hence redefine temperature more accurately<sup>b</sup>.

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<sup>b</sup>Dattani N S. & Puchalski M. (2015) *Physical Review Letters* (in press)