

## Improved empirical potential for the ground state of Be<sub>2</sub>

V. V. Meshkov<sup>a</sup>, A. V. Stolyarov<sup>a</sup>, R. J. Le Roy<sup>b</sup>

<sup>a</sup>Department of Chemistry, Lomonosov Moscow State University, 119991, Moscow, Russia,  
E-mail: meshkov@laser.chem.msu.ru

<sup>b</sup>Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

We have performed new direct-potential-fit (DPF) analyses of the rotationally resolved A<sup>1</sup>Π<sub>u</sub> (v' = 2, 3; J' = 1, 2) → X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> (v'' ∈ [0, 10]; J'' ∈ [0, 3]) stimulated emission pumping spectra of Be<sub>2</sub> [1]

using two quite different analytical potential energy functions which incorporate the correct theoretically-known long-range behavior in different ways. These functions are: the damped Morse/long-range (MLR) potential [2] and the Chebyshev polynomial expansion (CPE) potential [3]. In contrast with the potential energy function determined in the original DPF analysis of Merritt et al., both of our functions unambiguously support the existence of the v = 11 last vibrational level which is bound by only 0.50(5) cm<sup>-1</sup>. These empirical potentials predict the equilibrium distance r<sub>e</sub> = 2.444(1) and the dissociation energy D<sub>e</sub> = 934.8(0.3) cm<sup>-1</sup>, values which are both remarkably close (within the uncertainties) with the best ab initio estimates.

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[1] J. M. Merritt, V. E. Bondybey, M. C. Heaven, *Science* **2009**, *324*, 1548.

[2] R. J. Le Roy, C. C. Haugen, J. Tao, H. Li, *Molecular Physics* **2011**, *109*, 435-446.

[3] L. Busevica, I. Klinkare, O. Nikolayeva et al., *J. Chem. Phys.* **2011**, *134*, 104307.