AN IMPROVED EMPIRICAL POTENTIAL FOR THE HIGHLY MULTI-REFERENCE SEXTUPLY BONDED TRANSITION METAL BENCHAMRK MOLECULE Cr_2

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The ground electronic state of the chromium dimer dissociates into $^7Cr + {}^7Cr$ and therefore there are 12 open shells among its constituent atoms. It is considered the most difficult homonuclear diatomic for *ab initio* methods because of its highly multi-reference character. Therefore, every new multi-reference method must be tested against this benchmark system. However, the best empirical potential to compare with, was built based on an out-of-date method for representing experimental data. The photoelectron measurements of $v = 0 - 9$ were fitted to a Morse potential (an old function which has only one parameter controlling the shape from r_e to D_e), and also inverted using a semi-classical theory into a potential after combining these data with measurements from what was guessed to be $v = 24 - 43$. This bridging of a $\sim 2000\,cm^{-1}$ gap in data back in 1993 was a valiant spectroscopic analysis. However since 1993, there have been enormous improvements in the field of potentiology. In 2011 a Morse/long-range (MLR) function successfully bridged a gap of more than $5000\,cm^{-1}$ in experimental data[a], and in 2013 an experiment with $\pm 0.000\,02\,cm^{-1}$ resolution confirmed that the 2011 MLR predicted the energy levels in the very center of this gap correctly within $\sim 1\,cm^{-1}$,[b]. While *ab initio* methods have very recently been able to predict differences in energy levels correctly to within $1\,cm^{-1}$ for Li_2 [c] and to a lesser extent for BeH[d], *ab initio* methods have still not had this level of success for predicting binding energies.

The MLR function not only has more flexibility than the original Morse function, but it also converges mathematically to the correct long-range limit expected by the state-of-the-art theory. Fitting the data to an MLR potential function in the Schrödinger equation allows for a fully quantum mechanical treatment over the entire range of data. By avoiding a semi-classical treatment, and using this more flexible, more theoretically correct form, we improve the current best empirical potential. This vastly improves the experimental benchmarks against which emerging *ab initio* methods are tested. However, the lack of data for Cr_2 is still a big problem, so further experimental work on Cr_2 is desperately needed.

[a] Dattani & Le Roy (2011) Journal of Molecular Spectroscopy, **268**, 119, [b] Semczuk *et al.* (2013) Physical Review A, **88**, 062510., [c] Dattani (2015) http://arxiv.org/abs/1508.07184, [d] Dattani (2015) Journal of Molecular Spectroscopy **311**, 76.