A comparative study of CdH and N_2 systems in their ground electronic states between Hylleraas, Varandas and Aguado-Paniagua potentials

Judith P. Araújo, Ramon S. Silva and Maikel Y. Ballester[a]

[a]*Departamento de Física, Universidade Federal de Juiz de Fora, Brazil*
maikel.ballester@ufjf.edu.br

Egil Andersen Hylleraas (1898-1965) made numerous contributions to the development of Atomic and Molecular Physics [1]. In 1935, Hylleraas [2] focused his interests on potential energy curves (PECs) of diatomic species. He proposed a potential containing six fitting parameters [3]:

$$V_{HY} = F + -D - D\xi^2, \quad 1-\xi = \frac{(1+a)(1+c)(x+b)}{(1+b)(x+a)(x+c)},$$
$$x = e^{(1+k)\rho}, \quad \frac{1}{1+k} = \frac{1}{1+a} + \frac{1}{1+c} + \frac{1}{1+b}, \tag{1}$$
$$\rho = \frac{\hbar\omega_e}{2\sqrt{B_e D}} \frac{(R-R_e)}{R_e}$$

where D, B_e and $\hbar\omega_e$ are spectroscopic constants and R_e is the equilibrium distance. In this work, the evolution in the field of PECs is evaluated, comparing current methods with those proposed more than 80 years ago. For such, we have chosen analytic representations by Hylleraas [4], Varandas [5] and Aguado-Paniagua [6]. For comparisons, the diatomic systems CdH and N_2 both in their respective ground electronic states were selected. These species are the same systems previously used by Hylleraas to test his function [4]. *Ab initio* electronic energies calculated at multireference configuration interaction (MRCI) using AVXZ (X = Q,5,6) basis [7] set were fitted to the mentioned functions. For all studied cases, rovibrational levels, as well as spectroscopic constants, are calculated and compared with available literature data.

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References

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