

Potential energy Surface for the ground electronic state of SSiH

Delvany G. de Castro^a, Yu-zhi Song^b and Maikel Y. Ballester^{a1}

^a*Departamento de Física, Universidade Federal de Juiz de Fora, MG 36036-330, Brazil*

^b*School of Physics and Electronics, Shandong Normal University, Jinan 250014, China*

Sulfur-bearing molecular systems have attracted the interest of the astrophysical particularly after been observed in ISM and circumstellar regions [1]. This work presents an analytical function for the potential energy surface (PES) of the SSiH. The PES is constructed in the frame of the many-body expansion (MBE)[2]; dividing also each term into two-parts as proposed by Aguado and Paniagua [3]. *Ab initio* calculations, were carried out using Molpro 2012/2015 suite of programs [4]. Multi-reference configuration interaction with Davidson corrections, using the full valence complete-active-space self-consistent field wave function as reference was followed in the electronic structure calculations. Dunning basis sets AVTdZ and AVQdZ were used together with a three parameter scheme to extrapolate to the complete basis set limit. Topological features and exploratory dynamics calculations are discussed.

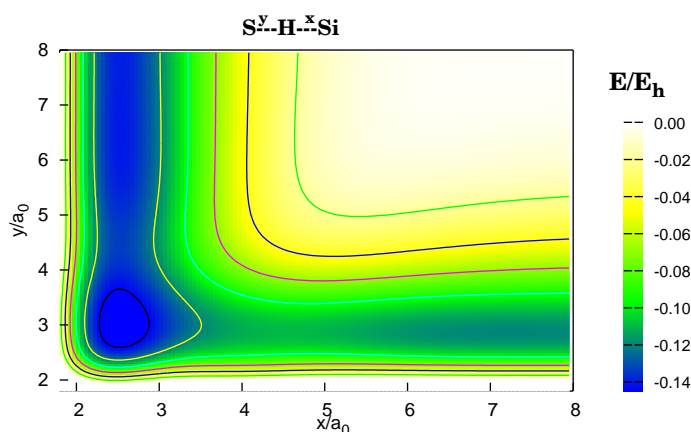


Figure 1: Contours plot for the analytically represented SSiH PES. The linear approach of the sulfur atom to the HSi molecule is depicted. Global minimum and saddle points can be viewed.

References

1. A. Fuente, *et al.* *Astron. & Astrophys.* 624, A105 (2019)
2. N. Murrell, S. Carter, S. C. Farantos, P. Huxley, and A. J. C. Varandas, *Molecular Potential Energy Functions* (Wiley, Chichester, 1984).
3. A. Aguado and M. Paniagua, *J. Chem. Phys.* 96 , 1265 (1992).
4. H.-J. Werner, P. J. Knowles, G. Knizia, F.R Manby and M. Schütz, M., *WIREs Comput Mol Sci*, 2, 242 (2012)

¹e-mail: maikel.ballester@ufjf.edu.br