

## HIGH ORDER VIBRONIC POTENTIALS FOR MOLECULES WITH JAHN-TELLER AND PSEUDO JAHN-TELLER COUPLINGS

KETAN SHARMA, *Quantum Theory Project, University of Florida, Gainesville, FL, USA*; OLEG A. VASILYEV, TERRY A. MILLER, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, USA*; JOHN F. STANTON, *Quantum Theory Project, University of Florida, Gainesville, FL, USA*.

Free radicals like  $\text{NO}_3$  and  $\text{CH}_3\text{O}$  often exhibit significant vibronic couplings. Past experimental and theoretical works on both these molecules have indicated the need for higher order potential energy surfaces than those available at the time of study, to enable a better understanding of the experimental results e.g. studying the vibronic structure of the  $\tilde{A}^2E''$  state of  $\text{NO}_3$  radical<sup>1</sup> and the spin-vibronic structure in the C-H stretch region of the  $\tilde{X}^2E$  state of  $\text{CH}_3\text{O}$  radical<sup>2</sup>. A typical problem with generating such potentials is the extremely high number of parameters required to represent them accurately. In this presentation, we talk about generating up to sixth order potential energy surfaces for molecules with three-fold symmetry. Molecular symmetry properties have been used to significantly reduce the number of independent parameters in the potential part of the corresponding spin-vibronic Hamiltonian matrices. Machine-learning-based methods have been developed to fit adiabatic potential energy surface data that have been obtained using electronic structure calculations. The improved quality of the new potentials is evidenced by comparing the predicted and observed values of spectral parameters. Improvements to the SOCJT3 software<sup>3</sup> used for solving the vibronic and spin-vibronic problems will also be discussed.

---

<sup>1</sup>T. Codd, M.-W. Chen, M. Roudjane, J. F. Stanton, and T. A. Miller, *The Journal of Chemical Physics* **142**, 184305 (2015).

<sup>2</sup>M. L. Weichman, L. Cheng, J. B. Kim, J. F. Stanton, and D. M. Neumark, *The Journal of chemical physics* **146**, 224309 (2017).

<sup>3</sup>K. Sharma, O. A. Vasilyev, T. A. Miller, and J. F. Stanton, *IOP Conf. Ser. Jahn-Teller Effect*, **In Press** (2024).