Abstract Submitted
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Computational method of molecular potentials from spectroscopic data[1] XUAN LI, CIAN MENZEL-JONES, MOSHE SHAPIRO, The University of British Columbia — We present a procedure that utilizes frequency-resolved fluorescence data from a reference potential to construct the corresponding potential energy surface and calculate its associated electronic transition dipole function. Our method is a fast and accessible alternative to an ab initio calculation with high accuracy. Compared to the RKR method, our procedure has the advantage to: (1) build a continuous potential above the dissociation limit, and (2) construct potentials with double minimums or local humps. In addition, we use the wavefunction of the calculated potential to construct the electronic transition dipole functions. We show the robustness of our procedure against insufficient or inaccurate fluorescence data through numerical simulations. Numerical simulations performed on both model systems and a diatomic Sodium molecule are presented.

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