Title:	A beyond Born-Oppenheimer treatment of five state molecular system NO3 and the photodetachment spectra of its anion
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Abstract:	A five-state multimode non-adiabatic dynamics has been performed on by constructing accurate diabatic potential energy surfaces (PESs) in vibronically coupled manifold using beyond Born-Oppenheimer (BBO) theory. In this article, we have considered the photodetachment of to the doublet states (, and) of and determined the vibronic couplings and conical intersections of the latter. Using ab initio calculated adiabatic PESs and Non-adiabatic Coupling Terms, we have carried out adiabatic-to-diabatic transformation (ADT) in five-state sub-Hilbert space to obtain ADT angles and thereby, constructed single-valued, smooth, symmetric and continuous diabatic PESs. The explicit analytic expressions for diabatic PESs and coupling elements are provided. Subsequently, we have performed nuclear dynamics starting from the electronic ground state of to simulate photodetachment spectra. The overall spectral profiles for and states show reasonably good agreement with experimental results and that of state with other theoretical calculations.
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