Title:	An ab initio investigation of non-adiabatic couplings and conical intersections among the lowest five electronic states of the NO3 radical
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Abstract:	In order to explore spectroscopic properties of a floppy molecule, it is necessary to compute accurate diabatic potential energy surfaces (PESs) around the Franck–Condon region of nuclear configuration space. In such cases, it is desirable to include the non-adiabatic coupling terms (NACTs) through Jahn–Teller (JT) and pseudo Jahn–Teller (PJT) effects as well as other accidental conical intersections (CIs) prevailing among the electronic states of the molecule. In this work, we investigate NACTs among the five lowest doublet electronic states of NO3 radical [and 22B2)], in which all those effects (JT, PJT and CIs) have prominent contributions. The study is carried out in terms of normal modes (Qis) of NO3 and the CIs (JT and accidental) are located in a plane of nuclear configuration space of two such coordinates (Qi and Qj). We have calculated ab initio adiabatic PESs and NACTs of those five states of NO3 at the MRCI level as functions of pairwise Qis. Further, to explore the nature of a given CI in terms of normal coordinates contributing to NACTs within a particular plane Qi-Qj, we have performed CP-MCSCF study computing analytic NACTs and characterised their contributions along various Qks.
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