Title:	Beyond Born-Oppenheimer treatment for the construction of triple-sheeted accurate diabatic Hamiltonian matrix of F+H2 system
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Abstract:	We intend to study the non-adiabatic interactions among the three lowest adiabatic states (12A′, 12A″, and 22A′) of F+H2 triatomic reactive system in hyperspherical coordinates for a fixed hyperradius at ρ = 7.5 bohr as functions of hyperangles, θ (0° ≤ θ ≤ 90°) and φ (0° ≤ φ ≤ 360°). The adiabatic potential energy surfaces are calculated using MRCI level of methodology whereas the non-adiabatic coupling terms between those states are calculated from the analytic gradient methods implemented in MOLPRO quantum chemistry package. The ground (12A′) and the first excited (12A″) states exhibit conical intersection (CI) and seam of CI along C2v geometries, whereas the first (12A″) and the second (22A′) excited states undergo Renner-Teller coupling at linear geometries. We carry out adiabatic-to-diabatic transformation (ADT) by solving ADT equations to obtain ADT angles for constructing single-valued, continuous and symmetric 3 × 3 diabatic potential energy matrix so that subsequent accurate scattering calculations can be performed
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