Title:	Jahn-Teller and coupled Jahn-Teller/Renner-Teller effects in the calculation of adiabatic-to-diabatic transformation angle for the lowest three 2A′ states of NH2 (NHH)
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.) Bear, M. (/jspui/browse?type=author&value=Bear%2C+M.)
Keywords:	adiabatic-to-diabatic transformation angle black hole Jahn-Teller non-adiabatic coupling term
Issue Date:	2015
Publisher:	Taylor & Francis.
Citation:	Molecular Physics, 113(5) pp. 436-446.
Abstract:	We report here on the first study of topological effects for the NHH system, as carried out by treating simultaneously the two dominant effects of this system, namely, the Jahn-Teller (JT) effect and the Renner-Teller (RT) effect. Both the effects were treated rigorously as demanded by the Born-Oppenheimer approach. No approximations were made and in those cases where convergence was required, it was achieved by including the required number of states. The study concentrates on calculating the privileged adiabatic-to-diabatic transformation (ADT) angle γ12, along closed contours, which is the only needed angle to carry out the ADT in the case of relatively low energies. For this purpose, three coupled A′-states are usually considered and only in the last two extreme cases, where the area in configuration space becomes relatively large, namely 15-35 Å2, we had also to include an A″ state (the second Δ-state), a situation that enforces the more elaborate (JT/RT) effect. In this paper, we also report on potential energies as calculated along the above-mentioned contours. Among them are considered the energies associated with the two adiabatic Δ-states, 1A′ and 1A″, of different symmetry and therefore are responsible for the RT effect. These states are expected to be degenerate along the collinear axis. It was revealed that these states, in contrast to the Renner theory, are not degenerate along a finite interval of the collinear axis at the vicinity of the JT conical intersection (JT-CI). In other words, the JT-CI annihilates the RT degeneracy along this interval.
Description:	Only IISERM authors are available in the record.
URI:	https://www.tandfonline.com/doi/full/10.1080/00268976.2014.948089 (https://www.tandfonline.com/doi/full/10.1080/00268976.2014.948089) http://hdl.handle.net/123456789/2971 (http://hdl.handle.net/123456789/2971)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2971/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/2971?mode=full)

(/jspui/handle/123456789/2971/statistics)