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Accurate global potential energy surfaces and ro-vibrational states of triatomic molecules ANTÓNIO VARANDAS, Departamento de Química, Universidade de Coimbra, 3004-535 Coimbra, Portugal — This presentation focus on two case systems. The first is ground-state hydrogen cyanide for which we report a global single-sheeted double many-body expansion (DMBE) potential energy surface that fits accurately the best available *ab initio* energies while reproducing with near spectroscopic accuracy all vibrational levels up to the saddle point for the isomerization process HCN $\rightleftharpoons$ HNC. The problem of assigning ro-vibrational levels having wave functions delocalized over the HCN and HNC minima is then discussed. The second system is triplet H_3^+, whose potential energy surface has two adiabatic sheets conically intersecting for nuclear arrangements with D_{3h} symmetry. Using highly accurate *ab initio* calculations, a global double-sheeted DMBE potential energy surface has been modeled which should be reliable within a few cm^{-1}. Ro- vibronic calculations both with the inclusion of the geometrical phase (GP) effect, and without it, have also been done. We will focus on the upper sheet case, as the GP effect plays there a key role. In this regard, we discuss the case of any homonuclear triatomic molecule subject to Jahn-Teller interaction. It will be shown that the GP effect can naturally be included in a generalization of the G quantum number previously derived by Watson. This generalized G will be demonstrated to provide an improved quantum number for classifying such cone states.

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