CALCULATIONS OF THE H_3^+ ROVIBRATIONAL SPECTRUM TO LEVELS NEAR THE BARRIER TO LINEARITY

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On the H_3^+ potential surface[a] the saddle point for linear configurations lies about 9930 cm^{-1} above the lowest vibrational level. For calculations of vibration-rotation energy levels near or above this energy, it is important that the wavefunctions should have the correct behavior at linear geometries. The present work describes calculations using hyperspherical harmonics[b] as the angular basis. Previous similar calculations of lower energy levels of H_3^+ have been described by Wolniewicz and Hinze[c]. Here the line intensities as well as wavenumbers for the $5\nu_2$ band will be discussed.

[a]W. Cencek, J. Rychlewski, R. Jaquet, and W. Kutzelnigg, J. Chem. Phys. 108, 2831–6 (1998)
[b]L. Wolniewicz, J. Chem. Phys. 90, 371–7 (1989)
[c]L. Wolniewicz and J. Hinze, J. Chem. Phys. 101, 9817–29 (1994)