

**Investigation of the highest bound ro-vibrational states of H_3^+ , DH_2^+ , HD_2^+ , D_3^+ , and T_3^+ :
Use of a non-direct product basis to compute the highest allowed $J>0$ states.**

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A Lanczos algorithm with a non-direct product basis was used to compute energy levels of H_3^+ , DH_2^+ , HD_2^+ , D_3^+ , and T_3^+ with total angular momentum J values as large as 46, 53, 66, 66, and 81. The energy levels are based on a modified potential surface of M. Pavanello et al (*J. Chem. Phys.* **2012**, 136,184303), that is better adapted to the ab initio energies near the dissociation limit [1, 2].

In this work we demonstrate that using the Lanczos algorithm it is possible to calculate energy levels of bound states of H_3^+ and its isotopologues up to highest allowed J values.

Iterative methods obviate the need to store the Hamiltonian matrix and therefore make it possible to use large basis sets. They are especially attractive when using a product basis. H_3^+ is extremely floppy and therefore not a good candidate for contracted basis methods. To use the two-step contracted approach [3] one must solve a vibrational-like problem for each K and then diagonalize in a basis of retained eigenfunctions of the vibrational-like problems. Due to the importance of Coriolis coupling, for $J > \approx 10$ the total number of retained vibrational-like eigenfunctions is large and the final diagonalization is costly.

Non-direct product basis functions are products of functions of a single variable, but with a shared index, and therefore efficient matrix-vector products are possible. In this paper we show that a non-direct product spherical oscillator basis works well for H_3^+ . We obtain energy levels that agree well with those of previous calculations (on the same surface) and we are also able to compute levels for larger values of J than was heretofore possible. The non-direct product basis provides a compact representation of the wave functions.

Now that excellent PESs are available for H_3^+ it is worthwhile to compute wave functions for high J . It is possible that calculations of this sort will enable us to begin to disentangle the tantalizing spectra of Carrington et al, that have motivated many researchers to study H_3^+ [4].

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