USING A NON-PRODUCT QUADRATURE GRID TO COMPUTE THE VIBRATIONAL SPECTRUM OF C_2H_4

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We present an accurate 12-D basis set calculation of the lowest 100 energy levels of the C_2H_4 molecule. A Smolyak non-product quadrature grid, a pruned product basis set, and the Lanczos algorithm are used. This scheme allows one to reduce the size of the basis set by almost 7 orders of magnitude (from 9×10^{12} to 1.3×10^6) and the size of the quadrature grid by almost 6 orders of magnitude (from 5.6×10^{13} to 1.52×10^8). Basis pruning and the nonproduct quadrature grid therefore enable us to solve a problem, numerically exactly, that would be impossible without these tools.