USING A NON-PRODUCT QUADRATURE GRID TO COMPUTE THE VIBRATIONAL SPECTRUM OF C$_2$H$_4$

GUSTAVO AVILA and TUCKER CARRINGTON JR., Chemistry Department, Queen’s University, Kingston, Ontario K7L 3N6, Canada.

We present an accurate 12-D basis set calculation of the lowest 100 energy levels of the C$_2$H$_4$ 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 $9 \times 10^{12}$ to $1.3 \times 10^6$) and the size of the quadrature grid by almost 6 orders of magnitude (from $5.6 \times 10^{13}$ to $1.52 \times 10^8$). Basis pruning and the nonproduct quadrature grid therefore enable us to solve a problem, numerically exactly, that would be impossible without these tools.