CONSTRUCTION OF NESTED CONTRACTED BASIS FUNCTIONS USING DIMENSIONALITY-REDUCTION TECHNIQUES IN CONJUNCTION WITH GROUP-THEORETICAL METHODS

MICHAËL REY, *Groupe de Spectrométrie Moléculaire et Atmosphérique UMR CNRS 7331, UFR Sciences BP 1039, 51687 Reims Cedex 2, France*; **TUCKER CARRINGTON, Jr.**, *Chemistry Department, Queen's University Chemistry Department, Queen's University, Kingston, Ontario K7L 3N6, Canada*

The construction of contracted basis functions for solving the time-independent Schrödinger equation is revisited[1]. First, an extensive use of symmetry *via* the irreducible tensor operator formalism allows a unified treatment of molecules belonging to both Abelian and non-Abelian molecular symmetry groups. Second, a suitable combination of pruned basis sets and Kronecker products with relevant reduction techniques based on a tree-like structure allows to control the memory cost during each contraction. The dimension of the matrices to be diagonalized is thus substantially reduced, making it still possible to use direct eigensolvers, even for molecules with more than 5 atoms.

As a validation test, the proposed method is used to compute the energy levels of CH_3CN (C_{3v}) and C_2H_4O (C_{2v}) and the results are compared to the best available calculations.

[1]M. Rey and T. Carrington, Jr., to be submitted

p-number: p099 **Submitted on Tue, 13 Jun 2023 15:28:13 +0200**