

about 25 times greater than in the one-dimensional version. In both cases, the velocity of the moving fraction is inversely proportional to the molecule length, and the diffusion coefficient is proportional to the molecule length. The fraction of trapped molecules decreases with N . The simulation allows for direct observation of the geometration effect.

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Computer-Oriented Treatment of High Symmetry in Quantum-Chemical Calculations of Correlated Electronic States

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Recent achievements in the synthesis of novel substances and materials raise specific problems in computational quantum chemistry demanding to consider electronic structure multiatomic molecular systems in excited and ionic states beyond one-electron approaches. The proposed computational treatment of problem of electron correlation with emphasis on the symmetry-induced degeneracy of molecular states is discussed. It is essentially based on the theory of symmetry molecular invariants that supposes (i) use of fixed reference symmetry base and (ii) determination of invariant expansions for two-electron integrals and energies. The method successively takes full advantage of the relations between the integrals defined on symmetry molecular orbitals (MO). Using the symmetry-similarity principle within the model with two-center electron - electron interaction a simple computational technique is elaborated enabling to represent each integral from complete set as an expansion of a few independent integrals [1,2].

The technique is specified for the most complicated case of icosahedral (I_h) symmetry which is inherent to fullerene C_{60} . It is considered for (i) the configurations ($t_{1u} + t_{1g}$), the symmetries of two lowest vacant MOs and (ii) for upper occupied h_u -shell. The reference symmetry basis sets (mostly with integer components) are presented enabling to obtain the most results in a mathematically rigorous form thus avoiding round-off errors. Energy functionals constructed for all multiplet states of multi-charged ions are reduced to simple form involving only five (h -shell) or six ($(t_{1u} + t_{1g})$ case) independent integrals (instead of 120 or 231, respectively, in the general case) thus enabling to reduce full-CI or multiconfigurational self-consistent-field calculations of multicharged ions within the corresponding orbital spaces.

Applications of the proposed approach are presented to the C_{60} anion states, which are the case in superconducting fullerenes K_3C_{60} and Rb_3C_{60} . Some effects of electron interactions within quasi- π -electron model with different interelectron potentials are considered [3].

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