

Abstract for the Trieste Conference on Chemical Evolution IV:
Physics of the Origin and Evolution of Life "Cyril Ponnamparuma Memorial",
Trieste, 4-8 September, 1995.

***Ab Initio* Calculation of Molecular Energies Including Parity Violating Interactions**

Ayaz Bakasov, Tae-Kyu Ha and Martin Quack

Laboratorium für Physikalische Chemie, ETH (Zentrum), CH-8092, Zürich, Switzerland

A new approach, RHF-CIS, based on the perturbation of the ground state RHF wave function by the CIS excitations, has been implemented for evaluations of energy of parity violating interaction in molecules, E_{pv} . The earlier approach, RHF-SDE, was based on the perturbation of the RHF ground states by the single-determinant "excitations" (SDE). The results obtained show the dramatic difference between E_{pv} values in the RHF-CIS framework and those in the RHF-SDE framework: the E_{pv} values of the RHF-CIS formalism are more than one order of magnitude greater compared to the RHF-SDE formalism as well as the corresponding tensor components. The maximal *total* value obtained for hydrogen peroxide in the RHF-CIS framework is $3.661 \times 10^{-19} E_H$ (DZ** basis set) while the maximal E_{pv} value for the RHF-SDE formalism is just $3.635 \times 10^{-20} E_H$ (TZ basis set). It is remarkable that both in the RHF-CIS and in the RHF-SDE approaches the diagonal tensor components of E_{pv} strictly follow the geometry of a molecule and are always different from zero at chiral conformations. The zeros of the total E_{pv} at chiral geometries are now found to be the results of the interplay between the diagonal tensor components values. We have carried out exhaustive analysis of the RHF-SDE formalism and found that it is not sufficiently accurate for studies of E_{pv} . To this end, we have completely reproduced the previous work, which has been done in the RHF-SDE framework, and developed it further, studying how the RHF-SDE results vary when changing size and quality of basis sets. This last resource doesn't save the RHF-SDE formalism for evaluations of E_{pv} from the general failure. Packages of FORTRAN routines called ENWEAK/RHFSDE-93 and ENWEAK/RHFCIS-94 have been developed which run on top of an *ab initio* MO package. We used 6-31G and 6-31G**, DZ and DZ**, TZ and TZ**, and (10s, 6p, **) basis sets. We will discuss the importance of the present results for possible measurement of the parity violating energy difference between enantiomers of chiral molecules.