

FIELDS OF APPLICABILITY OF FLOATING SPHERICAL GAUSSIAN ORBITALS, (FSGO), AND THE CHEMIST'S INVOLVEMENT WITH THE COMPUTER

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Some important aspects of the FSGO method, which have a wide range of applicability in Chemistry, are discussed in this paper. The following fields of study are dealt with in detail.

- (i) geometrical properties of molecules
- (ii) study of potential energy surfaces and reaction mechanisms;
- (iii) bond dissociation phenomena
- (iv) demonstration of the concepts of resonance, hybridisation, and delocalisation.
- (v) crystal structures and macromolecules

The work carried out in all the above areas where the FSGO method has been successfully utilized, is described.

Latter part of the paper explains the involvement of the computer, in the above work. Usefulness of the computer for chemists in general, is pointed out. It is suggested that chemists, students as well as professionals, must make the best use of the available computer facilities. Some examples of programming is also discussed.