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## A USEFUL, RECENT METHOD FOR STUDYING MOLECULAR STRUCTURE AND PROPERTIES\*

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This paper presents an introduction to the Floating Spherical Gaussian Orbital (FSGO) method as a means of evaluating structures and some properties of molecular systems. This FSGO concept is a sound ab-initio procedure, originated by A. A. Frost (U. S. A.) in 1967. The method uses normalised Floating Gaussian functions of the form;

$$\phi_i = \left\{ \frac{2\alpha_i}{\pi} \right\}^{\frac{3}{4}} \exp \left\{ -\alpha_i \frac{(\tau - R_i)^2}{i} \right\}$$

where the orbital exponent  $\alpha_i$  and the components of the orbital centre vector  $R_i$  are the variations parameters.

The biggest advantage of the method lies in its simplicity in

- (a) evaluation of component integrals
- (b) visualisation of the electron distribution and interpretation of the results.

(a):- increases speed and improves economy when compared to other methods. These facts enable us to extend the FSGO method to larger systems, than those that could be coped within Hartree-Fock-Self-Consistent Field (HF-SCF) calculations.

FSGO calculations have been made for a series of Molecular systems. These calculations show that the method predicts results which are remarkably consistent with experiment.

Some theoretical aspects of the FSGO method and the results for few simple molecules and their conclusions are discussed in this paper.

(\*This work was done at the chemical laboratories, University of Cambridge).