

# EVALUATION OF VIBRATIONAL FORCE CONSTANTS OF BONDS IN SIMPLE MOLECULES USING THE FLOATING SPHERICAL GAUSSIAN ORBITAL (FSGO) METHOD

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The Floating Spherical Gaussian Orbital (FSGO) method has been employed successfully in the calculation of energies and several other properties of simple molecules. In this study, the use of the FSGO method in its original form and also in certain modified forms to evaluate force constants of bonds for different modes of vibration of simple molecules, was investigated. Two of these molecules, of which the results are presented here, are ethylene ( $C_2H_4$ ) and Carbon dioxide ( $CO_2$ ). Symmetric vibration of the  $C=C$  bond in  $C_2H_4$  and symmetric and asymmetric vibrations of the  $C=O$  bonds in  $CO_2$  were studied.

Results show that the FSGO method produces values which are quite consistent with those obtained experimentally by spectroscopy. Further, the results confirm the fact that the FSGO method is very suitable for this type of extensive calculation of force constants, since its applicability could be conveniently extended to a large number of simple molecules.

## References:

1. Mallawaarachchi, W., 1976, A useful recent method for studying molecular structure and properties., Proc. SLAAS, (32nd Annual Sessions.)
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