HYBRIDISATION OF DELOCALISATION?

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In this paper, the shortcomings of using the criterion of hybridisation alone to explain bond lengths of some molecules is pointed out. The importance of delocalisation is also stressed. In this connection an analysis of the structural results for the cyanogen molecule (C_2N_2) and a series of other related molecules using the Floating Spherical Gaussian Orbital (FSGO) method [1,2], is presented. Calculations have been performed for the C_2N_2 molecule[1], considering it in the form of

(i) the conventional simple structure

(ii) a resonance hybrid of five canonical structures

This type of resonance calculations have not been attempted by using rigorous procedures such as the Hartree Fock method and seems possible only by employing a method such as the FSGO wkere the mathematics involved is fairly simple.

The results obtained provide a conclusive theoretical proof that delocalisation is as important as hybridisation in explaining bond ledgths of C_2N_2 and other related molecules. Further these results illustrate the versatility and the power of the FSGO method over the other quantum mechanical methods in its potential applicability to the explanation of molecular structures.

References

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

2. W. Mallawaarachchi, 1975, Ph. D. Thesis Cambridge, U. K.