A SIMPLE QUALITATIVE MODEL TO DETERMINE THE GEOMETRY OF TRIATOMICS

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Determination of the geometry of triatomics is usually discussed in terms of the models of Walsh, Pearson and Deb. However this can also be discussed using perturbation theory. This paper discusses a qualitative model based on simple molecular orbital and first order perturbation theory to determine whether a triatomic is bent or linear. The model was tested not only on stable ground state triatomic, but also on ions and excited states of triatomic, and the agreement with experiment was remarkable.

References:

1. Walsh, A. D (1953) J. Chem. Soc. 2260
2. Pearson, R. G. (1969) J. Amer. Chem. Soc. 91, 4947
3. Deb, B. M (1975) J. Chem. Educ. 52, 314