

The molecular orbital theory of V organic compounds, molecular orbital theory

Ali Sahandabadi

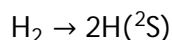
Kherad High School, Isar town Resalat street second Alley no.16, Urmia, Iran

Ali.Sahandabadi@yahoo.com

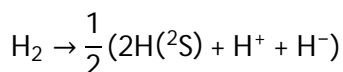
Abstract

The full hydrogenation of an organic molecule is divided to two stages. In the first stage, the molecule is broken to the simplest sources of itself which include similar components which was so-called link separation. In the second stage, I do the ab initio molecular orbital calculations of different multi-atomic molecules. Both increased and decreased basic groups are shown experimentally as linear combination of Gaussian-type functions to heat link separation. Instead, only the increased basic group is being succeeded in producing heat for sources hydrogenation.

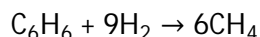
The energy of hydrogen decomposition with the lowest energy rate to its products



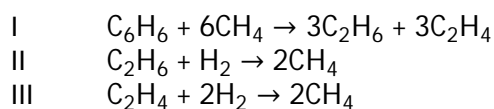
Is beyond Hartree-Fock theory because HF wave functions are analyzed to the combination of ions and atoms according to the equation



The anticipation goal of enthalpy change foe interaction is similar to



We use the Hess law to break the equation to the combination of



For the interaction of ideal gases with the Δn change in the number of gas moles, we have

$$\Delta H = \Delta U + RT\Delta n$$

They don't consider the zero-point vibrations, so, for example, in diatomic molecules the analytical constants of D_0 and D_e are related to

$$D_e = D_0 + \frac{1}{2} hc_0 \omega_e$$

So, we require calculating vibration frequencies which means doing a geometric optimization.

The rotational energy of $1/2 K_B T$ is in free rotational degree state.

There is two degree free rotation for a linear molecule and three degree rotation for a non linear molecule. Most vibration modes are crowded in T temperature. If the number of basic of vibration wave in a given mode is ω_e , so the related energy is $hc_0 \omega_e$. The approximate coordinate energies of all vibration states are

$$\varepsilon_v = \left(v + \frac{1}{2}\right) hc_0 \omega_e$$

The molecules fraction of N_v/N with energy of ϵ_v is provided by the well known Boltzmann formula as follow

$$\frac{N_v}{N} = \frac{\exp\left(-\frac{\epsilon_v}{k_B T}\right)}{\sum_v \exp\left(-\frac{\epsilon_v}{k_B T}\right)}$$

For both interactions, the logical experiment is accepted. In Benzene case, the bond energy separation (integral) is noted to the to the compared molecule energy with the pieces with pure single and double bonds. So, the internal energy change must be provided proper estimation to hyperergy.

References

- [1] McWeeny, R. and Sutcliffe, B.T. (1969) *Methods of Molecular Quantum Mechanics*, Academic Press, London.
- [2] Hoffmann, R. (1963) *J. Chem. Phys.* **39**, 1397.
- [3] Powell, M. J. D. (1985) (ed.), *Non-linear Optimization*, Macmillan, Basingstoke.
- [4] Pulay, P. (1969) *Molecular Physics* **2**, 197.
- [5] Pople, J. A., Head-Gordon, M., Fox, D. j., Raghavachari, K. and Curtiss, L. A. (1989) *J. Chem. Phys.* **90**, 5622.