



Comparison of the relative stabilities
of thiocarbonyl compounds
in gaseous state
(A molecular modeling study)

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Abstract

Carbonyl compounds and thiocarbonyl compounds are analogues where the oxygen of the former is replaced by sulfur in the later. Among the two type's thiocarbonyl compounds form the more reactive group.

The high reactivity of thiocarbonyl compounds is due to their weak carbon sulfur double bond. The weakness of the double bond arises due to the failure of sulfur to participate in $p\pi-p\pi$ Bonding

Overlap of the carbon 2p- orbital and sulfur 3p- orbital in the carbon sulfur double bond is less effective than the 2p-2p overlap in the carbon oxygen double bond. Therefore thiocarbonyl compounds are more reactive and less stable in comparison to oxygen analogues. They readily give carbon sulfur single bonds by enolization.

The above reactivity of thiocarbonyl compounds makes it interesting to investigate these compounds. Such investigations have made it possible to design many drugs through thiocarbonyl compounds.

Although, experiments cannot be completely replaced by theoretical calculations, they reveal valuable information about molecules and their reactivity. Therefore, theoretical calculations can supplement experiments and be used as a valuable tool in chemical investigations.

This thesis examines the order of stability of a series of thiocarbonyl compounds by performing theoretical calculations. Gaussian98W and Gauss view have been used to conduct the theoretical calculations of some selected thiocarbonyl compounds.