

A comparison of some properties of C=S and C=Se bond

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There are significant and interesting differences between compounds with thiocarbonyl and selenocarbonyl groups. The C=S bond length ($\sim 1.8 \text{ \AA}$) is considerably longer than C=S ($\sim 1.6 \text{ \AA}$) [1]. As a result, one would expect to be strengths to differ significantly. The π -bond also might be expect to be strongly affected in view of the orbital size mismatch between second and third row atoms. On the other hand, selenoamides are known to have larger rotational barriers than thioamides, where the barrier arises from the interaction nitrogen with the adjacent C=S or C=Se group [2]. The geometry optimizations for the ground state and, transition states, were carried out using Gaussian 03 program with B3LYP level of theory in combination of 6-311G (d,p) Basis set. One of the most important quantities that characterize a bond is the strength. This can be expressed either as the bond dissociation energy or the force constant for stretching the bond. The first refers to complete cleavage, and the latter to the effects of small deviations from the equilibrium geometry. Vibrational force constants are usually obtained via a normal coordinate analysis or a calculation of the vibrational frequencies. This presents problems because there is always coupling between the C=S (or C=Se) vibration with other vibrational modes. There is considerable no difference in electronegativity between selenium and sulfur [3], and therefore the charge distribution should be no different between selenocarbonyl and thiocarbonyl compound.

References

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