Theoretical Investigation of Telluro-ketones in View of Recent Synthetic Advances

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Carbonyl compounds are important species from chemical industry to bioscience. The chemistry of compounds having double bonds between carbon and heavier group 16 elements has also been studied extensively and their structures and properties have been systematically elucidated so far. However, the chemistry of compounds having heavier group 14 and 16 elements classified as "heavy ketones" has been a challenging field due to the difficulty in the stabilization of the very reactive double bonds. Thus in view of the limited literature of telluro-ketones and the recent synthetic advances, systematic investigations of X_2A=Te and XYA=Te (X,Y=H, F, Cl, Br, I and CN; A=C, Si and Ge) were carried out using the second order Møller-Plesset Perturbation theory (MP2) and the density functional theory (DFT). The endeavors of these studies were the determination of the structural and energetic parameters of the mentioned telluro-ketones. Further, this research work was extended to engage in the following query: Can the isolation of any of the monomeric *telluro*-ketones be aided by an energetic favorability on its potential energy surface (PES)? Thus reaction pathways for the isomerization and decomposition reactions of H_2A=Te and HFA=Te (A=C, Si and Ge) molecules on their singlet state PES were explored using MP2 level. In addition, to gain more confidence on the reactivity and thermodynamic stability of these telluro-ketones, the A=Te bond dissociation energies as well as the σ- and π-bond energies and their standard heats of formation ($\Delta H_f°$) were evaluated. In line with these studies we are currently investigating the stability of A=Te (C, Si and Ge) double bonds using a variety of bulky rigid protecting groups. Since experimental data are still lacking for the telluro-ketones, the findings of this research work should add to the literature and assist the experimental community in the synthesis, characterization and applications of these ketones.