ECCL

Electron Controlled Chemical Lithography
2009 Meeting

4th-9th June 2009
Istanbul, Turkey

ABSTRACT BOOKLET

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Studies of low energy electron interaction with furanose-structured alcohols

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Two furanose-structured alcohols related to some extent to deoxyribose molecule, 3-hydroxytetrahydrofuran (3HTHF, $C_4H_8O_2$) and α-tetrahydrofurfuryl alcohol (THFA, $C_5H_{10}O_2$), have been studied both experimentally and theoretically. Crossed electron/molecule beams technique together with quadrupole mass spectrometer has been used for electron induced positive ion formation studies. The mass spectra of 3HTHF and THFA determined at incident electron energy 70 eV were analyzed and for number of mass-charge ratios (m/q) the ionization efficiency curves have been measured. Thus, for 3HTHF 18 different m/q channels were analyzed experimentally, from which 6 were selected for deeper investigation on DFT level of theory and finally 5 for the G3MP2 method. The same was performed for THFA with 15 m/q channels experimentally, 5 on DFT and 4 on G3MP2 levels of theory. Theoretical calculations with Gaussian 03 program package led to more than 160 fragmentation reactions on B3LYP/6-311+G(2d,2p), only the energetically comparable to experimentally observed appearance energies were re-computed on G3MP2.

The experiment showed that although there were 18 and 15 m/q channels observed for 3HTHF and THFA respectively, only 10 of them for 3HTHF were abundant over 10% of the ionic yield of most intensive fragment and 6 for THFA. While the parent cation of 3HTHF occurred within its abundant ionic fragments, THFA cation had a weak signal only. Our theoretical conformational studies of neutral and cationic 3HTHF and THFA agree well with this experimental observation, for $3HTHF^+$ at least 2 stable conformers were found while for the cationic state of THFA partial dissociation the side CH_2OH chain group occurred. However the later process, dissociation of CH_2OH, seems to be a common feature for the most abundant fragmented ion of both molecules, the corresponding structures are the furanose closed ring cation with m/q=71 for THFA fragment and CH_2=CH-CH-OH^+ with m/q=57 for 3HTHF fragment. Additionally, fragmentations to cations with m/q=70, 58, 43 and 31 were studied theoretically for both molecules, except the 58 for THFA that was not observed. One could expect when looking at the chemical formulas of both molecules that the fragmented cationic structures can be oxygenated, either singly (possible products found for all discussed channels) or doubly (only the $C_2H_2O_2^+$ with m/q=58 fragmented from 3HTHF, but its second most abundant fragmented ion), or can be also cationic hydrocarbons. Only cationic hydrocarbon product found for our selected channels was the C_3H_7 cation with m/q=43, with corresponding neutrals COOH from 3HTHF and CH_2OH + CO from THFA, for the later the second most abundant cationic fragment.

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