

# Mass Spectra of New Heterocycles: XIII.\* Fragmentation of 2-(Prop-1-en-1-yl)-4,5-dihydro-1,3-thiazoles under Electron Impact and Chemical Ionization

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**Abstract**—Fragmentation of 2-(prop-1-en-1-yl)-4,5-dihydro-1,3-thiazoles synthesized from alkoxyallenes or propargylbenzene, isothiocyanates, and benzyl, allyl, or propargyl bromide has been studied under electron impact (70 eV) and chemical ionization (with methane as reactant gas). All compounds under electron impact give rise to stable molecular ions whose decomposition involves concurrent dihydrothiazole ring cleavage and elimination of substituents. The fragmentation pattern is largely determined by the nature of the substituent on C<sup>5</sup>. Chemical ionization of 4,5-dihydro-1,3-thiazole derivatives is typically accompanied by protonation and electrophilic addition with subsequent elimination of nitrile molecule. No substituent effect on the fragmentation pattern under chemical ionization has been revealed. Unlike electron impact and chemical ionization, the most abundant ion in the MALDI mass spectrum of 2-[(Z)-1-butoxyprop-1-en-1-yl]-4,4-dimethyl-5-phenyl-4,5-dihydro-1,3-thiazole is  $[M - H]^+$ .

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