(3-Iminio-1-propenyl)oxy-borates: New Acyclic Betaines from Enaminocarbonyl Compounds and Boron Trifluoride or Triphenylboron – Synthesis, Crystal Structure Analysis, and Quantum Chemical Calculations

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Adducts of various acyclic enaminoketones and enaminoaldehydes with the Lewis acids boron trifluoride and triphenylboron were prepared. The adducts were characterized by NMR (^{1}H, ^{13}C, ^{11}B) and IR spectroscopy, FAB-MS, and X-ray crystal structure analysis of the adducts of (*E*)-3-diethylamino-3-phenyl-2-propenal with BF_3 (**4a)** and BPh_3 (**5a**), respectively. The adduct formation occurs at the oxygen atom of the enaminocarbonyl compound and gives rise to a betainic structure with expressed equalization of the bond orders in the enaminocarbonyl moiety. The gas-phase structures of complexes **4a** and **5a** and of the corresponding free enaminoaldehyde were determined computationally by RHF and DFT methods, and a Natural Bond Orbital (NBO) analysis was undertaken.

Key words: Enaminocarbonyl Compounds, Boron, Betaines, Quantum Chemical Calculations