

**Paper ID: IT-04****Mechanistic Studies on Alicyclic and Heterocyclic Compounds Using Newer Synthetic Methodologies****Invited Talk**Warjeet S. Laitonjam<sup>1</sup>

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**Abstract**

An efficient method for the transformation of N-substituted-N'-benzoylthioureas to substituted N-benzoxazol-2-yl-amides using diacetoxyiodobenzene (DIB) will be described in this presentation. The transformation follows C–O bond formation leading to the benzoxazole derivative due to oxidative dehydrogenation by DIB, instead of the expected C–S bond formation of the benzothiazole moiety. The C–O bond formation leading to benzoxazole is due to consecutive acylation and deacylation in conjunction with the reduction of two moles of DIB. A plausible mechanism was proposed for the reaction, and density functional calculations were also performed to study the reaction mechanism. Unexpectedly, the reaction follows a different pathway leading to C–O bond formation between the carbonyl oxygen and the ortho-carbon of the aryl moiety, resulting in oxazole ring formation, which will be presented here.

A new approach for the conversion of aryl amines having no  $\alpha$ -methylene group to aryl nitriles using dimethyl carbonimidodithioates by intramolecular stabilization, particularly 1,2-carbon migration to give the products, will also be highlighted. Here, the conversion of a C–N bond to a C–C bond takes place.

**Keywords:** Heterocyclic synthesis, oxidative cyclization, reaction mechanism, hypervalent iodine reagents, aryl nitriles