

*Tripartite competition in topochemical AAC-conformational motion in crystal*

Hema K<sup>1</sup>, Kana Sureshan<sup>1</sup>

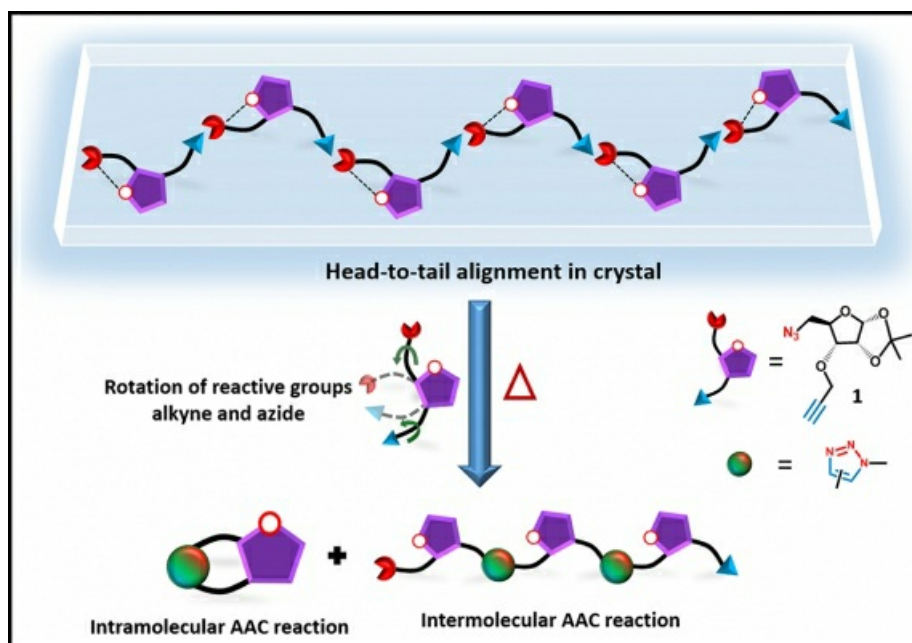
<sup>1</sup>*School Of Chemistry Indian Institute Of Science Education And Research, Thiruvananthapuram, India*  
E-mail: sruthihema@iisertvm.ac.in

Solid state reactions [1] (topochemical reactions) have incurred much attention in recent days. Designing a crystal suitable for topochemical reaction [2] is challenging since anticipating the orientation of the reactive partners [3] in the crystal lattice is difficult. Azide-alkyne cycloaddition is one of the reactions that could occur under topochemical conditions, provided the reactive groups attain proper orientation and proximity. We have synthesized 5-azido-3-O-propargyl-1,2-O-isopropylidene alpha-D-ribofuranose functionalized with alkyne and azide at pertinent positions for topochemical azide-alkyne cycloaddition (TAAC). The orientation of the reactive groups (alkyne and azide) in the crystal structure suggests the formation of 1,5-triazolyl linear polymer. Surprisingly, when crystals were heated, it underwent cycloaddition reaction yielding a mixture of the 1,5-intramolecular adduct and oligomers of different sizes and varying sequence of both 1,5-triazolyl and 1,4-triazolyl linkages. The macroscopic morphology of the crystal was unaffected even after the reaction. Although, molecules possess minimal motion in solids, the available space (voids) around the reactive motifs could allow the supple reactive motifs to rotate when they are thermally activated. To ascertain the topochemical nature of the reaction, alkyne-azide cycloaddition was done in solution states and the products obtained were compared.

[1] Schmidt, G. J. M. (1971). Pure Appl. Chem., 27, 647-678.

[2] Lange, R. Z., Hofer, G., Weber, T., Schlüter, A. D. (2017) J. Am. Chem. Soc., 139, 2053-2059.

[3] Mishra, M. K., Mukherjee, A., Ramamurty, U. & Desiraju, G. R. (2015). IUCr, 2, 653.-660.



**Keywords:** [competitive topochemical reaction](#), [conformational motion](#)