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Abstract:

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Pyrazolo[3,4-d]pyrimidines are a class of fused heterocyclic rings that possess a wide range of biological activity. Our molecule of interest is one such fused heterocyclic ring, 1H- Pyrazolo[3,4-d]pyrimidine-4-amine (1H-PPA), which is an Adenine isomer. The structural information and electronic properties of 1H-PPA has already been explored by Prabavathi et al. (Spectrochim. Acta A Mol. Biomol. Spectrosc., 2012, 96, 226–241). The radical isomers of 1H- PPA are yet to be explored. In our current work we have computationally explored the radical isomers of 1H-PPA by homolytic cleavage of either C-H or N-H bonds. The structural and electronic properties of the radical isomers are explored in details. Furthermore, Unimolecular decomposition pathways for 1H-PPA radicals are also carried out to explore their kinetic stabilities. A comparative study between 1H-PPA radical isomers and adenine radical isomers are also carried out to elucidate the effects of small structural changes in their stability order.

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