Title:	Computational and Matrix Isolation Infrared Spectroscopic Studies of 1H-Pyrazolo[3,4-d]pyrimidine-4-amine Radicals
Authors:	Kaur, Hunarpreet.
Keywords:	Infrared Spectroscopic Pyrimidine
Issue Date:	28-Jul-2021
Publisher:	IISERM
Abstract:	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.
URI:	http://hdl.handle.net/123456789/3883
Appears in Collections:	MS-16

Files in This Item:

File	Description	Size	Format	
It is under embargo period.docx		11.62 kB	Microsoft Word XML	View/Open

Show full item record