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Evaluating the Effect of Structural Reorientation to Thermochemical and Energetic Properties of 1,4-Diamino-3,6-Dinitropyrazolo[4,3- C]Pyrazole

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Abstract : 1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole (LLM-119) and its structural isomer 3,6-dinitropyrazolo[3,4-c]pyrazole-1,4(6H)-diamine were designed by structural reorientation of the fused pyrazole rings and their respective substituents (-NO2 and -NH2). Structural reorientation involves structural rearrangement which result in different structural isomers, employing this approach, six structural isomers of LLM-119 were achieved. The effect of structural reorientation (isomerisation and derivatives) on the enthalpy of formation, detonation properties, impact sensitivity, and density of these molecules is studied Computationally. The computational method used are detailed in the document and they yielded results that are close to the literature values with a relative error of 2% for enthalpy of formation, 2% for density, 0.05% for detonation velocity, and 4% for detonation pressure. The correlation of the structural reorientation to the calculated thermochemical and detonation properties of the molecules indicated that molecules with a -NO2 group attached to a Carbon atom and -NH2 connected to a Nitrogen atom maximize the enthalpy of formation and detonation velocity. The joining of pyrazole molecules has less effect on these parameters. It was seen that density and detonation pressure improved when both –NO2 or -NH2 functional groups were on the same side of the molecular structure. The structural reorientation gave rise to 3,4-dinitropyrazolo[3,4-c]pyrazole-1,6-diamine which exhibited optimal density and detonation performance compared to other molecules.

Keywords : LLM-119, fused rings, azole, structural isomers, detonation properties
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