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Kumaracoll - 629 180, Thuckalay, Kanyakumari District, Tamil Nadu, India

**National Conference on Recent Trends in Physics (NC RTP - 2022)**  
 12<sup>th</sup> May 2022

This is to certify that Dr. A. Rathi

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Participated/Presented a Paper entitled

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at National Conference on Recent Trends in Physics (NC RTP - 2022) on 12<sup>th</sup> May 2022 organised

by the Department of Physics, Noorul Islam Centre for Higher Education, Kumaracoll-629 180, Tamil Nadu.

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# **NATIONAL CONFERENCE ON RECENT TRENDS IN PHYSICS – 2022**

**(NCRTP-2022)**

**PROCEEDINGS**

**12<sup>th</sup> MAY 2022**



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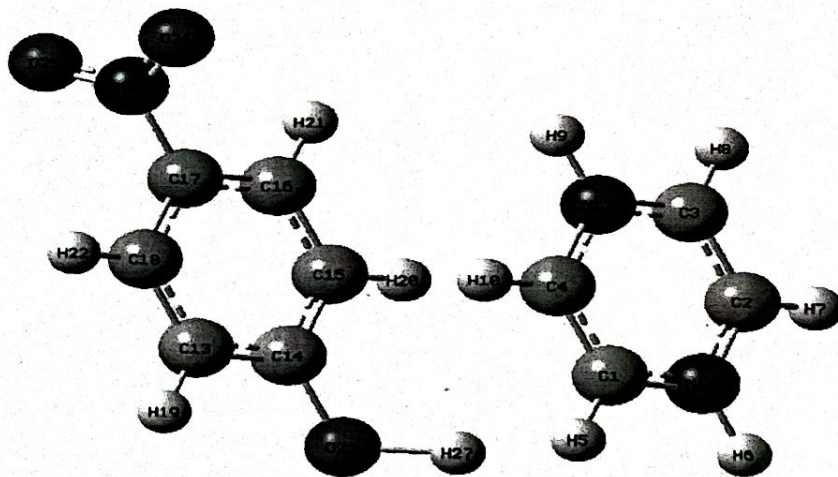
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**STRUCTURAL ANALYSIS OF PIPERAZINE 4-HYDROXYNITROBENZENE (P4HB)**R.Suja<sup>a</sup>, C.L.Shiny<sup>b</sup>, T. Joselin Beaula<sup>c</sup>, R.GanapathiRaman<sup>d</sup>, A.Rathika<sup>e\*</sup><sup>a</sup>Reg. No: 21213092132004, Research Scholar, Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode.<sup>b</sup>Reg. No: 20213082132003, Research Scholar, Department of Physics and Research Centre, Malankara Catholic College, Mariagiri.<sup>c</sup>Assistant Professor, Department of Physics and Research Centre, Malankara Catholic College, Mariagiri.<sup>d</sup>Associate Professor, Department of Physics, Noorul Islam Centre for Higher Education, Kumaracoil<sup>d</sup>Affiliated to Noorul Islam University, Kumaracoil - 629175.<sup>e\*</sup>Assistant Professor, Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode<sup>a,b,c,e</sup>Affiliated to Manonmaniam Sundaranar University, Tirunelveli - 627 012.

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**ABSTRACT**

Piperazine 4-hydroxynitrobenzene (P4HB) is an organic compound. Piperazine consist of a six-membered ring containing two opposing nitrogen atoms. 4-hydroxynitrobenzene is a phenolic compound that has a nitro group at the opposite position of the hydroxyl group on the benzene ring. The molecular structure of P4HB was optimized by B3LYP method with 6-311 G (d,p). Optimized geometrical parameters such as bond lengths, bond angles and dihedral angles have been compared with experimental values obtained from single XRD data. Bonding analysis was executed to establish charge transfer, conjugative interactions and the formation of intermolecular hydrogen bonding interactions. HOMO-LUMO energy gap indicates the possibility of a charge transfer within the molecule.



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