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National Conference on Recent Trends in Physics (NCRTP - 2022)

12th May 2022

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This is to certify that Dr. A. Rathi, Assistant Professor, Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode. has Participated/Presented a Paper entitled Structural Analysis of Piperazine 4-ethoxy-nitrobenzene (PHNB)

in the National Conference on Recent Trends in Physics (NCRTP - 2022) on 12th May 2022 organised by the Department of Physics, Noorul Islam Centre for Higher Education, Kumaracoil-629 180, Tamil Nadu.

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Kumaracoil, Thuckalay – 629 180

New Edition: 2022

ISBN: **978-93-91342-32-6**

Published by
JPS Publication

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STRUCTURAL ANALYSIS OF PIPERAZINE 4-HYDROXYNITROBENZENE (P4HB)

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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.