

Accepted Manuscript

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PII: S0167-7322(17)34815-8
DOI: doi:[10.1016/j.molliq.2017.11.150](https://doi.org/10.1016/j.molliq.2017.11.150)
Reference: MOLLIQ 8266
To appear in: *Journal of Molecular Liquids*
Received date: 10 October 2017
Revised date: 21 November 2017
Accepted date: 24 November 2017

Please cite this article as: Ishaat M. Khan, Sonam Shakya, Neelam Singh , Preparation, single-crystal investigation and spectrophotometric studies of proton transfer complex of 2,6-diaminopyridine with oxalic acid in various polar solvents. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2017.11.150](https://doi.org/10.1016/j.molliq.2017.11.150)

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Preparation, single-crystal investigation and spectrophotometric studies of proton transfer complex of 2,6-diaminopyridine with oxalic acid in various polar solvents

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ABSTRACT

Charge transfer complex (CT complex) of donor, 2,6-diaminopyridine (DAP) and π - acceptor, oxalic acid (OA) has been synthesized in acetonitrile at room temperature. The CT complex is formed through the transfer of lone pair electrons from 2,6-diaminopyridine to oxalic acid. The CT complex was characterized by elemental analysis, FTIR spectra single crystal studies, TGA-GTA, ^1H NMR and electronic absorption spectra in different solvents which indicate the CT interaction associated with proton migration from the acceptor to the donor followed by hydrogen bonding via $\text{N}^+ - \text{H} \cdots \text{O}^-$. It was found that formation of CT Complex is solvent dependent. Spectrophotometric data show the properties of complex in terms of formation constant (K_{CT}), molar extinction coefficient (ϵ_{CT}), energy of interaction (E_{CT}), ionization potential (I_{D}), resonance energy (R_{N}), free energy (ΔG), oscillator strength (f) and transition dipole moment (μ_{EN}). The stoichiometry of the CT complex was found to be 1:1 by a straight-line method between donor and acceptor with maximum absorption bands. The physical parameters of CT complex were evaluated by the Benesi–Hildebrand equation. The agreements between the spectroscopic results were also confirmed by single crystal X-ray of the resulting charge transfer complex.

Keywords: Charge transfer; Crystallography; ^1H -NMR; UV-visible; FTIR; TGA-DTA; Conductance.

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