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## Fluorescence, Photophysical Behaviour and DFT Investigation of E,E-2,5-bis[2-(3-pyridyl)ethenyl]pyrazine (BPEP)

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### Abstract

E,E-2,5-bis[2-(3-pyridyl)ethenyl]pyrazine (BPEP) has been prepared by aldol condensation between 2,5-dimethylpyrazine and pyridine-3-carboxaldehyde. It is characterized by IR, H-1 NMR, and C-13 NMR. The electronic absorption and emission properties of BPEP were studied in different solvents. BPEP displays a slight solvatochromic effect of the absorption and emission spectrum, indicating a small change in dipole moment of BPEP upon excitation. The dye solutions ( $1 \times 10^{-4}$  M) in CHCl<sub>3</sub>, EtOH and dioxane give laser emission in blue region upon excitation by a 337.1 nm nitrogen pulse ( $\lambda = 337$  nm). The tuning range, gain coefficient ( $\alpha$ ) and emission cross-section ( $\sigma(e)$ ) have been determined. Ground and excited states electronic geometric optimizations were performed using density functional theory (DFT) and time-dependent density functional theory (TD-DFT), respectively. A DFT natural bond analysis complemented the ICT. The simulated maximum absorption and emission wavelengths are in line the observed ones in trend, and are proportionally red-shifted with the increase of the solvent polarity. The stability, hardness and electrophilicity of BPEP in different solvents were correlated with the polarity of the elected solvents. BPEP dye displays fluorescence quenching by colloidal silver nanoparticles (AgNPs). The fluorescence data reveal that radiative and non-radiative energy transfer play a major role in the fluorescence quenching mechanism.

### Keywords

**Author Keywords:** [Photophysical properties](#); [Effect of solvent](#); [Fluorescence quenching](#); [E,E-2,5-bis\[2-\(3-pyridyl\)ethenyl\]pyrazine](#)

**KeyWords Plus:** [INTRAMOLECULAR CHARGE-TRANSFER](#); [SILVER NANOPARTICLES](#); [SPECTRAL BEHAVIOR](#); [LASER-DYES](#); [AB-INITIO](#); [SOLVENT](#); [PERFORMANCE](#); [ABSORPTION](#); [INTENSITY](#); [CONTINUUM](#)

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