Electronic Supplementary Information (ESI)

Tuning The Intra-molecular Charge Transfer (ICT) Process in Push-Pull Systems: Effect of Nitro group

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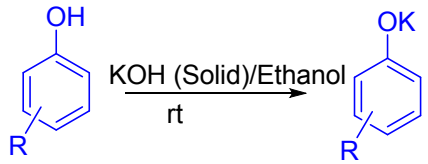
1. Synthesis of potassium salt of nitro-phenol derivative

Synthetic procedure:

Initially nitrophenol derivative is to be dissolved in methanol solvent. After that saturated solution of potassium carbonate (K_2CO_3) in water is to be added slowly because heat is generated. Resulting solution becomes fluorescent yellow and stirred at room temperature. Yellow colour solid is precipitated out from the solvent. Filtered and dried. Pure potassium salt of nitrophenol is obtained.



Mole ratio Phenol: K_2CO_3 = 1: 1

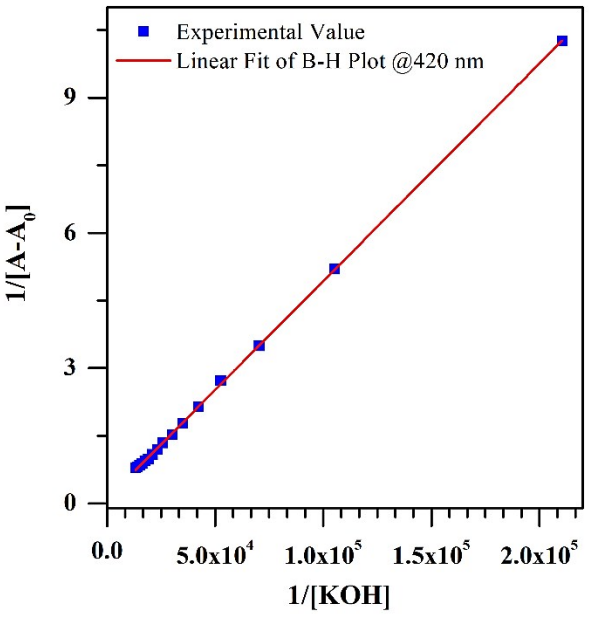


Figure 1a: B-H plot for KNP formation at 420 nm in ACN

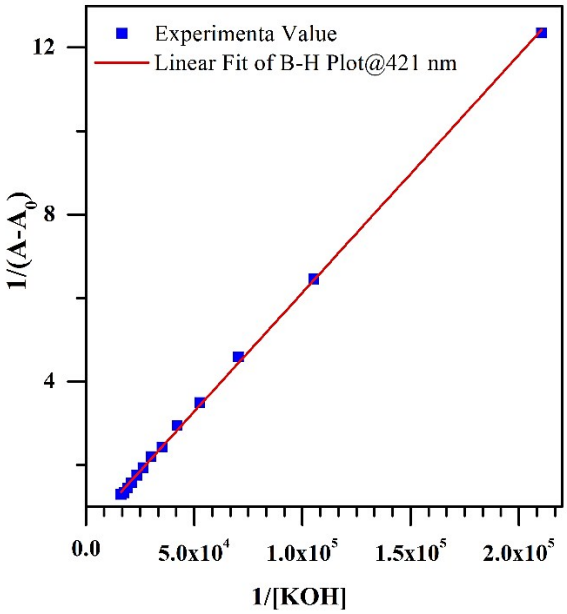


Figure 1b: B-H plot for KDNP formation at 421 nm in ACN

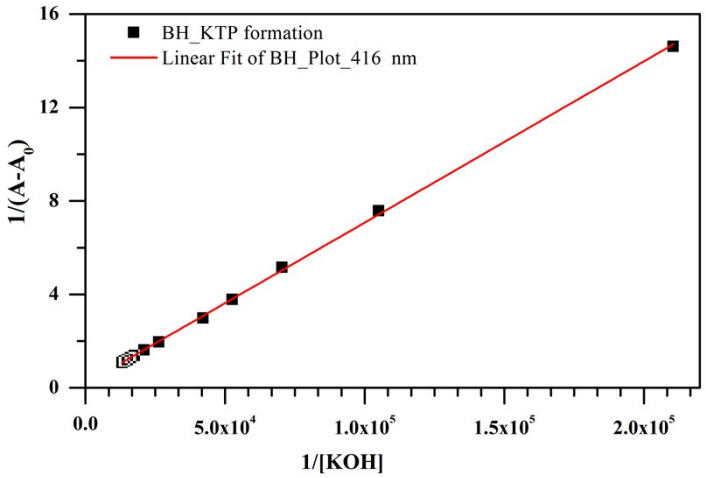


Figure 1c: B-H plot for KTNP formation at 435 nm in ACN

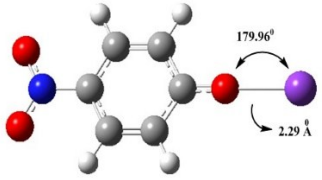


Figure 2a: Optimizes Structure of KNP (Lowest Energy)

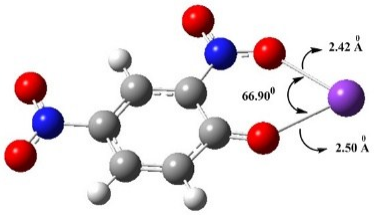


Figure 2b: Optimizes Structure of KDNP (Lowest Energy)

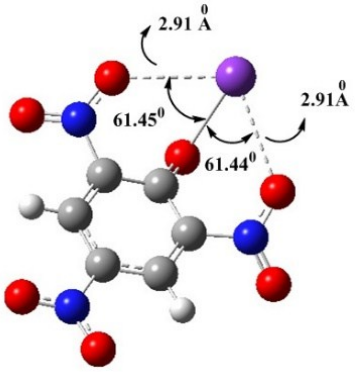


Figure 2c: Optimizes Structure of KTNP (Lowest Energy)

Table 1: Electronic Transition energy from Td-DFT Calculation with different functional

	B3LYP/6-311G (d, p)		CAM-B3LYP/6-311G (d, p)	
	GAS phase	ACN	GAS phase	ACN
HNP	295.3 nm (f = 0.2674)	324.9 nm (f = 0.3533)	270.9 nm (f = 0.0004)	283.5 nm (f = 0.3833)
HNP anion	351.7 nm (f = 0.4639)	367.6 nm (f = 0.5774)	349.0 nm (f = 0.5196)	356.0 nm (f = 0.6332)
KNP salt	468.29 nm (f = 0.0005)	375.9 nm (f = 0.5156)	363.7 nm (f = 0.0008)	354.3 nm (f = 0.5597)
HDNP	339.2 nm (f = 0.0518)	354.3 nm (f = 0.0693)	293.4 nm (f = 0.0801)	303.10 nm f=0.1093

HDNP anion	359.9 nm (f = 0.2873)	412.0 nm (f = 0.2594)	359.9 nm (f = 0.2873)	371.6 nm (f = 0.3485)
KDNP salt	402.1 nm (f = 0.1154)	418.6 nm (f = 0.1987)	352.1 nm (f = 0.1650)	365.0 nm (f = 0.2593)
HTNP	341.0 nm (f = 0.0589)	344.0 nm (f = 0.1087)	309.9 nm (f = 0.0191)	306.7 nm (f = 0.0678)
HTNP anion	451.2 nm (f = 0.0479)	437.9 nm (f = 0.1130)	418.6 nm (f = 0.0010)	410.8 nm (f = 0.0118)
KTNP salt	406.3 nm (f = 0.1222)	415.9 nm (f = 0.1606)	348.2 nm (f = 0.0994)	388.1 nm (f = 0.0154)

* f = Oscillator strength; nm = nanometre