

Supplemental Information

Fig. 1S. Electronic absorption spectra of (A) DNN, acceptor (1×10^{-4} M); (B) donor-acceptor CT complex (1×10^{-4} M + 1×10^{-4} M) and (C) DMP, donor (1×10^{-4} M) in methanol at room temperature.

Fig. 2S. Electronic absorption spectra of (A) DNN, acceptor (1×10^{-4} M); (B) donor-acceptor CT complex (1×10^{-4} M + 1×10^{-4} M) and (C) DMP, donor (1×10^{-4} M) in dichloromethane at room temperature.

Fig. 3S. Electronic absorption spectra of (A) DNN, acceptor (1×10^{-4} M); (B) donor-acceptor CT complex (1×10^{-4} M + 1×10^{-4} M) and (C) DMP, donor (1×10^{-4} M) in chloroform at room temperature.

Fig. 4S. TGA-DTA curve for 2,4-dinitro-1-naphthol.

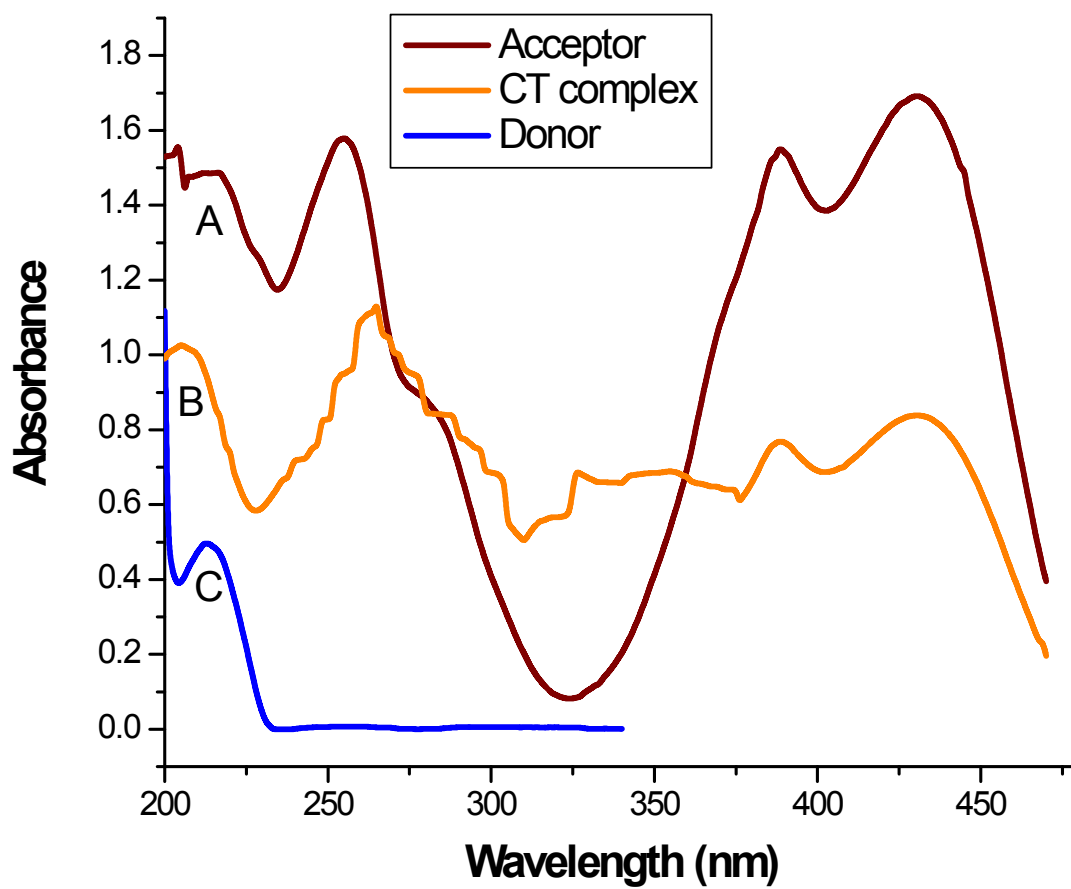


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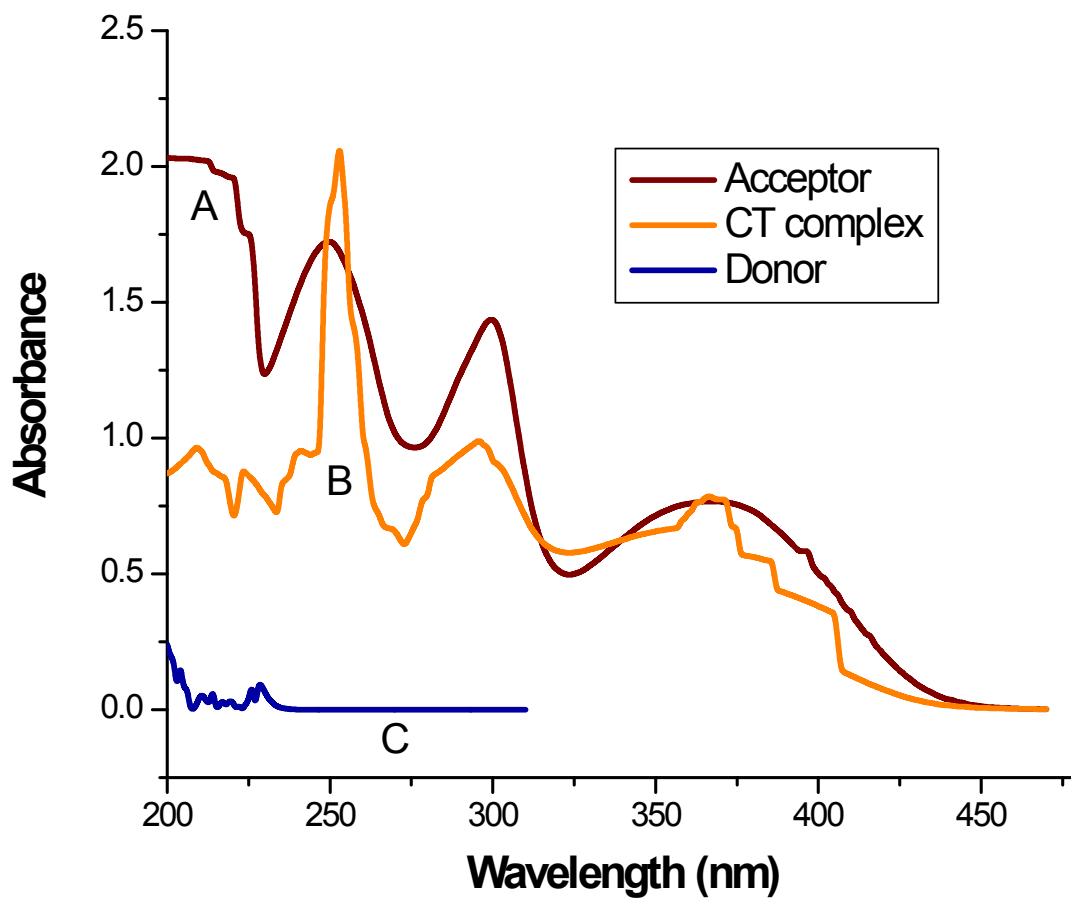


Fig. 2S. Electronic absorption spectra of (A) DNN, acceptor (1×10^{-4} M); (B) donor-acceptor CT complex (1×10^{-4} M + 1×10^{-4} M) and (C) DMP, donor (1×10^{-4} M) in dichloromethane at room temperature.

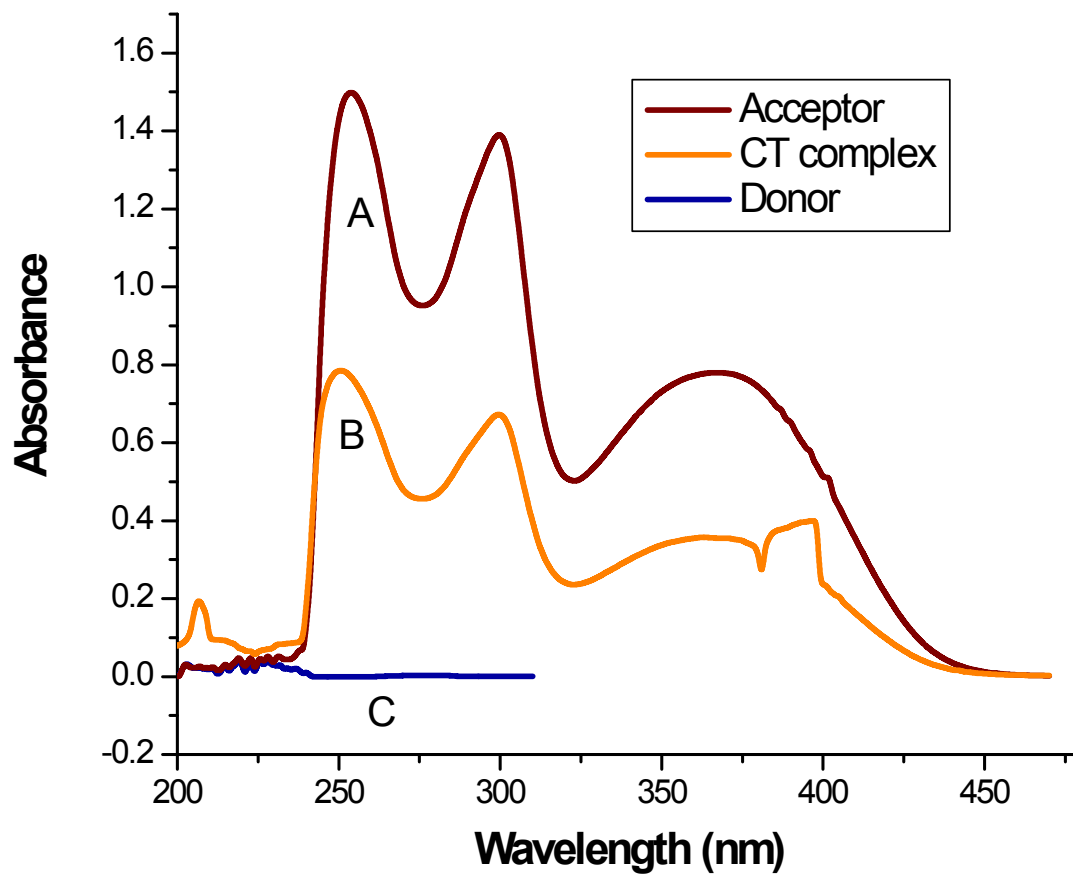


Fig. 3S. Electronic absorption spectra of (A) DNN, acceptor (1×10^{-4} M); (B) donor-acceptor CT complex (1×10^{-4} M + 1×10^{-4} M) and (C) DMP, donor (1×10^{-4} M) in chloroform at room temperature.

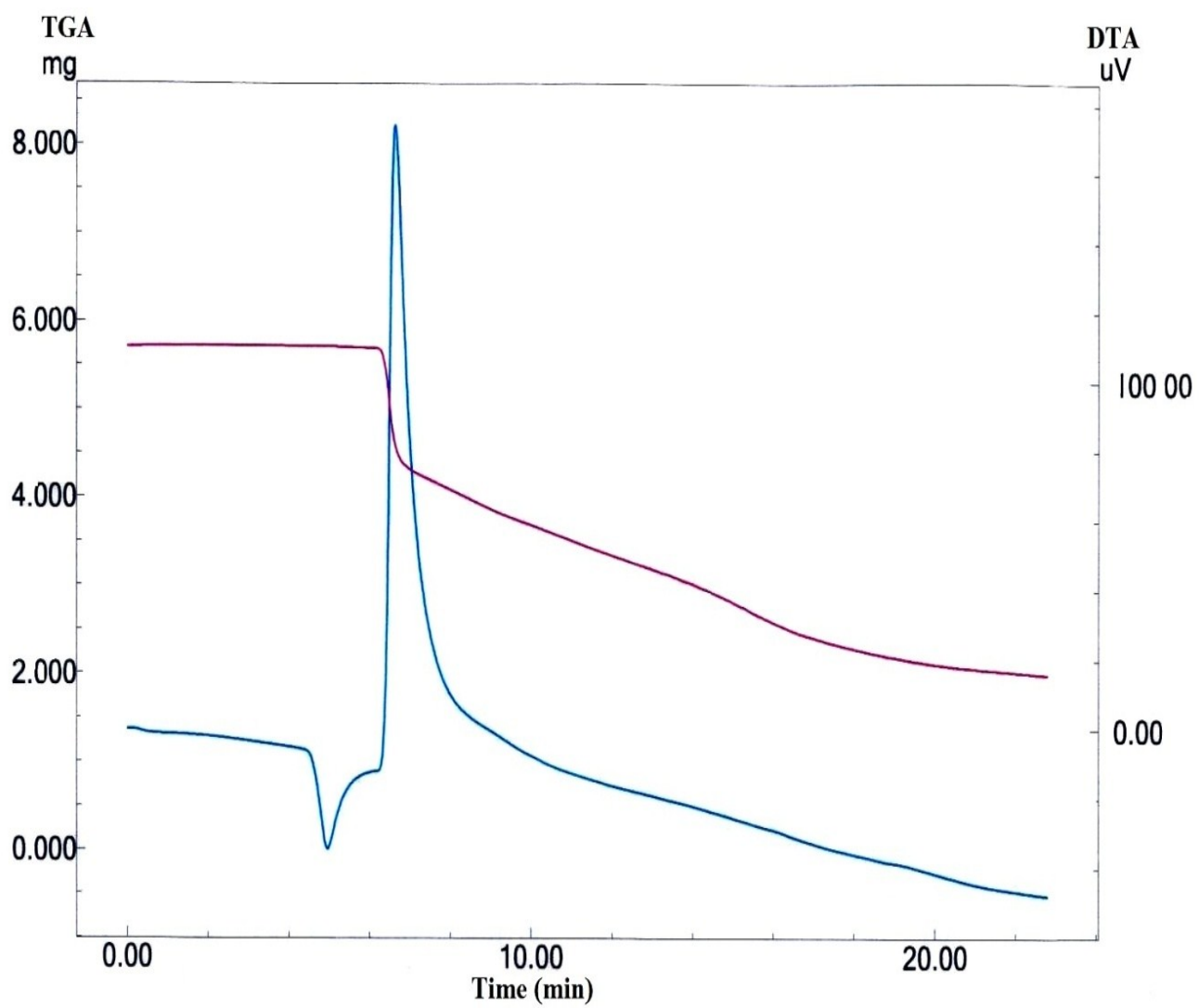


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Table 1S

Infrared Frequencies for 3,5-dimethylpyrazole (DMP), 2,4-dinitro-1-naphthol (DNN) and [(DMPH)⁺(DNN)⁻] CT complex.

Compound	Frequency	Assignments
3,5-dimethylpyrazole	3282	N-H
	3190	C-H
	2945	CH ₃
	1591(str)	C=C (ring)
	1480 (str)	C-N
	1150	N-N
	1019	C-H in plane <i>def</i>
	781	C-H out of plane bending
2,4-dinitro-1-naphthol	3093	-OH
	3083-2369	C-H (Ar)
	1797, 1627, 1583	C=C (benzene ring)
	1353(sy, str), 765(wag)	Ar-NO ₂
[(DMPH) ⁺ (DNN) ⁻] CT complex	3225	O--H---N
	3119, 2365	C-H (Ar)
	3000	CH ₃
	1601	C=C (ring)
	1575	C=N ⁺ --H
	1531, 1444, 1388	C=C (benzene ring)
	1496	C-N
	1349(sy, str), 746(wag)	Ar-NO ₂
	1222	N-N
	1087	C-H in plane <i>def</i>
849	C-H out of plane bending	

Str, stretching; sy, symmetric; wag, wagging; *def*, deforming; Ar, aromatic

Table 2S

Gaussian curve analysis for the CT spectrum of DMP with DNN in different solvents.

Solvent	Area of the curve (<i>A</i>)	Width of the curve (<i>w</i>)	Centre of the curve (<i>x_c</i>)	<i>y</i>₀
Chloroform	35.31 ± 2.99	61.55 ± 4.69	279.25 ± 1.96	0.16 ± 0.01
DCM	19.91 ± 1.88	11.74 ± 1.23	252.46 ± 0.60	0.53 ± 0.02
Methanol	11.98 ± 1.21	24.06 ± 2.57	266.14 ± 1.22	0.68 ± 0.01
Acetonitrile	22.37 ± 3.39	68.58 ± 10.22	248.38 ± 4.17	0.56 ± 0.01