

Electronic Supporting Information for

Tuning the strength of intramolecular charge-transfer of triene-based nonlinear optical dyes for electrooptics and optofluidic laser

Jieyun Wu,^{*a} Wen Wang,^a Chaoyang Gong,^a Qing Li,^a Zhonghui Li,^{*b} Guowei Deng,^b Xiaoling Zhang,^b Kaixin Chen,^a Yuan Gong,^{*a} and Kin seng Chiang^{a,c}

^aSchool of communication and information engineering, key Laboratory of Optical Fiber Sensing and Communications, university of electronic science and technology of china, Chengdu, China. *E-mail: jieyunwu@uestc.edu.cn (J. Wu); ygong@uestc.edu.cn (Y. Gong).

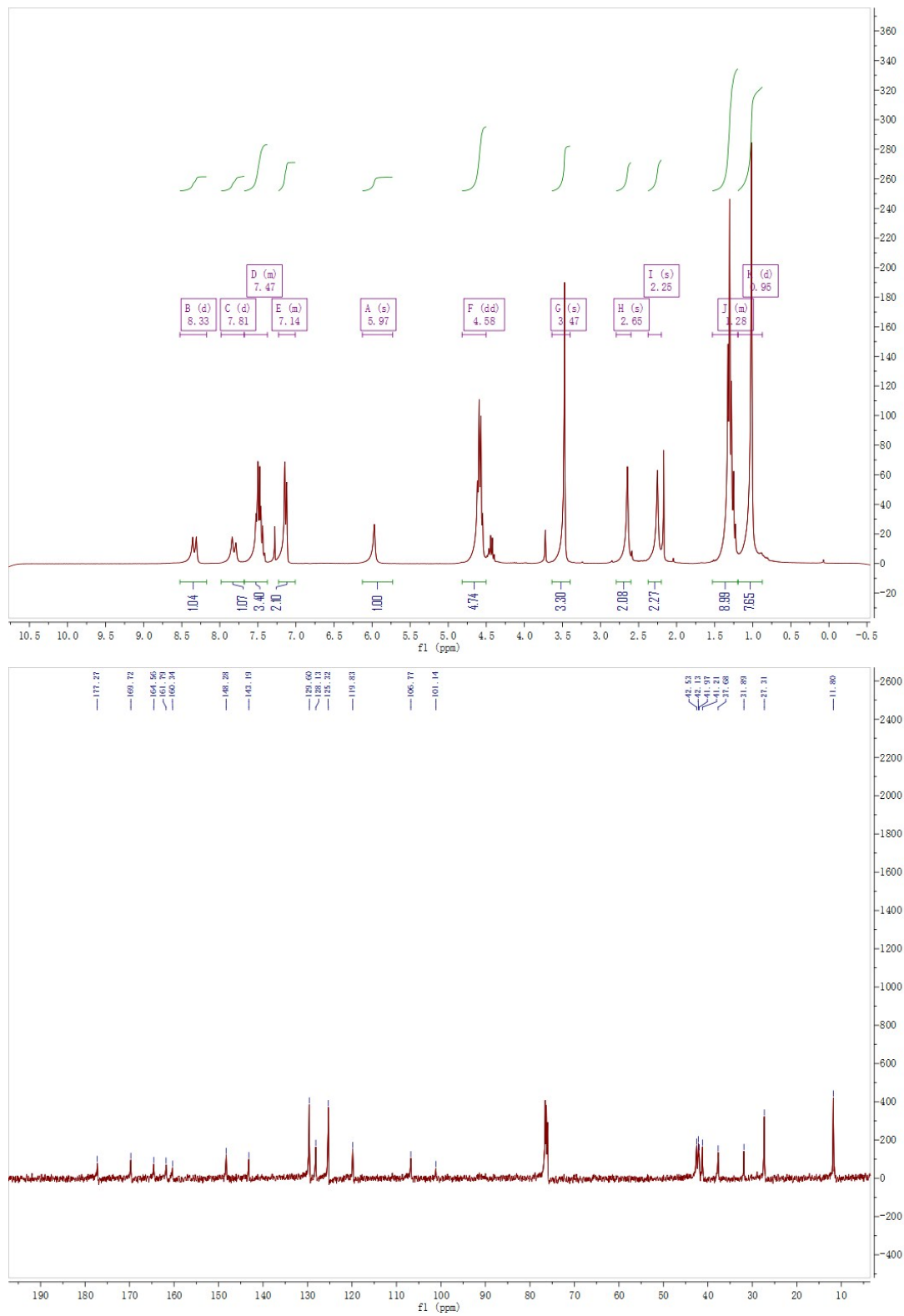
^bCollege of Chemistry and Life Science, Institute of Functional Molecules, Chengdu Normal University, Chengdu, China. *E-mail: zhonghli@sohu.com (Z. Li)

^cDepartment of Electronic Engineering, City University of Hong Kong, Hong Kong, China.

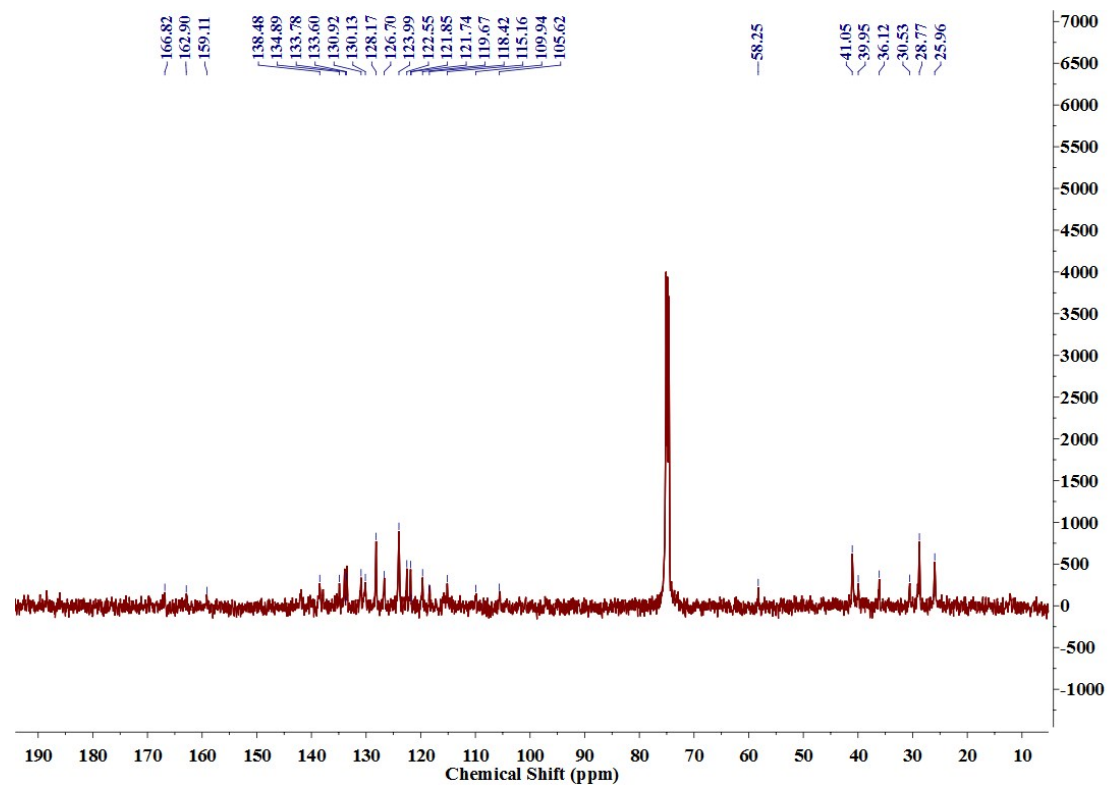
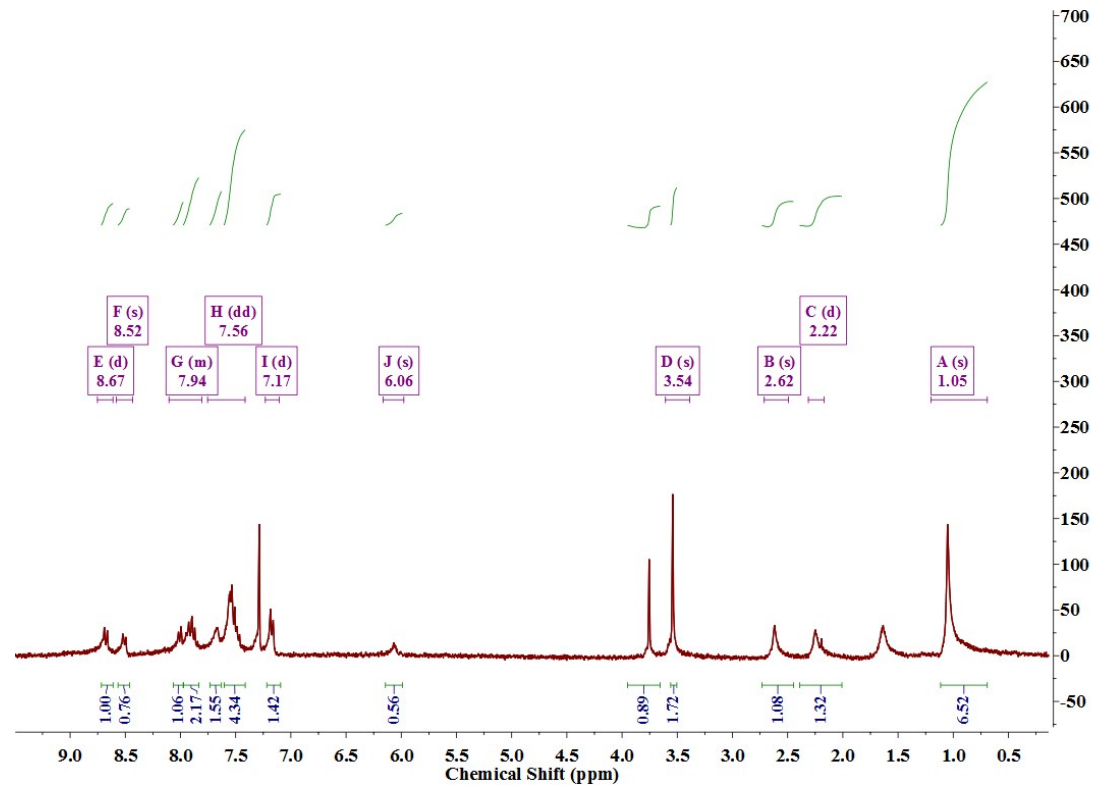
1. ¹H NMR and ¹³C NMR spectra of dyes 1-4
2. Crystal data of dye 3
3. Thermal gravity analysis of dyes 1-4
4. Fluorescent decay spectra of dyes 1-4

1. ¹H NMR and ¹³C NMR spectra of dyes 1-4

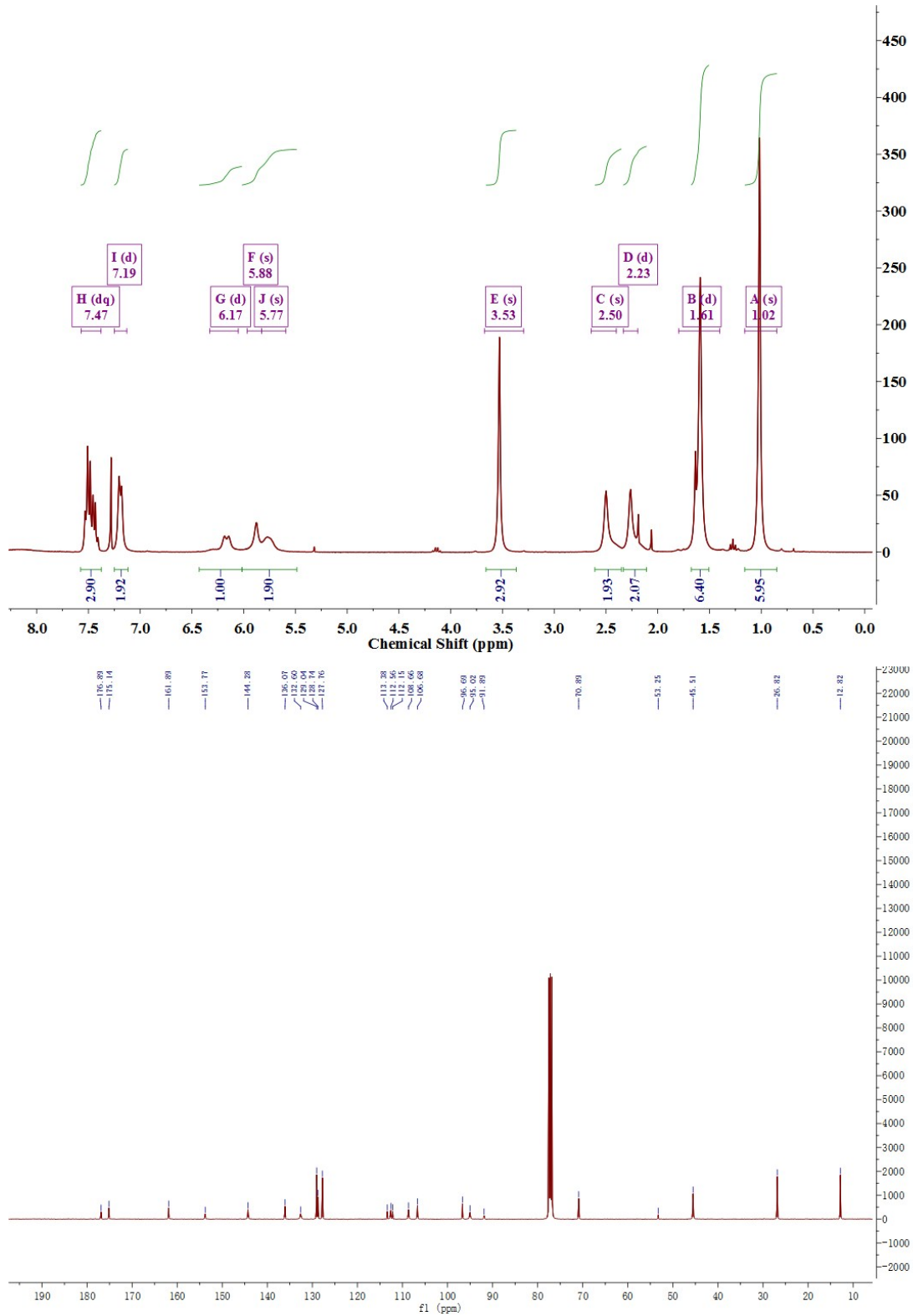
Dye 1:



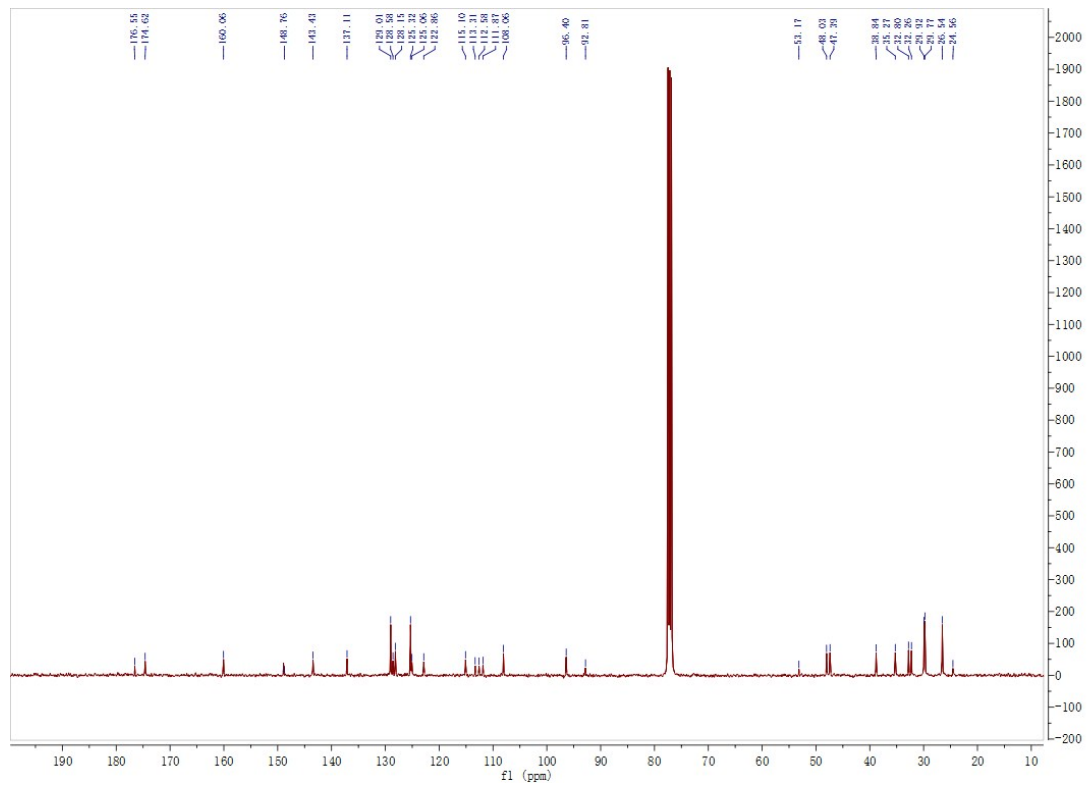
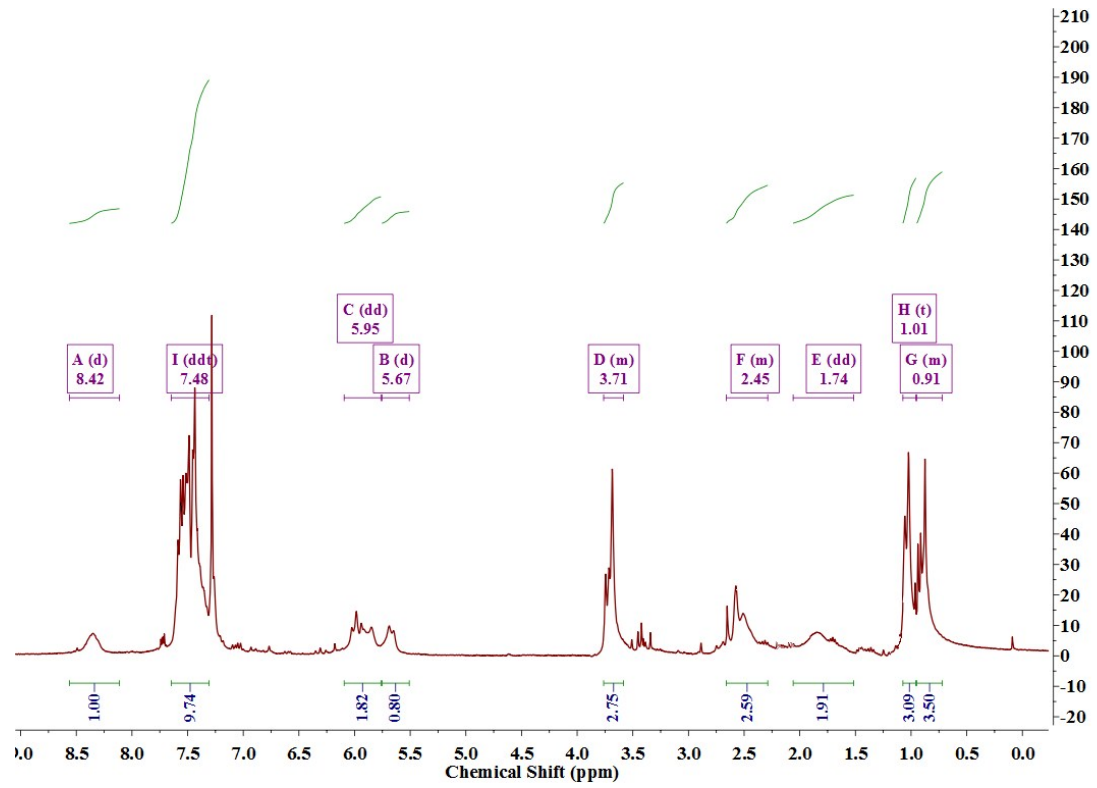
Dye 2:



Dye 3:

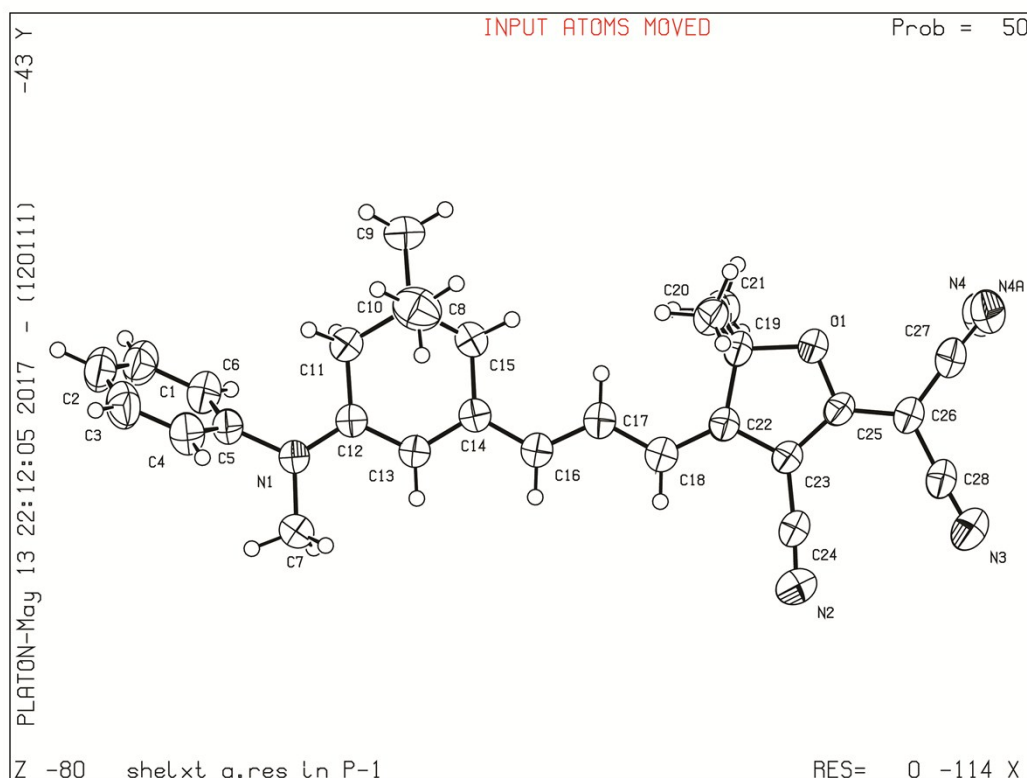


Dye 4:



2. Crystal data of dye 3

Intensity data of dye 3 (CCDC 1549946) were collected at room temperature on a Bruker PLATFORM diffractometer equipped with a SMART APEX II CCD area detector and a graphite-monochromated Mo $K\alpha$ radiation source, using ω scans at 6 different ϕ angles with a frame width of 0.3° and an exposure time of 25 second per frame. Face-indexed numerical absorption corrections were applied. Structure solution and refinement were carried out with use of the SHELXTL (version 6.12) program package.[1]

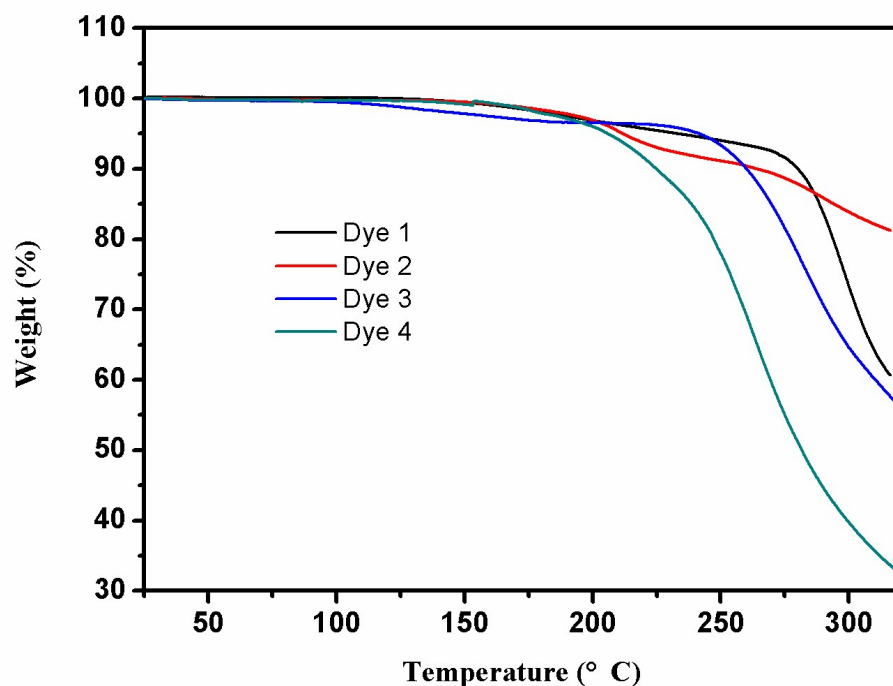


Bond precision:	C-C = 0.0030 Å			Wavelength=0.71073
Cell:	a=6.2564(5)	b=11.3834(10)	c=17.9585(15)	
	alpha=97.453(2)	beta=94.502(2)	gamma=96.730(2)	
Temperature:	296 K			
Data completeness:	0.998	Theta(max):	25.781	
R(reflections):	0.0483(2800)	wR2(reflections):	0.1463(4801)	
S = 1.012	N _{par} = 307			
	Calculated			Reported
Volume	1253.73(18)			1253.73(18)
Space group	P -1			P -1
Hall group	-P 1			-P 1
Moiety formula	C ₂₈ H ₂₈ N ₄ O			C ₂₈ H ₂₈ N ₄ O

Sum formula	C ₂₈ H ₂₈ N ₄ O	C ₂₈ H ₂₈ N ₄ O
Mr	436.54	436.54
Dx,g cm ⁻³	1.156	1.156
Z	2	2
Mu (mm ⁻¹)	0.072	0.072
F000	464.0	464.0
F000'	464.16	
h,k,l _{max}	7,13,21	7,13,21
N _{ref}	4813	4801

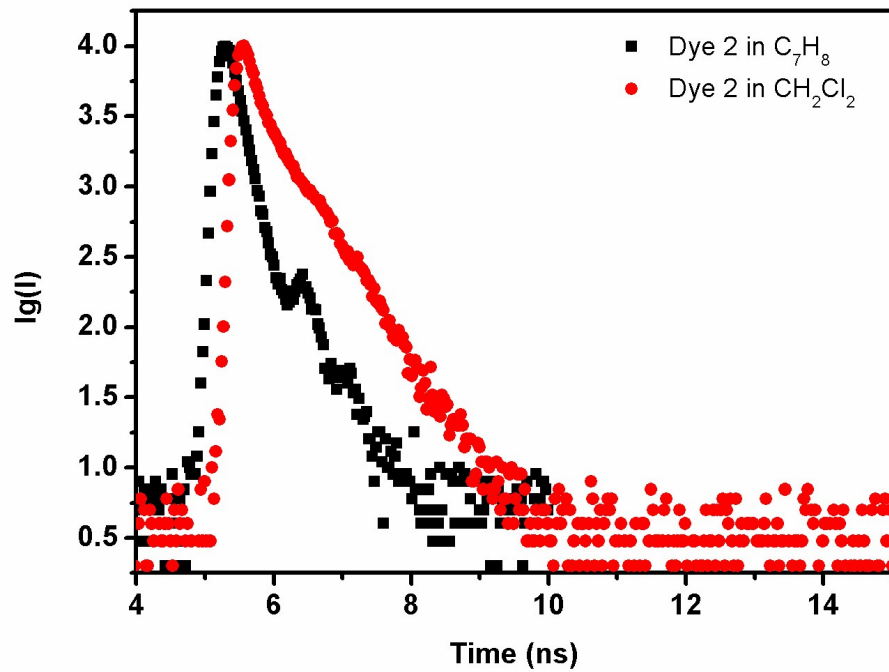
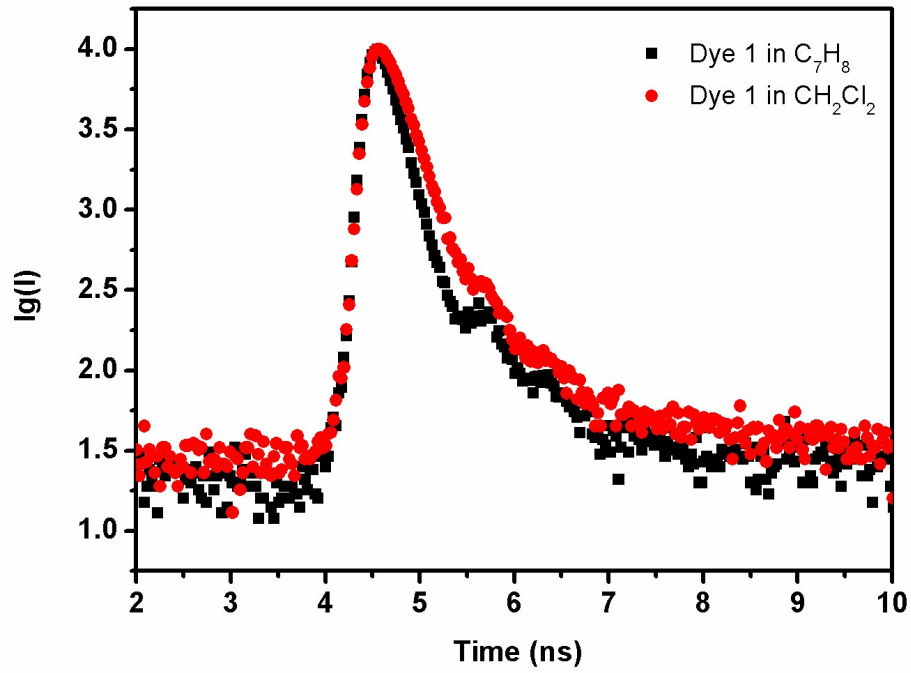
3. Thermal gravity analysis of dyes 1-4

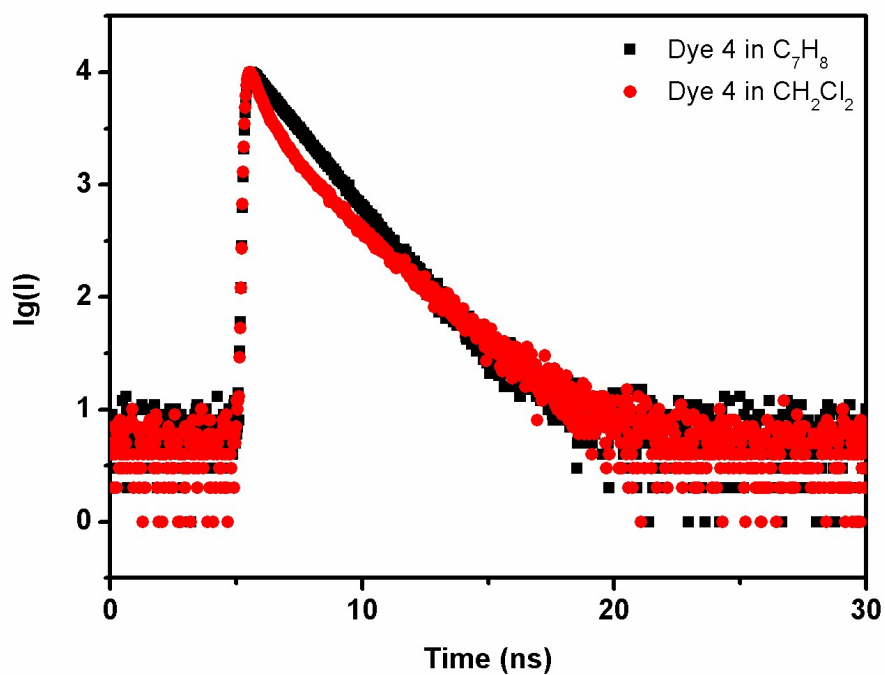
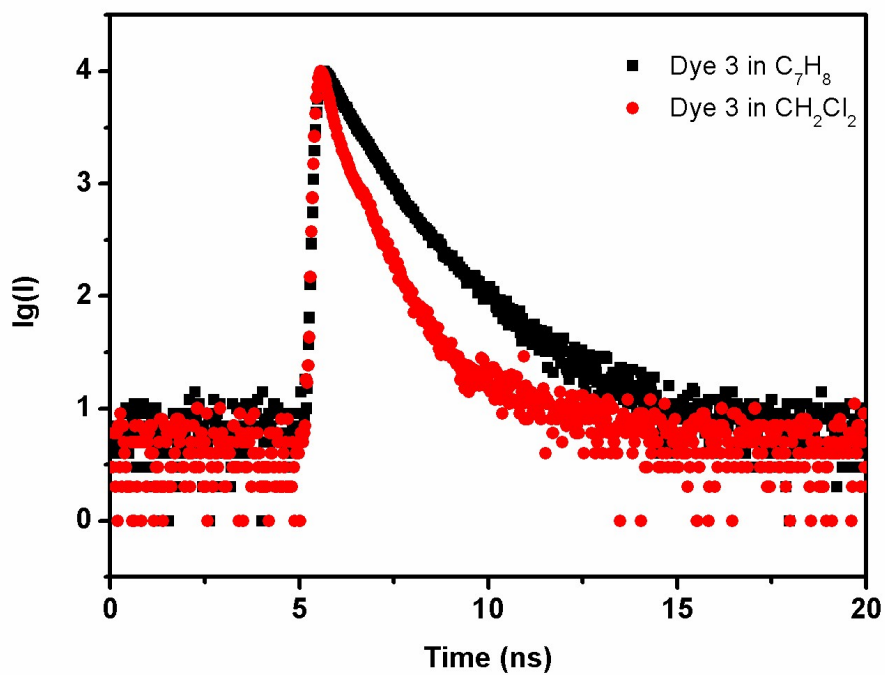
The TGA was determined by TA5000-2950TGA (TA co) with a heating rate of 10 °C min⁻¹ under the N₂ atmosphere.



4. Fluorescent decay spectra of dyes 1-4

Fluorescence lifetime was measured on a Fluorolog-3 spectrofluorometer (Horiba JobinYvon) with a Delta Diode (505 nm, D-505, Horiba Scientific; 635 nm, D-635, Horiba Scientific) as the excitation source and a picosecond photon detection module (PPD-850, Horiba Scientific) as the detector. The excited wavelengths are 505 nm dye 1 and 635 nm for dyes 2-4.





[1]. G.M. Sheldrick, SHELXTL, Version 6.12, Bruker AXS Inc., Madison, WI, 2001.