

Electronic Supplementary information for:

1,2-Bis[(2,5-dimethyl)dithioene[3,2-*b*,2,3-*d*]thiophene]perfluorocyclopentene: Synthesis and Photochromic Reactions in Solution and LB Films

Hui Lin^{a,b}, Wei Xu^{*a} and Daoben Zhu^{*a}

^a Beijing National Laboratory for Molecular Science, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, 100190, China; Fax 086-010-62569349; Tel 086-010-82617790; wxu@iccas.ac.cn, zhudb@iccas.ac.cn

^b Academy of Sciences, and Graduate School of Chinese Academy of Sciences, Beijing 100049, P. R. China

1 HPLC chromatograms of two isomers

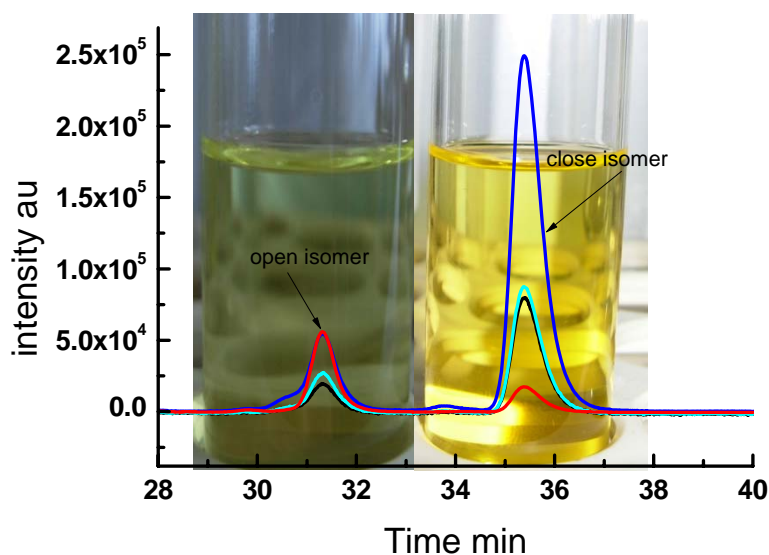


Fig 1 high pressure Liquid chromatogram of two isomer BDDTP eluted by solution (petroleum:ethyl acetate=50:1) under UV light irradiation of 380nm until the photostationary state is reached

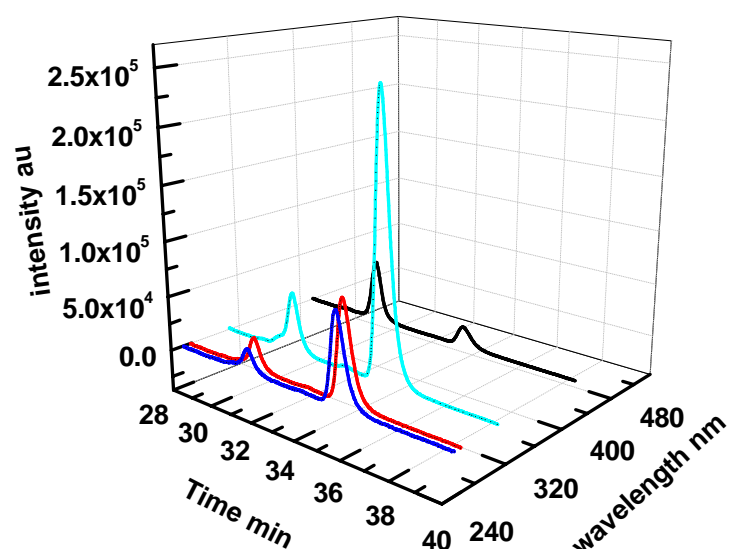


Fig 2 high pressure Liquid chromatogram of two isomers detected at the wavelength of 254,262,308,418nm under UV light irradiation of 380nm until the photostationary state is reached

3 Conversion ratio at the photostationary state determined by HPLC

HPLC is a convenient way to measure the ratio since the ring-open and closed forms of compound BDDTP are easy to be separated by silica gel column chromatography. The ratios of ring-open forms before and after under UV irradiation of 380nm until the photostationary state is reached is 65.7%, ($(71211.5-24420.4)/71211.5=65.7\%$). The ratio is consistent with data measured by ^1H NMR. Under Vis irradiation of 500nm until the photostationary state is reached, close isomers convert to open isomers reversely.

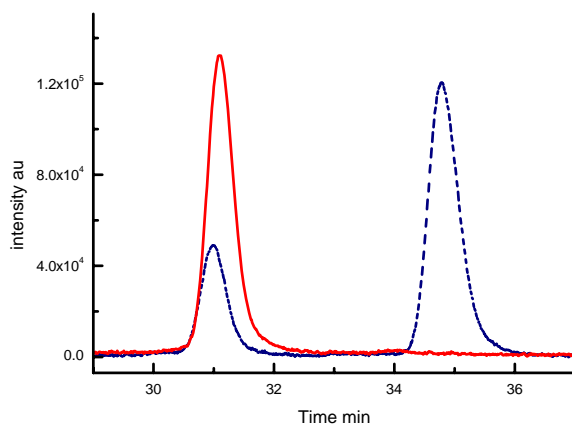


Fig 3 high pressure Liquid chromatogram of BDDTP, Photostationary state (state line), under UV

light irradiation of 380nm until the photostationary state is reached (dash line) eluent by solution (petroleum :ethyl acetate=50:1)

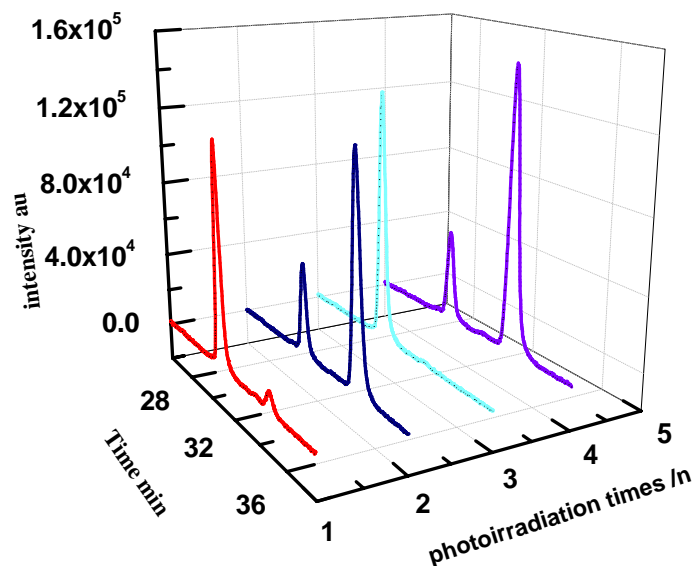


Fig 4 HPLC chromatograph of BDDTP in n-hexane detected by wavelength of 308nm, 1) before photoirradiation, 2) UV photoirradiation of 380nm wavelength until the photostationary state is reached, 3) Vis photoirradiation of 500nm wavelength until the photostationary state is reached, 4) second UV photoirradiation of 380nm wavelength until the photostationary state is reached

Table S- 1 X-ray crystallographic data of BDDTP

Empirical formula	$C_{25}H_{14}F_6S_6$
Formula weight	620
Temperature(K)	113
Crystal system	monoclinic
Space group	$C 2/c$
a(Å)	29.925(4)
b(Å)	6.9672(8)
c(Å)	23.953(3)
α	90.00

β	99.850(7)
γ	90.00
Volume (\AA^3)	4920.43
Z	8
Density <small>calcd.</small> (g cm^{-3})	1.676
Goodness of fit on F^2	1.097
$R1(I > 2\sigma(I))$	0.0750
$wR2(\text{all data})$	0.0908
