SUPPORTING INFORMATION FOR

Efficient Synthesis of 3,4-Diphenyl-Substituted Maleimides from Readily Prepared Diphenylfumaronitrile Derivatives

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Three CIF files in separate files:

i5823cif: bis(4-methoxyphenyl)fumaronitrile

i5852cif: bis(4-bromophenyl)fumaronitrile

ic9246cif: bis(3-trifluoromethylphenyl)fumaronitrile

General

The quantum yields of red emitting fluorene derivatives were determined by integrating-sphere method described by de Mello *et al.* on vacuum deposited thin films.[s1] HeCd laser beam (325 or 442 nm) interacts with a liquid or solid sample located inside an integrating sphere with internal diffuse white reflectance coating. Through a baffle-blocked opening, the uniformly scattered radiation is coupled to a fused-silica fiber and is detected by a spectrally-calibrated spectrometer-CCD system. We estimate the error of ϕ_f by repeated measurements on several dyes with known ϕ_f values. Nile Red (in 1,4-dioxane) was one of the fluorescent dyes and the corresponding ϕ_f was determined as 67±5%, which was quite close to the literature value of 68%.[s2]

References

s1. de Mello, J. C.; Wittmann, H. F.; Friend, R. H. *Adv. Mater.* **1997**, *9*, 230.

s2. Sarkar, N.; Das, K.; Narayan, D.; Bhattachartta, K. *Langmuir* **1994**, *10*, 326.

X-ray Crystal Structure Determinations.

Single crystals of bis(4-bromophenyl)fumaronitrile, bis(3-trifluoromethylphenyl)fumaronitrile and bis(4-methoxyphenyl)fumaronitrile suitable for X-ray diffraction studies were grown by slowly evaporation of solutions of chloroform/hexane, diethyl ether/methanol, and dichloromethane containing the fumaronitriles, respectively. Data collection was carried out on a Nonius KappaCCD diffractometer for bis(3-trifluoromethylphenyl)fumaronitrile, and Enraf-nonius CAD4 diffractometer for bis(4-bromophenyl)fumaronitrile and bis(4-methoxyphenyl)fumaronitrile. The radiation of Mo Kα radiation (λ •= 0.7107 Å) was used for three crystals. Details of the structure determination of both compounds are given in Table S1.

For bis(3-trifluoromethylphenyl)fumaronitrile, the chosen crystals were mounted on a glass fiber. Cell parameters were retrieved and refined using *DENZO-SMN* software[s3a] on all reflections. Data reduction was performed with the *DENZO-SMN* software.[s3a] An empirical absorption was based on the symmetry-equivalent reflections and applied the data using the *SORTAV* program.[s3b] Using *SHELXTL* program on PC computer made the structure analysis. The structure was solved using the *SHELXS-90* program[s3c] and refined using *SHELXL-97* program[s3d] by full-matrix least squares on F^2 values. All of non-hydrogen atoms are refined anisotropically. Hydrogen atoms attached to the carbons were fixed at calculated positions and refined using a riding mode. For bis(4-bromophenyl)fumaronitrile and bis(4-methoxyphenyl)fumaronitrile, unit cell parameters were obtained by a least-squares fit to the automatically centered settings for 25 reflections. Intensity data were collected by using $\omega/2\theta$ scan mode. Corrections were made for Lorentz

and polarisation effects. The structures were solved by direct methods *SHELX-97*.[10d] All non-hydrogen atoms were located from the difference Fourier maps and were refined by full-matrix least-squares procedures. Hydrogen atoms were calculated and refined with an overall isotropic temperature factor. Calculations and full-matrix least-squares refinements were performed utilizing the *WINGX* program package.[s3e]

Reference

s3. (a) Otwinowski, Z.; Minor, W. Proceeding of X-ray Diffraction Data Collected in Oscillation Method. In *Mehtods in Enzymology, Vol. 276: Macromolecular Crystallography, Part A*; Carter, C. W.; Jr., Sweet, R. M. Eds.; Academic Press: New York, 1997; pp. 307-326. (b) Blessing, R. H., *Acta Cryst., Sect. A* **1995**, *51*, 33. (c) Sheldrick, G. M., *Acta Cryst., Sect. A* **1990**, *46*, 467. (d) Sheldrick, G.. M., *SHELXL-97*, University of Göttingen, Germany, 1997. (e) Farrugia, L. J. *J. Appl. Cryst.* **1999**, *32*, 837.

Table S1. Crystallographic Data for bis(4-bromophenyl)fumaronitrile (A), bis(3-trifluoromethylphenyl)fumaronitrile (B), and bis(4-methoxyphenyl)fumaronitrile (C)

	A	B	C
Chemical formula	$C_{16}H_8Br_2N_2$	$C_{18}H_8F_6N_2$	$C_{18}H_{14}N_2O_2$
Formula Weight	434.01	366.26	290.31
Temperature (K)	300(2)	150(1)	300(2)
Space group	*P*-1	$P2_1/n$	$P2_1/n$
a (Å)	7.9926(9)	8.0331(10)	3.907(1)
b (Å)	9.4626(12)	11.967(2)	23.189(2)
c (Å)	10.6914(15)	8.7219(13)	8.020(1)
α (°)	92.131(11)	90	90
β (°)	110.063(10)	115.331(7)	97.83(1)
γ (°)	74.017(10)	90	90
V (Å^3)	728.70(16)	758.34(19)	719.8
Z	2	2	2
ρ_{calc} (g/cm^3)	1.769	1.604	1.339
μ (mm^{-1})	5.552	0.148	0.089
F(000)	376	368	304
λ (Mo Kα) (Å)	0.71073	0.71073	0.71073
$R(F_o)^a(I > 2\sigma(I))$	0.0259	0.0507	0.0319
$R_w(F_o)^b(I > 2\sigma(I))$	0.0569	0.1121	0.0811
Reflection collected	2758	3717	1454
Unique reflections	2559	1330	1263
Absorption correction	Psi-scan	Semi-emperical from equivalents	Psi-scan
Refinement on	F^2	F^2	F^2
Parameters refined	182	119	101
Goodness-of-fit on F^2	1.047	1.046	1.070

[a] $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $R_w = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$.

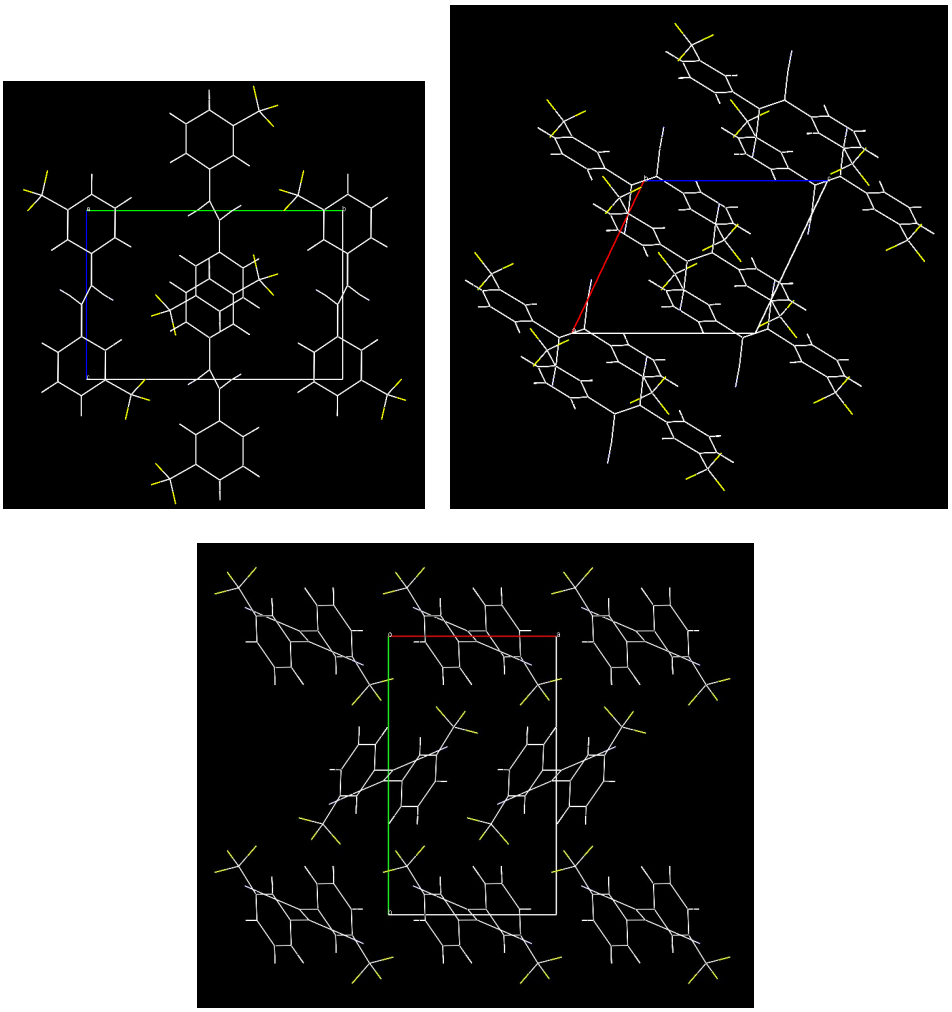

FIGURE S1. Crystal packing diagrams of bis(3-trifluoromethylphenyl)fumaronitrile viewing along *a*-axis (top left), *b*-axis (top right), and *c*-axis (bottom).

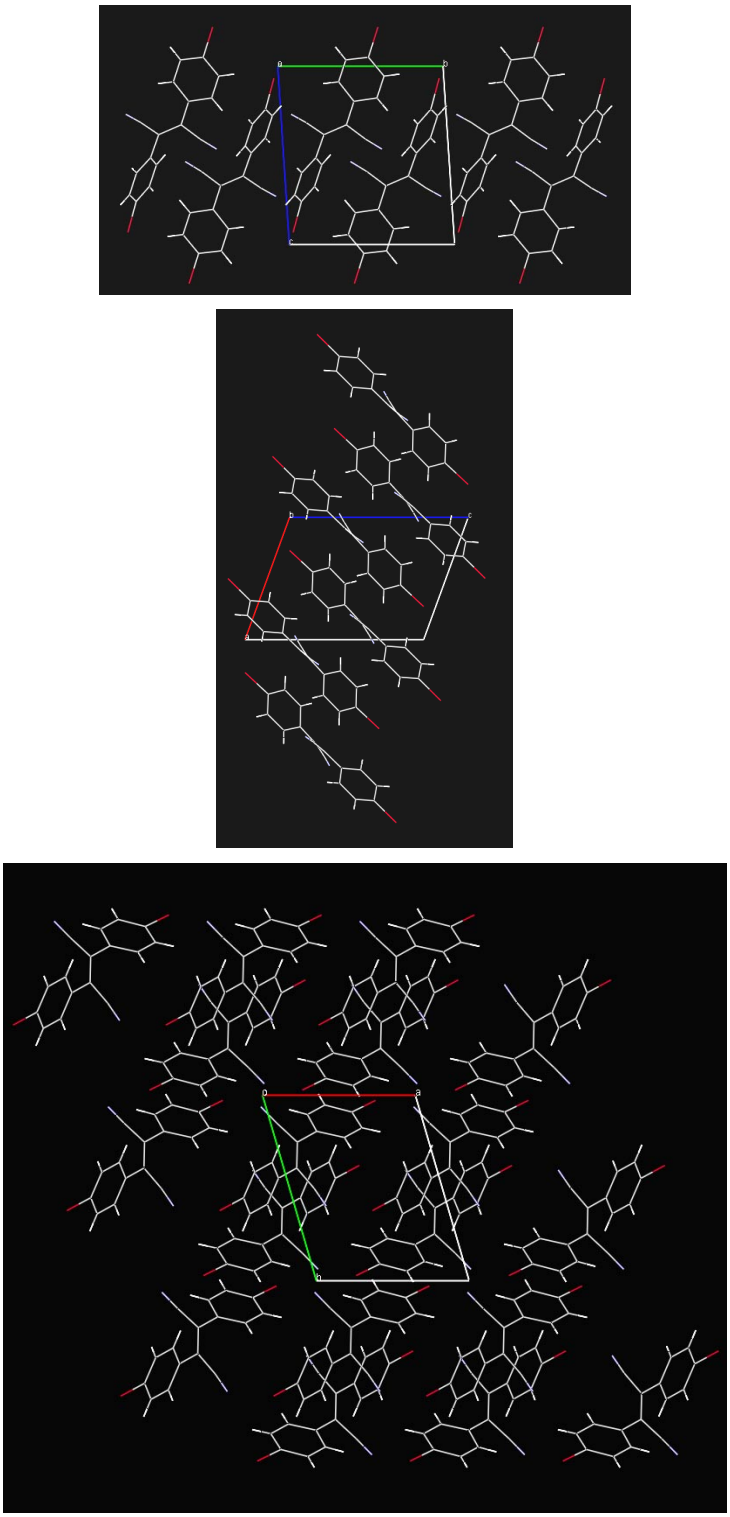

FIGURE S2. Crystal packing diagrams of bis(4-bromophenyl)fumaronitrile viewing along *a*-axis (top), *b*-axis (center), and *c*-axis (bottom).