Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Bimolecular Photoactivation of NBD Fluorescence

Sherif Shaban Ragab,[a,b] Subramani Swaminathan,[a] Jaume Garcia-Amorós,[a] Burjor Captain[a] and Françisco M. Raymo*[,a]

a Laboratory for Molecular Photonics, Department of Chemistry, University of Miami, 1301 Memorial Drive, Coral Gables, Florida, 33146-0431, USA

b Department of Photochemistry, Chemical Industries Research Division, National Research Centre (NRC), El-Tahrir Street, Dokki, Giza, 12622, Egypt

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Crystallographic Analysis. Yellow single crystals of **6** were obtained from a CH_2Cl_2/hexane solution of the compound, after the slow evaporation of the solvent. The data crystal was glued onto the end of a thin glass fiber. X-ray intensity data were measured with a Bruker SMART APEX2 CCD-based diffractometer, using Mo Kα radiation (λ = 0.71073 Å).[S1] The raw data frames were integrated with the SAINT+ program by using a narrow-frame integration algorithm. Corrections for Lorentz and polarization effects were also applied with SAINT+. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the program SADABS. The structure was solved by a combination of direct methods and difference Fourier syntheses and refined by full-matrix least-squares on F^2 with the SHELXTL software package.[S2] Compound **6** crystallized in the monoclinic crystal system and the systematic absences in the data were consistent with the unique space group $P2_1/c$. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in geometrically-idealized positions and included as standard riding atoms during the least-squares refinements. Crystal data, data collection parameters and results of the analysis are listed in Table S1. Crystallographic data were deposited with the Cambridge Crystallographic Data Centre (CCDC No. 1033127). Copies of this information may be obtained free of charge from: The Director, CCDC12 Union Road, Cambridge CB2 1EZ, UK [fax: +44(1223) 336−033; e−mail: deposit@ccdc.cam.ac.uk; www.http://www.ccdc.cam.ac.uk].

S1 Apex2 Version 2.2-0 and SAINT+ Version 7.46A; Bruker Analytical X-ray System, Inc., Madison, Wisconsin, USA, 2007.

S2 (*a*) Sheldrick, G. M. SHELXTL Version 6.1; Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, 2000. (*b*) G. M. Sheldrick, *Acta Cryst*., 2008, **A64**, 112–122.

Table S1. Crystallographic Data for **6**.

Empirical Formula	$C_{16}H_{17}NO_4S$
Formula Weight	319.37
Crystal System	Monoclinic
Lattice Parameters:	
a (Å)	15.7805(9)
b (Å)	5.0908(3)
c (Å)	21.0600(13)
β (°)	110.851(1)
V (Å^3)	1468.32(17)
Space Group	$P2_1/c$ (# 14)
Z Value	4
ρ_{calc} (g cm^{-3})	1.342
μ (Mo Kα) (mm^{-1})	0.222
T (K)	296
$2\Theta_{max}$ (°)	56.0
No. Obs. ($I > 2\sigma(I)$)	2912
No. Parameters	202
Goodness of Fit	1.038
Max. Shift in Cycle	0.003
*Residuals**: R1; wR2	0.0380; 0.0949
Absorption Correction, Max/min	Multi-Scan 0.9912/0.9245
Largest Peak in Final Diff. Map (e$^-$ Å^{-3})	0.227

$w = 1/\sigma^2(F_{obs})$; GOF = $[\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/(n_{data}-n_{vari})]^{1/2}$.

* $R = \Sigma_{hkl}(||F_{obs}|-|F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$

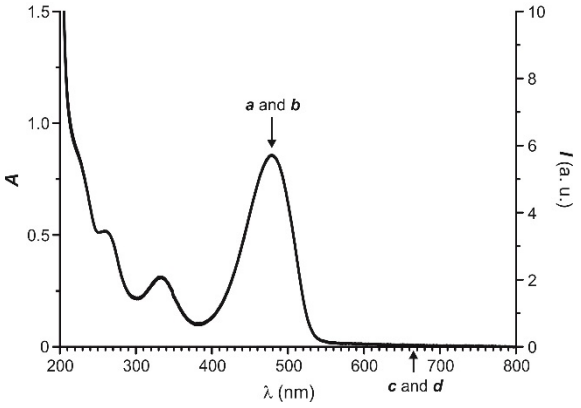

Fig. S1. Absorption (***a*** and ***b***) and emission (***c*** and ***d***) spectra of a solution of **1** [10 μM, MeCN:PBS (95:5 v/v), 25 °C, λ_{Ex} = 440 nm] before (***a*** and ***c***) after (***b*** and ***d***) illumination at λ_{Ac} (350 nm, 2.48 mW cm^{-2}) for 60 min.