Уральский федеральный университет имени первого Президента России Б.Н.Ельцина

THE OPTICAL PROPERTIES OF 1*H*-THIENO[3,4-*d*]-1,2,3-TRIAZOLIUM-OLATES

Alexander K. Eltyshev, Nadezhda V. Chernyshova, and Nataliya P. Belskaya[1]

[1]*Ural Federal University, 19, Mira St., Yekaterinburg, 620002, Russian Federation*

a.k.eltyshev@urfu.ru

1 INTRODUCTION

Organic small molecule fluorophores have been widely studied because of the simple procedures for their synthesis and purification. Moreover, they have structures with ease of modification and functionalization and also demonstrate high stability along with good absorption coefficients [1-5]. Significant attention has been directed on the design and synthesis of thiophene-based materials with tunable fluorescent and sensitivity towards the microenvironment. Various mono-cyclic assembles or fused thiophenes have been obtained for applications in biology for cellular imaging, fluorescent probes and full-color displays [6-9]. Additionally, they have significant applications in material science as organic light-emitting diodes (OLEDs), organic photovoltaic cells (OPVs), fuel-sensitized solar cells (DSSCs), and organic field-effect transistors (OFETs) [8,10].

2 SYNTHESIS

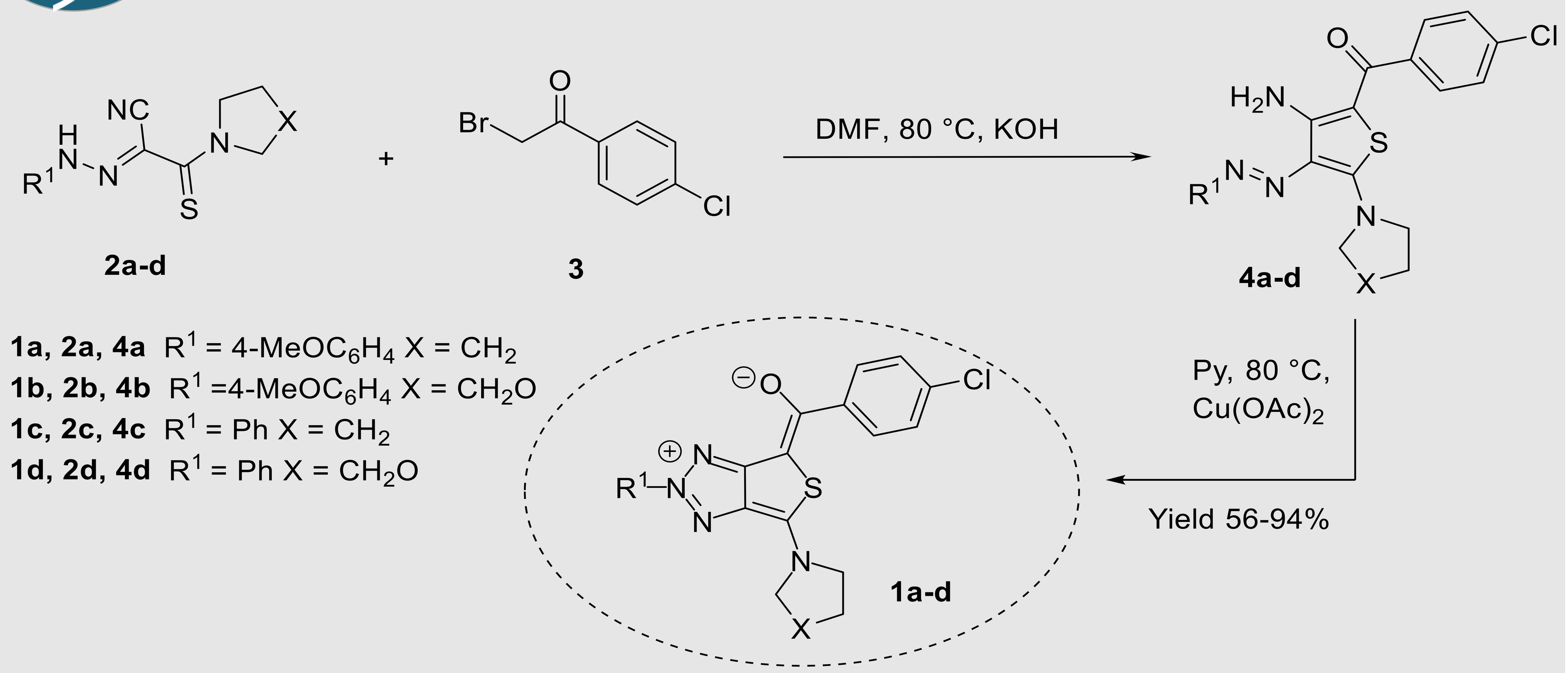

FIGURE 1. The synthetic route to 1H-thieno[3,4-d][1,2,3]triazolium-olate 1a-d.

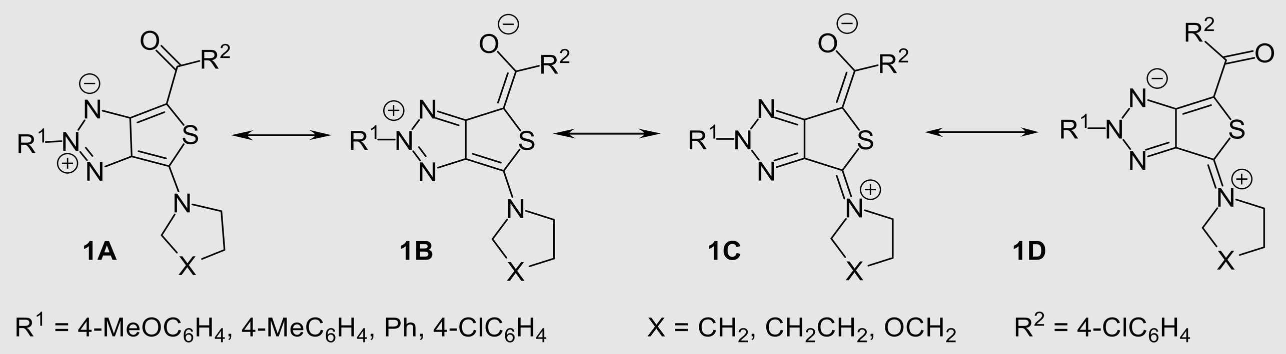

FIGURE 2. Structure of 1H-thieno[3,4-d]-1,2,3-triazolium-olates.

3 FLUORESCENCE in $CHCl_3$

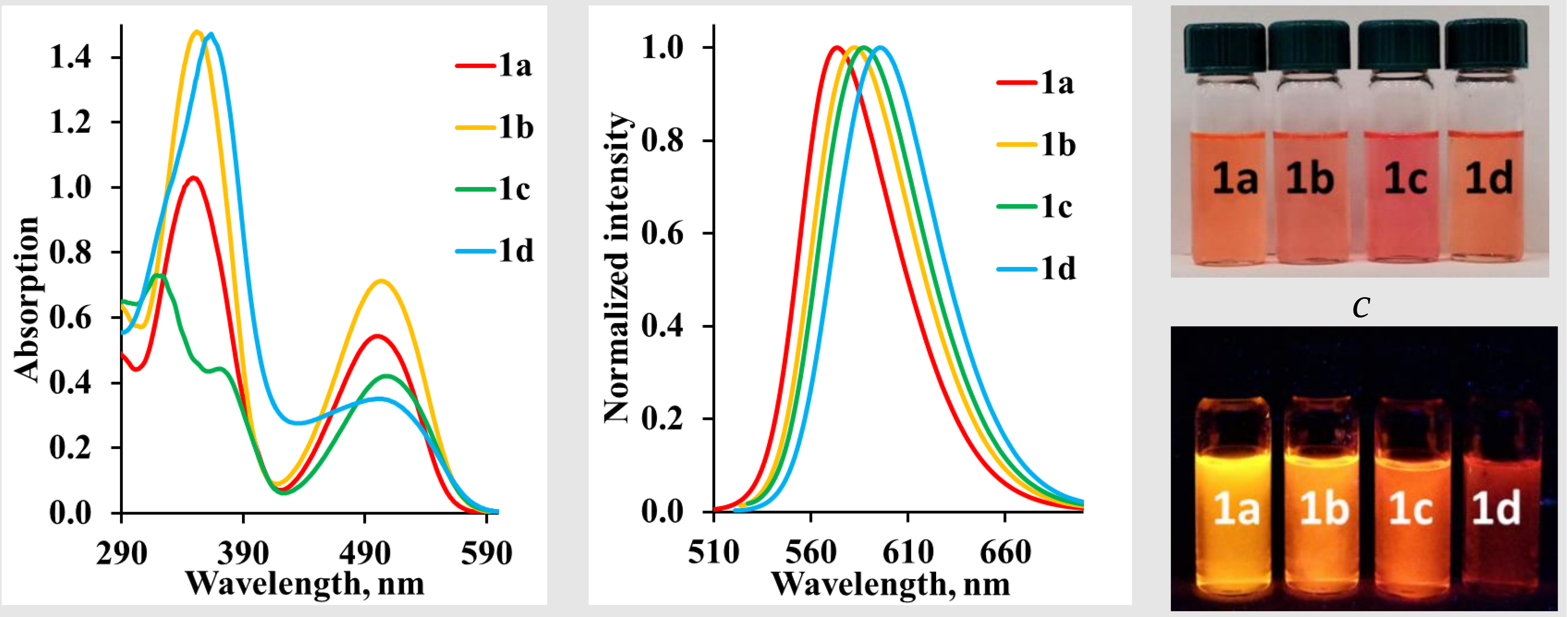

FIGURE. 3 (a) Absorption (5×10^{-5} M) and emission (1×10^{-6} M) spectra of thieno[3,4-d]-1,2,3-triazolium-olates **1a–d** in $CHCl_3$. Photographs of TTMs **1a–d** in $CHCl_3$ under irradiation with (c) sunlight and (d) a hand-held UV lamp at an emission wavelength of 380 nm

Entry	Compound	λ_{abs}, nm	ε, L·mol^{-1}·cm^{-1}	λ_{em}, nm	QY, %	Stokes shift, nm/cm^{-1}
1	1a	349, 501	19500, 10300	574	25. 9	73/2538
2	1b	352, 504	29100, 14000	583	20.9	79/2689
3	1c	371, 508	8600, 8100	588	17.6	80/2678
4	1d	364, 501	29600, 7100	596	17.2	95/3182

TABLE 1. Photophysical properties of TTMs **1a–d** in dilute solution in $CHCl_3$: Absorption (λ_{abs})^a and fluorescence (λ_{em})^b wavelengths, Stokes shifts (SS), molar absorption coefficients (ε_{max}), and fluorescence quantum yields (QY)^c.

4 SOLVATO(FLUORO)CHROMISM

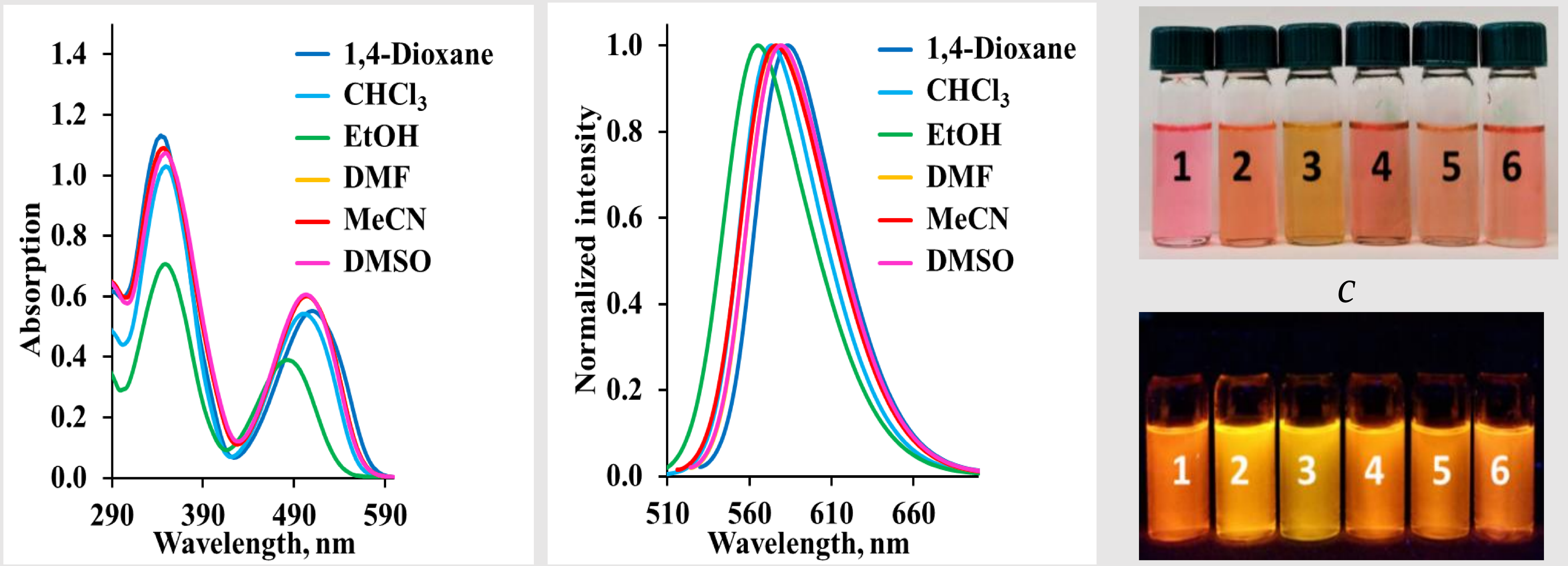

FIGURE 4. Absorption (c = 5×10^{-5} mol L^{-1}) (a) and emission (c = 5×10^{-6} mol L^{-1}) (b) spectra of TTM **1d** in different solvents at room temperature. Photographs of the solutions compound **1a** in different solvents (1 – 1,4-Dioxane, 2 – $CHCl_3$, 3 – EtOH, 4 – DMF, 5 – MeCN, 6 – DMSO) under irradiation with (c) sunlight and (d) a hand-held UV lamp at an emission wavelength of 380 nm.

5 DMSO/H_2O MIXTURES

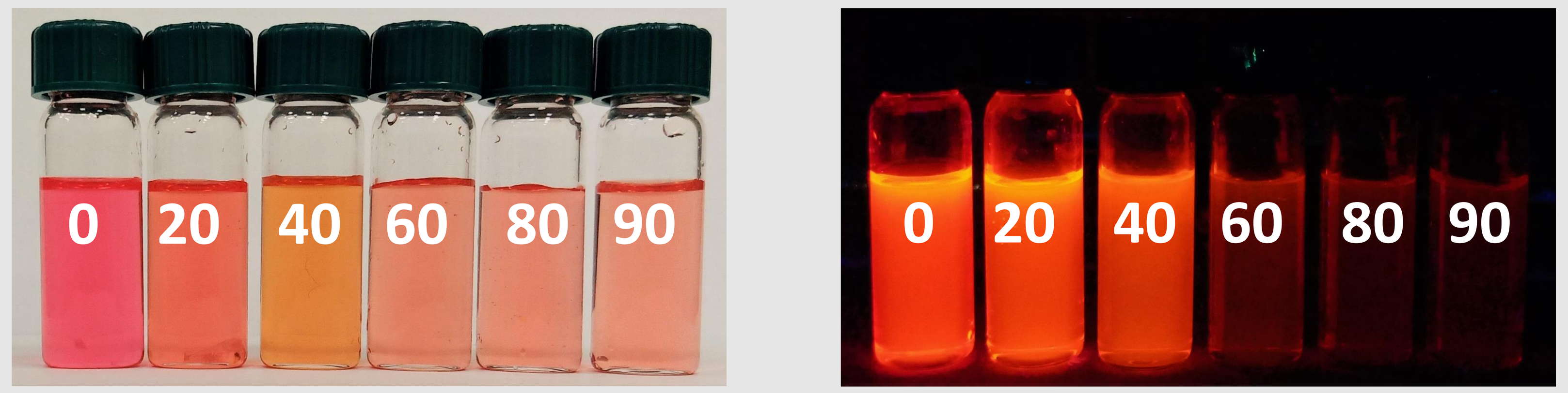

FIGURE 5. Photographs of the solutions of compound **1a** in DMSO/H_2O mixtures under irradiation with (c) sunlight and (d) a hand-held UV lamp at an emission wavelength of 380 nm.

1. M. Vendrell, D. Zhai, J. C. Er and Y-T. Chang, Chem. Rev. **112**, 4391–4420 (2012).
2. H. Kobayashi, M. Ogawa, R. Alford, P. L. Choyke and Y. Urano, Chem. Rev. **110**, 2620–2640 (2010).
3. L. Yuan, W. Lin, K. Zheng, L. He and W. Huang, Chem. Soc. Rev. **42**, 622–661 (2013).
4. J. Fan, M. Hu, P. Zhan and X. Peng, Chem. Soc. Rev. **42**, 29–43 (2013).
5. N. P. Belskaya, I. Kostova and Z. Fan, Targets Heterocycl. Syst. **23**, 116-142, (2019).
6. M. E. Cinar and T. Ozturk, Chem. Rev. **115**, 3036–3140 (2015).
7. B. S. Ong, Y. Wu, Y. Li, P. Liu and H. Pan, Chem. Eur. J. **14**, 4766–4778 (2018).
8. K. I. Lugovik, A. K. Eltyshev, E. Benassi and N. P. Belskaya, Chem. Asian J. **12**, 2410–2425 (2017).
9. K. I. Lugovik, A. K. Eltyshev, P. O. Suntsova, L. T. Smoluk, A. V. Belousova, M. V. Ulitko, A. S. Minin, P. A. Slepukhin, E. Benassi and N. P. Belskaya, Org. Biomol. Chem. **16**, 5150–5162, 2018.
10. M. S. M. Li, K. Chu, J. T. Price, N. D. Jones and Zh. Ding, ChemElectroChem **3**, 2170–2178 (2016).

This work was supported by the Russian Found of Basic Research [Reference # 19-33-90184].