Supplementary Materials

Effects of Difluorophenyl Substituents on Structural, Redox, and Magnetic Properties of Blatter Radicals

Dmitry Gulyaev[1], Andrey Serykh[1], Evgeny Tretyakov*[,1], Anna Akyeva[1], Mikhail Syroeshkin[1], Dmitry Gorbunov[2], Svetlana Maltseva[2], Nina Gritsan*[,2], Galina Romanenko[3] and Artem Bogomyakov[3]

[1] N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky Ave. 47, Moscow 119991, Russian Federation; refihis@ioc.ac.ru (D.G.); andreyser200@mail.ru (A.S.); anna.kozmenkova@gmail.com (A.A.); syroeshkin@ioc.ac.ru (M.S.)

[2] V. V. Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of Russian Academy of Sciences, Institutskaya Str. 3, Novosibirsk 630090, Russian Federation; dmitry.e.gorbunov@gmail.com (D.G.); lana.maltseva04@gmail.com (S.M.)

[3] International Tomography Center, Siberian Branch of Russian Academy of Sciences, Institutskaya Str. 3a, Novosibirsk 630090, Russian Federation; romanenk@tomo.nsc.ru (G.R.); bus@tomo.nsc.ru (A.B.)

* Correspondence: tretyakov@ioc.ac.ru (E.T.); gritsan@kinetics.nsc.ru (N.G.)

Table of Contents:

Cyclic voltammetry

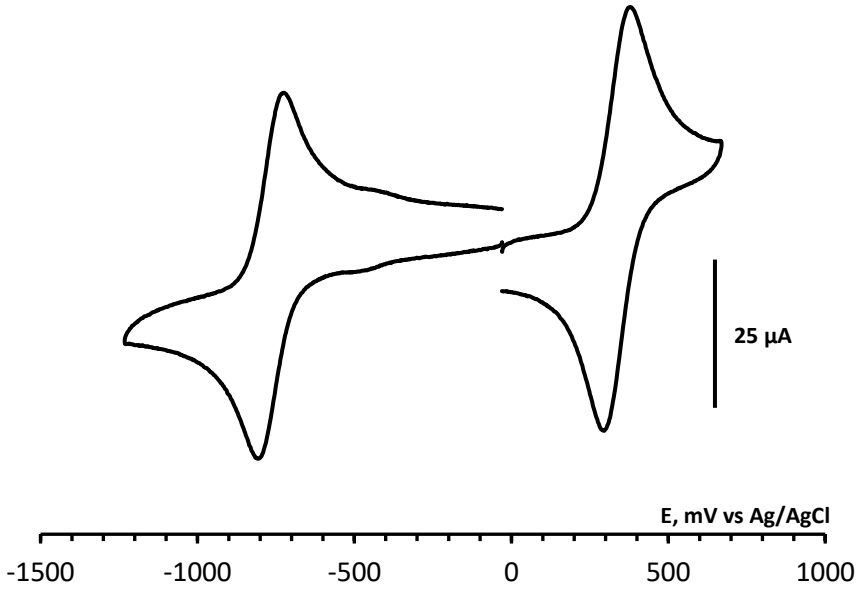


Figure S1. CV curves of oxidation and reduction of **1b** (3×10^{-3} M) in 0.1 M Bu_4NBF_4/MeCN on a glassy carbon disk electrode at a potential sweep rate of 0.1 V/s.

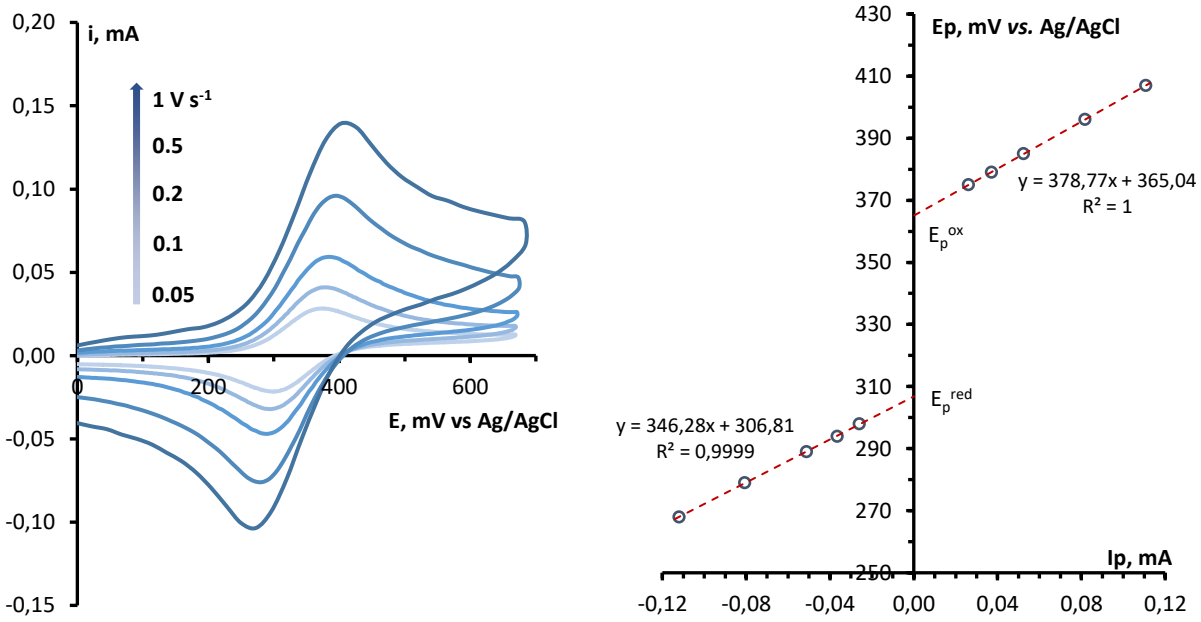


Figure S2. (left) CV curves of the oxidation of **1b** (3×10^{-3} M) in 0.1 M Bu_4NBF_4/MeCN on a glassy carbon disk electrode at potential sweep rates of 0.05, 0.10, 0.20, 0.50, and 1.00 V/s. (right) Dependences of the potentials of the peaks of oxidation and reciprocal reduction on the current at the peak for the corresponding process.

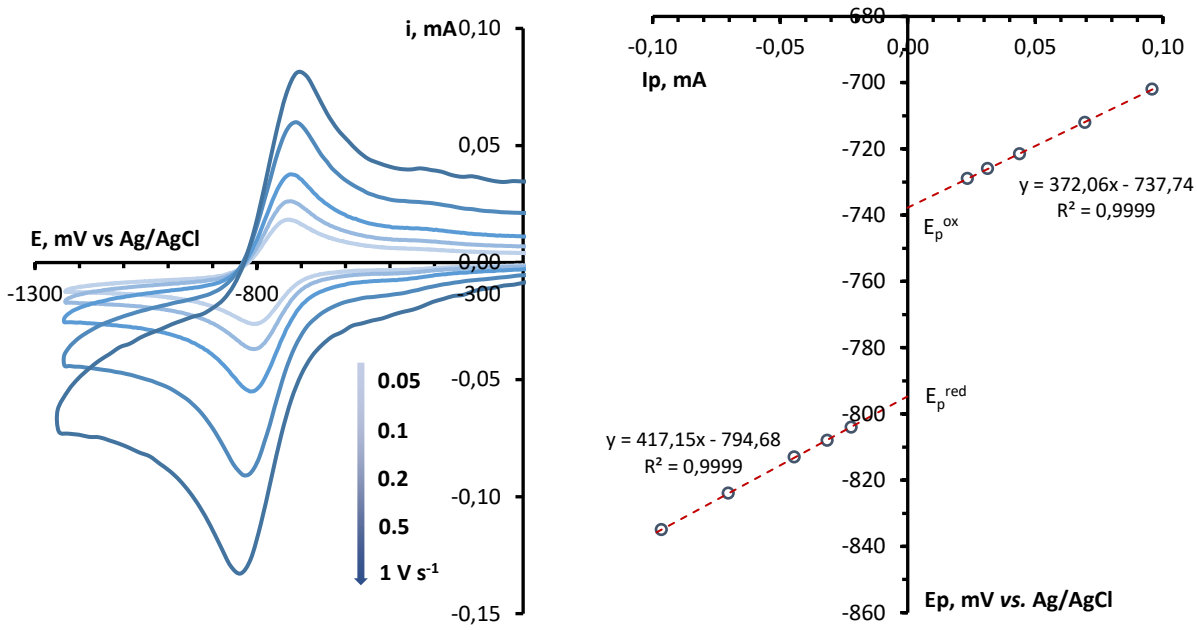


Figure S3. CV curves of reduction of **1b** (3×10^{-3} M) in 0.1 M Bu_4NBF_4/MeCN on a glassy carbon disc electrode at potential sweep rates of 0.05, 0.10, 0.20, 0.50, and 1.00 V/s. (right) Plots of reduction and reciprocal oxidation peak potentials versus peak current for the respective process.

CW ESR Spectroscopy

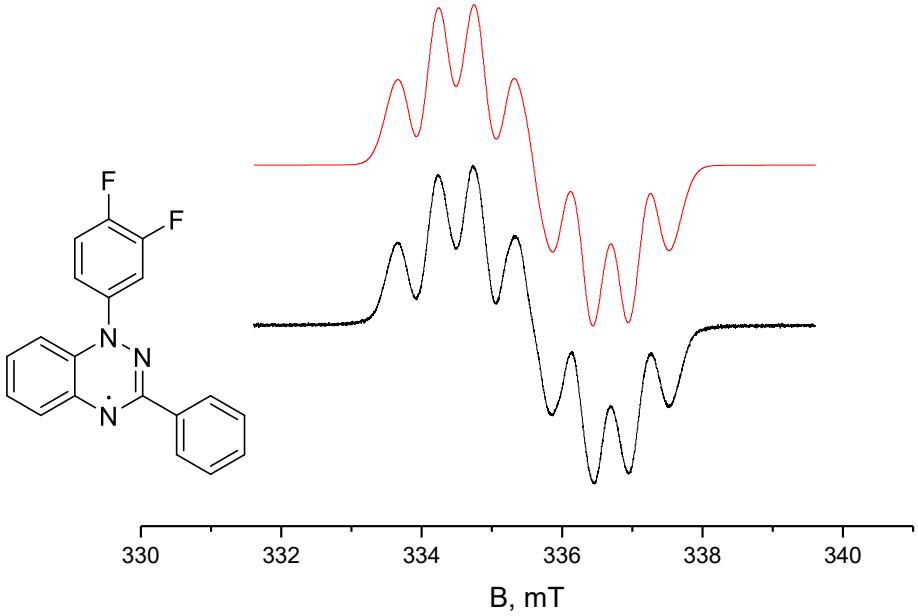


Figure S4. The EPR spectrum of radical **1a** (black) in toluene solution (~10^{-5} M) at 298 K and its modeling (red).

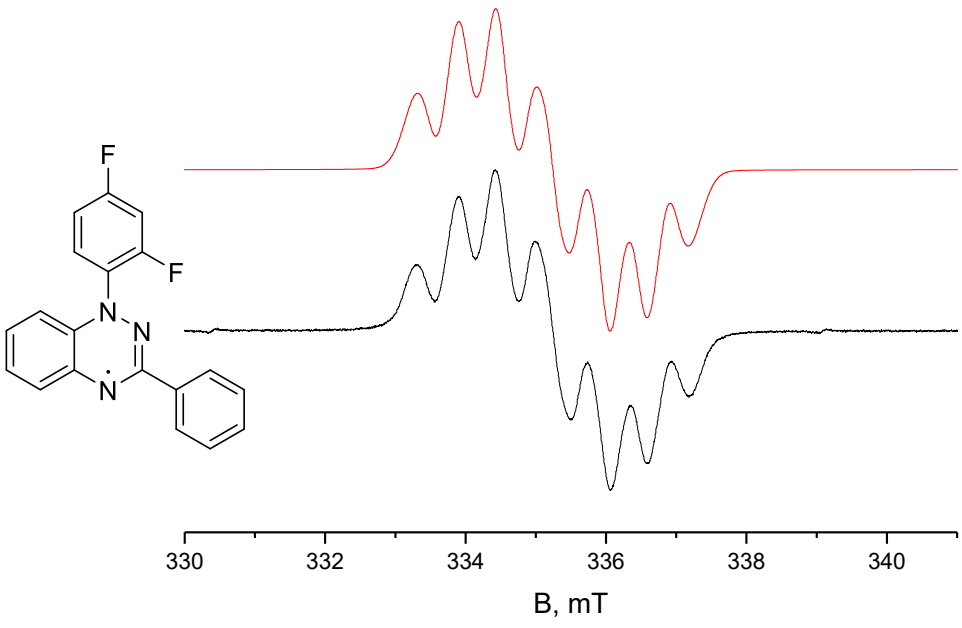


Figure S5. The EPR spectrum of radical **1b** (black) in toluene solution (~10^{-5} M) at 298 K and its modeling (red).

Near-UV and Visible Spectroscopy

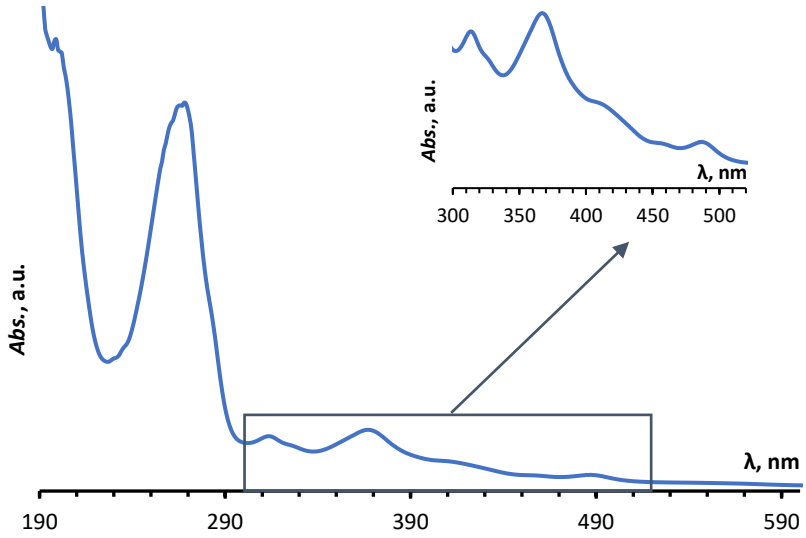
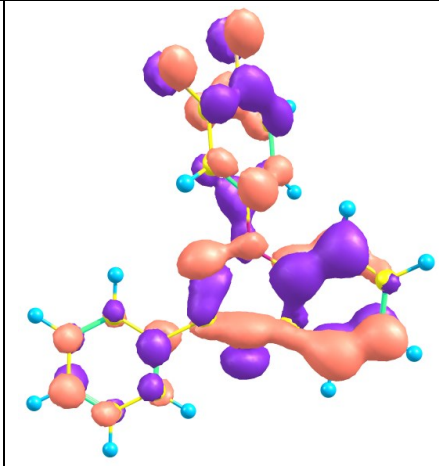
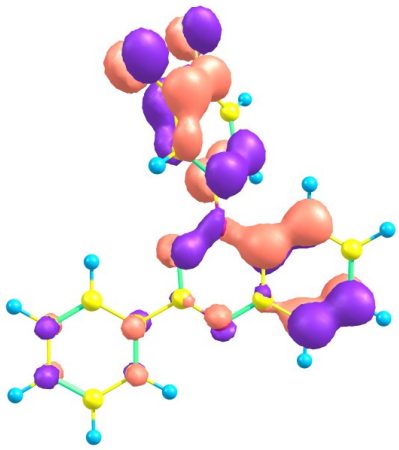
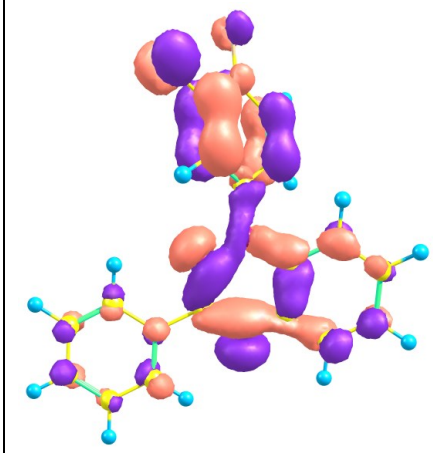
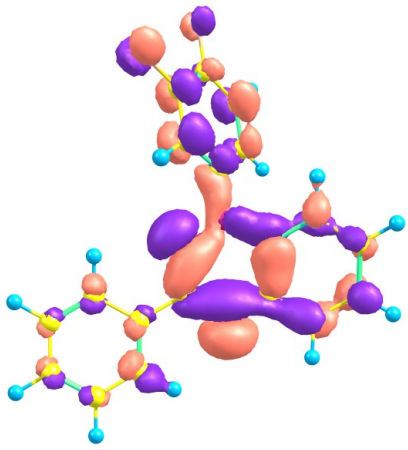
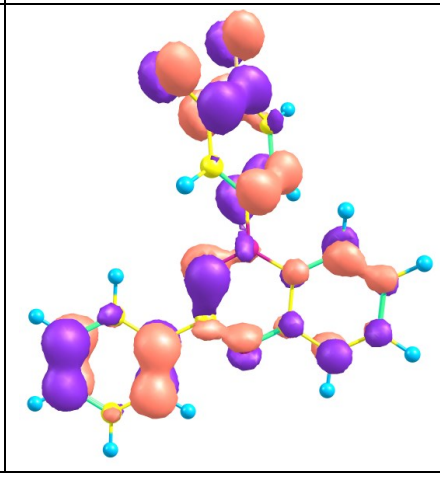
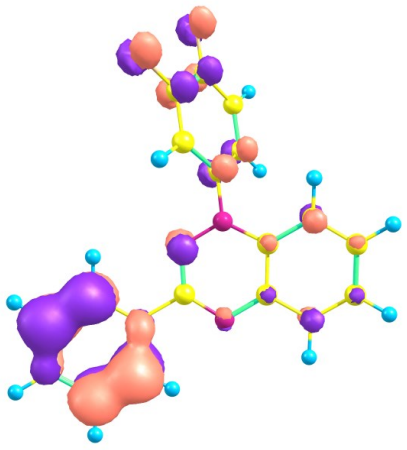
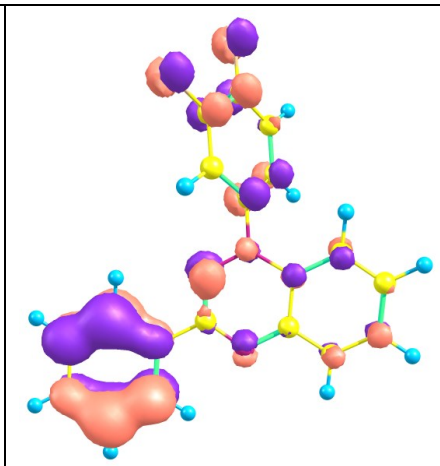
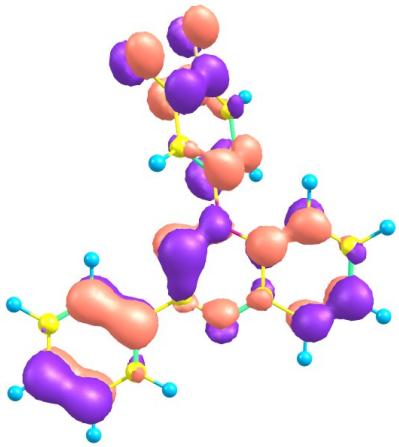
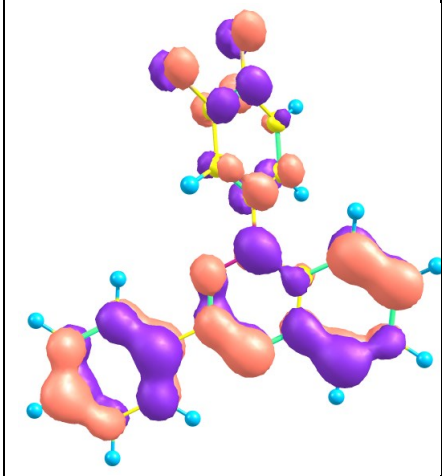
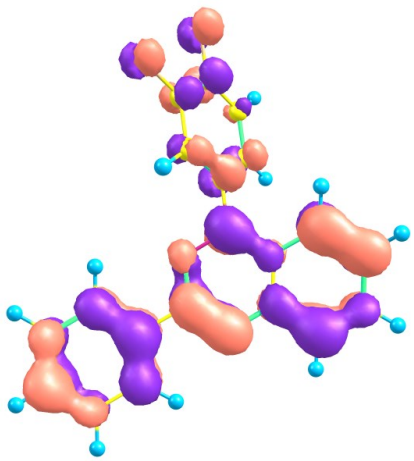
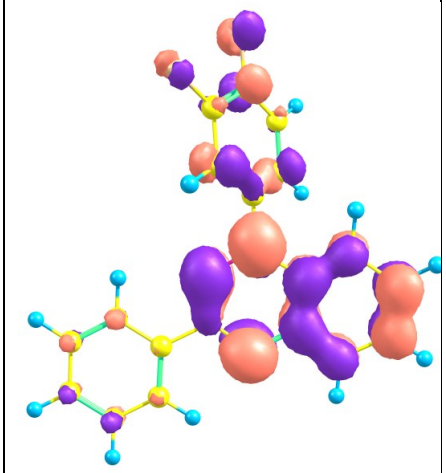
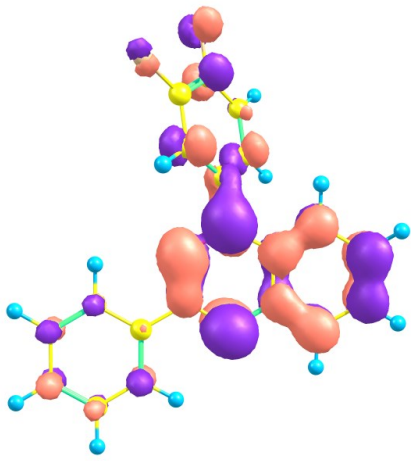
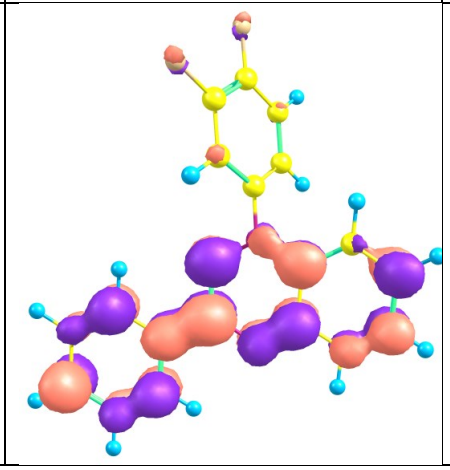
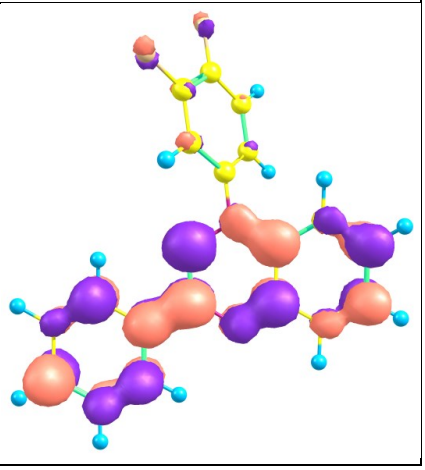


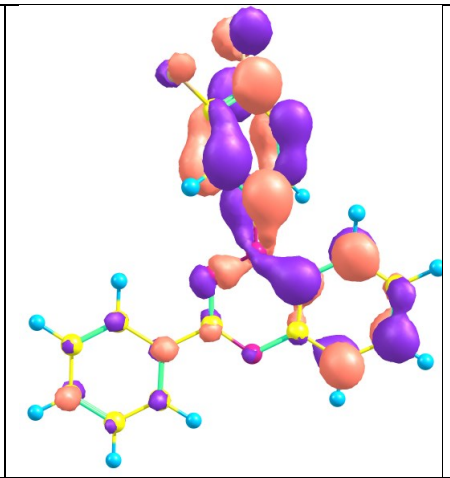
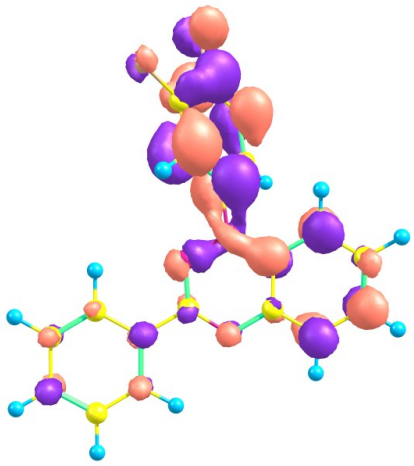
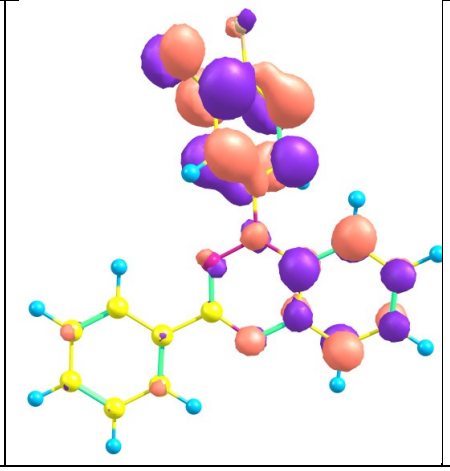
Figure S6. The experimental electronic absorption spectrum of an acetonitrile solution of radical **1b** (10^{-4} M) recorded at room temperature [the inset shows enlarged spectra of **1b**].

Quantum-chemical calculations

Table S1. A series of higher occupied and lower unoccupied MOs of α and β type and their energies for radical **1a**.

α type molecular orbitals (MOs)		β type molecular orbitals (MOs)	
numbers, occupation, energies		numbers, occupation, energies	
MO-78 Occ. E= -7.42 eV		MO-78 Occ. E= -7.30 eV	
MO-79 Occ. E= -7.38 eV		MO-79 Occ. E= -7.23 eV	
MO-80 Occ. E= -7.15 eV		MO-80 Occ. E= -7.10 eV	

MO-81 Occ. E= -7.06 eV		MO-81 Occ. E= -6.95 eV	
MO-82 Occ. E= -6.60 eV		MO-82 Occ. E= -6.33 eV	
MO-83 Occ. E= -4.86 eV		MO-83 Unocc. E= -2.87 eV	
MO-84 Unocc. E= -1.71 eV		MO-84 Unocc. E= -1.57 eV	

MO-85 Unocc. E= -1.04 eV		MO-85 Unocc. E= -0.96 eV	
MO-86 Unocc. E= -0.93 eV		Unocc. E= -0.87 eV