Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Photo-controllable Third-Order Nonlinear Optical (NLO) Switch based on Rhodamine B Salicylaldehyde Hydrazone metal Complex

Qi Feng,[1] Yuanyuan Li,[2] Guang Shi,[3] Lili Wang,[1] Wenjing Zhang,[1] Kai Li,*[,1] Hongwei Hou*[,1] and Yinglin Song*[,3]

1 College of Chemistry and Molecular Engineering, Zhengzhou University, Henan 450001, P. R. China

2 School of Chemistry and Chemical Engineering, Henan University of Technology, Henan 450001, P. R. China

3 Department of Applied Physics, Harbin Institute of Technology, Harbin 150001, P.R. China

*Correspondence and requests for materials should be addressed to K. L. (likai@zzu.edu.cn), H. W. H. (houhongw@zzu.edu.cn) or (ylsong@hit.edu.cn.).

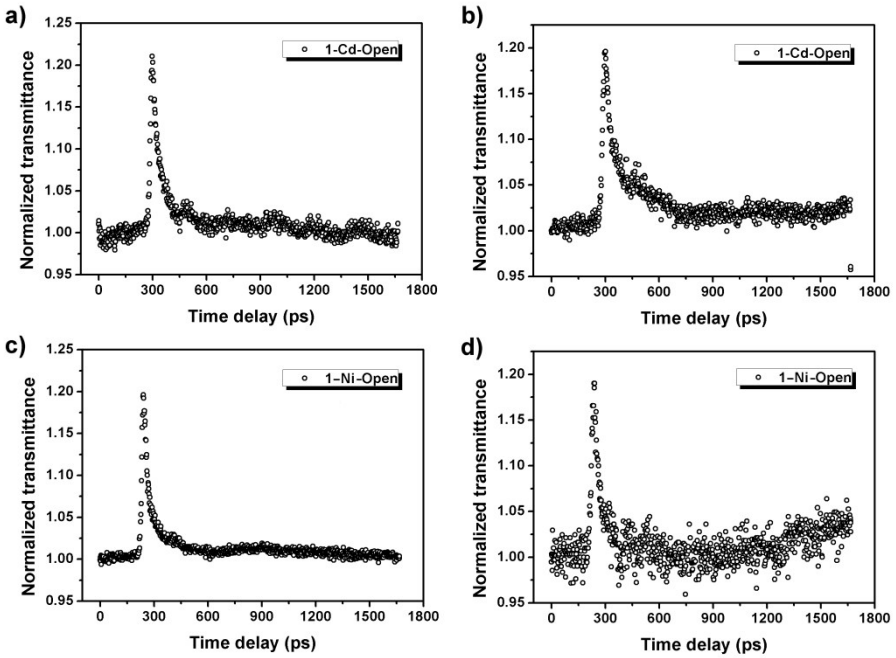

Figure S1. a), c) Open aperture and b), d) close aperture PO-pump-probe results of **1-Cd-Open** and **1-Ni-Open**. Conditions: [**1-Cd**] = [**1-Ni**] = 5×10^{-5} mol/L in THF solution, 2 mm quartz cells.

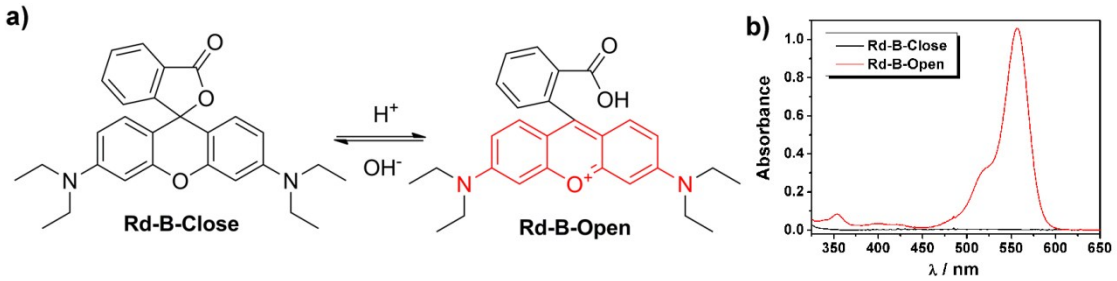

Figure S2. a) The known tautomerism of **Rd-B** in the presence of acid or base and b) the corresponding absorption spectra. Conditions: [**Rd-B**] = 5×10^{-5} mol/L in THF solution, 2 mm quartz cells.

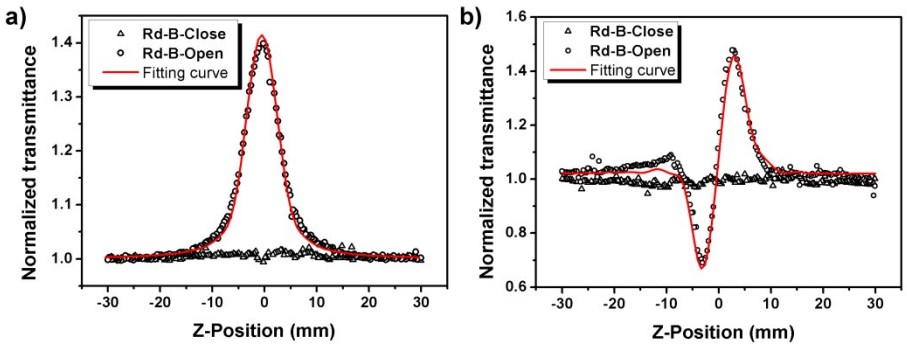

Figure S3. a) open-aperture and b) closed-aperture top-hat Z-scan results of **Rd-B-Close** and **Rd-B-Open**. Conditions: [**Rd-B**] = 5×10^{-5} mol/L in THF solution, 2 mm quartz cells.

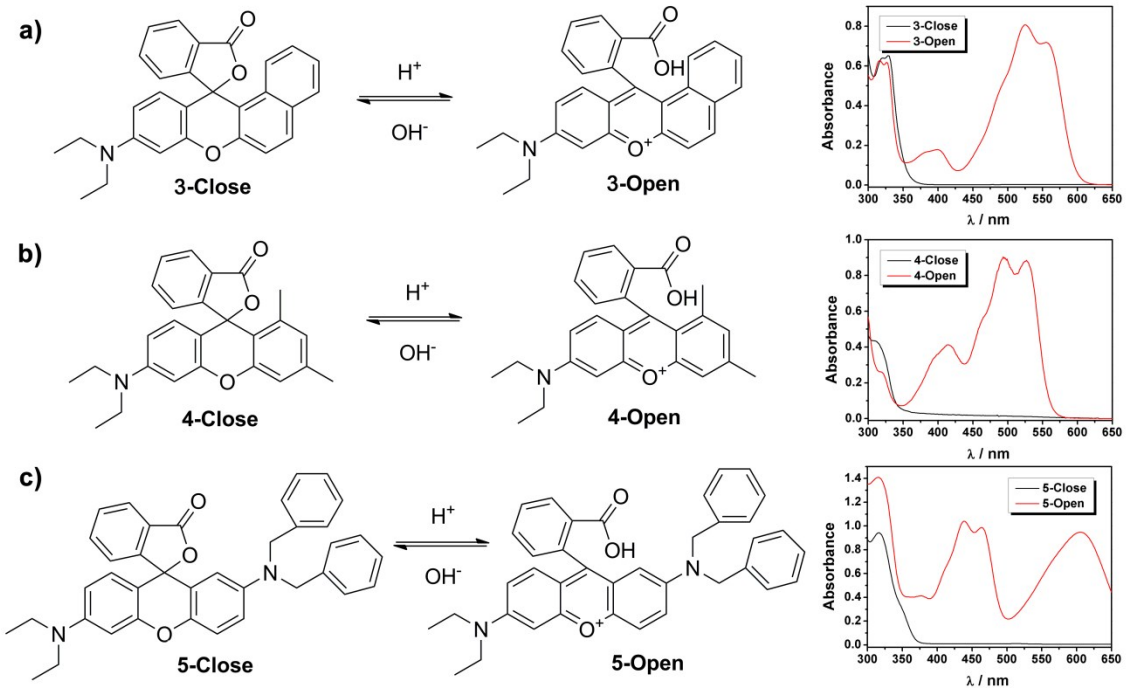

Figure S4. The known tautomerism and corresponding absorption spectra of **3-5** in the presence of acid or base. Conditions: [**3**] = 5×10^{-4} mol/L, [**4**] = 5×10^{-4} mol/L, [**5**] = 5×10^{-4} mol/L in THF solution, 2 mm quartz cells. The conjugations of **3-5** are adjusted by the addition of TFA and TEA.

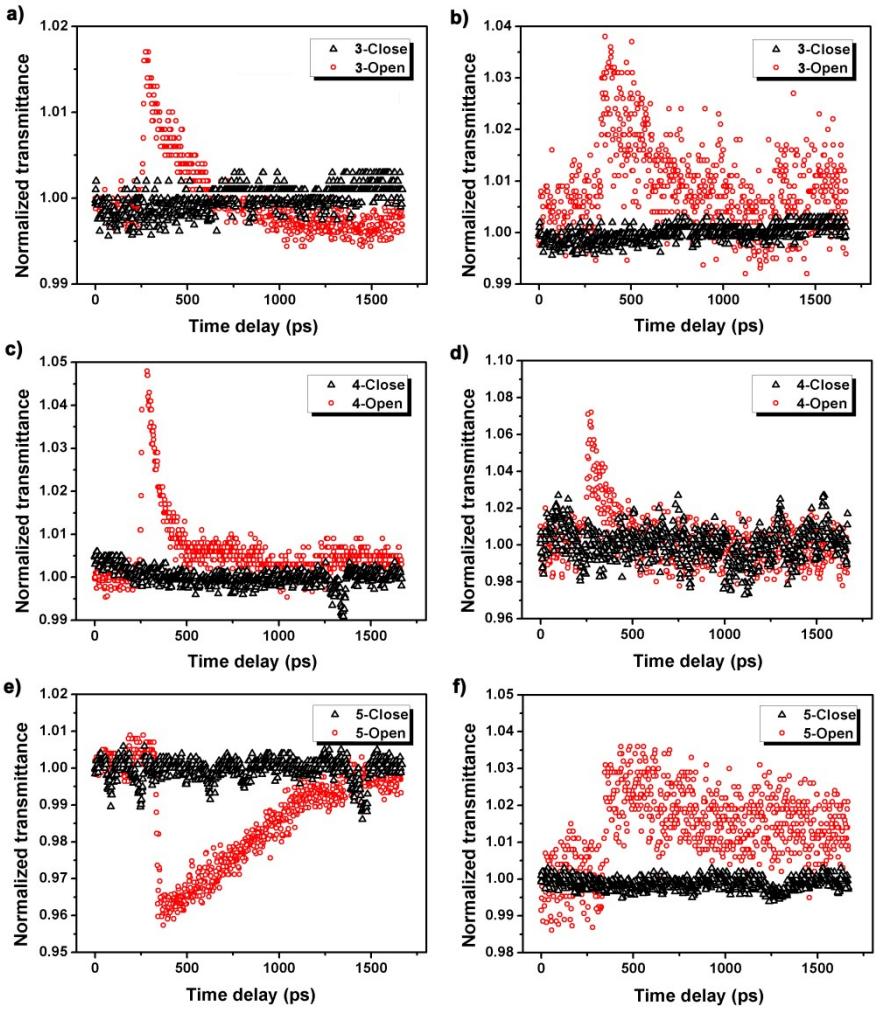

Figure S5. a), c) and e) open-aperture and b), d) and f) close-aperture PO-pump-probe results of **3-5**. Conditions: [**3**] = 5×10^{-4} mol/L, [**4**] = 5×10^{-4} mol/L, [**5**] = 5×10^{-4} mol/L in THF solution, 2 mm quartz cells. The conjugations of **3-5** are adjusted by the addition of TFA and TEA.

Table S1. Values of energies, oscillator strengths and dominant contributions of the respective molecular orbitals of **Rd-B-Open** for $S_0 \rightarrow S_n$.

State	Energy (ev)	Oscillator strength	Major MO → MO contributions (%)
S_1	3.0042	1.0011	HOMO → LUMO (100)
S_2	3.6957	0.0057	HOMO-2 → LUMO (20) HOMO-1 → LUMO (80)
S_3	4.3915	0.2010	HOMO-2 → LUMO (69) HOMO-1 → LUMO (20) HOMO → LUMO+2 (8) HOMO → LUMO+4 (3)
S_4	4.5199	0.0027	HOMO-4 → LUMO (3) HOMO-3 → LUMO (97)
S_5	4.7084	0.0011	HOMO-5 → LUMO (65) HOMO-4 → LUMO (22) HOMO-1 → LUMO+2 (5) HOMO → LUMO+5 (8)
S_6	4.7888	0.0585	HOMO-2 → LUMO (3) HOMO → LUMO+1 (97)

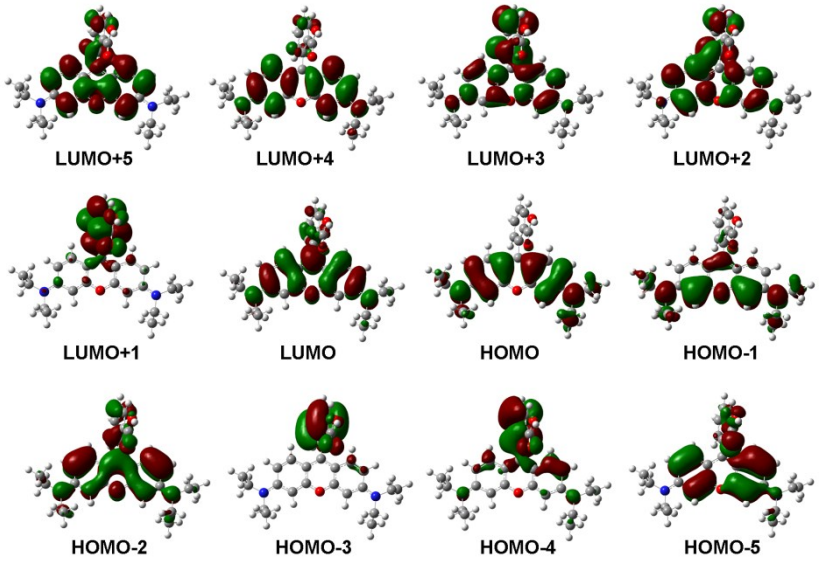

Figure S6. Calculated orbital energy diagram of **Rd-B-Open**.

Table S2. Values of energies, oscillator strengths and dominant contributions of the respective molecular orbitals of **1-Zn-Open** for $S_0 \rightarrow S_n$.

State	Energy (ev)	Oscillator strength	Major MO → MO contributions (%)
S_1	2.3705	0.0141	HOMO → LUMO (100)
S_2	2.9062	0.9184	HOMO → LUMO+1 (94) HOMO → LUMO+2 (6)
S_3	2.9859	0.1189	HOMO-7 → LUMO (32) HOMO-3 → LUMO (63) HOMO-2 → LUMO (5)
S_4	3.3840	0.0250	HOMO-7 → LUMO (3) HOMO-1 → LUMO (91) HOMO-1 → LUMO+1 (6)
S_5	3.6346	0.0171	HOMO-2 → LUMO (3) HOMO-2 → LUMO+1 (17) HOMO-1 → LUMO (5) HOMO-1 → LUMO+1 (70) HOMO-1 → LUMO+2 (5)
S_6	3.6957	0.1314	HOMO-9 → LUMO (18) HOMO-7 → LUMO (12) HOMO-2 → LUMO (12) HOMO → LUMO+1 (4) HOMO → LUMO+2 (51) HOMO → LUMO+3 (3)

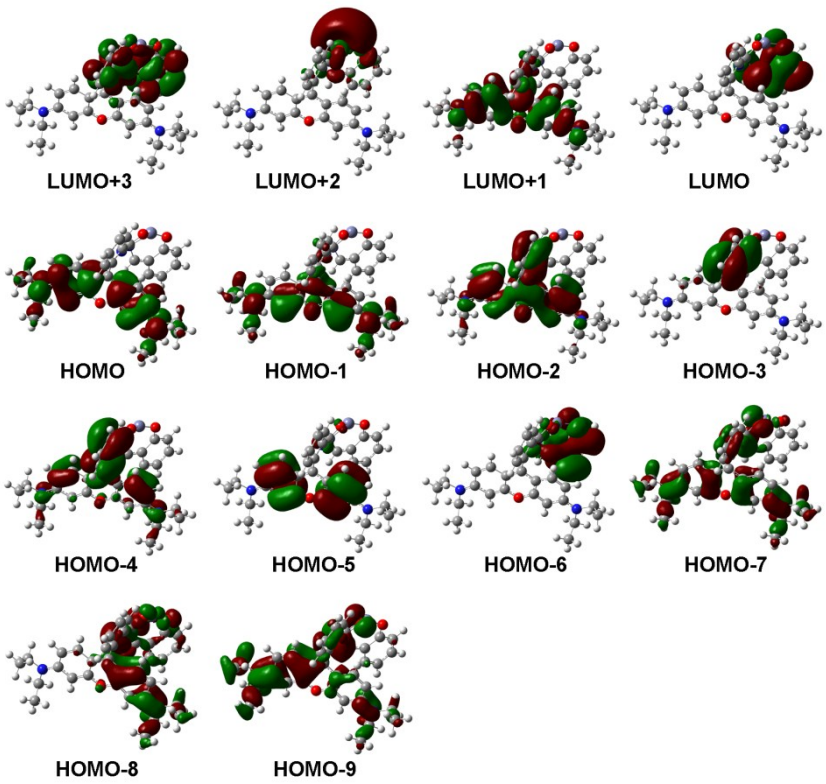

Figure S7. Calculated orbital energy diagram of **1-Zn-Open**.

Table S3. The influence of different wavelength light to the color change of **1-Zn**.[a]

Wavelength/nm	365	400	425	450	475	500	550	600	650
Color change of **1-Zn**	Yes	Yes	Yes	Yes	No	No	No	No	No

[a] Light of different wavelengths are produced by a CEL-HXF300 xenon light source with different optical filters.