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Photochromism and fluorescence modulation of pyrazolone derivatives in the solid state

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Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{26}H_{19}N_5F_6SO \cdot CH_3CH_2OH$
Formula weight	609.59
Temperature	293(2) *K*
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P2(1)/c*
Unit cell dimensions	*a* =8.2512(3) Å α = 90.00º *b*=30.1101(10) Å β=102.2120(10) º *c*=11.6340(5) Å γ=90.00 º
Volume	2825.00(18) Å^3
Z	4
Calculated density	1.433 mg/m^3
Absorption coefficient	1.90 mm^{-1}
F(000)	1256
Crystal size	0.54 × 0.39 × 0.15 mm
Theta range for data collection	3.08–25.50º
Limiting indices	$-9 \le h \le 9$, $-36 \le k \le 36$, $-14 \le l \le 14$
Reflections collected / unique	23076 / 5230 [R_{int} = 0.0370]
Absorption correction	Empirical
Max. and min. transmission	0.922 and 0.968
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5230 / 5 / 392
Goodness-of-fit on F^2	1.080
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0716, wR_2 = 0.1338
R indices (all data)	R_1 = 0.1092, wR_2 = 0.1559
Extinction coefficient	0.0066(5)
Largest diff. peak and hole	0.595 and -0.499 e Å^{-3}

Table S2. Selected Bond Lengths (Å) and Bond Angles (º) of B

S–C(23)	1.675(4)	N(3)–C(16)	1.306(4)
O–C(7)	1.256(4)	N(3)–N(4)	1.377(4)
N(1)–N(2)	1.385(4)	N(4)–C(23)	1.369(5)
N(1)–C(7)	1.391(4)	N(5)–C(23)	1.315(5)
N(1)–C(6)	1.418(4)	N(5)–C(24)	1.458(5)
N(2)–C(9)	1.349(4)		
N(2)-N(1)-C(7)	108.6(3)	N(2)-C(9)-C(8)	109.4(3)
N(2)-N(1)-C(6)	121.2(3)	N(2)-C(9)-C(10)	119.5(3)
C(7)-N(1)-C(6)	127.6(3)	N(5)-C(18)-N(4)	116.7(3)
C(9)-N(2)-N(1)	108.8(3)	N(5)-C(18)-S	124.6(3)
N(1)-C(7)-C(8)	106.6(3)	N(4)-C(18)-S	118.7(3)