

Table S1. Excitation energies and oscillator strengths:

Excited State 1:	7.004-A	0.5648 eV	2195.17 nm	f=0.0000	<S**2>=12.012
Excited State 2:	7.004-A	0.5656 eV	2191.95 nm	f=0.0001	<S**2>=12.012
Excited State 3:	7.004-A	1.0073 eV	1230.89 nm	f=0.0000	<S**2>=12.013
Excited State 4:	7.004-A	1.0126 eV	1224.39 nm	f=0.0001	<S**2>=12.013
Excited State 5:	7.003-A	1.1632 eV	1065.89 nm	f=0.0000	<S**2>=12.012
Excited State 6:	7.003-A	1.1645 eV	1064.66 nm	f=0.0001	<S**2>=12.012
Excited State 7:	7.005-A	1.5699 eV	789.74 nm	f=0.0000	<S**2>=12.016
Excited State 8:	7.005-A	1.5703 eV	789.55 nm	f=0.0001	<S**2>=12.016
Excited State 9:	7.004-A	1.8356 eV	675.44 nm	f=0.0000	<S**2>=12.014
Excited State 10:	7.004-A	1.8451 eV	671.96 nm	f=0.0002	<S**2>=12.014
Excited State 11:	7.004-A	2.1177 eV	585.46 nm	f=0.0000	<S**2>=12.015
Excited State 12:	7.004-A	2.1409 eV	579.11 nm	f=0.0033	<S**2>=12.014
Excited State 13:	7.054-A	3.6703 eV	337.81 nm	f=0.0000	<S**2>=12.188
Excited State 14:	7.053-A	3.6709 eV	337.75 nm	f=0.0001	<S**2>=12.186
Excited State 15:	7.074-A	3.7033 eV	334.80 nm	f=0.0754	<S**2>=12.259
Excited State 16:	7.073-A	3.7044 eV	334.70 nm	f=0.0001	<S**2>=12.256
Excited State 17:	7.047-A	3.7197 eV	333.32 nm	f=0.0010	<S**2>=12.164
Excited State 18:	7.045-A	3.7248 eV	332.86 nm	f=0.0000	<S**2>=12.160
Excited State 19:	7.050-A	3.8985 eV	318.03 nm	f=0.0023	<S**2>=12.177
Excited State 20:	7.047-A	3.8993 eV	317.97 nm	f=0.0000	<S**2>=12.166
Excited State 21:	7.448-A	3.9902 eV	310.72 nm	f=0.0043	<S**2>=13.617
Excited State 22:	7.452-A	3.9923 eV	310.56 nm	f=0.0000	<S**2>=13.634
Excited State 23:	7.485-A	4.0340 eV	307.35 nm	f=0.0036	<S**2>=13.755
Excited State 24:	7.493-A	4.0346 eV	307.30 nm	f=0.0000	<S**2>=13.788

Excited State 25: 7.062-A 4.1696 eV 297.36 nm f=0.0000 <S**2>=12.217
Excited State 26: 7.059-A 4.1706 eV 297.28 nm f=0.0023 <S**2>=12.206
Excited State 27: 7.088-A 4.1784 eV 296.73 nm f=0.0000 <S**2>=12.311
Excited State 28: 7.091-A 4.1866 eV 296.14 nm f=0.0344 <S2>=12.320**
Excited State 29: 7.065-A 4.2360 eV 292.69 nm f=0.0269 <S2>=12.229**
Excited State 30: 7.113-A 4.2384 eV 292.53 nm f=0.0000 <S**2>=12.398
Excited State 31: 7.140-A 4.2470 eV 291.94 nm f=0.0000 <S**2>=12.495
Excited State 32: 7.207-A 4.2671 eV 290.56 nm f=0.0052 <S**2>=12.735
Excited State 33: 7.097-A 4.3371 eV 285.87 nm f=0.0030 <S**2>=12.344
Excited State 34: 7.063-A 4.3472 eV 285.20 nm f=0.0000 <S**2>=12.220
Excited State 35: 7.267-A 4.3697 eV 283.74 nm f=0.0000 <S**2>=12.952
Excited State 36: 7.156-A 4.3904 eV 282.40 nm f=0.0000 <S**2>=12.551
Excited State 37: 7.146-A 4.3905 eV 282.39 nm f=0.0000 <S**2>=12.515
Excited State 38: 7.226-A 4.3926 eV 282.26 nm f=0.0007 <S**2>=12.803
Excited State 39: 7.053-A 4.4525 eV 278.46 nm f=0.0001 <S**2>=12.186
Excited State 40: 7.066-A 4.4527 eV 278.45 nm f=0.0174 <S**2>=12.231

Table S2. Crystallographic data of **1**.

Empirical formula	$C_{50}H_{78}O_4N_{10}S_2Co_2$
Formula weight	1065.20
Temperature	293(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
a , Å	10.562(4)
b , Å	14.568(6)
c , Å	17.808(7)
β , deg	98.219(8)
Volume, Å ³	2711.9(19)
Z	2
D_{calc} (mg m ⁻³)	1.304
μ (Mo $K\alpha$) (mm ⁻¹)	0.740
F(000)	1132
Total reflections	28323
Unique reflections (R_{int})	4622 ($R_{\text{int}} = 0.1010$)
Observed reflections [$F_o > 4\sigma(F_o)$]	3192
R indices [$F_o > 4\sigma(F_o)$] ^b R_1 , wR_2	0.0431, 0.0889
Goodness-of-fit on F^{2a}	1.004
Largest diff. Peak and hole, $e.\text{Å}^{-3}$	0.262, -0.281

^aGoodness-of-fit $S = [\sum w(F_o^2 - F_c^2)^2 / (n-p)]^{1/2}$, where n is the number of reflections and p the number of parameters. ^b $R_1 = \sum \|F_o\| - \|F_c\| / \sum \|F_o\|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$