Supporting Information

Luminescence Tunable Europium and Samarium Complexes: Reversible On/Off Switching and White-Light Emission

Jing Chen, [a,b,c] Ziyu Xie, [a,b,c] Lingyi Meng, [a,c,e] Ziying Hu, [a,c,d] Xiaofei Kuang, [a,c] Yiming Xie[b] and Can-Zhong Lu [a,b,c] *

[a] CAS Key Laboratory of Design and Assembly of Functional Nanostructures, and Fujian Provincial Key Laboratory of Nanomaterials, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P.R. China

[b] Fujian Key Laboratory of Photoelectric Functional Materials (Huaqiao University), Xiamen, Fujian 361021, P.R. China

[c] Xiamen Institute of Rare-earth Materials, Haixi Institutes, Chinese Academy of Sciences, Xiamen 361021, P.R. China

[d] College of Chemistry, New Campus, Fuzhou University, Fuzhou, 350116, P.R. China

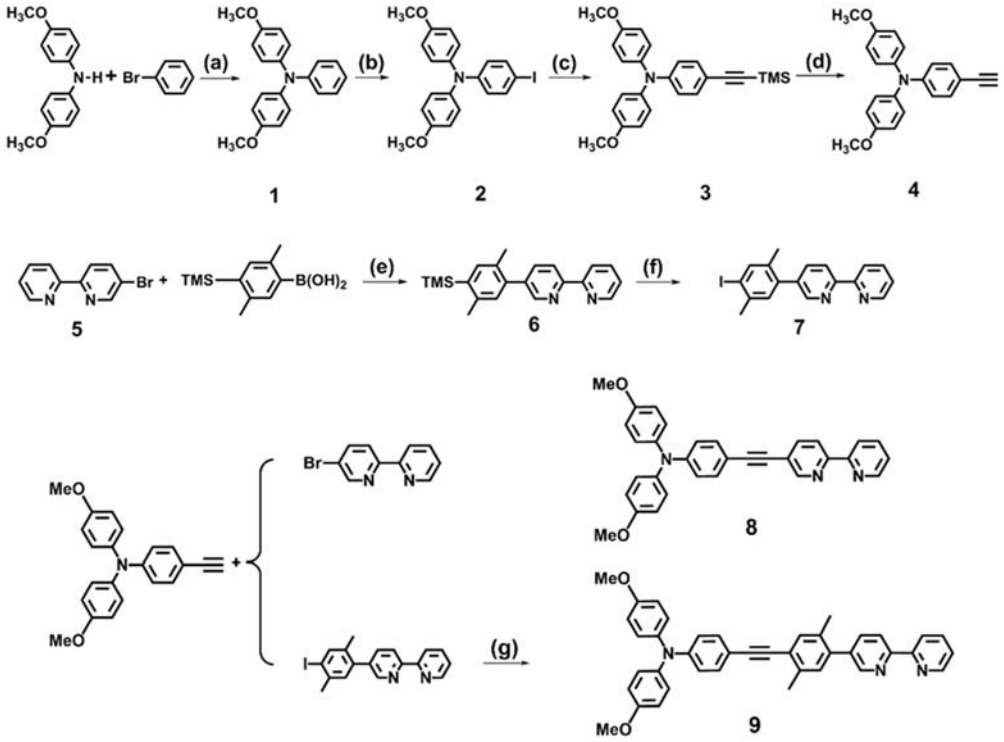
[e] Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Xiamen, P.R. China

Corresponding Author: Can-Zhong Lu

Email: czlu@fjirsm.ac.cn

Table of Contents

1. Synthesis and product characterization data



Scheme S1. Synthesis routes for the ligands $\mathbf{L_1}$ (8) and $\mathbf{L_2}$ (9). (a) $P(^tBu)_3H^+BF_4^-$, $Pd(dba)_2$, ^{t}BuOK, toluene; (b) NIS, DMF; (c) TMS-C≡C-H, CuI, $Pd(PPh_3)_2Cl_2$, Et_3N, THF; (d) KOH, MeOH, CH_2Cl_2; (e) Na_2CO_3, $Pd(PPh_3)_4$, THF, H_2O; (f) ICl, CH_3CN, CH_2Cl_2; (g) $Pd(PPh_3)_4$, CuI, THF, $^iPr_2NH$.

Full synthetic details:

Organic compounds **1**, **2**, **3** and **4** in Scheme S1 were synthesized following the published paper.[1]

N,N-bis(4-methoxyphenyl)-phenylaniline (**1**). 4,4'-dimethoxydiphenylamine (4.58 g, 20 mmol), bromobenzene (2.1 ml, 20 mmol), tri-t-butylphosphonium tetrafluoroborate (232 mg, 0.8 mmol), ^{t}BuOK (3.34 g, 30 mmol), and bis(dibenzylideneacetone)palladium (464 mg, 0.8 mmol) were added into dry toluene (200 ml). Under an inert atmosphere, the reaction mixture was stirred at 80 °C for 24 hour. And then, distilled water was added to quench the reaction and the mixture was extracted with CH_2Cl_2. The organic phases was dried with anhydrous Na_2SO_4, and the solvent was evaporated resulting in an oily compounds. The pure compound was separated by chromatography on silica gel, using a mixture of CH_2Cl_2 and cyclohexane (1:2, v: v) as the eluent. The product was obtained as a white solid (5.5 g, 90 %). ^{1}H NMR ($CDCl_3$,

400 MHz) δ = 7.25-7.10 (m, 2 H), 7.13-7.09 (m, 4 H), 7.03-7.00 (m, 2 H), 6.94-6.86 (m, 5 H), 3.83 (s, 6 H). ESI-MS (m/z): 305.3 (M^+). Elemental analysis: Anal. Calc. for $C_{20}H_{19}NO_2$ (%): C, 78.66; H, 6.27; N, 4.59. Found: C, 78.70; H, 6.25; N, 4.50.

4-iodo-*N,N*-bis(4-methoxyphenyl)aniline (**2**).[2] Molecule **1** (1.95 g, 6.4 mmol) and *N*-iodosuccinimide (1.5 g, 6.5 mmol) were added in 10 ml DMF and stirred for 3 hours at room temperature. Then, aqueous $NaHCO_3$ solution was added to quench the reaction. After extracting the compounds with CH_2Cl_2, the combined organic phases were dried over anhydrous Na_2SO_4. Yellow solid products were obtained by removing solvents under reduced pressure (2.1 g, 76 %). ^{1}H NMR ($CDCl_3$, 400 MHz) δ= 7.42-7.40 (m, 2 H), 7.04-7.01 (m, 4 H), 6.84-6.78 (m, 4 H), 6.69-6.67 (m, 2H), 3.79 (s, 6 H). ESI-MS (m/z): 432.1 ($M+H^+$). Elemental analysis: Anal. Calc. for $C_{20}H_{18}INO_2$ (%): C, 55.70; H, 4.21; N, 3.25. Found: C, 55.58; H, 4.18; N, 3.28.

N,N-bis(4-methoxyphenyl)-N-(4-trimethylsilylethynylphenyl)amine (**3**). To a flask with molecule **2** (1.6 g, 3.7mmol), CuI (70 mg, 10 mol-%), Pd $(PPh_3)_2Cl_2$ (130 mg, 5 mol-%), triethylamine (20 ml), THF (40 ml) and trimethylsilylacetylene (0.55 ml, 3.8 mmol) were added. After de-oxygenating with three freeze-pump-thaw cycles, the reaction mixture was stirred at 60 °C for 24 hours, and then the solvents were removed on rotary evaporator. Pure yellow solids (1.34 g, 90 %) were obtained by column chromatography on silica gel with a eluent of CH_2Cl_2/cyclohexane (1:2, v: v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ= 7.25-7.23 (m, 2 H), 7.06-7.02 (m, 4 H), 6.86-6.77 (m, 6 H), 3.80 (s, 6 H), 0.23 (s, 9 H). ESI-MS (m/z): 401.2 (M^+). Elemental analysis: Anal. Calc. for $C_{25}H_{27}NO_2Si$ (%): C, 74.77; H, 6.78; N, 3.49. Found: C, 74.69; H, 6.82; N, 3.51.

N,N-bis(4-methoxyphenyl)-N-(4-ethynylphenyl)amine (**4**). Molecule **3** (1.34 g, 3.34 mmol) and KOH (0.19 g, 3.4 mmol) were dissolved in a mixture of methanol (20 ml) and CH_2Cl_2 (20 ml), under N_2, and the mixture was stirred at room temperature for 2 hours. After removing the solvents, the crude product was purified by a silica gel column with a eluent of 1:1 (v: v) CH_2Cl_2 and cyclohexane. A brownish solid products was obtained (0.91 g, 81 %). ^{1}H NMR (Acetone-*d6*, 400 MHz) = 7.59-7.86 (m, 2 H), 7.72-7.68 (m, 4 H), 7.56-7.52 (m, 4 H), 7.38-

7.36 (m, 2H), 4.41 (s, 6 H), 4.06 (s, 1 H). ESI-MS (m/z): 329.2 (M^+). Elemental analysis: Anal. Calc. for $C_{22}H_{19}NO_2$ (%): C, 80.22; H, 5.81; N, 4.25. Found: C, 80.31; H, 5.87; N, 4.22.

5-Bromo-2,2'-bipyridine (**5**). Following a published protocol, [3] bromo-2-iodopyridine (1.44 g, 5 mmol) and $pd(pph_3)_4$ (116 mg, 0.10 mmol) were dissolved in 15 ml dry THF and the solution was de-oxygenated. And then, a 0.5 M 2-pyridylzinc bromide in THF solution (15 ml, 7.5 mmol) was added into the above solvent drop by drop. After stirring at room for 24 hours, saturated Na_2CO_3 aqueous solution was added to dissolve the precipitate. Extract the product with Et_2O, and the combined organic phases were dried over anhydrous $NaSO_4$, and the solvents were evaporated. The crude products were purified on silica gel column. The eluent was pentane/ Et_2O/Et_3N mixture solution with ratio of 200:100:3 (v: v: v). This afforded the white pure solid products (1.15g, 89%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ[ppm] 8.71 (dd, J= 2.4, 0.6 Hz, 1H), 8.66(ddd, J = 4.8, 1.9, 0.9Hz, 1H), 8.36 (td, J = 8.0, 1.0 Hz, 1H), 8.31 (dd, J = 8.5, 0.7Hz, 1H), 7.95-7.90 (m, 1H), 7.80 (td, J = 7.8, 1.8 Hz, 1H), 7.31 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H). ESI-MS (m/z): 235.1($M+H^+$). Elemental analysis: Anal. Calc. for $C_{10}H_7BrN_2$ (%): C, 51.09; H, 3.00; N, 11.92. Found: C, 51.03; H, 2.95; N, 11.97.

Compound **6**. Following to the paper.[4] To a flask with a de-oxygenated mixture solvents of 20 ml (THF/H_2O=1:1, v: v), 5-Bromo-2,2'-bipyridine (**5**) (1.0 g, 4.25 mmol), 4-(trimethylsilyl)phenylboronic acid (1.04 g, 4.68 mmol), Na_2CO_3 (1.35 g, 12.8 mmol) and $Pd(PPh_3)_4$ (246 mg, 0.21 mmol) were added and the reaction mixture was refluxed for 2 days. After cooling down to room temperature, extracted the products with CH_2Cl_2, and the combined organic phase was dried over Na_2SO_4. Evaporated the solvents and the crude solid products were purified on silica gel column with the eluent of a 2:1 (v: v) mixture of pentane and Et_2O. This afford the pure product as a white solid (1.2 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ[ppm] 8.71–8.68 (m, 2H), 8.46-8.42 (m, 2H), 7.86-7.78 (m, 2H), 7.40 (s, 1H), 7.34-7.31 (m, 1H), 7.10 (s, 1H), 2.48 (s, 3H), 2.31 (s, 3H), 0.37 (s, 9H). ESI-MS (m/z): 332.1. Elemental analysis: Anal. Calc. for $C_{21}H_{24}N_2Si$ (%): C, 75.85; H, 7.28; N, 8.42. Found: C, 75.82; H, 7.24; N, 8.49.

Compound **7**. [5] Compound **6** (500 mg, 1.51 mmol) was dissolved in a mixture solvents of 25

ml acetonitrile and 10 ml dichloromethane, after bubbling the solution with nitrogen for a few minutes and keeping it at 0 ºC, ICl (748 mg, 4.58mmol) was added. And the reaction mixture was permitted to be warmed to room temperature with stirring overnight. Then, an aqueous solution of Na_2SO_4 (100 ml) was added and extracted the products with dichloromethane. The organic phase was dried over Na_2SO_4, filtered and the crude product was collected by evaporating the solvents. A yellow solid product was purified by silica gel column chromatographies using a mixture of pentane/ether (2:1) as the eluate (210 mg, 36%). ^{1}H NMR (400 MHz, $CDCl_3$): δ[ppm] 8.73 (d, J = 4.8Hz, 1H), 8.65 (d, J = 2.1Hz, 1H), 8.51 (dd, J = 12.3, 8.1 Hz , 2H), 7.90 (t, J = 7.8Hz, 1H), 7.81–7.79 (m, 2H), 7.38 (dd, J = 6.5, 5.0 Hz, 1H), 7.13 (s, 1H), 2.45 (s, 3H), 2.24 (s, 3H). ESI-MS (m/z):386.1. Elemental analysis: Anal. Calc. for $C_{18}H_{15}IN_2$ (%): C, 55.98; H, 3.91; N, 7.25. Found: C, 55.95; H, 3.97; N, 7.18.

Molecule **8 (L_1)**. Molecule **4** (164 mg, 0.5 mmol), 5-bromo-2,2'-bipyridine **5** (116 mg, 0.5 mmol), CuI (9.5 mg, 0.05mmol), and $Pd(PPh_3)_4$ (28.8 mg, 0.025 mmol) were added to de-oxygenated mixture of THF (12 ml) and diisopropylamine (3 ml). The reaction mixture was heated to 80 °C for 24 hours. After solvent removal, chromategraphy on a silica gel column with an eluent comprised of a 100:100:2 (v: v: v) mixture of CH_2Cl_2, cyclohexane, and triethylamine gave an orange solid (0.20 g, 83 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ[ppm] 8.77 (d, J = 1.5 Hz, 1H), 8.68 (d, J = 4.0 Hz, 1H), 8.39 (dd, J = 11.3, 8.1 Hz, 2H), 7.89 (dd, J = 8.3, 2.1 Hz, 1H), 7.85-7.79 (m, 1H), 7.37-7.28(m, 3H), 7.12-7.06 (m, 4H), 6.86 (d, J = 8.9, 6H), 3.83(s, 6H). ESI-HRMS (m/z): 506.1839 $[M+Na]^+$. IR (KBr) υ_{max}: 3045 (w), 3005 (w), 2950 (w), 2930 (w), 2904 (w), 2832 (w), 2203 (w), 2170 (w), 1600 (w), 1585 (w), 1569 (w), 1542 (w), 1504 (s), 1456 (m), 1436 (w), 1337 (m), 1287 (m), 1236 (s), 1179 (w), 1163 (w), 1139 (m), 1102 (w), 1028 (s), 822 (s), 795 (s), 766 (w), 746 (s), 716 (w), 694 (w), 649 (w), 618 (w), 576 (s), 534 (w). Elemental analysis: Anal. Calc. for $C_{32}H_{25}N_3O_2$ (%): C, 79.48; H, 5.21; N, 8.69. Found: C, 79.46; H, 5.23; N, 8.71.

Molecule **9 (L_2)**. Molecule **4** (131 mg, 0.4 mmol), molecule **7** (144 mg, 0.375 mmol), CuI (7.6 mg, 0.04 mmol), and Pd $(PPh_3)_4$ (23 mg, 0.02 mmol) were added to deoxygenated mixture of THF (15 ml) and diisopropylamine (5 ml). The reaction mixture was heated to 80 °C for 24 hours. After solvent removal, chromatography on a silica gel column with an eluent comprised

of a 100:100:2 (v: v: v) mixture of CH_2Cl_2, cyclohexane, and triethylamine gave an yellow products (202mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$): δ [ppm] 8.70 (d, J = 4.7 Hz, 1H), 8.66 (d, J = 2.1 Hz, 1H), 8.44(dd, J = 8.0, 5.4 Hz, 2H), 7.86-7.76 (m, 2H), 7.42 (s,1H), 7.32 (td, J = 6.0, 5.3, 1.2 Hz, 3H), 7.13 (s, 1H), 7.09-7.04 (m, 4H), 6.85 (td, J = 6.8, 2.0 Hz, 6H), 3.80 (s, 6H), 2.50 (s, 3H), 2.27 (s, 3H). ESI-HRMS (m/z): 610.2460 $[M+Na]^+$. IR (KBr) υ_{max}: 3035 (w), 2996 (w), 2952 (w), 2931 (w), 2915 (w), 2833 (w), 2200 (w), 1599 (w), 1586 (w), 1570 (w), 1549 (w), 1506 (s), 1459 (m), 1439 (w), 1322 (m), 1287 (m), 1243 (s), 1178 (w), 1164 (w), 1107 (w),1038 (m), 829 (m), 798 (m), 762 (w), 749 (w), 723 (w), 655 (w), 639 (w),622 (w), 581 (w), 530 (w). Elemental analysis: Anal. Calc. for $C_{40}H_{33}N_3O_2$ (%): C, 81.75; H, 5.66; N, 7.15. Found: C, 81.70; H, 5.69; N, 7.08.

Ln(tta)$_3$(H$_2$O)$_2$ (Ln = Eu, Sm) were synthesized according to the literature.[6] And they are characterized by FR-IR, ^{1}H NMR and elemental analysis.

Eu(tta)$_3$(H$_2$O)$_2$: ^{1}H NMR (500 MHz, DMSO-*d6*) δ [ppm] 7.46 (s, 3H), 6.50 (s, 3H), 6.32 (s, 3H), 3.70(s, 3H). Elemental analysis: Anal. Calc. for $C_{24}H_{16}EuF_9O_8S_3$ (%): C, 33.85; H, 1.89; S, 11.30. Found: C, 33.96; H, 1.90; S, 11.68. IR (KBr) υ_{max}: 3650 (w), 3612 (w), 3184 (w), 3115 (w), 3092 (w), 1599 (s), 1579 (s), 1536 (s), 1508 (m), 1460 (m), 1408 (s), 1355 (s), 1300 (s), 1284 (s), 1248 (m), 1231 (m), 1185 (s), 1135 (s), 1081(w), 1060 (m), 1037(w), 1011 (w), 929 (s), 860 (s), 787 (s), 767 (w), 752 (w), 714 (s), 693 (w), 681 (w), 642 (s), 604 (w), 578 (s), 562 (w).

Sm(tta)$_3$(H$_2$O)$_2$: ^{1}H NMR (400 MHz, DMSO-*d6*) δ [ppm] 8.15 (s, 3H), 7.87(s, 3H), 7.34 (s, 3H), 7.22 (s, 3H). Elemental analysis: Anal. Calc. for $C_{24}H_{16}SmF_9O_8S_3$ (%): C, 33.92; H, 1.90; S, 11.32. Found: C, 33.46; H, 1.96; S, 11.44. IR (KBr) υ_{max}: 3650 (w), 3612 (w), 3184 (w), 3115 (w), 3092 (w), 1601 (s), 1582 (s), 1539 (s), 1508 (m), 1459 (w), 1445 (w), 1435 (w), 1408 (s), 1356 (s), 1300 (s), 1293 (s), 1288 (s), 1248 (m), 1231 (w), 1188 (s), 1132 (s), 1080(w), 1061 (m), 1037(w), 1011 (w), 929 (s), 861 (s), 788 (s), 767 (w), 750 (w), 736 (m), 724 (w), 712 (s), 694 (w), 682 (w), 642 (s), 604 (w), 580 (s), 537 (w).

Complex 1 ($C_{56}H_{37}F_9N_3O_8S_3Eu$). **L$_1$** (48 mg, 0.1mmol), Eu(tta)$_3$ • 2H$_2$O (86 mg, 0.1 mmol) were dissolved in a mixture solvents of DCM (20 ml) and ethanol (20 ml), the solution was

bubbled with N_2 for several minutes and refluxed overnight. The orange crude products were obtained by removing the solvents. And pure compound were separated by recrystallizing the solids in small amount of DCM and ethanol (71 mg, yield of 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 14.33(s, 1H), 12.74(s, 1H), 10.00-9.84(m, 3H), 9.42 (s, 1H), 8.27(s, 1H), 7.74(s, 3H), 6.50(s, 3H),7.21(d, J = 8.7 Hz, 4H), 7.05(d, J = 8.3 Hz, 2H), 6.96-6.94(m, 6H), 6.18(s, 3H), 3.87(s, 6H), 3.13(s, 3H). EI-HRMS (m/z): 1322.0706 $[M+Na]^+$. Elemental analysis: Anal. Calc.: C, 51.78; H, 2.87; N, 3.23. Found: C, 51.98; H, 2.91; N, 3.29. IR (KBr) υ_{max}: 3088 (w), 3043 (w), 2998 (w), 2951 (w), 2929 (w), 2902 (w), 2833 (w), 2208 (w), 2178 (w), 1622 (w), 1595 (s), 1536 (s), 1502 (s), 1462, 1411(s), 1354 (w), 1305 (s), 1282 (s), 1238 (s), 1183 (s), 1133 (s), 1063, 1035, 1006, 932 (m), 860 (w), 829 (m), 783 (s), 769 (w), 740 (w), 718 (m), 683 (w), 661 (w), 640 (m), 604 (w), 580 (m), 539 (w).

Complex 2 (**C_{56} H_{37} F_9 N_3 O_8 S_3 Sm**) was synthesized following the same procedure for the preparation of complex **1** with 69 % yield, replacing $Eu(tta)_3 \cdot 2H_2O$ with $Sm(tta)_3 \cdot 2H_2O$. ^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.49 (s, 1H), 8.28 (s, 1H), 7.82 (d, J = 3.1 Hz, 3H), 7.70-7.64 (m, 3H), 7.46(d, J = 4.7 Hz, 3H), 7.39 (s, 3H), 7.27-7.25 (m, 3H), 7.22 (s, 1H), 7.12-7.06 (m, 7H), 6.89-6.84 (m, 6H), 3.83 (s, 6H). EI-HRMS (m/z): 1299.0869 $[M+H]^+$. Elemental analysis: Anal. Calc.: C, 51.84; H, 2.87; N, 3.24; S, 7.41. Found: C, 51.34; H, 3.05; N, 3.26; S, 7.52. IR (KBr) υ_{max}: 3110 (w), 3077 (w), 3045 (w), 3000 (w), 2964 (w), 2932 (w), 2917 (w), 2837 (w), 2217 (w), 2187 (w), 1620 (w), 1594 (s), 1536 (m), 1504 (s), 1463 (w), 1406 (m), 1357 (w), 1304 (s), 1283 (s), 1242 (s), 1226 (s), 1179 (s), 1132 (s), 1085 (w), 1061 (w), 1034 (m), 933 (w), 861 (w), 827 (w), 787 (s), 765 (w), 746 (w), 719 (w), 693 (w), 681 (w), 659 (w), 638 (m), 604 (w), 579 (m).

Complex 3 (C_{64} H_{45} F_9 N_3 O_8 S_3 Eu). L_2 (130 mg, 0.22 mmol), $Eu(tta)_3 \cdot 2H_2O$ (188 mg, 0.22 mmol) were dissolved in a mixture solvents of DCM (10 ml) and ethanol (10 ml), the solution was bubbled with N_2 for several minutes and refluxed overnight. The orange crude products were obtained by removing the solvents. And pure compounds were separated by recrystallizing the solids in small amount of DCM and ethanol (200 mg, yield of 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 14.16-14.02 (m, 2H), 9.88(s, 1H), 9.65-9.49 (m, 3H), 8.60 (s, 1H), 8.02 (s, 1H), 7.75 (s, 3H), 7.45 (d, 3H), 7.13 (d, J = 7.9 Hz,3H), 7.00 (s, 2H), 6.95-6.88

(m, 5H), 6.55 (s, 3H), 6.31 (s, 3H), 3.83 (s, 6H), 3.16 (s, 3H), 2.88 (s, 3H) 2.64 (s, 3H). EI-HRMS (m/z): 1322.0706 $[M+Na]^+$. Elemental analysis: Anal. Calc.: C, 54.78; H, 3.23; N, 2.99. Found: C, 54.76; H, 3.29; N, 3.02. IR (KBr) υ_{max}: 3115 (w), 3090 (w), 3077 (w), 3042 (w), 2991 (w), 2959 (w), 2932 (w), 2908 (w), 2837 (w), 2197 (w), 2161 (w), 1594 (s), 1537 (m), 1467 (w), 1407 (s), 1356 (w), 1298 (s), 1235 (s), 1184 (s), 1132 (s), 1085 (w), 1061 (w), 1034 (m), 1009 (w), 964 (w), 933 (w), 890 (w), 860 (w), 823 (m), 788 (m), 765 (w), 747 (w), 718 (m), 683 (w), 660 (w), 642 (m), 607 (w), 579 (m), 533 (w).

2. Crystal data, data collection and structural refinement details.

Table S1. Crystal data, data collection and structural refinement details for $\mathbf{L_1}$, complexes **1** and **2**.

Compound	$\mathbf{L_1}$	**1**	**2**
Formula	$C_{32}H_{25}N_3O_2$	$C_{56}H_{37}F_9N_3O_8S_3Eu$	$C_{56}H_{37}F_9N_3O_8S_3Sm$
fw	483.55	1299.03	1297.43
Temperature/K	200(2)	200(2)	200(2)
Radiation	Mo Kα (λ =0.71073)	Mo Kα (λ =0.71073)	Mo Kα (λ =0.71073)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a /Å	11.3327(5)	9.7881(3)	9.7815(10)
b /Å	25.7208(11)	20.5676(6)	20.612(2)
c /Å	17.6708(8)	26.9306(8)	26.931(3)
ß	99.008(2)	97.813(1)	97.579(3)
volume ($Å^3$)	5087.3(4)	5371.3(3)	5382.3(10)
Z	8	4	4
D_c (g/cm^3)	1.263	1.606	1.601
F_{000}	2032	2600	2596
μ (mm^{-1})	0.08	1.374	1.297
crystal size (mm)	0.191×0.116×0.042	0.705×0.156×0.133	0.116×0.062×0.037
2θ range for data collection /°	4.66 to 54.82	4.22 to 74.11	4.64 to 56.06
Reflections collected	172870	399538	153721
Independent reflections	12164	27535	12907
Goodness-of-fit on F^2	1.035	1.046	1.095
R_{int}	0.080	0.0707	0.1573
R_1, wR_2 [I > 2σ(I)]	0.0640, 0.1650	0.0484, 0.1352	0.0839, 0.2087
R_1, wR_2 [all date]	0.1123, 0. 2009	0.0705, 0.1525	0.1313, 0.2421
Largest diff. peak/hole / e $Å^{-3}$	0.358/-0.317	2.937/-1.586	2.936/-2.379

3. Selected bond lengths and bond angles.

Table S2. Selected bond lengths and angles of $\mathbf{L_1}$, complexes **1** and **2**.

Compound	$\mathbf{L_1}$	**1**	**2**
Ln-N/Å		2.627(2), 2.598(2)	2.641(6), 2.613(6)
Ln-O/Å		2.377(2), 2.355(2) 2.3499(19), 2.361(2) 2.396(2), 2.361(2)	2.363(5), 2.363(6) 2.383(6), 2.372(5) 2.407(6), 2.372(5)
C≡C/Å	1.200(4), 1.197(3)	1.198(4)	1.193(12)
C-C≡C angles/°	174.9(3), 176.2(3) 176.5(3), 178.4(3)	176.0(3), 174.7(3)	176.4(9),174.3(10)
O-Ln-O angles/°		O7-Eu-O8, 71.47(7) O5-Eu-O6, 72.39(8) O3-Eu-O4, 70.78(7)	O7-Sm-O8, 71.37(19) O5-Sm-O6, 70.23(19) O3-Sm-O4, 72.1(2)
N-Ln-N angles/°		61.60(6)	61.29(19)

4. X-ray single crystal structure of complex 2.

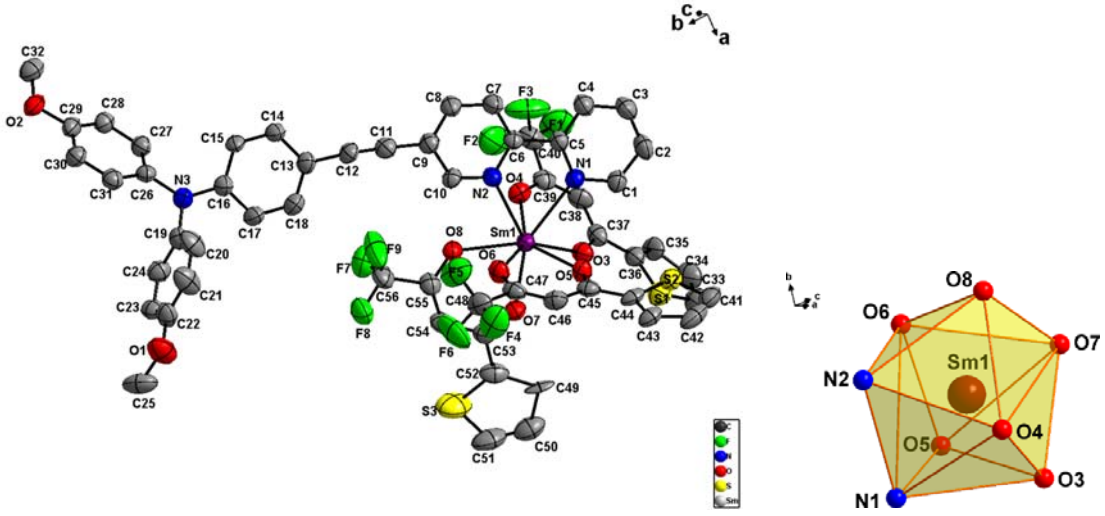


Figure S1. ORTEP of $Sm(tta)_3L_1$(**2**) (left) (Hydrogen atoms are omitted for clarity, thermal ellipsoids are shown at the 50% probability.); coordination polyhedron of the central Sm atom in **2** (right), coordinating N atoms from the $\mathbf{L_1}$ ligand, and O atoms from tta ligands.

5. Absorption and emission spectral data of ligands in different solvents.

Table S3. UV-vis absorption and emission spectra data of $\mathbf{L_1}$ in different solvents (the concentration is about 2×10^{-5} M).

Solvent	Abs. λ_{max} /nm (ε/$M^{-1}cm^{-1}$)	Em. λ_{max}/nm (λ_{ex}= ~380nm)	Stokes shift / cm^{-1}
CH_2Cl_2	298 (86643) , 384 (91596)	576	8681
CH_3Cl	299 (29812), 387 (30025)	547	7425
Toluene	299 (35044), 386 (35334)	473	4765
THF	297 (36802), 383(39045)	545	7693
DMF	297 (31916), 382 (33470)	440, 626	3451, 10135
DMSO	299 (31215), 385 (32844)	444, 632	3452, 10151
EAC	295 (34322), 379 (37278)	538	7798
C_2H_5OH	296 (7687), 384 (7825)	585	8948
CH_3OH	295 (9654), 382 (10005)	442, 603	3553, 9594
CH_3CN	294 (65295), 376 (75350)	434, 645	3555, 11091
Acetone	379 (38326)	602	9773

Table S4. UV-vis absorption and emission spectra data of $\mathbf{L_2}$ in different solvents (the concentration is about 2×10^{-5} M).

Solvent	Abs. λ_{max} /nm (ε/$M^{-1}cm^{-1}$)	Em. λ_{max}/nm (λ_{ex}= ~360nm)	Stokes shift/cm^{-1}
CH_2Cl_2	295 (39975), 366 (37630)	544	8940
CH_3Cl	296 (42348), 368 (41758)	497	7053
Toluene	296 (40805), 367 (38818)	445	4776
THF	294 (43948), 366 (42235)	510	7714
DMF	294 (35159), 365 (34794)	606	10895
DMSO	296 (37560), 367 (37110)	615	10987
EAC	292 (37953), 362 (38205)	497	7503
C_2H_5OH	293 (14968), 364 (13156)	509	7826
CH_3OH	293 (25807), 362 (24684)	514	8169
CH_3CN	292 (38894), 360 (39525)	620	11649
Acetone	361 (44664)	580	10459

6. DFT calculation results of ligands.

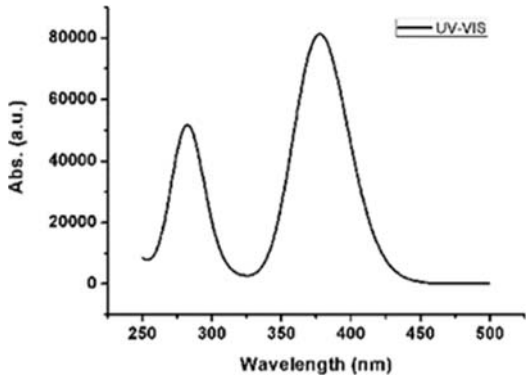


Figure S2. The calculated absorption spectra of ligand $\mathbf{L_1}$ by TD-DTF methodology with G09 program using the single crystal structure of $\mathbf{L_1}$ without optimization.

Table S5. The HOMO and LUMO energy levels of the ligand $\mathbf{L_1}$ and $\mathbf{L_2}$ with their band gaps, singlet and triplet energy levels calculated by DTF methodology with G09 program using their optimized structures.

Ligand	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)	Eg (eV)	S_1 (eV)	T_1 (eV)
$\mathbf{L_1}$	-5.98	-4.97	-1.86	-0.86	3.11	2.32	2.18
$\mathbf{L_2}$	-5.87	-4.90	-1.65	-1.15	3.25	2.47	2.25

7. Emission spectra of ligands in different solvents.

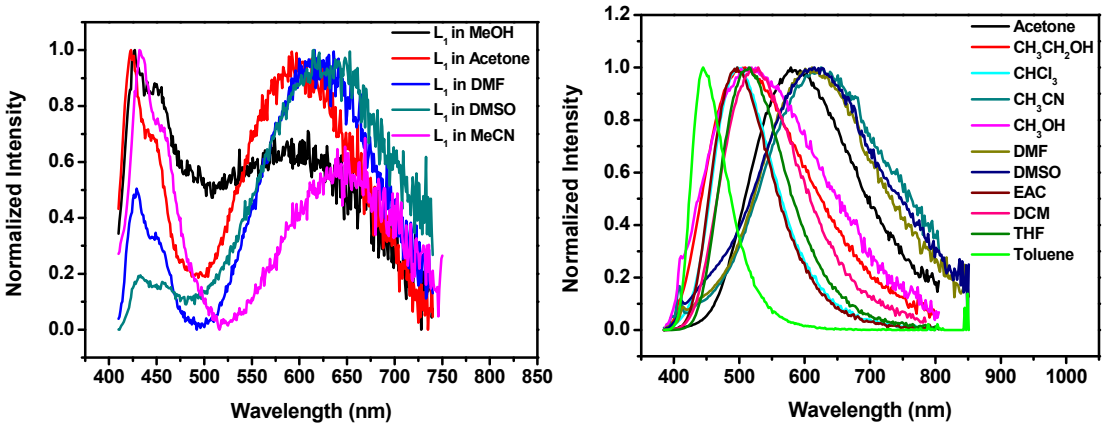


Figure S3. Emission spectra of $\mathbf{L_1}$ (left) and $\mathbf{L_2}$ (right) in different solvents (the concentration is about 2×10^{-5} M) at room temperature (λ_{ex} = ~ 380 nm for $\mathbf{L_1}$, λ_{ex} = ~ 360 nm for $\mathbf{L_2}$, taken from the maximum values from the corresponding absorption spectra in different solvents).

8. UV-vis absorption spectra of complex 2 in different solvents.

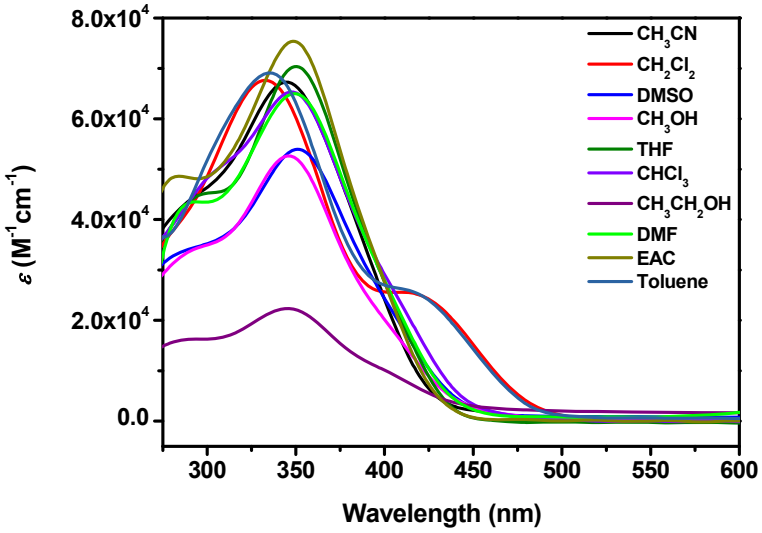


Figure S4. UV-vis absorption spectra of complex **2** in different solvents (the concentration is about 2×10^{-5} M).

9. Absorption spectra for 1 and 3 obtained by TD-DFT calculation.

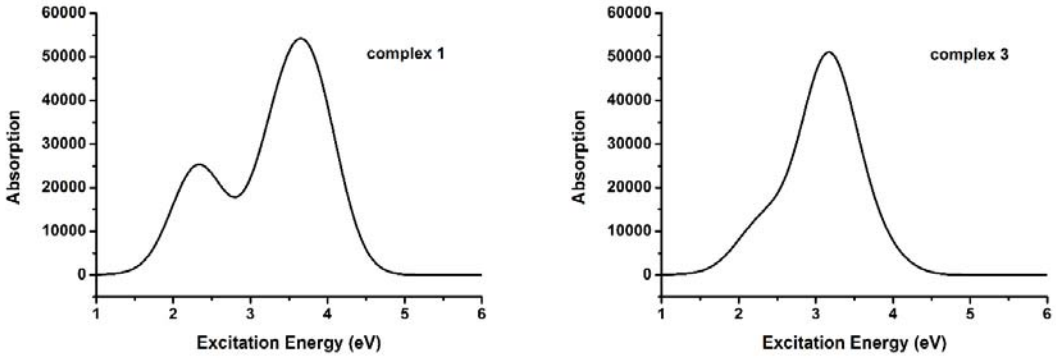


Figure S5. Absorption spectra of complexes **1** and **3** calculated by TD-DTF methodology with G09 program using their optimized structures.

10. Solid state PL properties of complexes 1, 2 and 3.

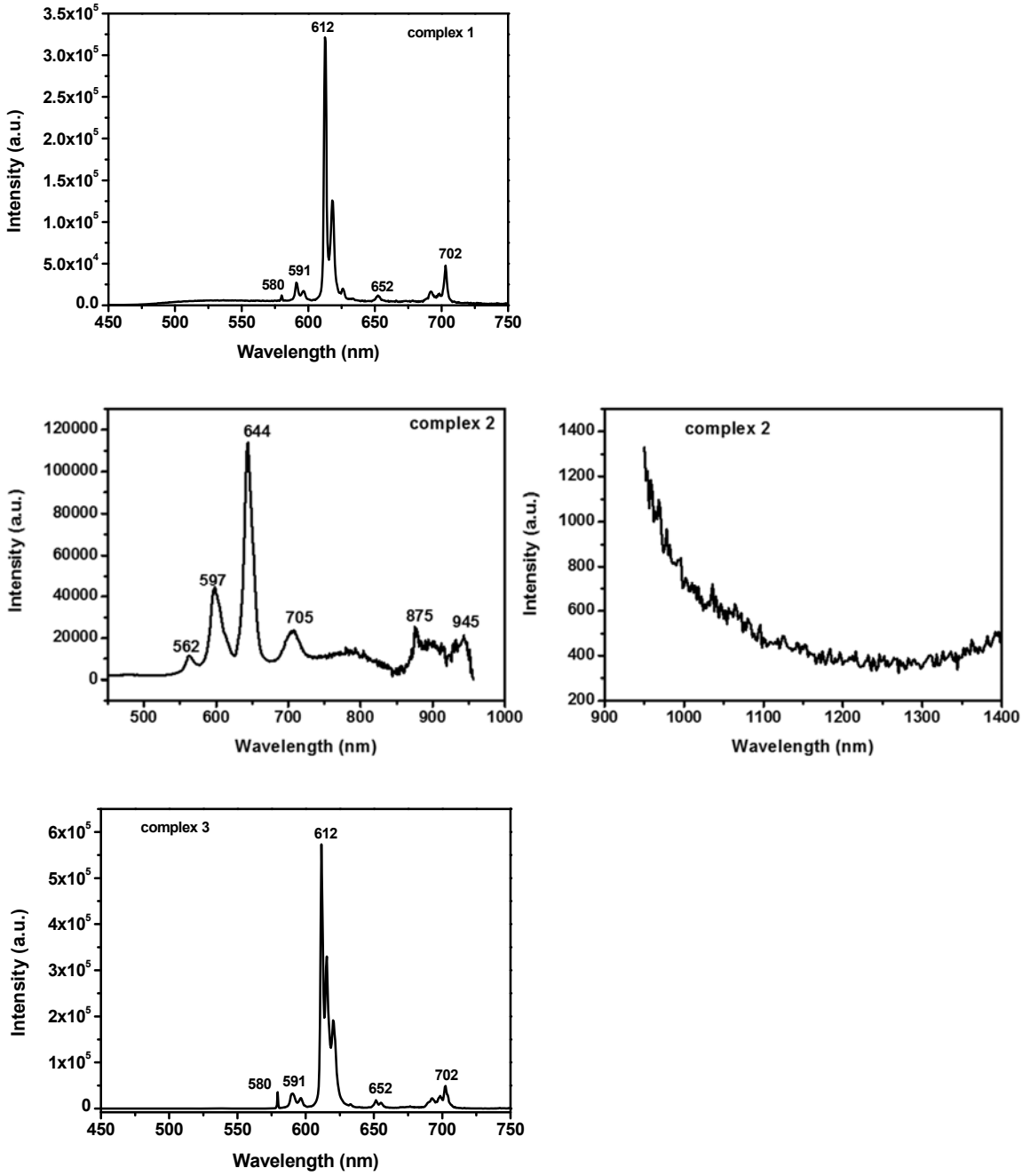


Figure S6. Emission spectra of complexes **1**, **2** and **3** in solid state at room temperature with excitation wavelength of 340 nm. For the emission spectra of complex **2**, the detector was changed for the range from 950 to 1400 nm.

11. Room temperature emission spectra of complex 2 in CH_3CN.

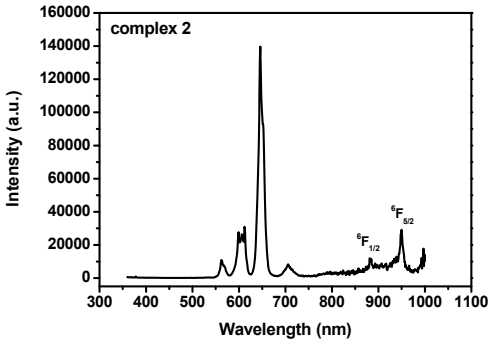


Figure S7. Emission spectra of complex **2** in CH_3CN at room temperature (λ_{ex} = 340 nm, the concentration is about 2×10^{-5} M).

12. Absorption and emission spectral data of complexes 1, 2 and 3 in different solvents.

Table S6. UV-vis absorption and emission spectral data of **1**, **2** and **3** in different solvents. The data belong to the emission of Eu^{3+} or Sm^{3+} are bold fonts. (λ_{ex} = ~ 340 nm, concentration of the samples are 2×10^{-5} M)

	1		**2**		**3**	
Solvents	**Abs. λ_{max}/nm ε/M^{-1}cm^{-1}**	**Em. λ_{max}/nm**	**Abs. λ_{max}/nm ε/M^{-1}cm^{-1}**	**Em. λ_{max}/nm**	**Abs. λ_{max}/nm ε/M^{-1}cm^{-1}**	**Em. λ_{max}/nm**
Acetone	341 (65255)	**588, 594, 612, 651, 702**	341 (70640)	**561, 598, 645, 705**	343 (90503)	**595, 612, 655, 702**
C_2H_5OH	294 (54118), 343 (75831)	**580, 592, 613, 650, 701**	291 (16292), 344 (22355)	434, **563, 598, 645, 705**	291 (22215), 344 (33096)	**579, 592, 614, 650, 702**
CH_3OH	295 (44610), 343 (66443)	**579, 589, 612, 651, 703**	344 (52717)	436, **564, 599, 645, 705**	292 (42177), 344 (70190)	**580, 590, 612, 650, 702**
DMF	297 (46460), 343 (72639)	**579, 591, 613, 652, 702**	297 (43599), 346 (65010)	437, **563, 598, 645, 705**	294 (49283), 346 (84608)	**580, 593, 612, 651, 702**
DMSO	300 (45360), 348 (71180)	**579, 592, 611, 650, 700**	301 (35433), 349 (53982)	439, **563, 597, 644, 702**	294 (50640), 350 (84815)	**579, 592, 612, 650, 701**
EAC	294 (49103), 343 (74762)	534, **579, 596, 612, 650, 702**	294 (48564), 348 (75250)	532, **598, 645**	292 (54797), 344 (89356)	493, **579, 592, 612, 650, 702**
THF	295 (50357), 348 (74372)	535, **579, 594, 613, 650, 702**	296 (45365), 348 (70285)	543, **598, 645**	294 (58572), 348 (93100)	505, **579, 589, 612, 651, 701**
CH_3CN	296 (48526), 341 (71671)	**579, 595, 612, 655, 701**	295 (25122), 340 (67254)	**560, 598, 645, 704**	292 (54001), 343 (86790)	**595, 612, 652, 702**
CH_2Cl_2	332 (66645), 412 (26053)	554, **580, 594, 612, 652, 702**	333 (67730), 408 (25553)	411, 427, 464, **565, 599, 645**	341 (93306)	530, **580, 591, 612, 651, 702**
$CHCl_3$	302 (49796), 342 (66067)	537, **579, 590, 613, 650, 703**	302 (48516), 344 (65344)	542, **645**	297 (57952), 343 (79860)	497, **580, 592, 612, 650, 702**
Toluene	334 (62962)	469, **580, 591, 612, 651, 702**	336 (69163), 405 (26173)	474, **645**	341 (81246)	445, **580, 591, 612, 652, 703**

13. PL decay curves of complexes 1, 2 and 3 in different solvents.

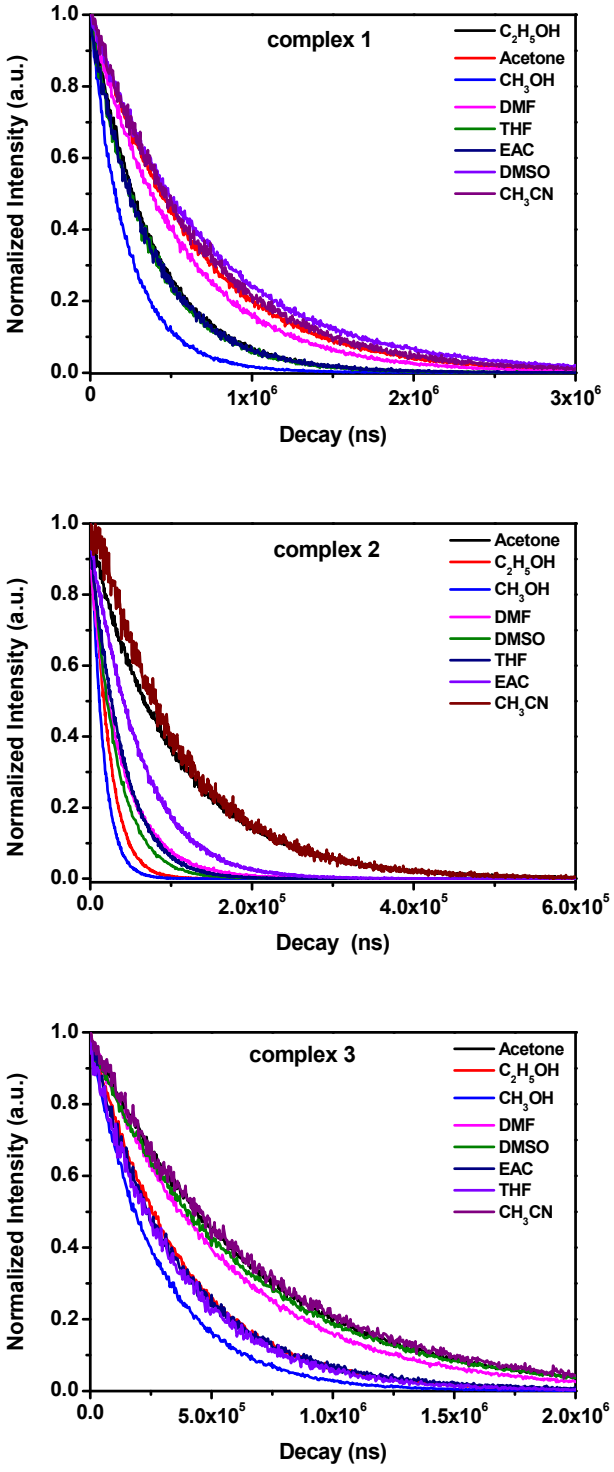


Figure S8. Luminescence decay curves of the complexes **1**, **2** and **3** in different solvents. (λ_{ex} = 340 nm, λ_{em} = 612 nm for **1** and **3**, and λ_{em} = 645 nm for **2**, the concentration of the solvents are all 2×10^{-5} M).

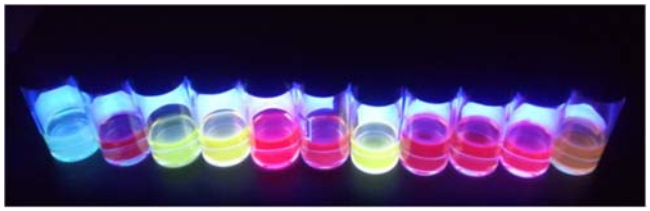
14. Lifetimes of complexes 1, 2 and 3 in different solvents.

Table S7. Summary of the emission lifetimes (τ_{obs}) of the complexes (λ_{ex}= 340 nm, λ_{em}= 612 nm for **1** and **3**, λ_{em}= 645 nm for **2**) in different solvents (concentration of the samples are 2×10^{-5} M).

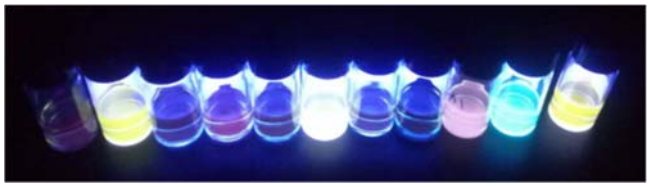
Solvents	τ_{obs} for **1**/μs	τ_{obs} for **2**/μs	τ_{obs} for **3**/μs
Acetone	620	102	630
C_2H_5OH	368	21	366
CH_3OH	232	16	279
DMF	546	38	548
DMSO	712	30	610
EAC	364	59	364
THF	357	38	355
CH_3CN	646	104	646

15. The Pictures of ligands L_1, L_2, complexes 1, 2 and 3 in dark irradiated with 365 nm UV lamp.

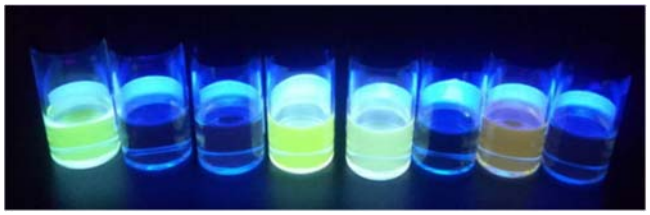
(a) **L_1** in EAC, CH_3CN, CH_3Cl, DMF, THF, Toluene, acetone, ethanol, DCM, DMSO and methanol (from left to right).



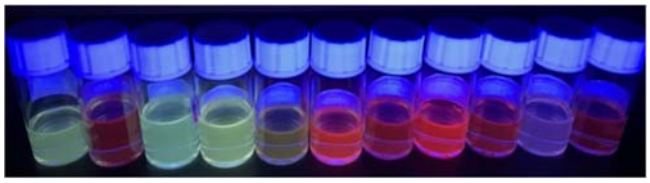
(b) **1** in toluene, methanol, EAC, THF, CH_3CN, DMF, CH_3Cl, DMSO, ethanol, acetone and DCM (from left to right).



(c) **2** in CH_3CN, CH_3Cl, DMF, acetone, ethanol, EAC, DMSO, methanol, DCM, Toluene, THF (from left to right).



(d) $\mathbf{L_2}$ in DCM, CH_3Cl, CH_3CN, methanol, ethanol, EAC, acetone, DMSO, DMF, THF, toluene (from left to right).



(e) **3** in CH_3Cl, DMSO, EAC, THF, DCM, acetone, DMF, CH_3CN, ethanol, toluene, and methanol (from left to right).

Figure S9. The pictures of $\mathbf{L_1}$ (a), **1** (b), **2** (c), $\mathbf{L_2}$ (d) and **3** (e) in different solvents irradiated by 365 nm UV lamp in dark.

16. CIE coordinates data of 1, 2 and 3 in different solvents.

Table S8. The CIE coordinates data of complex **1** in different solvents with concentration of 2×10^{-5} M.

Solvent	Excitation Wavelength (λ_{ex})	CIE coordinates			Emission Intensity
		x	y	T_c	
Acetone	340	0.347	0.331	4821	2.040E+005
CH_3CH_2OH	294	0.322	0.241	6639	3.367E+005
	343	0.338	0.341	5265	3.464E+005
	397	0.486	0.497	2963	1.324E+005
CH_3CN	270	0.554	0.445	2162	2.435E+005
	294	0.587	0.412	2367	3.188E+005
	340	0.387	0.415	4098	2.178E+005
	390	0.518	0.480	2538	1.784E+005
CH_3OH	294	0.543	0.456	2241	2.200E+005
	342	0.567	0.432	2143	2.000E+005
	394	0.570	0.429	2151	6.939E+004
$CHCl_3$	302	0.317	0.257	6951	2.413E+005
	344	0.322	0.356	5945	2.227E+005
	399	0.325	0.378	5800	3.487E+005
DCM	275	0.349	0.384	4963	8.561E+004
	333	0.417	0.394	3272	1.232E+005
	411	0.269	0.269	9043	1.812E+005
DMF	299	0.387	0.388	3898	1.002E+005
	345	0.374	0.323	3708	3.220E+005
	398	0.291	0.430	6855	8.757E+004
DMSO	298	0.305	0.342	6825	1.898E+005
	349	0.449	0.441	3092	2.097E+005
	397	0.313	0.487	6036	6.852E+004
EAC	294	0.301	0.219	15776	2.180E+005
	343	0.309	0.333	6681	2.30E+005
	398	0.290	0.339	7717	4.274E+005
THF	296	0.309	0.228	10004	2.599E+005
	348	0.311	0.308	6798	2.304E+005
	397	0.293	0.308	8098	3.423E+005
Toluene	334	0.359	0.379	4653	3.100E+005
	400	0.354	0.394	4848	2.502E+006

Table S9. The CIE coordinates data of complex **2** in different solvents with concentration of 2×10^{-5} M.

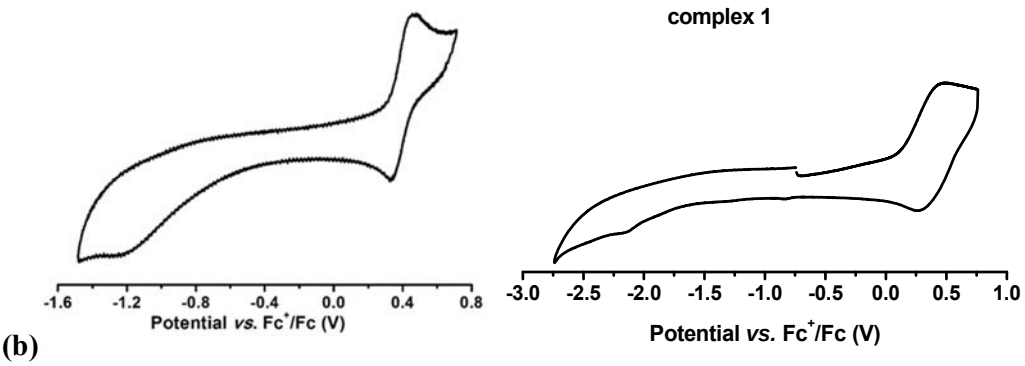
Solvent	Excitation Wavelength (λ_{ex})	CIE coordinates			Emission Intensity
		x	y	T_c	
Acetone	340	0.356	0.396	4798	6.466E+004
CH_3CH_2OH	290	0.384	0.450	4324	3.637E+004
	342	0.417	0.308	2343	3.554E+005
	395	0.376	0.392	4229	6.953E+004
CH_3CN	270	0.302	0.275	8229	2.279E+004
	294	0.390	0.391	3856	3.179E+004
	340	0.363	0.316	4052	6.601E+004
	390	0.425	0.321	2364	2.063E+004
	490	0.298	0.410	6703	1.750E+003
CH_3OH	294	0.186	0.031	2139	4.320E+003
	344	0.327	0.365	5744	3.403E+004
	396	0.306	0.289	7480	6078E+003
	398	0.370	0.383	4330	1.065E+005
$CHCl_3$	275	0.317	0.393	6070	7.032E+003
	300	0.304	0.275	7997	3.002E+004
	344	0.379	0.344	3780	1.128E+005
DCM	270	0.411	0.408	3522	3.982E+004
	334	0.341	0.300	4916	3.142E+004
	406	0.388	0.394	3930	7.302E+004
	426	0.336	0.331	5313	4.014E+004
DMF	296	0.412	0.426	3625	3.275E+004
	349	0.327	0.446	5700	3.383E+005
DMSO	297	0.367	0.284	3425	2.432E+004
	349	0.262	0.260	16298	2.456E+005
	400	0.454	0.352	2295	5.088E+004
EAC	294	0.349	0.402	5019	1.036E+005
	344	0.372	0.231	2145	2.470E+005
THF	296	0.358	0.412	4804	1.030E+005
	347	0.378	0.359	3931	1.193E+005
	396	0.361	0.391	4640	1.039E+005
Toluene	355	0.330	0.353	5590	3.729E+004
	404	0.351	0.370	4869	3.091E+004
	480	0.134	0.084	8814	2.302E+003

Table S10. The CIE coordinates data of complex **3** in different solvents with concentration of 2×10^{-5} M.

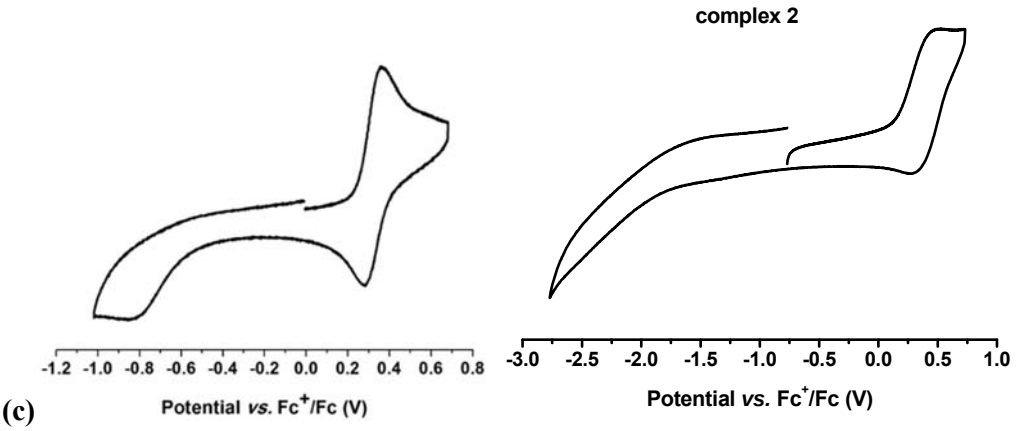
Solvent	Excitation Wavelength (λ_{ex})	CIE coordinates			Emission Intensity
		x	y	T_c	
Acetone	342	0.334	0.416	5491	3.663E+005
CH_3CH_2OH	292	0.524	0.474	2450	6.201E+004
	345	0.390	0.575	4627	2.908E+005
CH_3CN	292	0.334	0.284	5309	2.802E+005
	342	0.324	0.354	5870	4.975E+005
CH_3OH	293	0.358	0.381	4665	9.442E+004
	346	0.355	0.285	4034	1.147E+005
$CHCl_3$	299	0.295	0.367	7137	1.068E+005
	343	0.312	0.305	6749	4.339E+004
DCM	277	0.307	0.265	7977	2.489E+004
	341	0.343	0.367	5131	1.072E+005
DCM	277	0.307	0.265	7977	2.489E+004
	341	0.343	0.367	5130	1.072E+005
DMF	294	0.388	0.327	3297	2.031E+004
	347	0.358	0.412	4793	2.159E+005
DMSO	296	0.343	0.461	5306	7.345E+004
	351	0.332	0.265	5424	1.094E+005
EAC	293	0.384	0.342	3584	1.744E+005
	344	0.325	0.306	5881	4.549E+004
THF	293	0.372	0.326	3806	1.404E+005
	348	0.333	0.318	5465	4.276E+004
Toluene	284	0.344	0.375	5127	6.284E+004
	342	0.342	0.369	5158	2.444E+005

17. Electrochemistry study of complexes 1, 2 and 3.

(a)



(b)



(c)

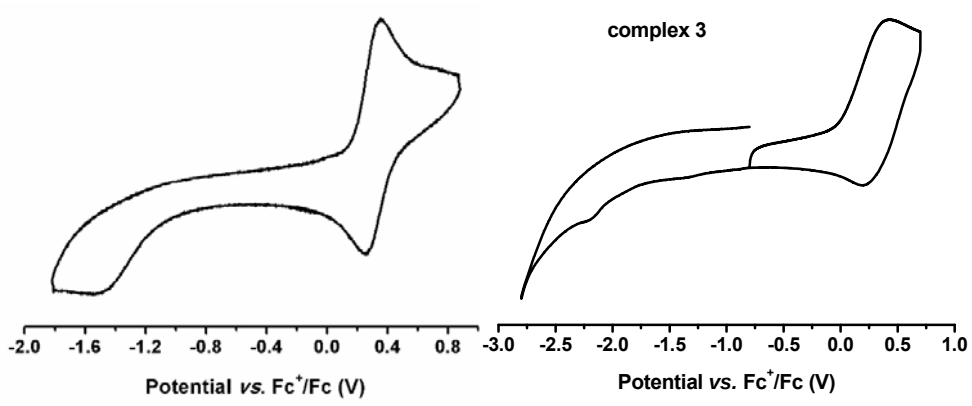


Figure S10. Cyclic voltammograms of complexes **1** (a), **2** (b) and **3** (c) in CH_3CN (0.1 mol•dm^{-3} Bu_4NPF_6, RT, v= 0.1 V • s^{-1}).

18. Absorption spectra for complexes 1, 2, 3 and their oxidized forms.

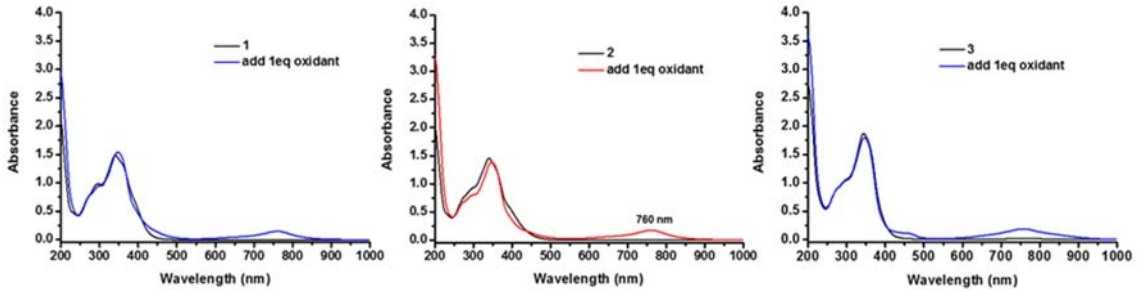


Figure S11. The UV-vis absorption spectra of complexes **1**, **2** and **3** in their neutral forms and radical cations (oxidized by 1 eq CAN) in CH_3CN solution.

19. PL decay curves of $Eu(tta)_3bpy$ and $Sm(tta)_3bpy$.

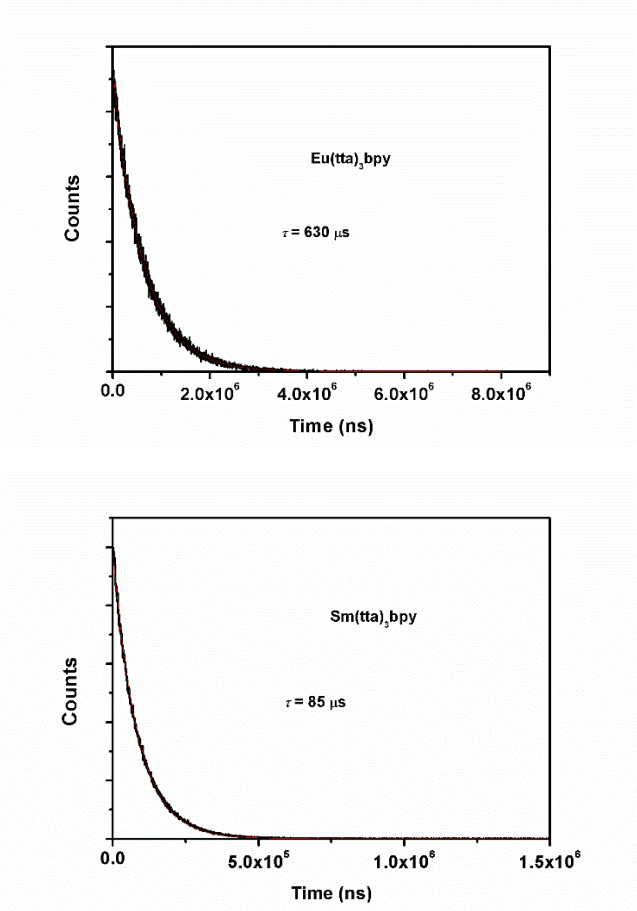


Figure S12. Emission decay curves for $Eu(tta)_3bpy$ and $Sm(tta)_3bpy$ in CH_3CN (λ_{ex} = 340 nm, the concentration is about 2×10^{-5} M).

20. The emission spectra of the Gd-complex in solid state at 77K.

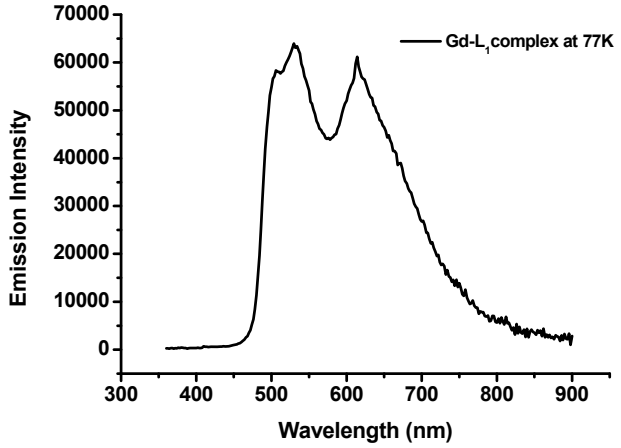


Figure S13. The emission spectra of the GdL_1 complex in solid state at 77K.

The triplet energy of **L_1** was determined from the emission spectra of GdL_1 complex at 77K, the low wavelength peak at 506 nm (19762 cm^{-1}) was used to calculate.

21. Intersystem crossing and energy transfer processes in 2 and $2^{\bullet+}$.

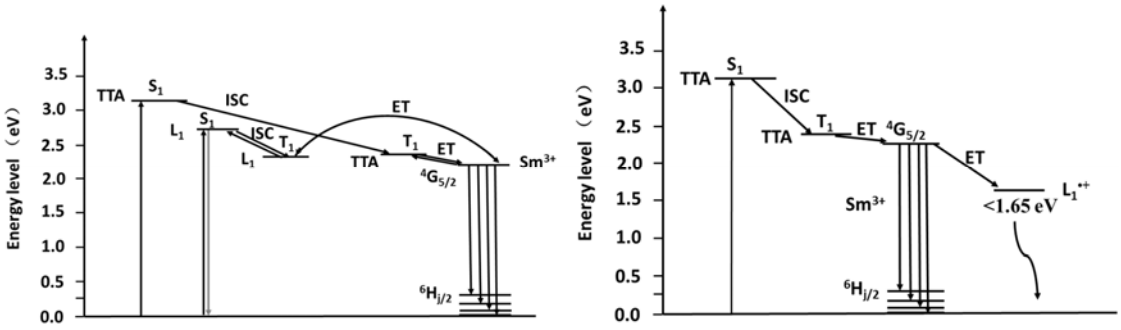


Figure S14. Intersystem crossing (ISC) and energy transfer (ET) processes in **2** (left) and **$2^{\bullet+}$** (right). We only focus on the emission of Sm^{3+} in visible region (NIR emission of Sm^{3+} are not discussed here).

22. Cartesian coordinates of all the optimized geometries.

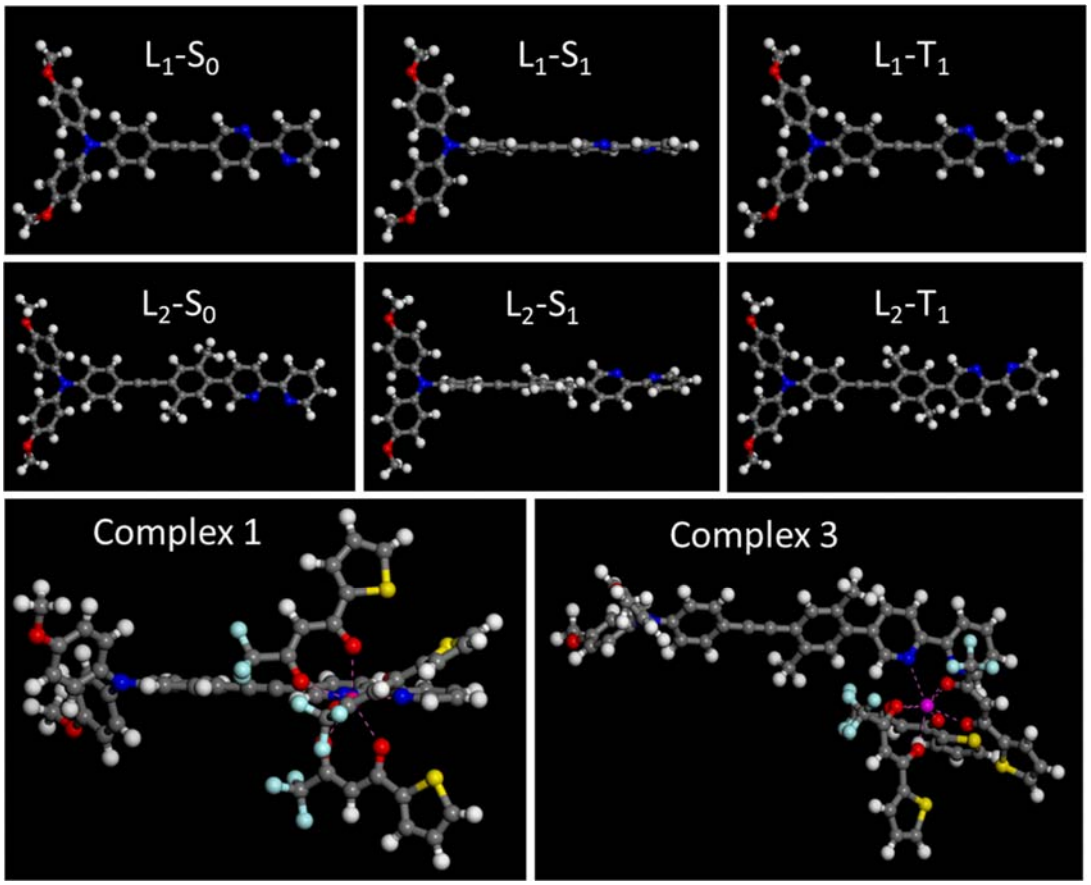


Figure S15. The optimized structures of **L1** (S_0, S_1 and T_1) , L_2 (S_0, S_1 and T_1), complexes 1(S_0) and 2 (S_0). (color code: blue for N, grey for C, red for O, white for H, and light blue for F; view along Z axis).

TITLE Cartesian coordinates of **L1** (S_0)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	10.911	-1.025	-0.477	C
HETATM	2	H	0	11.422	-1.893	-0.888	H
HETATM	3	C	0	11.639	0.048	0.033	C
HETATM	4	H	0	12.723	0.029	0.026	H
HETATM	5	C	0	10.933	1.133	0.546	C
HETATM	6	H	0	11.457	1.991	0.954	H
HETATM	7	C	0	9.545	1.102	0.529	C
HETATM	8	H	0	8.947	1.918	0.914	H
HETATM	9	C	0	8.900	-0.021	-0.006	C

HETATM	10	C	0	7.417	-0.101	-0.045	C
HETATM	11	C	0	6.768	-1.222	-0.580	C
HETATM	12	H	0	7.362	-2.037	-0.969	H
HETATM	13	C	0	5.385	-1.257	-0.596	C
HETATM	14	H	0	4.857	-2.113	-1.003	H
HETATM	15	C	0	4.656	-0.172	-0.077	C
HETATM	16	C	0	5.409	0.905	0.436	C
HETATM	17	H	0	4.893	1.768	0.849	H
HETATM	18	C	0	3.240	-0.149	-0.060	C
HETATM	19	C	0	2.028	-0.123	-0.040	C
HETATM	20	C	0	0.610	-0.095	-0.011	C
HETATM	21	C	0	-0.152	-1.148	-0.551	C
HETATM	22	H	0	0.357	-1.990	-1.007	H
HETATM	23	C	0	-1.536	-1.122	-0.523	C
HETATM	24	H	0	-2.094	-1.943	-0.958	H
HETATM	25	C	0	-2.227	-0.041	0.056	C
HETATM	26	C	0	-1.469	1.014	0.598	C
HETATM	27	H	0	-1.974	1.854	1.058	H
HETATM	28	C	0	-0.086	0.987	0.560	C
HETATM	29	H	0	0.476	1.808	0.992	H
HETATM	30	C	0	-4.387	-1.226	0.124	C
HETATM	31	C	0	-4.084	-2.242	1.044	C
HETATM	32	H	0	-3.256	-2.109	1.732	H
HETATM	33	C	0	-4.826	-3.410	1.078	C
HETATM	34	H	0	-4.595	-4.198	1.786	H
HETATM	35	C	0	-5.910	-3.590	0.209	C
HETATM	36	C	0	-6.230	-2.579	-0.699	C
HETATM	37	H	0	-7.062	-2.684	-1.384	H
HETATM	38	C	0	-5.464	-1.414	-0.742	C

HETATM 39 H 0 -5.716 -0.637 -1.455 H

HETATM 40 C 0 -7.690 -5.010 -0.520 C

HETATM 41 H 0 -8.066 -5.995 -0.250 H

HETATM 42 H 0 -8.481 -4.268 -0.369 H

HETATM 43 H 0 -7.393 -5.014 -1.575 H

HETATM 44 C 0 -4.339 1.224 0.089 C

HETATM 45 C 0 -5.333 1.478 1.046 C

HETATM 46 H 0 -5.553 0.728 1.798 H

HETATM 47 C 0 -6.037 2.671 1.035 C

HETATM 48 H 0 -6.807 2.873 1.772 H

HETATM 49 C 0 -5.757 3.653 0.077 C

HETATM 50 C 0 -4.764 3.413 -0.876 C

HETATM 51 H 0 -4.526 4.148 -1.635 H

HETATM 52 C 0 -4.074 2.201 -0.871 C

HETATM 53 H 0 -3.313 2.018 -1.621 H

HETATM 54 C 0 -6.262 5.826 -0.784 C

HETATM 55 H 0 -6.953 6.627 -0.529 H

HETATM 56 H 0 -5.234 6.201 -0.718 H

HETATM 57 H 0 -6.460 5.490 -1.807 H

HETATM 58 N 0 9.580 -1.069 -0.501 N

HETATM 59 N 0 6.733 0.943 0.453 N

HETATM 60 N 0 -3.631 -0.016 0.094 N

HETATM 61 O 0 -6.581 -4.771 0.332 O

HETATM 62 O 0 -6.500 4.794 0.160 O

END

TITLE Cartesian coordinates of **L_1** (S_1)

REMARK 1 File created by GaussView 5.0.8

HETATM 1 C 0 10.833 -0.190 -1.068 C

HETATM 2 H 0 11.353 -0.297 -2.020 H

HETATM 3 C 0 11.561 -0.047 0.111 C

HETATM	4	H	0	12.646	-0.042	0.097	H
HETATM	5	C	0	10.838	0.086	1.302	C
HETATM	6	H	0	11.354	0.200	2.251	H
HETATM	7	C	0	9.457	0.072	1.261	C
HETATM	8	H	0	8.854	0.172	2.155	H
HETATM	9	C	0	8.800	-0.077	0.017	C
HETATM	10	C	0	7.347	-0.097	-0.070	C
HETATM	11	C	0	6.679	-0.247	-1.310	C
HETATM	12	H	0	7.277	-0.351	-2.207	H
HETATM	13	C	0	5.308	-0.259	-1.357	C
HETATM	14	H	0	4.786	-0.375	-2.302	H
HETATM	15	C	0	4.555	-0.120	-0.151	C
HETATM	16	C	0	5.327	0.024	1.041	C
HETATM	17	H	0	4.805	0.133	1.990	H
HETATM	18	C	0	3.163	-0.118	-0.118	C
HETATM	19	C	0	1.937	-0.113	-0.081	C
HETATM	20	C	0	0.541	-0.098	-0.042	C
HETATM	21	C	0	-0.242	-0.215	-1.228	C
HETATM	22	H	0	0.266	-0.331	-2.178	H
HETATM	23	C	0	-1.624	-0.194	-1.186	C
HETATM	24	H	0	-2.195	-0.293	-2.105	H
HETATM	25	C	0	-2.287	-0.054	0.038	C
HETATM	26	C	0	-1.552	0.062	1.223	C
HETATM	27	H	0	-2.067	0.181	2.172	H
HETATM	28	C	0	-0.170	0.037	1.186	C
HETATM	29	H	0	0.394	0.134	2.107	H
HETATM	30	C	0	-4.449	-1.222	0.096	C
HETATM	31	C	0	-3.861	-2.374	0.670	C
HETATM	32	H	0	-2.875	-2.307	1.108	H
HETATM	33	C	0	-4.538	-3.570	0.683	C
HETATM	34	H	0	-4.101	-4.451	1.138	H
HETATM	35	C	0	-5.814	-3.685	0.097	C
HETATM	36	C	0	-6.388	-2.563	-0.519	C
HETATM	37	H	0	-7.341	-2.630	-1.027	H
HETATM	38	C	0	-5.712	-1.353	-0.517	C
HETATM	39	H	0	-6.144	-0.512	-1.043	H
HETATM	40	C	0	-7.669	-5.110	-0.416	C
HETATM	41	H	0	-7.910	-6.152	-0.223	H
HETATM	42	H	0	-8.418	-4.467	0.054	H
HETATM	43	H	0	-7.649	-4.934	-1.495	H
HETATM	44	C	0	-4.382	1.225	0.078	C
HETATM	45	C	0	-5.675	1.403	0.638	C
HETATM	46	H	0	-6.174	0.569	1.113	H
HETATM	47	C	0	-6.275	2.639	0.648	C

HETATM	48	H	0	-7.248	2.785	1.103	H
HETATM	49	C	0	-5.619	3.760	0.101	C
HETATM	50	C	0	-4.324	3.606	-0.426	C
HETATM	51	H	0	-3.785	4.450	-0.834	H
HETATM	52	C	0	-3.715	2.367	-0.423	C
HETATM	53	H	0	-2.715	2.264	-0.818	H
HETATM	54	C	0	-5.687	6.113	-0.343	C
HETATM	55	H	0	-6.421	6.899	-0.185	H
HETATM	56	H	0	-4.774	6.347	0.211	H
HETATM	57	H	0	-5.466	6.026	-1.409	H
HETATM	58	N	0	9.505	-0.206	-1.136	N
HETATM	59	N	0	6.638	0.036	1.090	N
HETATM	60	N	0	-3.747	-0.011	0.076	N
HETATM	61	O	0	-6.380	-4.903	0.161	O
HETATM	62	O	0	-6.295	4.918	0.154	O
END							

TITLE Cartesian coordinates of **L_1** (T_1)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	10.866	-0.945	-0.544	C
HETATM	2	H	0	11.397	-1.752	-1.046	H
HETATM	3	C	0	11.577	0.069	0.099	C
HETATM	4	H	0	12.661	0.064	0.105	H
HETATM	5	C	0	10.846	1.080	0.727	C
HETATM	6	H	0	11.353	1.891	1.241	H
HETATM	7	C	0	9.463	1.036	0.688	C
HETATM	8	H	0	8.851	1.794	1.159	H
HETATM	9	C	0	8.828	-0.030	0.014	C
HETATM	10	C	0	7.377	-0.120	-0.053	C
HETATM	11	C	0	6.727	-1.191	-0.731	C
HETATM	12	H	0	7.344	-1.944	-1.204	H
HETATM	13	C	0	5.365	-1.251	-0.774	C
HETATM	14	H	0	4.854	-2.059	-1.285	H
HETATM	15	C	0	4.587	-0.223	-0.127	C
HETATM	16	C	0	5.353	0.817	0.528	C

HETATM	17	H	0	4.812	1.618	1.030	H
HETATM	18	C	0	3.224	-0.203	-0.113	C
HETATM	19	C	0	1.979	-0.169	-0.087	C
HETATM	20	C	0	0.615	-0.132	-0.050	C
HETATM	21	C	0	-0.193	-1.141	-0.693	C
HETATM	22	H	0	0.308	-1.936	-1.233	H
HETATM	23	C	0	-1.559	-1.098	-0.645	C
HETATM	24	H	0	-2.137	-1.862	-1.151	H
HETATM	25	C	0	-2.240	-0.051	0.036	C
HETATM	26	C	0	-1.461	0.956	0.672	C
HETATM	27	H	0	-1.963	1.749	1.212	H
HETATM	28	C	0	-0.095	0.922	0.636	C
HETATM	29	H	0	0.482	1.686	1.145	H
HETATM	30	C	0	-4.393	-1.217	0.133	C
HETATM	31	C	0	-4.006	-2.267	0.982	C
HETATM	32	H	0	-3.129	-2.152	1.608	H
HETATM	33	C	0	-4.737	-3.440	1.030	C
HETATM	34	H	0	-4.447	-4.252	1.687	H
HETATM	35	C	0	-5.885	-3.598	0.240	C
HETATM	36	C	0	-6.283	-2.554	-0.601	C
HETATM	37	H	0	-7.162	-2.644	-1.227	H
HETATM	38	C	0	-5.536	-1.379	-0.654	C
HETATM	39	H	0	-5.846	-0.580	-1.319	H
HETATM	40	C	0	-7.705	-5.008	-0.404	C
HETATM	41	H	0	-8.047	-6.007	-0.141	H
HETATM	42	H	0	-8.489	-4.282	-0.162	H
HETATM	43	H	0	-7.492	-4.970	-1.478	H
HETATM	44	C	0	-4.326	1.234	0.066	C
HETATM	45	C	0	-5.398	1.470	0.942	C

HETATM	46	H	0	-5.701	0.697	1.638	H
HETATM	47	C	0	-6.063	2.683	0.928	C
HETATM	48	H	0	-6.888	2.876	1.605	H
HETATM	49	C	0	-5.672	3.701	0.047	C
HETATM	50	C	0	-4.604	3.475	-0.827	C
HETATM	51	H	0	-4.282	4.235	-1.527	H
HETATM	52	C	0	-3.945	2.247	-0.817	C
HETATM	53	H	0	-3.126	2.074	-1.505	H
HETATM	54	C	0	-6.036	5.930	-0.738	C
HETATM	55	H	0	-6.725	6.737	-0.499	H
HETATM	56	H	0	-5.009	6.267	-0.559	H
HETATM	57	H	0	-6.151	5.657	-1.792	H
HETATM	58	N	0	9.540	-1.009	-0.595	N
HETATM	59	N	0	6.654	0.868	0.565	N
HETATM	60	N	0	-3.638	-0.012	0.082	N
HETATM	61	O	0	-6.534	-4.786	0.367	O
HETATM	62	O	0	-6.388	4.855	0.120	O

END

TITLE Cartesian coordinates of **L**$_2$ (S$_0$)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	-8.051	-3.663	0.033	C
HETATM	2	C	0	-7.012	-3.471	-0.881	C
HETATM	3	C	0	-6.312	-2.264	-0.896	C
HETATM	4	C	0	-6.614	-1.244	0.007	C
HETATM	5	C	0	-7.656	-1.449	0.924	C
HETATM	6	C	0	-8.369	-2.637	0.931	C
HETATM	7	N	0	-5.895	-0.012	-0.009	N
HETATM	8	C	0	-6.637	1.207	-0.014	C
HETATM	9	C	0	-4.489	0.001	-0.014	C
HETATM	10	C	0	-3.753	-1.028	0.602	C
HETATM	11	C	0	-2.368	-1.016	0.593	C
HETATM	12	C	0	-1.649	0.025	-0.023	C
HETATM	13	C	0	-2.390	1.054	-0.635	C
HETATM	14	C	0	-3.775	1.042	-0.636	C

HETATM	15	C	0	-6.338	2.236	0.880	C
HETATM	16	C	0	-7.062	3.428	0.875	C
HETATM	17	C	0	-8.123	3.597	-0.018	C
HETATM	18	C	0	-8.438	2.561	-0.906	C
HETATM	19	C	0	-7.701	1.388	-0.910	C
HETATM	20	C	0	-0.230	0.040	-0.025	C
HETATM	21	C	0	0.983	0.057	-0.028	C
HETATM	22	C	0	2.404	0.084	-0.031	C
HETATM	23	C	0	3.153	-0.916	0.631	C
HETATM	24	C	0	4.540	-0.824	0.588	C
HETATM	25	C	0	5.221	0.212	-0.069	C
HETATM	26	C	0	4.472	1.203	-0.738	C
HETATM	27	C	0	3.083	1.113	-0.703	C
HETATM	28	C	0	6.706	0.206	-0.039	C
HETATM	29	C	0	7.429	-0.938	-0.417	C
HETATM	30	N	0	8.753	-1.044	-0.386	N
HETATM	31	C	0	9.466	0.012	0.029	C
HETATM	32	C	0	8.849	1.204	0.429	C
HETATM	33	C	0	7.465	1.297	0.395	C
HETATM	34	C	0	10.951	-0.137	0.059	C
HETATM	35	N	0	11.434	-1.339	0.405	N
HETATM	36	C	0	12.756	-1.495	0.442	C
HETATM	37	C	0	13.669	-0.485	0.140	C
HETATM	38	C	0	13.167	0.759	-0.224	C
HETATM	39	C	0	11.789	0.938	-0.267	C
HETATM	40	C	0	5.114	2.332	-1.513	C
HETATM	41	C	0	2.470	-2.042	1.361	C
HETATM	42	O	0	-8.903	4.713	-0.102	O
HETATM	43	C	0	-8.634	5.792	0.777	C
HETATM	44	O	0	-8.807	-4.794	0.129	O
HETATM	45	C	0	-8.534	-5.867	-0.758	C
HETATM	46	H	0	-6.745	-4.239	-1.596	H
HETATM	47	H	0	-5.516	-2.119	-1.617	H
HETATM	48	H	0	-7.906	-0.666	1.631	H
HETATM	49	H	0	-9.176	-2.800	1.637	H
HETATM	50	H	0	-4.277	-1.838	1.096	H
HETATM	51	H	0	-1.824	-1.818	1.081	H
HETATM	52	H	0	-1.863	1.864	-1.127	H
HETATM	53	H	0	-4.316	1.842	-1.126	H
HETATM	54	H	0	-5.524	2.110	1.586	H
HETATM	55	H	0	-6.795	4.204	1.582	H
HETATM	56	H	0	-9.263	2.705	-1.595	H
HETATM	57	H	0	-7.950	0.598	-1.609	H
HETATM	58	H	0	5.125	-1.577	1.108	H

HETATM	59	H	0	2.492	1.860	-1.223	H
HETATM	60	H	0	6.893	-1.813	-0.779	H
HETATM	61	H	0	9.441	2.033	0.799	H
HETATM	62	H	0	6.974	2.203	0.737	H
HETATM	63	H	0	13.107	-2.484	0.731	H
HETATM	64	H	0	14.736	-0.674	0.187	H
HETATM	65	H	0	13.835	1.575	-0.482	H
HETATM	66	H	0	11.368	1.890	-0.573	H
HETATM	67	H	0	6.037	2.018	-2.004	H
HETATM	68	H	0	5.365	3.182	-0.870	H
HETATM	69	H	0	4.434	2.705	-2.282	H
HETATM	70	H	0	1.841	-2.630	0.686	H
HETATM	71	H	0	1.813	-1.665	2.150	H
HETATM	72	H	0	3.197	-2.716	1.818	H
HETATM	73	H	0	-8.756	5.498	1.826	H
HETATM	74	H	0	-9.364	6.562	0.534	H
HETATM	75	H	0	-7.625	6.192	0.628	H
HETATM	76	H	0	-8.682	-5.573	-1.803	H
HETATM	77	H	0	-7.514	-6.246	-0.629	H
HETATM	78	H	0	-9.243	-6.652	-0.502	H
END							

TITLE Cartesian coordinates of **L₂** (S_1)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	-7.923	3.771	-0.021	C
HETATM	2	C	0	-6.642	3.620	0.539	C
HETATM	3	C	0	-6.020	2.387	0.532	C
HETATM	4	C	0	-6.662	1.249	-0.006	C
HETATM	5	C	0	-7.941	1.422	-0.596	C
HETATM	6	C	0	-8.553	2.654	-0.602	C
HETATM	7	N	0	-6.010	0.017	-0.011	N
HETATM	8	C	0	-6.692	-1.200	-0.032	C
HETATM	9	C	0	-4.551	-0.001	0.008	C
HETATM	10	C	0	-3.832	0.156	-1.185	C
HETATM	11	C	0	-2.451	0.138	-1.171	C
HETATM	12	C	0	-1.718	-0.033	0.044	C
HETATM	13	C	0	-2.485	-0.188	1.240	C
HETATM	14	C	0	-3.867	-0.174	1.219	C
HETATM	15	C	0	-6.069	-2.349	-0.565	C
HETATM	16	C	0	-6.720	-3.568	-0.588	C
HETATM	17	C	0	-8.012	-3.691	-0.048	C
HETATM	18	C	0	-8.624	-2.562	0.529	C
HETATM	19	C	0	-7.983	-1.345	0.537	C
HETATM	20	C	0	-0.324	-0.048	0.062	C

HETATM	21	C	0	0.903	-0.060	0.076	C
HETATM	22	C	0	2.298	-0.074	0.105	C
HETATM	23	C	0	3.080	0.109	-1.079	C
HETATM	24	C	0	4.455	0.088	-0.971	C
HETATM	25	C	0	5.155	-0.121	0.246	C
HETATM	26	C	0	4.373	-0.298	1.427	C
HETATM	27	C	0	2.994	-0.264	1.330	C
HETATM	28	C	0	6.619	-0.124	0.218	C
HETATM	29	C	0	7.334	0.755	-0.636	C
HETATM	30	N	0	8.649	0.811	-0.761	N
HETATM	31	C	0	9.407	-0.024	-0.020	C
HETATM	32	C	0	8.809	-0.944	0.857	C
HETATM	33	C	0	7.431	-0.995	0.973	C
HETATM	34	C	0	10.878	0.064	-0.176	C
HETATM	35	N	0	11.355	0.510	-1.353	N
HETATM	36	C	0	12.673	0.593	-1.511	C
HETATM	37	C	0	13.605	0.242	-0.535	C
HETATM	38	C	0	13.117	-0.212	0.688	C
HETATM	39	C	0	11.744	-0.299	0.873	C
HETATM	40	C	0	4.985	-0.449	2.804	C
HETATM	41	C	0	2.407	0.305	-2.411	C
HETATM	42	O	0	-8.726	-4.828	-0.011	O
HETATM	43	C	0	-8.162	-6.029	-0.542	C
HETATM	44	O	0	-8.609	4.925	-0.074	O
HETATM	45	C	0	-8.024	6.115	0.458	C
HETATM	46	H	0	-6.123	4.463	0.975	H
HETATM	47	H	0	-5.030	2.285	0.951	H
HETATM	48	H	0	-8.420	0.591	-1.095	H
HETATM	49	H	0	-9.515	2.796	-1.079	H
HETATM	50	H	0	-4.363	0.297	-2.122	H
HETATM	51	H	0	-1.902	0.265	-2.097	H
HETATM	52	H	0	-1.963	-0.327	2.179	H
HETATM	53	H	0	-4.424	-0.303	2.142	H
HETATM	54	H	0	-5.070	-2.269	-0.968	H
HETATM	55	H	0	-6.214	-4.420	-1.021	H
HETATM	56	H	0	-9.597	-2.683	0.990	H
HETATM	57	H	0	-8.450	-0.504	1.033	H
HETATM	58	H	0	5.037	0.195	-1.881	H
HETATM	59	H	0	2.402	-0.370	2.234	H
HETATM	60	H	0	6.781	1.477	-1.232	H
HETATM	61	H	0	9.417	-1.651	1.411	H
HETATM	62	H	0	6.980	-1.746	1.610	H
HETATM	63	H	0	13.008	0.958	-2.480	H
HETATM	64	H	0	14.669	0.330	-0.727	H

HETATM	65	H	0	13.796	-0.482	1.492	H
HETATM	66	H	0	11.344	-0.615	1.829	H
HETATM	67	H	0	5.877	0.170	2.926	H
HETATM	68	H	0	5.281	-1.481	3.022	H
HETATM	69	H	0	4.266	-0.157	3.572	H
HETATM	70	H	0	1.761	1.190	-2.407	H
HETATM	71	H	0	1.763	-0.545	-2.664	H
HETATM	72	H	0	3.140	0.424	-3.212	H
HETATM	73	H	0	-7.951	-5.925	-1.609	H
HETATM	74	H	0	-8.918	-6.795	-0.393	H
HETATM	75	H	0	-7.250	-6.304	-0.005	H
HETATM	76	H	0	-7.831	6.012	1.529	H
HETATM	77	H	0	-7.098	6.366	-0.066	H
HETATM	78	H	0	-8.759	6.898	0.294	H
END							

TITLE Cartesian coordinates of **L₂** (T_1)
REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	-7.965	3.717	0.051	C
HETATM	2	C	0	-6.850	3.520	0.872	C
HETATM	3	C	0	-6.182	2.298	0.858	C
HETATM	4	C	0	-6.601	1.258	0.022	C
HETATM	5	C	0	-7.720	1.466	-0.802	C
HETATM	6	C	0	-8.393	2.674	-0.783	C
HETATM	7	N	0	-5.904	0.020	0.003	N
HETATM	8	C	0	-6.642	-1.194	-0.025	C
HETATM	9	C	0	-4.503	-0.003	0.009	C
HETATM	10	C	0	-3.751	0.980	-0.701	C
HETATM	11	C	0	-2.387	0.962	-0.703	C
HETATM	12	C	0	-1.643	-0.050	0.020	C
HETATM	13	C	0	-2.426	-1.036	0.739	C
HETATM	14	C	0	-3.790	-1.010	0.724	C
HETATM	15	C	0	-6.246	-2.251	-0.850	C
HETATM	16	C	0	-6.956	-3.449	-0.872	C
HETATM	17	C	0	-8.091	-3.604	-0.070	C
HETATM	18	C	0	-8.496	-2.544	0.754	C
HETATM	19	C	0	-7.781	-1.360	0.781	C
HETATM	20	C	0	-0.281	-0.072	0.025	C
HETATM	21	C	0	0.965	-0.085	0.023	C
HETATM	22	C	0	2.336	-0.116	0.033	C
HETATM	23	C	0	3.127	0.863	-0.677	C
HETATM	24	C	0	4.496	0.763	-0.612	C
HETATM	25	C	0	5.187	-0.257	0.096	C
HETATM	26	C	0	4.408	-1.225	0.809	C

HETATM	27	C	0	3.035	-1.131	0.768	C
HETATM	28	C	0	6.655	-0.245	0.074	C
HETATM	29	C	0	7.367	0.974	0.164	C
HETATM	30	N	0	8.685	1.096	0.118	N
HETATM	31	C	0	9.429	-0.016	-0.019	C
HETATM	32	C	0	8.832	-1.280	-0.119	C
HETATM	33	C	0	7.452	-1.393	-0.074	C
HETATM	34	C	0	10.906	0.154	-0.075	C
HETATM	35	N	0	11.372	1.283	-0.633	N
HETATM	36	C	0	12.691	1.455	-0.696	C
HETATM	37	C	0	13.622	0.534	-0.217	C
HETATM	38	C	0	13.140	-0.633	0.367	C
HETATM	39	C	0	11.766	-0.827	0.442	C
HETATM	40	C	0	5.031	-2.311	1.658	C
HETATM	41	C	0	2.453	1.946	-1.470	C
HETATM	42	O	0	-8.861	-4.724	-0.017	O
HETATM	43	C	0	-8.504	-5.834	-0.828	C
HETATM	44	O	0	-8.694	4.863	-0.012	O
HETATM	45	C	0	-8.311	5.959	0.806	C
HETATM	46	H	0	-6.498	4.300	1.535	H
HETATM	47	H	0	-5.327	2.148	1.506	H
HETATM	48	H	0	-8.053	0.674	-1.463	H
HETATM	49	H	0	-9.254	2.843	-1.420	H
HETATM	50	H	0	-4.280	1.740	-1.265	H
HETATM	51	H	0	-1.834	1.704	-1.268	H
HETATM	52	H	0	-1.901	-1.796	1.308	H
HETATM	53	H	0	-4.348	-1.751	1.285	H
HETATM	54	H	0	-5.375	-2.133	-1.485	H
HETATM	55	H	0	-6.621	-4.243	-1.527	H
HETATM	56	H	0	-9.373	-2.681	1.377	H
HETATM	57	H	0	-8.098	-0.554	1.433	H
HETATM	58	H	0	5.087	1.482	-1.171	H
HETATM	59	H	0	2.437	-1.844	1.328	H
HETATM	60	H	0	6.818	1.901	0.310	H
HETATM	61	H	0	9.440	-2.165	-0.276	H
HETATM	62	H	0	6.992	-2.366	-0.202	H
HETATM	63	H	0	13.024	2.382	-1.159	H
HETATM	64	H	0	14.685	0.731	-0.298	H
HETATM	65	H	0	13.822	-1.376	0.770	H
HETATM	66	H	0	11.365	-1.713	0.921	H
HETATM	67	H	0	5.926	-1.963	2.177	H
HETATM	68	H	0	5.321	-3.187	1.068	H
HETATM	69	H	0	4.321	-2.658	2.412	H
HETATM	70	H	0	1.813	2.567	-0.834	H

HETATM	71	H	0	1.805	1.527	-2.247	H
HETATM	72	H	0	3.184	2.597	-1.953	H
HETATM	73	H	0	-8.536	-5.579	-1.893	H
HETATM	74	H	0	-9.246	-6.602	-0.620	H
HETATM	75	H	0	-7.509	-6.213	-0.574	H
HETATM	76	H	0	-8.370	5.705	1.870	H
HETATM	77	H	0	-7.298	6.302	0.569	H
HETATM	78	H	0	-9.021	6.754	0.587	H

END

TITLE Cartesian coordinates of complex **1** (S_0)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	Eu	0	-8.884	2.267	13.248	Eu
HETATM	2	S	0	-5.317	-1.075	14.758	S
HETATM	3	S	0	-4.743	4.622	15.265	S
HETATM	4	F	0	-10.974	-2.915	11.680	F
HETATM	5	F	0	-11.368	-1.111	10.534	F
HETATM	6	F	0	-12.304	-1.393	12.475	F
HETATM	7	F	0	-9.464	1.685	18.968	F
HETATM	8	F	0	-11.186	2.119	17.719	F
HETATM	9	F	0	-10.200	0.189	17.576	F
HETATM	10	F	0	-13.671	3.331	12.086	F
HETATM	11	F	0	-13.830	5.324	12.939	F
HETATM	12	F	0	-13.665	3.596	14.243	F
HETATM	13	O	0	-7.631	0.265	13.633	O
HETATM	14	O	0	-10.147	0.409	12.484	O
HETATM	15	O	0	-7.180	3.114	14.738	O
HETATM	16	O	0	-9.567	1.878	15.455	O
HETATM	17	O	0	-8.867	4.631	12.866	O
HETATM	18	O	0	-11.132	3.077	13.191	O
HETATM	19	N	0	-9.241	2.483	10.608	N
HETATM	20	N	0	-6.753	2.436	11.646	N
HETATM	21	C	0	-10.493	2.494	10.163	C
HETATM	22	H	0	-11.264	2.289	10.894	H
HETATM	23	C	0	-10.840	2.752	8.821	C
HETATM	24	C	0	-9.779	2.982	7.931	C
HETATM	25	H	0	-9.986	3.189	6.887	H
HETATM	26	C	0	-8.475	2.945	8.396	C
HETATM	27	H	0	-7.665	3.125	7.701	H
HETATM	28	C	0	-8.222	2.693	9.749	C
HETATM	29	C	0	-6.853	2.618	10.313	C
HETATM	30	C	0	-5.708	2.703	9.511	C
HETATM	31	H	0	-5.789	2.840	8.441	H
HETATM	32	C	0	-4.452	2.598	10.094	C

HETATM	33	H	0	-3.560	2.659	9.480	H
HETATM	34	C	0	-4.361	2.405	11.467	C
HETATM	35	H	0	-3.404	2.312	11.968	H
HETATM	36	C	0	-5.540	2.331	12.199	C
HETATM	37	H	0	-5.527	2.190	13.272	H
HETATM	38	C	0	-7.781	-0.986	13.502	C
HETATM	39	C	0	-6.690	-1.841	13.995	C
HETATM	40	C	0	-4.566	-2.604	15.031	C
HETATM	41	H	0	-3.606	-2.651	15.526	H
HETATM	42	C	0	-5.325	-3.646	14.568	C
HETATM	43	H	0	-5.030	-4.685	14.649	H
HETATM	44	C	0	-6.537	-3.210	13.978	C
HETATM	45	H	0	-7.270	-3.885	13.557	H
HETATM	46	C	0	-8.918	-1.590	12.911	C
HETATM	47	H	0	-8.961	-2.664	12.817	H
HETATM	48	C	0	-9.991	-0.841	12.446	C
HETATM	49	C	0	-11.168	-1.580	11.783	C
HETATM	50	C	0	-6.992	3.171	15.988	C
HETATM	51	C	0	-5.756	3.828	16.448	C
HETATM	52	C	0	-3.613	5.085	16.484	C
HETATM	53	H	0	-2.735	5.656	16.216	H
HETATM	54	C	0	-3.988	4.657	17.729	C
HETATM	55	H	0	-3.414	4.847	18.627	H
HETATM	56	C	0	-5.212	3.941	17.708	C
HETATM	57	H	0	-5.668	3.517	18.593	H
HETATM	58	C	0	-7.888	2.655	16.957	C
HETATM	59	H	0	-7.646	2.745	18.004	H
HETATM	60	C	0	-9.088	2.049	16.608	C
HETATM	61	C	0	-9.989	1.508	17.733	C
HETATM	62	C	0	-9.688	5.589	12.772	C
HETATM	63	C	0	-9.122	6.928	12.545	C
HETATM	64	C	0	-9.734	8.152	12.387	C
HETATM	65	H	0	-10.808	8.289	12.413	H
HETATM	66	C	0	-8.818	9.214	12.187	C
HETATM	67	H	0	-9.110	10.247	12.045	H
HETATM	68	C	0	-7.516	8.787	12.195	C
HETATM	69	H	0	-6.623	9.383	12.070	H
HETATM	70	C	0	-11.095	5.440	12.863	C
HETATM	71	H	0	-11.731	6.306	12.768	H
HETATM	72	C	0	-11.688	4.199	13.059	C
HETATM	73	C	0	-13.227	4.123	13.090	C
HETATM	74	S	0	-7.385	7.086	12.449	S
HETATM	75	C	0	-12.197	2.792	8.434	C
HETATM	76	C	0	-13.378	2.839	8.161	C

HETATM 77 C 0 -14.764 2.893 7.882 C
HETATM 78 C 0 -15.706 2.881 8.930 C
HETATM 79 C 0 -15.249 2.959 6.562 C
HETATM 80 C 0 -17.063 2.927 8.671 C
HETATM 81 H 0 -15.356 2.829 9.955 H
HETATM 82 C 0 -16.606 3.011 6.299 C
HETATM 83 H 0 -14.544 2.979 5.738 H
HETATM 84 C 0 -17.547 2.993 7.348 C
HETATM 85 H 0 -17.764 2.903 9.496 H
HETATM 86 H 0 -16.950 3.073 5.274 H
HETATM 87 N 0 -18.923 3.039 7.084 N
HETATM 88 C 0 -19.836 3.586 8.038 C
HETATM 89 C 0 -19.624 4.847 8.595 C
HETATM 90 C 0 -20.978 2.868 8.420 C
HETATM 91 C 0 -20.512 5.381 9.529 C
HETATM 92 H 0 -18.749 5.419 8.305 H
HETATM 93 C 0 -21.876 3.399 9.330 C
HETATM 94 H 0 -21.158 1.887 7.994 H
HETATM 95 C 0 -21.649 4.659 9.900 C
HETATM 96 H 0 -20.308 6.359 9.945 H
HETATM 97 H 0 -22.760 2.848 9.631 H
HETATM 98 C 0 -19.451 2.553 5.850 C
HETATM 99 C 0 -20.330 3.331 5.097 C
HETATM 100 C 0 -19.120 1.272 5.381 C
HETATM 101 C 0 -20.877 2.853 3.906 C
HETATM 102 H 0 -20.599 4.321 5.448 H
HETATM 103 C 0 -19.643 0.798 4.190 C
HETATM 104 H 0 -18.447 0.649 5.960 H
HETATM 105 C 0 -20.530 1.582 3.441 C
HETATM 106 H 0 -21.561 3.485 3.354 H
HETATM 107 H 0 -19.392 -0.191 3.824 H
HETATM 108 O 0 -22.586 5.085 10.794 O
HETATM 109 O 0 -20.996 1.018 2.290 O
HETATM 110 C 0 -22.401 6.347 11.416 C
HETATM 111 H 0 -22.398 7.161 10.683 H
HETATM 112 H 0 -23.248 6.473 12.088 H
HETATM 113 H 0 -21.472 6.377 11.996 H
HETATM 114 C 0 -21.903 1.762 1.493 C
HETATM 115 H 0 -21.452 2.694 1.133 H
HETATM 116 H 0 -22.140 1.127 0.641 H
HETATM 117 H 0 -22.824 1.993 2.039 H
END

TITLE Cartesian coordinates of complex **2** (S_0)

REMARK 1 File created by GaussView 5.0.8

HETATM	1	C	0	-12.155	1.597	1.489	C
HETATM	2	C	0	-11.068	2.424	1.168	C
HETATM	3	C	0	-11.013	2.983	-0.110	C
HETATM	4	C	0	-12.002	2.716	-1.057	C
HETATM	5	C	0	-13.083	1.897	-0.724	C
HETATM	6	C	0	-13.152	1.345	0.561	C
HETATM	7	N	0	-10.057	2.698	2.136	N
HETATM	8	C	0	-11.421	4.081	3.642	C
HETATM	9	C	0	-11.826	4.440	4.916	C
HETATM	10	C	0	-11.267	3.821	6.042	C
HETATM	11	C	0	-10.303	2.826	5.863	C
HETATM	12	C	0	-9.916	2.455	4.576	C
HETATM	13	C	0	-10.458	3.078	3.451	C
HETATM	14	C	0	-7.741	3.442	2.415	C
HETATM	15	C	0	-6.399	3.349	2.090	C
HETATM	16	C	0	-5.940	2.425	1.131	C
HETATM	17	C	0	-6.897	1.594	0.518	C
HETATM	18	C	0	-8.240	1.679	0.846	C
HETATM	19	C	0	-8.693	2.607	1.801	C
HETATM	20	O	0	-14.109	1.578	-1.566	O
HETATM	21	O	0	-11.727	4.255	7.250	O
HETATM	22	C	0	-14.091	2.105	-2.882	C
HETATM	23	C	0	-11.199	3.662	8.426	C
HETATM	24	C	0	-4.563	2.341	0.800	C
HETATM	25	C	0	-3.383	2.283	0.527	C
HETATM	26	C	0	-1.476	1.262	-0.666	C
HETATM	27	C	0	-0.110	1.279	-0.917	C
HETATM	28	C	0	0.762	2.215	-0.340	C
HETATM	29	C	0	0.246	3.176	0.555	C
HETATM	30	C	0	-1.122	3.158	0.813	C
HETATM	31	C	0	-1.997	2.233	0.220	C
HETATM	32	C	0	2.862	0.898	-0.670	C
HETATM	33	N	0	4.127	0.721	-1.050	N
HETATM	34	C	0	4.840	1.778	-1.486	C
HETATM	35	C	0	4.267	3.051	-1.535	C
HETATM	36	C	0	2.947	3.226	-1.144	C
HETATM	37	C	0	2.197	2.133	-0.703	C
HETATM	38	N	0	6.591	0.213	-2.029	N
HETATM	39	C	0	7.807	-0.096	-2.489	C
HETATM	40	C	0	8.737	0.862	-2.876	C
HETATM	41	C	0	8.381	2.201	-2.768	C
HETATM	42	C	0	7.115	2.528	-2.301	C
HETATM	43	C	0	6.226	1.507	-1.946	C

HETATM	44	C	0	1.113	4.185	1.275	C
HETATM	45	C	0	-2.367	0.237	-1.316	C
HETATM	46	Eu	0	5.152	-1.728	-0.919	Eu
HETATM	47	C	0	10.763	-5.484	-0.691	C
HETATM	48	C	0	11.329	-4.838	0.377	C
HETATM	49	C	0	10.535	-3.758	0.835	C
HETATM	50	C	0	9.374	-3.592	0.112	C
HETATM	51	S	0	9.254	-4.790	-1.154	S
HETATM	52	C	0	8.284	-2.614	0.249	C
HETATM	53	C	0	8.357	-1.637	1.276	C
HETATM	54	C	0	7.342	-0.712	1.480	C
HETATM	55	O	0	7.335	-2.696	-0.583	O
HETATM	56	O	0	6.244	-0.610	0.871	O
HETATM	57	C	0	4.525	-8.395	-0.537	C
HETATM	58	C	0	3.495	-8.395	0.367	C
HETATM	59	C	0	3.126	-7.086	0.762	C
HETATM	60	C	0	3.878	-6.103	0.155	C
HETATM	61	S	0	5.062	-6.803	-0.923	S
HETATM	62	C	0	3.828	-4.641	0.279	C
HETATM	63	C	0	2.876	-4.048	1.147	C
HETATM	64	C	0	2.784	-2.673	1.307	C
HETATM	65	O	0	4.657	-3.980	-0.413	O
HETATM	66	O	0	3.476	-1.770	0.759	O
HETATM	67	C	0	7.971	-4.087	-6.604	C
HETATM	68	C	0	6.806	-4.148	-7.323	C
HETATM	69	C	0	5.684	-3.722	-6.569	C
HETATM	70	C	0	6.004	-3.340	-5.284	C
HETATM	71	S	0	7.719	-3.512	-4.997	S
HETATM	72	C	0	5.160	-2.838	-4.189	C
HETATM	73	C	0	3.755	-2.767	-4.386	C
HETATM	74	C	0	2.897	-2.289	-3.407	C
HETATM	75	O	0	5.747	-2.492	-3.124	O
HETATM	76	O	0	3.181	-1.878	-2.249	O
HETATM	77	C	0	7.537	0.356	2.573	C
HETATM	78	F	0	7.504	1.591	2.027	F
HETATM	79	F	0	8.713	0.245	3.230	F
HETATM	80	F	0	6.558	0.292	3.491	F
HETATM	81	C	0	1.716	-2.122	2.268	C
HETATM	82	F	0	0.894	-1.270	1.619	F
HETATM	83	F	0	2.286	-1.442	3.278	F
HETATM	84	F	0	0.939	-3.082	2.818	F
HETATM	85	C	0	1.391	-2.224	-3.723	C
HETATM	86	F	0	1.075	-2.679	-4.954	F
HETATM	87	F	0	0.950	-0.945	-3.652	F

HETATM	88	F	0	0.680	-2.939	-2.834	F
HETATM	89	H	0	-12.215	1.155	2.477	H
HETATM	90	H	0	-10.185	3.631	-0.374	H
HETATM	91	H	0	-11.920	3.166	-2.038	H
HETATM	92	H	0	-13.994	0.707	0.805	H
HETATM	93	H	0	-11.853	4.575	2.779	H
HETATM	94	H	0	-12.571	5.213	5.069	H
HETATM	95	H	0	-9.855	2.321	6.710	H
HETATM	96	H	0	-9.176	1.672	4.446	H
HETATM	97	H	0	-8.065	4.172	3.148	H
HETATM	98	H	0	-5.685	4.008	2.572	H
HETATM	99	H	0	-6.571	0.864	-0.215	H
HETATM	100	H	0	-8.950	1.016	0.366	H
HETATM	101	H	0	-13.206	1.773	-3.437	H
HETATM	102	H	0	-14.126	3.200	-2.879	H
HETATM	103	H	0	-14.985	1.719	-3.369	H
HETATM	104	H	0	-11.409	2.587	8.464	H
HETATM	105	H	0	-11.700	4.154	9.257	H
HETATM	106	H	0	-10.119	3.823	8.508	H
HETATM	107	H	0	0.299	0.548	-1.607	H
HETATM	108	H	0	-1.537	3.879	1.511	H
HETATM	109	H	0	2.354	0.015	-0.306	H
HETATM	110	H	0	4.827	3.901	-1.902	H
HETATM	111	H	0	2.492	4.207	-1.216	H
HETATM	112	H	0	8.033	-1.154	-2.543	H
HETATM	113	H	0	9.711	0.559	-3.242	H
HETATM	114	H	0	9.079	2.985	-3.042	H
HETATM	115	H	0	6.832	3.568	-2.206	H
HETATM	116	H	0	1.281	5.088	0.677	H
HETATM	117	H	0	2.093	3.778	1.530	H
HETATM	118	H	0	0.636	4.505	2.203	H
HETATM	119	H	0	-3.144	0.712	-1.923	H
HETATM	120	H	0	-2.881	-0.372	-0.567	H
HETATM	121	H	0	-1.792	-0.431	-1.960	H
HETATM	122	H	0	11.150	-6.337	-1.229	H
HETATM	123	H	0	12.275	-5.125	0.820	H
HETATM	124	H	0	10.811	-3.128	1.671	H
HETATM	125	H	0	9.223	-1.602	1.919	H
HETATM	126	H	0	4.998	-9.249	-1.000	H
HETATM	127	H	0	3.020	-9.296	0.736	H
HETATM	128	H	0	2.333	-6.878	1.469	H
HETATM	129	H	0	2.197	-4.676	1.702	H
HETATM	130	H	0	8.965	-4.355	-6.930	H
HETATM	131	H	0	6.753	-4.485	-8.351	H

HETATM 132 H 0 4.678 -3.695 -6.965 H
HETATM 133 H 0 3.333 -3.092 -5.324 H
END

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