Supporting information

Synthesis, crystal structures and two-photon absorption properties of triphenylamine cyanoacetic acid derivative and its organooxotin complexes

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Table S1. Selection bond lengths (Å) and angles (º) of Z1

Bond	Length(Å)	Bond	Angles/(º)
Sn(1)-O(1)	2.039(7)	O(1)-Sn(1)-C(31)	108.5(4)
Sn(1)-C(31)	2.101(11)	O(1)-Sn(1)-C(27)	105.6(4)
Sn(1)-O(1)#1	2.164(6)	O(1)-Sn(1)-O(1)#1	76.4(3)
Sn(2)-O(1)	2.019(7)	O(1)-Sn(1)-O(2)	88.1(3)
Sn(2)-C(22)	2.170(13)	C(31)-Sn(1)-O(2)	85.8(4)
O(1)-Sn(1)#1	2.164(6)	C(23)-Sn(2)-C(22)	138.1(5)
C(45)-N(3)	1.417(16)	O(1)-Sn(2)-O(3)	93.3(3)
N(2)-C(20)	1.111(16)	Sn(2)-O(1)-Sn(1)#1	119.2(3)
C(37)-N(4)	1.158(18)	Sn(1)-O(1)-Sn(1)#1	103.6(3)

Table S2. Selection bond lengths (Å) and angles (º) of Z2

Bond	Length(Å)	Bond	Angles/(º)
Sn(1)-O(2)	2.131(3)	O(2)-Sn(1)-C(23)	100.33(16)
Sn(1)-C(23)	2.137(5)	O(2)-Sn(1)-C(30)	90.07(16)
Sn(1)-C(30)	2.140(5)	C(23)-Sn(1)-C(30)	112.69(19)
Sn(1)-C(35)	2.148(6)	O(2)-Sn(1)-C(35)	94.93(18)
Sn(1)-O(3)	2.432(4)	C(23)-Sn(1)-C(35)	126.20(2)
O(1)-C(22)	1.196(7)	O(2)-Sn(1)-O(3)	175.25(15)
O(3)-C(41)	1.234(7)	C(30)-Sn(1)-O(3)	86.38(17)

Table S3. Selection bond lengths (Å) and angles (º) of Z3

Bond	Length(Å)	Bond	Angles/(º)
Sn(1)-O(2)	2.120(5)	O(2)-Sn(1)-C(5B)	99.0(5)
Sn(1)-C(5A)	2.200(15)	O(2)-Sn(1)-C(9B)	95.0(4)
Sn(1)-C(4A)	2.090(6)	C(5A)-Sn(1)-C(9B)	123.0(6)
Sn(2)-O(4)	2.102(3)	O(4)-Sn(2)-C(13A)	97.0(4)
Sn(2)-C(13A)	2.050(16)	O(4)-Sn(2)-C(17A)	92.0(2)
Sn(3)-O(8)	2.110(3)	C(17A)-Sn(2)-C(13B)	130.0(4)

Sn(3)-C(1D)	2.200(2)	O(8)-Sn(3)-C(1C)	102.0(6)
Sn(4)-O(6)	2.112(3)	O(8)-Sn(3)-C(5C)	92.0(4)
Sn(4)-C(1E)	2.120(7)	O(6)-Sn(4)-C(1E)	98.0(2)
N(1)-C(23)	1.390(5)	C(1E)-Sn(4)-C(9F)	130.0(4)

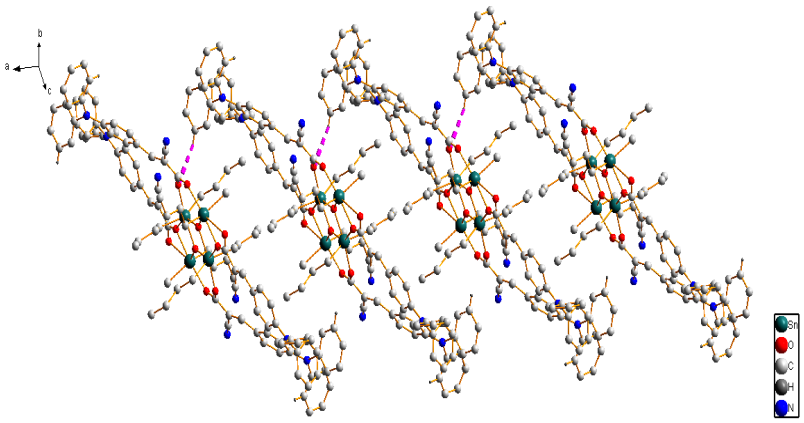

Figure S1. 1D packing diagram of Z1

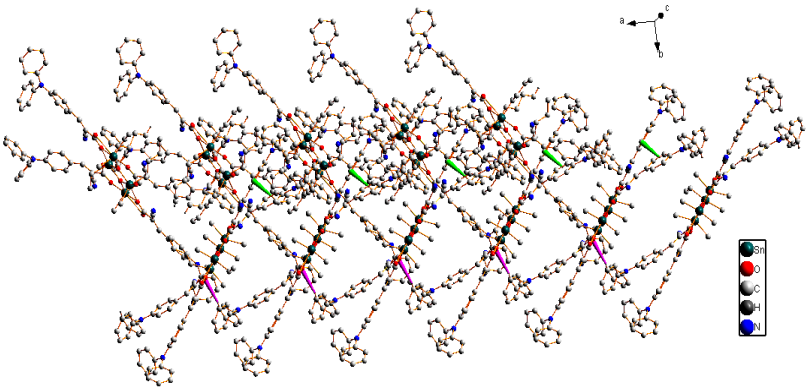

Figure S2. 2D packing diagram of Z1

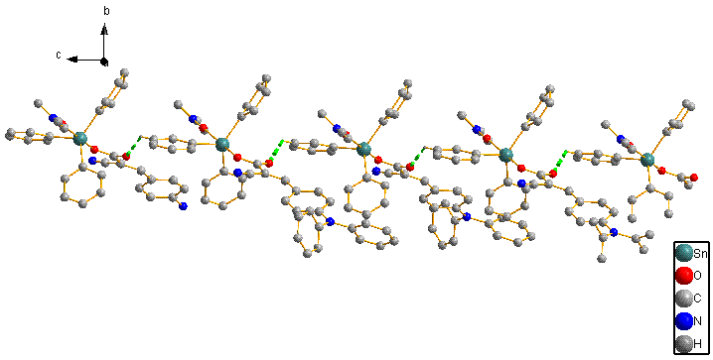

Figure S3. 1-D packing diagram of Z2

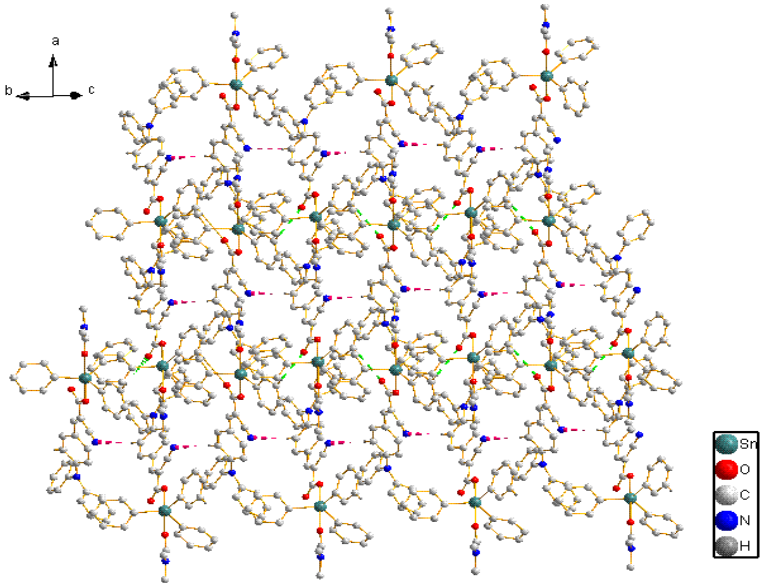

Figure S4. 2D packing diagram of Z2

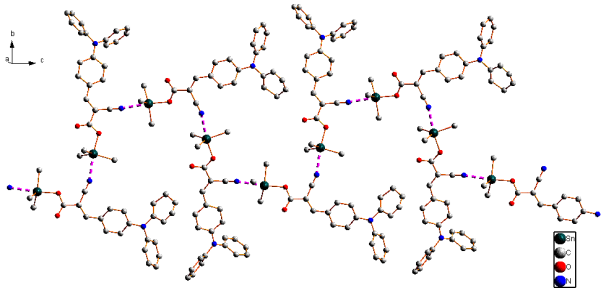

Figure S5. 1D packing diagram of Z3

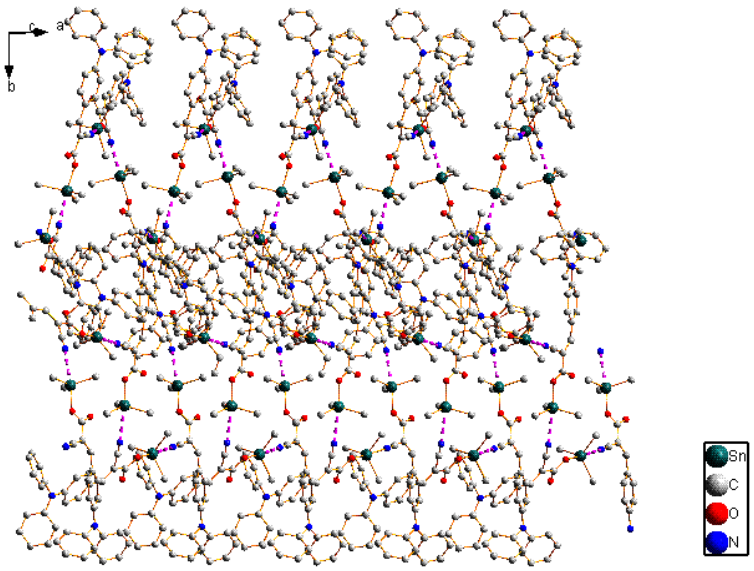

Figure S6. 2D Packing program of Z3

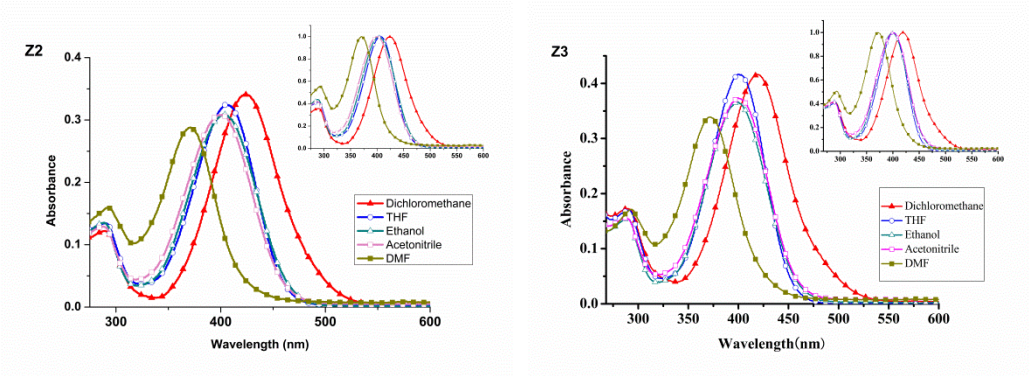

Figure S7. UV-vis absorption spectra of Z2 and Z3 (inset: Normalized absorption)

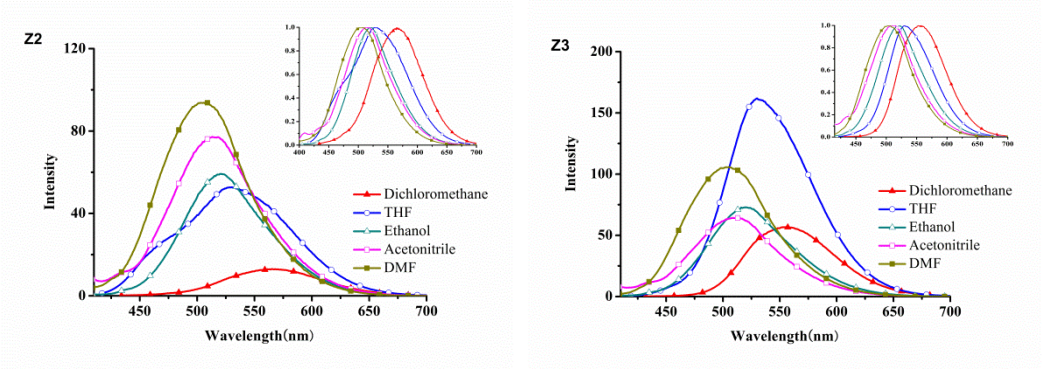

Figure S8. Single-photon excited fluorescence spectra (SPEF) of Z2 and Z3 (inset: Normalized intensity)

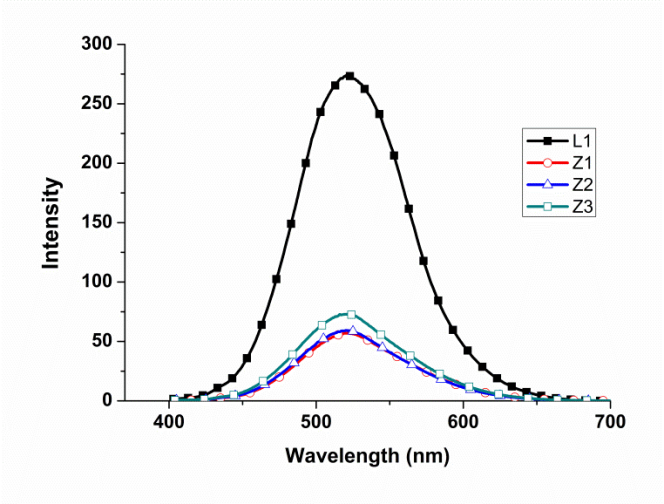

Figure S9. The SPEF of L1 and Z1-Z3 in C_2H_5OH solution

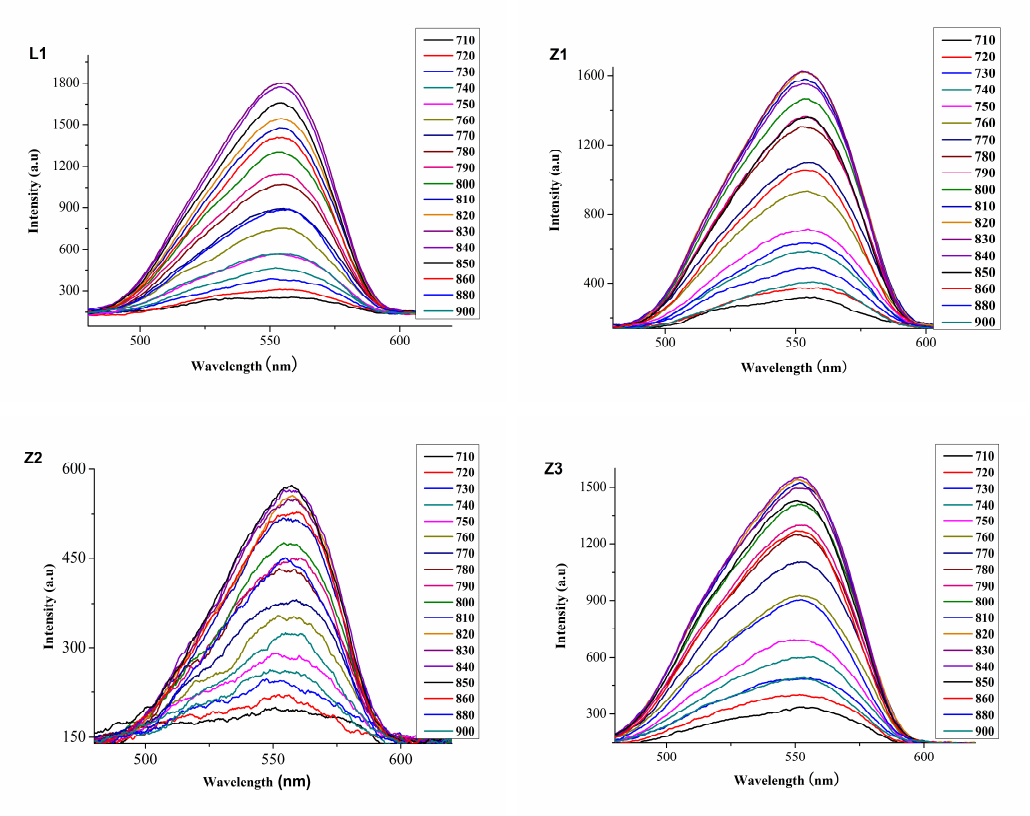

Figure S10. Two-photon exited fluorescence (TPEF) of L1 and Z1-Z3 in THF solution

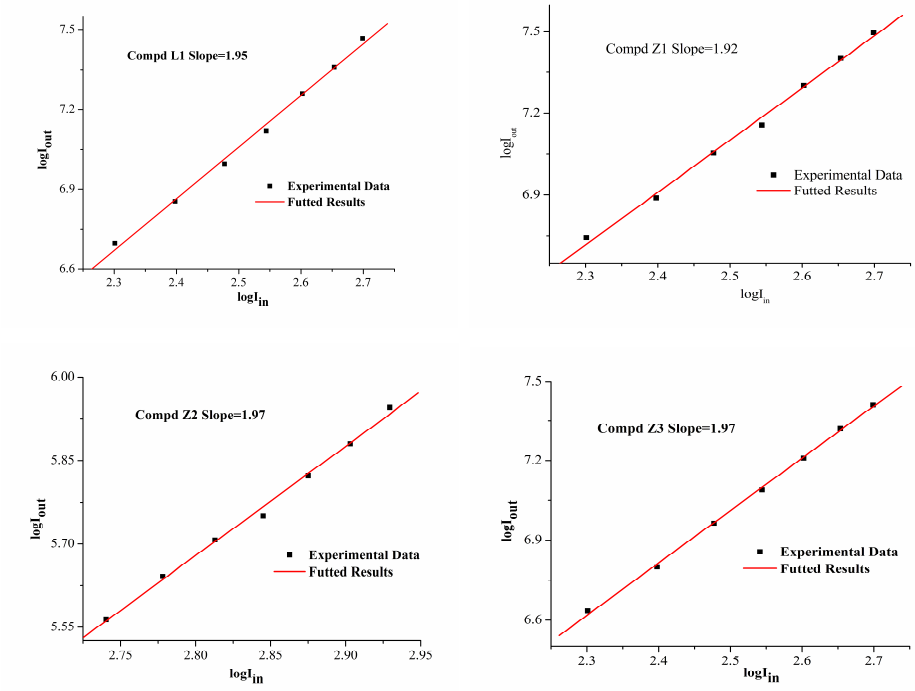

Figure S11. Output fluorescence (Iout) vs. the square of input laser power (Iin) for L1, and Z1-Z3 in THF solution.

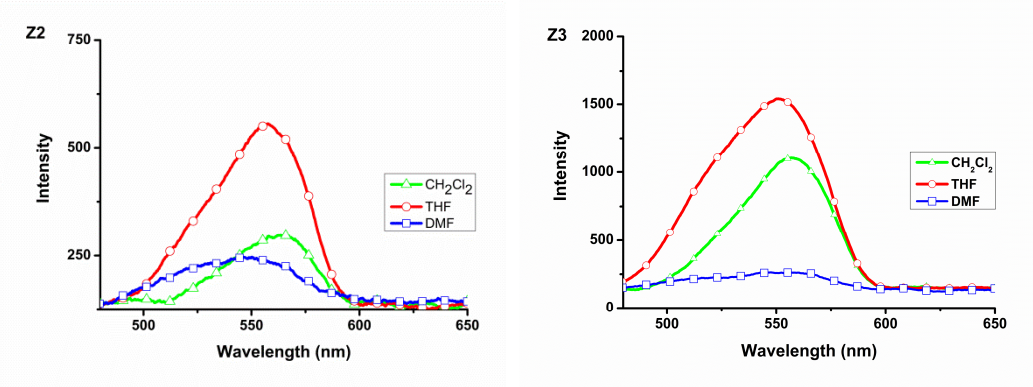

Figure S12. Two-photon exited fluorescence (TPEF) of Z2 and Z3 in different solutions

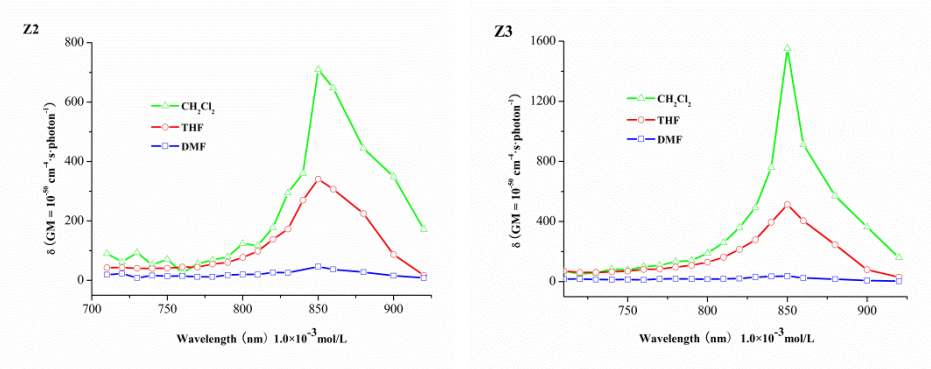

Figure S13. TPA cross-sections of Z2 and Z3 in different solutions

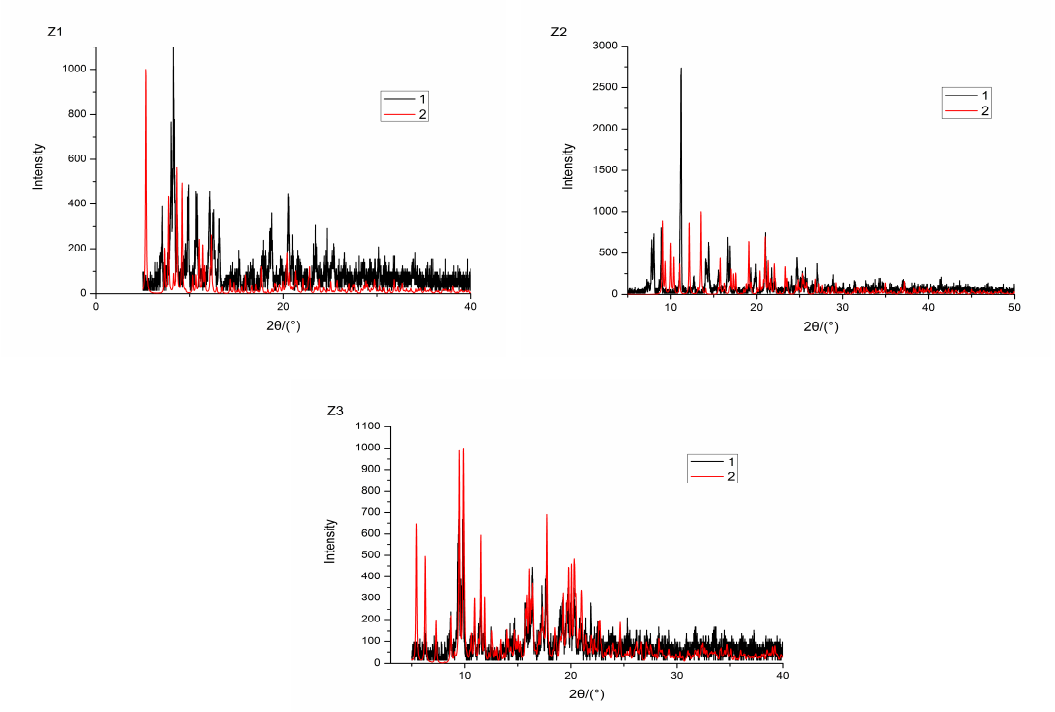

Figure S14. PXRD of three complexes in experimental (1) and theoretical (2)