Supporting information for

Two chiral Co^{III} and Ni^{II} complexes with the identical ligands presenting different nonlinear optical responses

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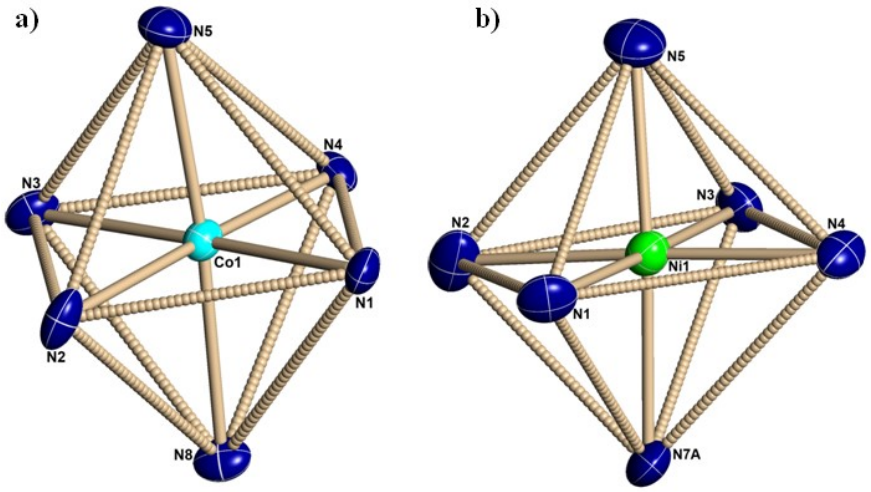

Fig. S1 Coordination geometries of Co1 in **1** (a) and Ni1 in **2** (b).

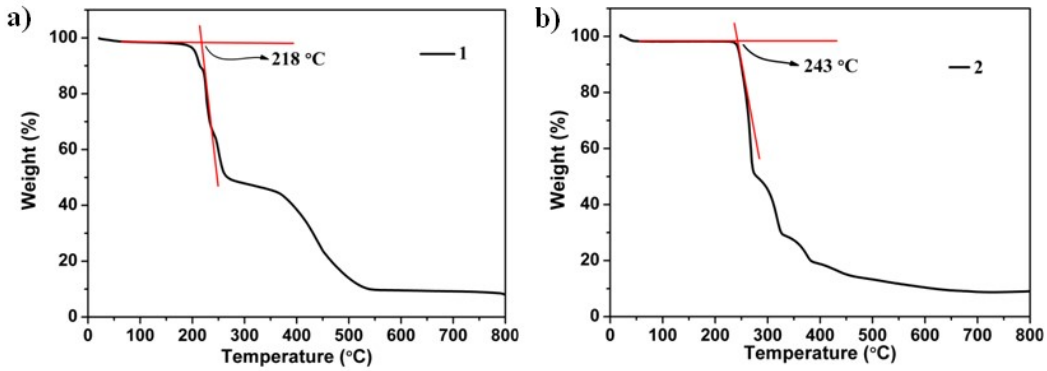

Fig. S2 Thermogravimetric analyses of **1** (a) and **2** (b).

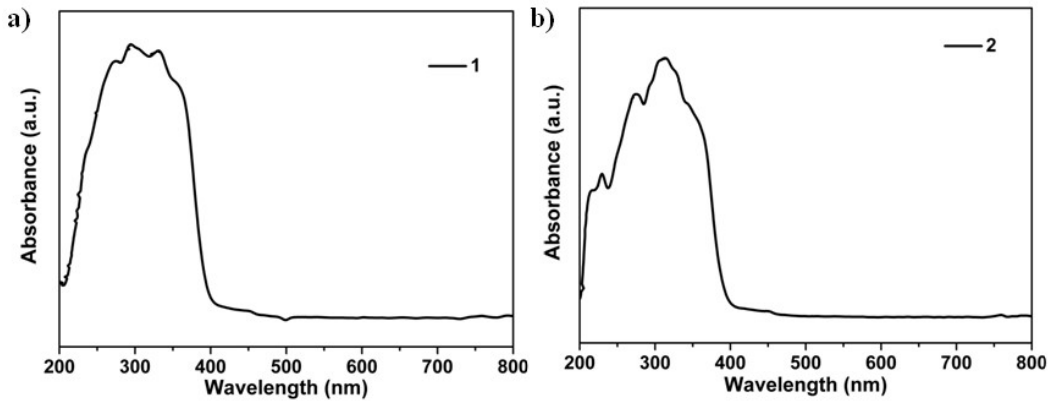

Fig. S3. UV-vis diffuse reflectance spectra of **1** (a) and **2** (b).

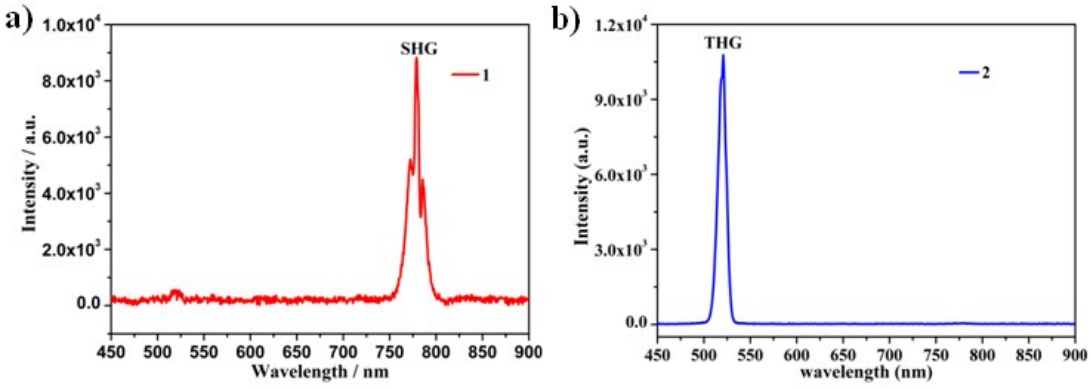

Fig. S4 (a) SHG spectrum of **1**. (b) THG spectrum of **2**. Under the excitation at λ = 1550 nm (T_{int} = 0.5 s) at room temperature.

Table S1 Crystallographic data and structure refinement parameters for **1** and **2**.

Complexes	**1**	**2**
Chemical formula	$C_{28}H_{33}N_{10}O_{4.5}ClCo$	$C_{28}H_{33}N_7O_{4.5}ClNi$
Formula weight	676.02	633.75
Crystal system	triclinic	monoclinic
Space group	*P*1	*Cc*
a (Å)	7.2172(16)	31.575(2)
b (Å)	9.066(2)	6.0167(12)
c (Å)	13.516(3)	17.2771(15)
α (deg)	89.015(3)	90
β (deg)	78.749(4)	116.709(3)
γ (deg)	73.930(3)	90
V (Å^3)	832.8(3)	2932.1(7)
Z	1	2
D_c (g cm^{-3})	1.348	1.436
μ (mm^{-1})	0.645	0.801
F(000)	351	1324
Reflections collected	4211	7520
Independent reflections	3533	4010
Data/restraints/parameters	3533/3/406	4010/3/379
GOF	1.006	1.079
$R_1[I >= 2\sigma(I)]$[a]	0.0567	0.0468
$wR_2[I >= 2\sigma(I)]$[b]	0.1203	0.1165
Flack parameter	0.03(2)	0.015(13)
CCDC	2342450	2342453

[a]$R_1 = \sum||Fo|-|Fc||/\sum|Fo|$. [b]$wR_2 = [\sum w(Fo^2 - Fc^2)^2/\sum w(Fo^2)^2]^{1/2}$

Table S2 Selected bond lengths (Å) and angles (°) for **1** and **2**.

Bond lengths for **1**					
Co(1)─N(1)	1.930(8)	Co(1)─N(2)	1.959(7)	Co(1)─N(3)	1.964(8)
Co(1)─N(4)	1.925(6)	Co(1)─N(5)	1.944(8)	Co(1)─N(8)	1.959(7)
Bond lengths for **2**					
Ni(1)─N(1)	2.118(5)	Ni(1)─N(2)	2.067(6)	Ni(1)─N(3)	2.071(5)
Ni(1)─N(4)	2.176(6)	Ni(1)─N(5)	2.172(6)	Ni(1)─N(7A)	2.183(5)
Symmetry code for A: x, y + 1, z					
Bond angles for **1**					
N(1)-Co(1)-N(2)	85.6(3)	N(3)-Co(1)-N(4)	87.0(3)	N(1)-Co(1)-N(4)	96.1(3)
N(3)-Co(1)-N(2)	91.3(3)	N(5)-Co(1)-N(8)	175.3(4)		
Bond angles for **2**					
N(1)-Ni(1)-N(2)	78.5(2)	N(3)-Ni(1)-N(4)	82.3(2)	N(1)-Ni(1)-N(4)	101.4(2)
N(3)-Ni(1)-N(2)	94.8(2)	N(5)-Ni(1)-N(7A)	173.7(2)		
Symmetry code for A: x, y + 1, z					

Table S3 Calculated dipole moments of **1** and **2**.

Complex	**1**	**2**
μ_{total} (D)	16.1663	26.8221
x	0.5789	–8.2162
y	–16.0616	–23.5702
z	1.7440	–9.8167

Table S4 The coordinates of the calculated structure for **1**.

	x	*y*	*z*
C	3.9910	6.3730	–2.3380
C	2.7570	6.3710	–3.0020
H	1.9910	6.6580	–2.5600
C	2.6800	5.9350	–4.3250
H	1.8620	5.9140	–4.7660
C	3.8400	5.5340	–4.9780
H	3.8030	5.2640	–5.8680
C	5.0530	5.5350	–4.3010
H	5.8230	5.2530	–4.7410
C	5.1340	5.9390	–3.0250
H	5.9560	5.9300	–2.5920
C	4.0830	9.3070	–1.3910
C	3.2880	10.1710	–2.1340
H	2.3750	10.0100	–2.2110
C	3.8520	11.2720	–2.7600
H	3.3230	11.8450	–3.2680
C	5.1750	11.5080	–2.6310
H	5.5420	12.2580	–3.0410
C	6.0140	10.6550	–1.8940
H	6.9270	10.8190	–1.8350
C	5.4480	9.5690	–1.2620
H	5.9790	9.0070	–0.7460
C	2.3430	7.2930	5.8100
C	3.0940	7.5200	6.9380
H	4.0000	7.3080	6.9260
C	2.5480	8.0490	8.0880
H	3.0750	8.1880	8.8420

C	1.2130	8.3660	8.0990
H	0.8400	8.7330	8.8670
C	0.4020	8.1500	6.9780
H	–0.5040	8.3610	6.9940
C	0.9920	7.6080	5.8390
H	0.4710	7.4550	5.0840
C	2.3810	4.3110	5.0790
C	3.5450	3.9110	5.6870
H	4.3340	4.3650	5.4970
C	3.5760	2.8530	6.5710
H	4.3720	2.6060	6.9860
C	2.3790	2.1550	6.8360
H	2.3890	1.4350	7.4240
C	1.1810	2.5300	6.2270
H	0.3900	2.0770	6.4120
C	1.1980	3.5970	5.3400
H	0.4120	3.8430	4.9080
C	4.1170	6.8270	–0.9100
H	5.0690	6.9270	–0.7010
C	3.4180	8.1790	–0.6480
H	2.4680	8.1260	–0.8800
C	2.9560	6.6860	4.6240
H	3.8870	6.4790	4.8520
C	2.3290	5.4070	4.0710
H	1.3850	5.5950	3.8850
Cl	5.3150	2.1130	1.6110
Co	3.2460	6.7340	1.7730
N	3.5230	5.8810	0.0640
H	4.0640	5.1820	0.1660

H	2.7440	5.5840	–0.2490
N	3.5910	8.4120	0.8230
H	3.0230	9.0390	1.0980
H	4.4190	8.6900	0.9890
N	2.9830	7.6950	3.4670
H	3.6440	8.2770	3.5880
H	2.2160	8.1450	3.4410
N	2.9920	5.1090	2.7740
H	2.4910	4.5440	2.3040
H	3.7800	4.7230	2.9220
N	1.3240	6.8980	1.5250
N	0.7920	6.6940	0.5050
N	0.2900	6.5760	–0.4540
N	5.1910	6.7280	2.0050
N	5.6470	6.1530	2.9140
N	6.1890	5.6650	3.8070
O	3.9320	1.7280	1.7500
O	6.0490	1.7410	2.7860
O	5.8870	1.4850	0.4440
O	5.3680	3.5320	1.4760
O	8.4610	3.6030	0.6290
H	7.7230	3.2500	0.8600
H	8.4250	4.4430	0.7540

Table S5 The coordinates of the calculated structure for **2**.

	x	*y*	*z*
C	10.3030	2.7330	1.7890
C	10.0410	3.7570	0.9660
H	10.0860	4.6320	1.2780
C	9.7080	3.5070	–0.3360
H	9.5680	4.2240	–0.9120
C	9.5670	2.2060	–0.8290
H	9.3170	2.0550	–1.7120
C	9.8140	1.1590	0.0170
H	9.7470	0.2850	–0.2950
C	10.1610	1.4020	1.3550
H	10.2980	0.6950	1.9430
C	8.4820	2.3300	4.0580
C	7.4530	3.2420	4.1020
H	7.6290	4.1310	4.3110
C	6.1430	2.8390	3.8370
H	5.4540	3.4580	3.8950
C	5.8550	1.5110	3.4800
H	4.9850	1.2450	3.2830
C	6.8760	0.6380	3.4360
H	6.6950	–0.2450	3.2100
C	8.1910	0.9950	3.7090
H	8.8710	0.3620	3.6610
C	13.7980	3.6540	9.4520
C	13.8000	2.3580	10.0440
H	13.5530	1.6190	9.5360
C	14.1470	2.1970	11.3050
H	14.1540	1.3380	11.6620

C	14.4930	3.2490	12.1110
H	14.7540	3.1030	12.9920
C	14.4540	4.5320	11.5940
H	14.6460	5.2600	12.1400
C	14.1260	4.7310	10.2740
H	14.1210	5.5940	9.9270
C	16.0980	3.8250	7.3790
C	16.5400	2.6350	7.9870
H	15.9220	1.9600	8.1550
C	17.8380	2.4420	8.3370
H	18.1060	1.6670	8.7770
C	18.7380	3.4230	8.0240
H	19.6280	3.3030	8.2630
C	18.3830	4.5720	7.3740
H	19.0250	5.2060	7.1460
C	17.0540	4.7680	7.0660
H	16.7960	5.5520	6.6360
C	10.7420	2.9930	3.1890
H	10.9120	3.9570	3.2130
C	9.8930	2.7450	4.3720
H	9.7580	3.6530	4.7170
C	13.5000	3.8450	7.9980
H	13.1470	4.7600	8.0210
C	14.6930	4.0470	7.0150
H	14.6720	5.0170	6.8740
Cl	10.5020	0.2410	9.9040
N	12.0600	2.3710	3.5400
H	12.7220	2.6940	3.0420
H	12.0390	1.4840	3.4710

N	10.3700	2.0490	5.5530
H	10.4390	1.1700	5.4340
H	9.8840	2.2260	6.2800
N	12.3210	3.1460	7.6180
H	11.6070	3.5730	7.9310
H	12.3320	2.3290	7.9730
N	14.3040	3.5430	5.6900
H	14.7980	2.8270	5.4990
H	14.4850	4.1660	5.0810
N	12.8880	0.9700	5.8740
N	12.3430	–0.0240	5.5920
N	11.7110	–0.8940	5.3460
Ni	12.2010	3.0060	5.5560
O	9.8420	–0.9980	10.2430
O	11.2710	0.0320	8.6950
O	11.4050	0.6060	10.9900
O	9.5240	1.2730	9.6680
O	9.6460	3.8720	7.7200
H	9.7010	3.5970	6.9190
H	10.4080	4.1300	7.9870