Supporting Information for

Two temperature-induced 1D Cu^{II} chain enantiomeric pairs showing different magnetic properties and nonlinear optical responses

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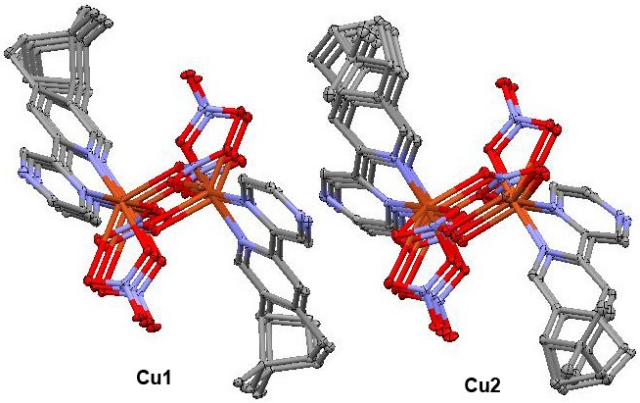

Fig. S1. The topologies of 1D helical Cu1 and Cu2 chains in ***S*-1-Cu** running along the crystallographic *b*-axis. Color code: Cu, orange; N, blue; O, red; C, gray. H atoms are omitted for clarity.

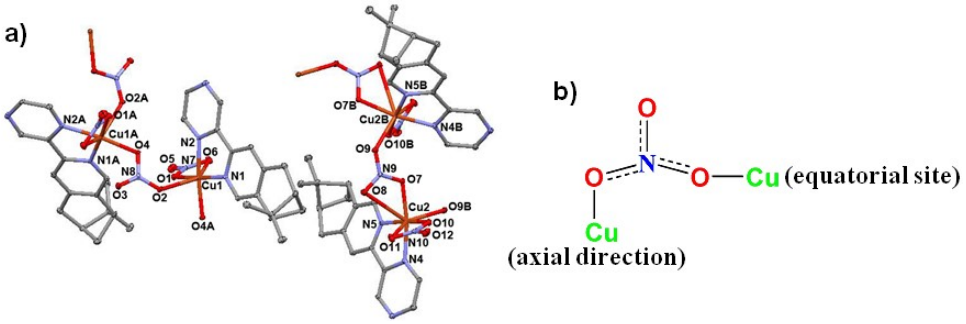

Fig. S2. (a) The coordination fashions of Cu^{II} ions in ***S*-1-Cu** (symmetry codes: A = $-x$, y + 1/2, $-z$; B = $-x$ + 1, y + 1/2, $-z$ + 1), and H atoms are removed for clarity. (b) The bridging fashion of the NO_3^- anion in ***S*-1-Cu**.

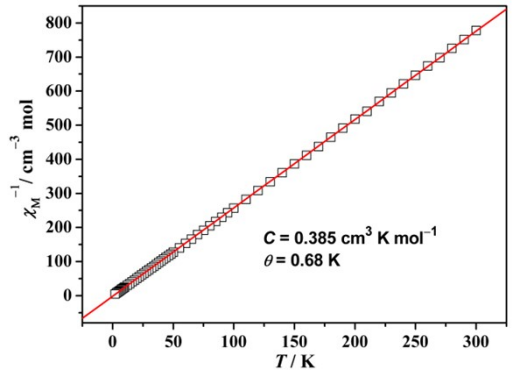

Fig. S3. χ_M^{-1} vs. *T* plot of ***S*-1-Cu**, the solid red lines represent the best fitting to the data.

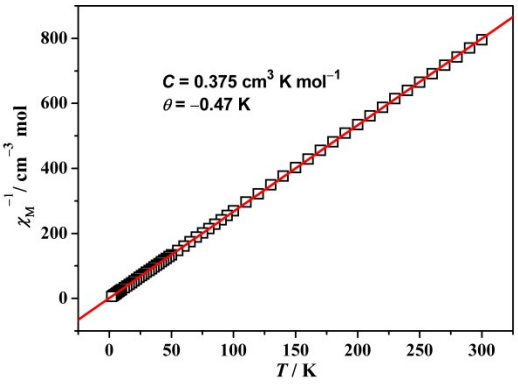

Fig. S4. χ_M^{-1} vs. *T* plot of ***S*-2-Cu**, the solid red lines represent the best fitting to the data.

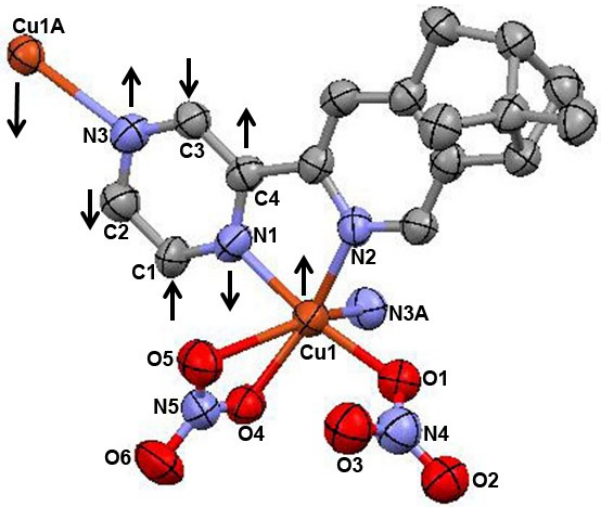

Fig. S5. Schematic representation of the spin polarization mechanism between two adjacent Cu^{II} spin centers bridged by a pyrazine (pyz) moiety in ***S*-2-Cu**.

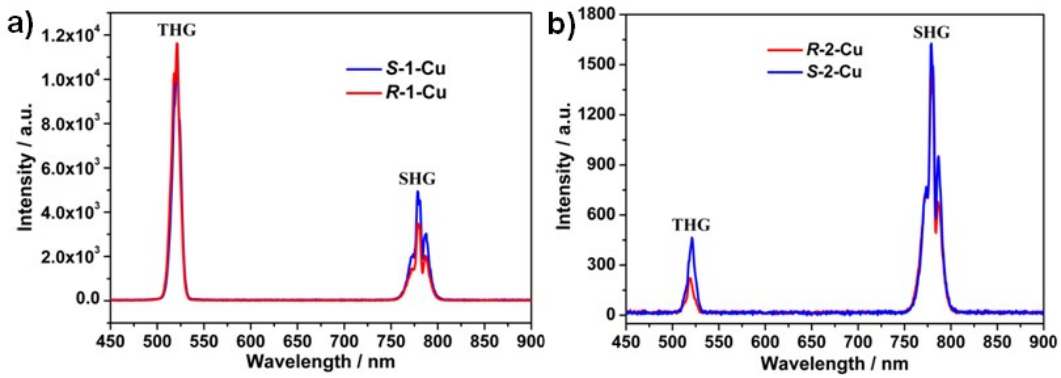

Fig. S6 THG and SHG spectra of ***S*-1-Cu/*R*-1-Cu** (a) and ***S*-2-Cu/*R*-2-Cu** (b) based on crystalline samples under excitation at λ = 1550 nm (T_{int} = 0.5 s).

Table S1 Crystallographic data and structure refinement parameters for ***S*-1-Cu/ *R*-1-Cu** and ***S*-2-Cu/*R*-2-Cu** enantiomeric pairs.

Complex	***R*-1-Cu**	***S*-1-Cu**	***R*-2-Cu**	***S*-2-Cu**
Chemical formula	$C_{16}H_{17}N_5O_6Cu$	$C_{16}H_{17}N_5O_6Cu$	$C_{16}H_{17}N_5O_6Cu$	$C_{16}H_{17}N_5O_6Cu$
Formula weight	438.88	438.88	438.88	438.88
Crystal system	monoclinic	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	10.4167(9)	10.4166(9)	11.307(3)	10.5166(3)
b (Å)	9.0382(8)	9.0426(8)	12.101(3))	12.0542(5)
c (Å)	19.3517(16)	19.3600(18)	13.657(3)	14.3380(4)
β (deg)	105.2740(10)	105.247(2)	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$
V(Å^3)	1757.6(3)	1759.4(3)	1868.6(8)	1817.62(10)
Z	4	4	4	4
D_c(g cm^{-3})	1.659	1.657	1.560	1.604
μ (mm^{-1})	1.290	1.289	1.213	2.115
F(000)	900	900	900	900
Reflections collected	16980	17024	9089	7422
Independent reflections	7876	8143	4285	2782
Data/restraints/parameters	7876/1/510	8143/1/510	4285/0/256	2782/0/256
GOF	1.011	1.033	1.034	1.100
R_1 [$I >= 2\sigma$ (I)][a]	0.0416	0.0453	0.0472	0.0451
wR_2 [$I >= 2\sigma$ (I)][b]	0.0798	0.0911	0.1191	0.1009
Flack parameter	0.033(14)	0.020(15)	0.02(2)	0.03(5)
CCDC	2216907	2216908	2216909	2216910

[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) for ***R*-1-Cu/*S*-1-Cu** and ***R*-2-Cu/*S*-2-Cu**.

Bond lengths for ***R*-1-Cu**

Cu(1)─O(1)	1.966(4)	Cu(1)─O(2)	2.000(3)	Cu(1)─O(4A)	2.238(3)
Cu(2)─O(7)	1.990(3)	Cu(2)─O(10)	1.975(3)	Cu(2)─O(9B)	2.309(3)
Cu(1)─N(1)	1.982(4)	Cu(1)─N(2)	2.005(4)	Cu(2)─N(4)	2.004(4)
Cu(2)─N(5)	2.010(3)				

Symmetry Codes for A: $-x, y - 1/2, -z + 1$; B: $-x + 1, y + 1/2, -z + 2$

Bond lengths for ***S*-1-Cu**

Cu(1)─O(1)	1.977(4)	Cu(1)─O(2)	2.317(3)	Cu(1)─O(4A)	2.418(4)
Cu(2)─O(7)	2.002(4)	Cu(2)─O(10)	1.969(4)	Cu(2)─O(9B)	2.281(3)
Cu(1)─N(1)	2.010(5)	Cu(1)─N(2)	2.008(4)	Cu(2)─N(4)	2.003(4)
Cu(2)─N(5)	1.989(4)				

Symmetry Codes for A: $-x, y + 1/2, -z$; B = $-x + 1, y + 1/2, -z + 1$

Bond lengths for ***R*-2-Cu**

Cu(1)─O(1)	1.974(4)	Cu(1)─O(4)	1.978(4)	Cu(1)─N(1)	1.994(4)
Cu(1)─N(2)	2.000(4)	Cu(1)─N(3A)	2.350(4)		

Symmetry Codes for A: $x + 1/2, -y + 1/2, -z + 2$

Bond lengths for ***S*-2-Cu**

Cu(1)─O(1)	1.965(3)	Cu(1)─O(4)	1.986(3)	Cu(1)─N(1)	2.007(3)
Cu(1)─N(2)	1.999(4)	Cu(1)─N(3A)	2.535(6)		

Symmetry Codes for A: $x + 1/2, -y + 1/2, -z + 2$

Table S3 Selected bond angles (°) for ***R*-1-Cu**/***S*-1-Cu** and ***R*-2-Cu**/***S*-2-Cu**.

Bond angles for ***R*-1-Cu**

O(1)-Cu(1)-O(2)	90.47(14)	O(1)-Cu(1)-N(2)	93.86(16)	O(2)-Cu(1)-N(1)	93.50(15)
N(1)-Cu(1)-N(2)	81.41(17)	O(7)-Cu(2)-O(10)	90.00(13)	O(7)-Cu(2)-N(5)	92.44(14)
O(10)-Cu2-N(4)	95.82(14)	N(4)-Cu(2)-N(5)	81.54(15)		

Bond angles for ***S*-1-Cu**

O(1)-Cu(1)-O(2)	84.14(14)	O(1)-Cu(1)-N(2)	95.95(17)	O(2)-Cu(1)-N(1)	100.51(15)
N(1)-Cu(1)-N(2)	81.49(18)	O(7)-Cu(2)-O(10)	90.16(15)	O(7)-Cu(2)-N(5)	93.24(16)
O(10)-Cu2-N(4)	94.57(16)	N(4)-Cu(2)-N(5)	81.35(17)		

Bond angles for ***R*-2-Cu**

O(1)-Cu(1)-O(4)	88.76(15)	O(4)-Cu(1)-N(1)	96.57(16)	O(1)-Cu(1)-N(2)	94.19(15)
N(1)-Cu(1)-N(2)	80.47(16)				

Bond angles for ***S*-2-Cu**

O(1)-Cu(1)-O(4)	92.43(14)	O(4)-Cu(1)-N(1)	93.87(17)	O(1)-Cu(1)-N(2)	96.11(15)
N(1)-Cu(1)-N(2)	80.72(18)				