# Canted Antiferromagnetic Behaviors in Isostructural Co(II) and Ni(II) Frameworks with Helical lvt Topology

Qipu Lin, Jian Zhang, Xinyi Cao, Yuangen Yao*, Zhaoji Li, Lei Zhang and Zhangfeng Zhou

*State Key Laboratory of Structural Chemistry, Fujian institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, P.R. China, yyg@fjirsm.ac.cn*

**Table S1**. Crystal Data and Structure Refinements for Complexes **1Co** and **2Ni**.

| | | |
|---|---|---|
| Formula | $C_{12}H_{12}N_8CoO_3$ | $C_{12}H_{12}N_8NiO_3$ |
| Formula weight | 375.23 | 374.99 |
| Space group | *I*4(1)/a(No.88) | *I*4(1)/a(No.88) |
| *a*(Å) | 15.6671(2) | 15.5470(10) |
| *b*(Å) | 15.6671(2) | 15.5470(10) |
| *c*(Å) | 12.6333(2) | 12.4988(13) |
| *α*(º) | 90 | 90 |
| *β*(º) | 90 | 90 |
| *γ*(º) | 90 | 90 |
| *V*(Å$^3$) | 3100.95(7) | 3021.1(4) |
| *Z* | 8 | 8 |
| $D_{calc}$(g cm$^3$) | 1.607 | 1.649 |
| *μ*(Mo*K*α)( mm$^{-1}$) | 1.138 | 1.316 |
| Crystal size(mm) | 0.22×0.16×0.10 | 0.20×0.15×0.10 |
| *F*(000) | 1528 | 1536 |
| Reflections collected | 8265 | 11479 |
| Independent reflections | 1476($R_{int}$=0.0307) | 1735 ($R_{int}$=0.0321) |
| Observed data[$I$ >2σ($I$)] | 1372 | 1634 |
| Data/restraints/parameters | 1476 / 6 / 112 | 1735 / 6 / 112 |
| GOF on $F^2$ | 1.003 | 1.007 |
| $R_1$, w$R_2$ ($I$ >2σ($I$))[a] | 0.0416, 0.0899 | 0.0392, 0.0979 |
| $R_1$, w$R_2$ ( all data )[a] | 0.0459, 0.0921 | 0.0416, 0.1000 |

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$, $wR_2 = \{\sum w[(F_o)^2 - (F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$.

**Table S2**. Important Bond Lenghts (Å) and angles (deg) for **1Ni** and **2Co**.

| | | | |
|---|---|---|---|
| **1Co** | | | |
| Co(1)-N(1)#1 | 2.109(2) | Co(1)-O(71) | 2.161(2) |
| Co(1)-N(1) | 2.109(2) | Co(1)-O(71)#1 | 2.161(2) |
| Co(1)-N(3)#2 | 2.130(2) | N(3)-Co(1)#4 | 2.130(2) |
| Co(1)-N(3)#3 | 2.130(2) | | |
| N(1)#1-Co(1)-N(1) | 180.00(10) | N(3)#2-Co(1)-O(71) | 88.98(9) |
| N(1)#1-Co(1)-N(3)#2 | 89.39(9) | N(3)#3-Co(1)-O(71) | 91.02(9) |
| N(1)-Co(1)-N(3)#2 | 90.61(9) | N(1)#1-Co(1)-O(71)#1 | 78.63(8) |
| N(1)#1-Co(1)-N(3)#3 | 90.61(9) | N(1)-Co(1)-O(71)#1 | 101.37(8) |
| N(1)-Co(1)-N(3)#3 | 89.39(9) | N(3)#2-Co(1)-O(71)#1 | 91.02(9) |
| N(3)#2-Co(1)-N(3)#3 | 180.0 | N(3)#3-Co(1)-O(71)#1 | 88.98(9) |
| N(1)#1-Co(1)-O(71) | 101.37(8) | O(71)-Co(1)-O(71)#1 | 180.0 |
| N(1)-Co(1)-O(71) | 78.63(8) | | |
| **2Ni** | | | |
| Ni(1)-N(1)#1 | 2.0654(18) | Ni(1)-O(71) | 2.1184(17) |
| Ni(1)-N(1) | 2.0654(18) | Ni(1)-O(71)#1 | 2.1184(17) |
| Ni(1)-N(3)#2 | 2.1132(18) | N(3)-Ni(1)#4 | 2.1132(18) |
| Ni(1)-N(3)#3 | 2.1132(18) | | |
| N(1)#1-Ni(1)-N(1) | 180.00(9) | N(3)#2-Ni(1)-O(71)#1 | 89.36(7) |
| N(1)#1-Ni(1)-N(3)#2 | 90.74(7) | N(3)#3-Ni(1)-O(71)#1 | 90.64(7) |
| N(1)-Ni(1)-N(3)#2 | 89.26(7) | N(1)#1-Ni(1)-O(71) | 99.69(7) |
| N(1)#1-Ni(1)-N(3)#3 | 89.26(7) | N(1)-Ni(1)-O(71) | 80.31(7) |
| N(1)-Ni(1)-N(3)#3 | 90.74(7) | N(3)#2-Ni(1)-O(71) | 90.64(7) |
| N(3)#2-Ni(1)-N(3)#3 | 180.00(9) | N(3)#3-Ni(1)-O(71) | 89.36(7) |
| N(1)#1-Ni(1)-O(71)#1 | 80.31(7) | O(71)#1-Ni(1)-O(71) | 180.00(9) |
| N(1)-Ni(1)-O(71)#1 | 99.69(7) | | |

Symmetry transformations used to generate equivalent atoms:
**1Co**: #1 -x+1/2,-y+1/2,-z+1/2; #2 y+1/4,-x+1/4,z+1/4; #3 -y+1/4,x+1/4,-z+1/4.
**2Ni**: #1 -x,-y+1,-z; #2 -y+1/4,x+1/4,-z+1/4; #3 y-1/4,-x+3/4,z-1/4; #4 -y+3/4,x+1/4,z+1/4.

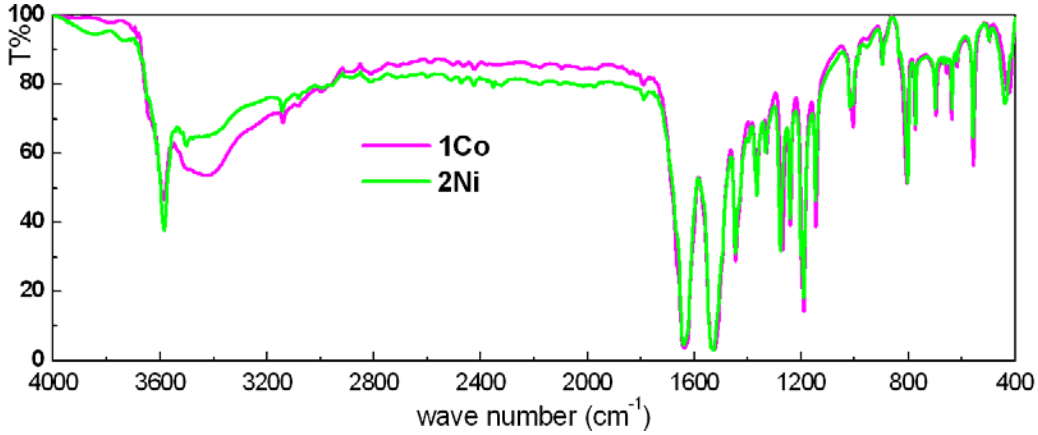


**Figure S1**. IR spectra of **1Co** (magenta), **2Ni** (green).

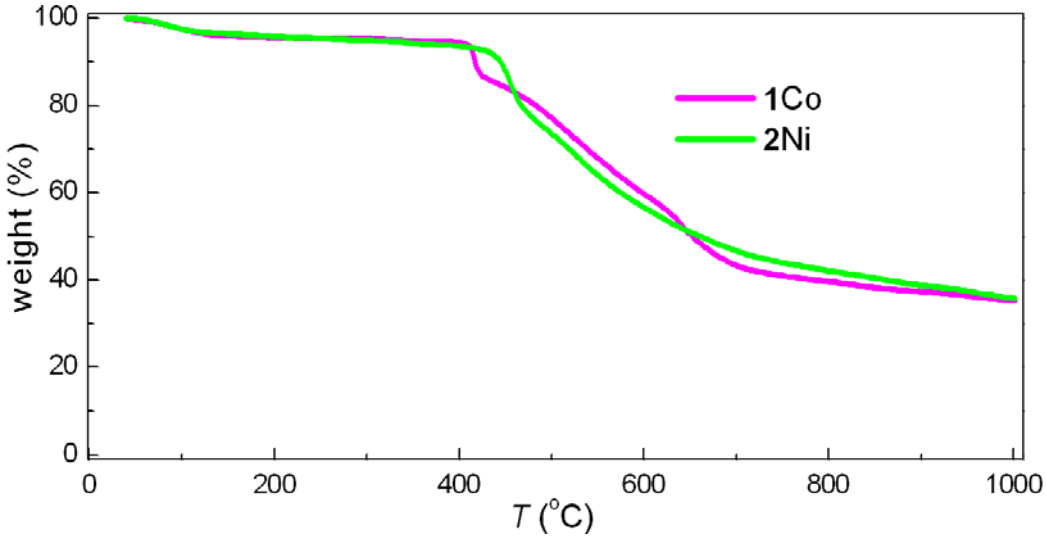


**Figure S2**. The TG curves of **1Co** (magenta), **2Ni** (green).

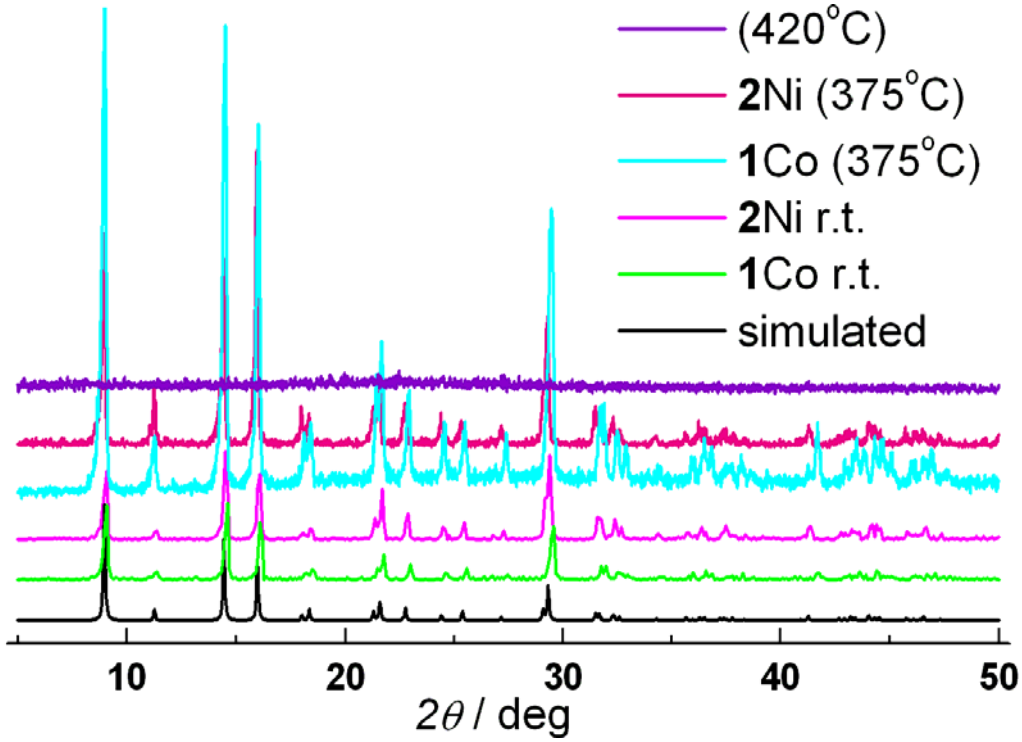


**Figure S3**. Simulated and measured XRD powder patterns for **1Co**, **2Ni** before and after heated to 375 and 420℃, respectively.

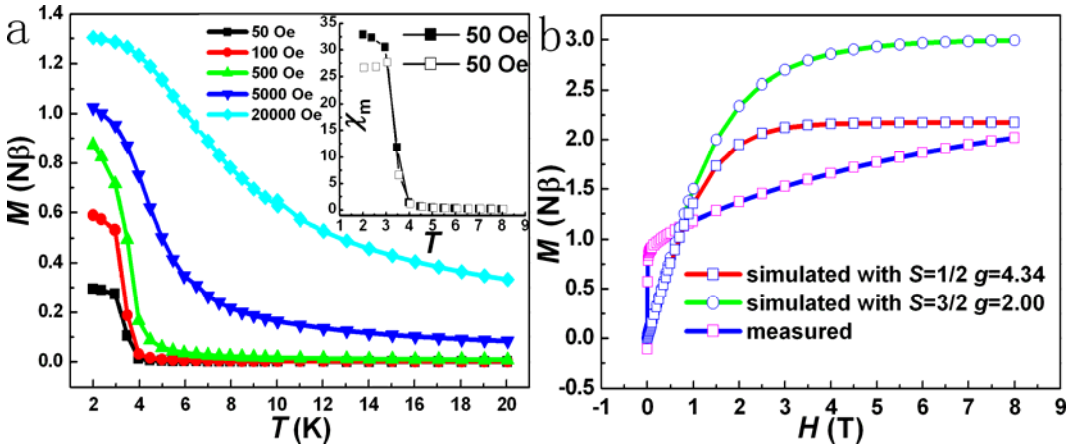


**Figure S4**. left: Plots of *M* vs. *T* under various fields (inset: FC and ZFC (*H* = 100 Oe) magnetization); right: Isothermal magnetization (measured and simulated) at 2 K for **1Co**.

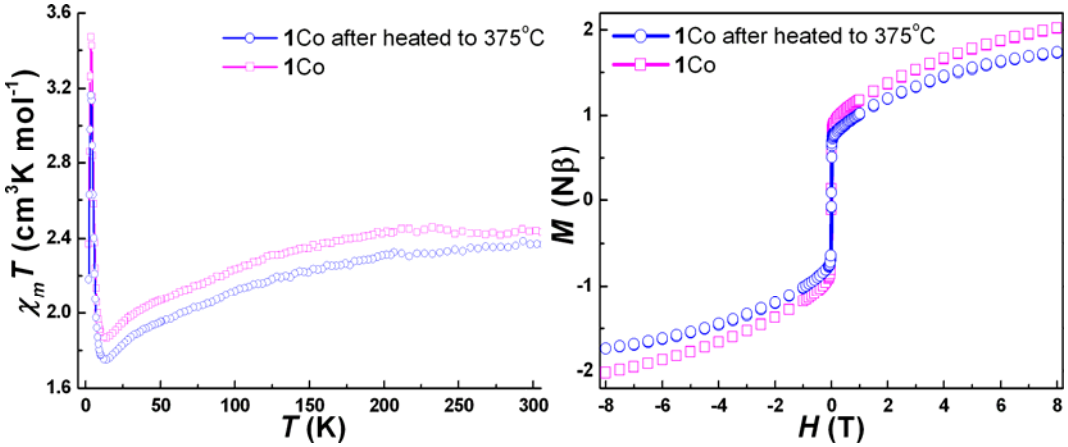


**Figure S5**. left: Plots of $\chi_m T$ vs. $T$; right: Isothermal magnetization for **1Co** before and after heated to 375℃, respectively.

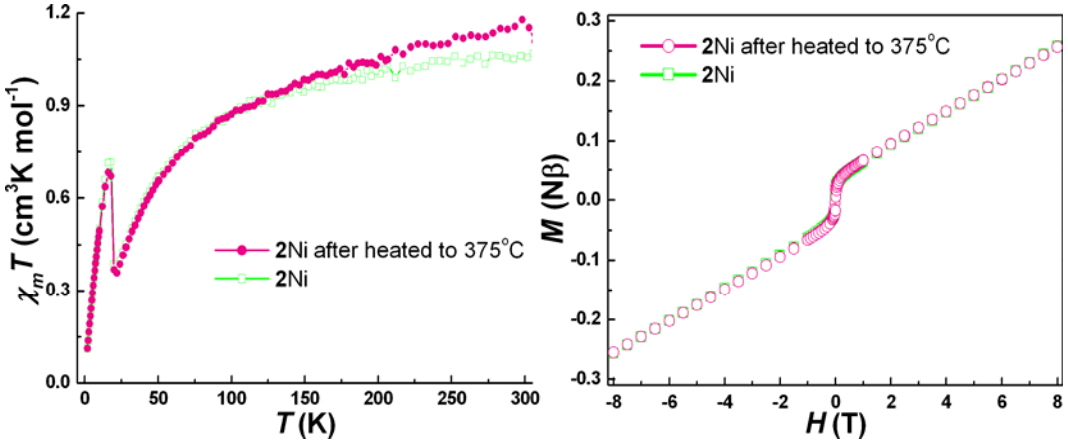


**Figure S6**. left: Plots of $\chi_m T$ vs. $T$; right: Isothermal magnetization for **2Ni** before and after heated to 375℃, respectively.