

Supporting Materials

Title:

Structural phase transition driven by spin-lattice interaction in a Quasi-one-dimensional Spin System of [1-(4'-iodobenzyl)pyridinium][Ni(mnt)₂]

X. M. Ren ^{*§} T. Akutagawa [§] S. Nishihara [‡] T. Nakamura ^{*§} W. Fujita [⊥]
K. Awaga [‡]

Research Institute for Electronic Science, Hokkaido University, Sapporo 060-0812, Japan
and CREST, Japan Science and Technology Corporation (JST), Kawaguchi 332-0012,
Japan

Department of Chemistry, Graduate School of Science, Nagoya University, Chikusa-ku,
Nagoya 464-8602, Japan

Research Center of Materials Science, Nagoya University, Chikusa-ku, Nagoya, 464-
8602, Japan

Tel: 0081 11-706-2849

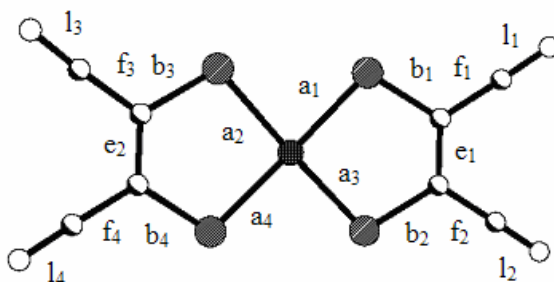
Fax: 0081 11-706-4972

Email: xmren@es.hokudai.ac.jp; tnaka@imd.es.hokudai.ac.jp

This supporting material includes the information:

- ✚ Table S1 bond lengths (Å) in an anion for **1** and **2**
- ✚ Figure S1 the single crystal magnetic susceptibility of **1**.
- ✚ Figure S2 Magnetic susceptibility of **2**.

Table S1 bond distances (Å) in an anion for **1** and **2**



	1 (293 K)	1 (100 K) *	1 (100)**	2 (293K)	2 (100K)
a ₁	2.1554(14)	2.143(9)	2.123(10)	2.1821(13)	2.1879(12)
a ₂	2.1627(14)	2.103(9)	2.133(10)	2.1815(13)	2.1871(12)
a ₃	2.1515(14)	2.150(10)	2.143(9)	2.1744(13)	2.1824(12)
a ₄	2.1489(14)	2.144(9)	2.137(9)	2.1871(13)	2.1946(12)
b ₁	1.724(5)	1.70(3)	1.67(4)	1.726(4)	1.744(4)
b ₂	1.722(5)	1.70(4)	1.69(4)	1.733(5)	1.737(4)
b ₃	1.727(5)	1.74(3)	1.75(3)	1.729(5)	1.740(4)
b ₄	1.715(5)	1.69(3)	1.73(3)	1.739(5)	1.744(4)
e ₁	1.363(7)	1.42(5)	1.46(5)	1.351(6)	1.350(6)
e ₂	1.384(6)	1.49(4)	1.34(5)	1.359(6)	1.350(6)
f ₁	1.435(7)	1.40(4)	1.42(5)	1.421(6)	1.434(5)
f ₂	1.442(7)	1.40(5)	1.43(4)	1.424(6)	1.441(5)
f ₃	1.431(8)	1.45(4)	1.35(5)	1.422(6)	1.442(6)
f ₄	1.436(7)	1.49(4)	1.34(5)	1.425(7)	1.433(5)
l ₁	1.146(7)	1.16(4)	1.12(5)	1.144(6)	1.150(5)
l ₂	1.148(7)	1.20(4)	1.07(4)	1.142(7)	1.143(5)
l ₃	1.149(7)	1.13(4)	1.17(5)	1.131(7)	1.144(5)
l ₄	1.143(7)	1.16(4)	1.20(5)	1.135(7)	1.149(5)

* and ** indicate the anion containing Ni(1) and Ni(2), respectively.

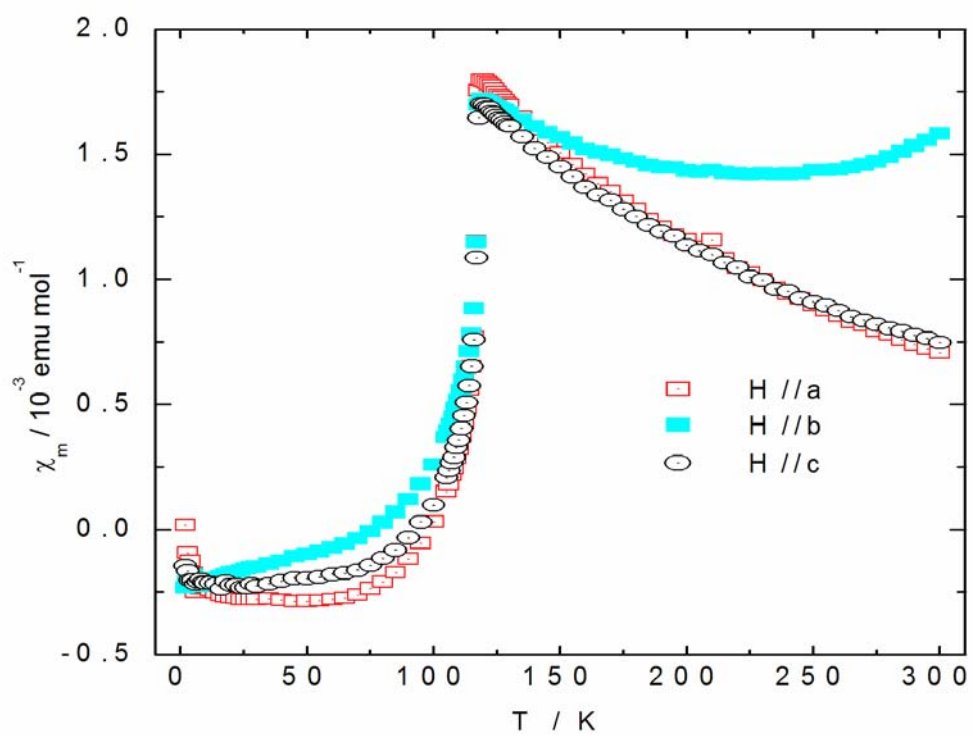


Figure S1. Single crystal magnetic susceptibilities of **1** (applied magnetic field is parallel to *a*-, *b*- and *c*-axis of the crystal, respectively).

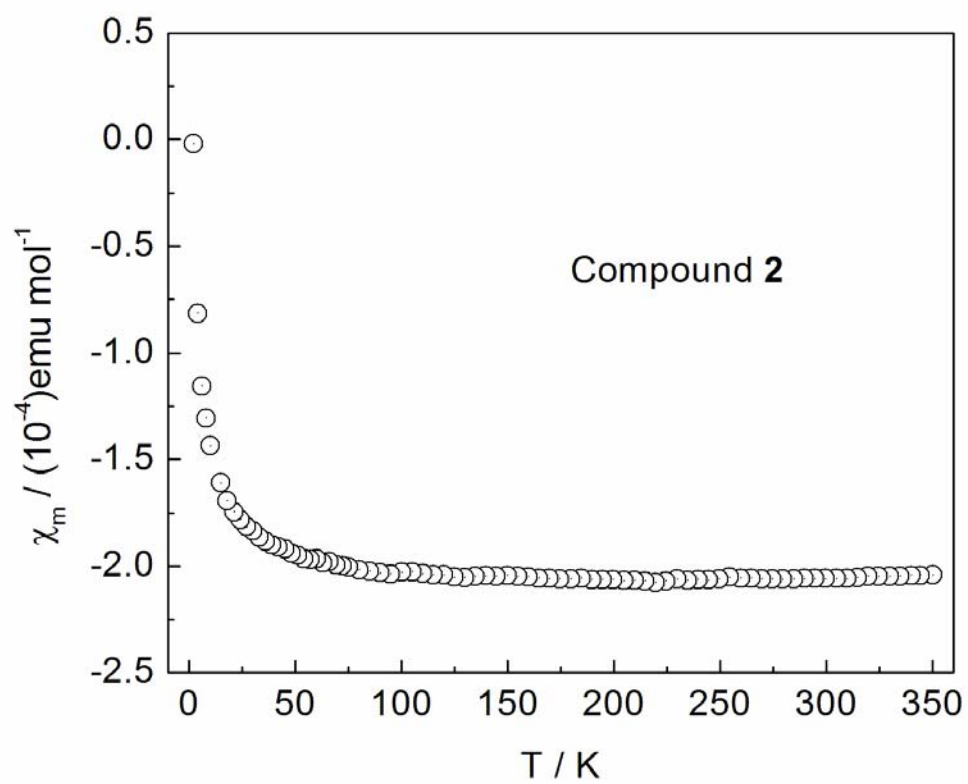


Figure S2 temperature dependent magnetic susceptibility of compound **2**.