Supplementary Materials: Spin-Crossover Behavior of a Hofmann-Type-Like Complex Fe(4,4′-bipyridine)Ni(CN)$_4$·*n*H$_2$O Depending on Guest Species

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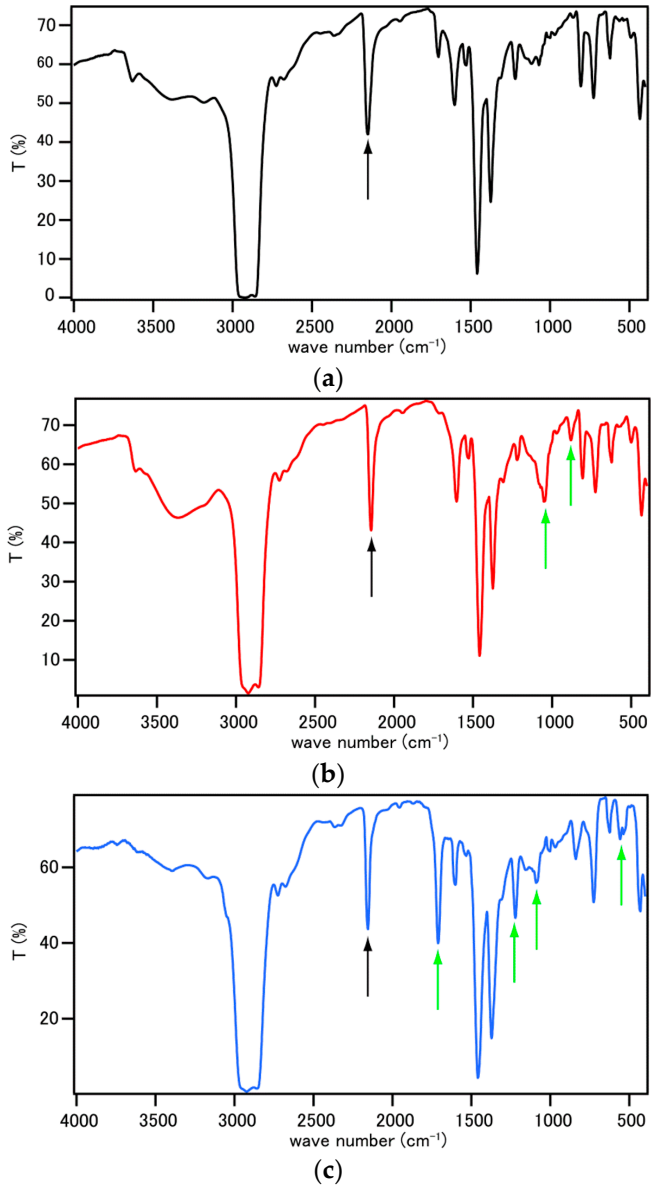

Figure S1. (**a**) Infrared (IR) spectra of Fe(bpy)Ni(CN)$_4$·*n*H$_2$O (*n* = 2.5) (**1**); (**b**) **2** (**1** exposed to ethanol vapor) and (**c**) **3** (**1** exposed to acetone vapor). Stretching band of band C≡N is marked with black arrow. Characteristic signals of included guest compounds are marked with green arrows.

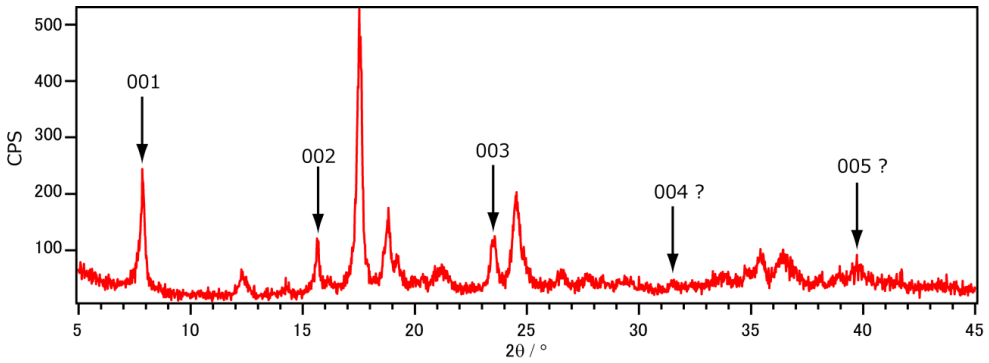

Figure S2. Powder X-ray diffraction pattern of Fe(bpy)Ni(CN)$_4$·nH$_2$O (n = 2.5) (**1**). A series of 00l reflections indicated corresponds to the spacing of 11.3 Å, which agrees with the length of a bpy molecule working as a bridging ligand.

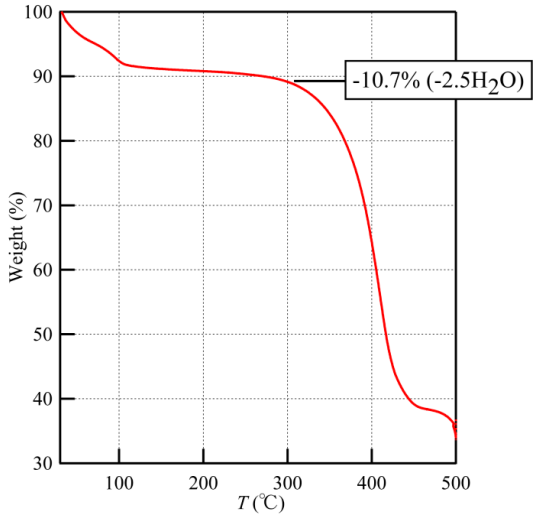

Figure S3. Thermogravimetry (TG) curve of Fe(bpy)Ni(CN)$_4$·nH$_2$O (n = 2.5) (**1**).

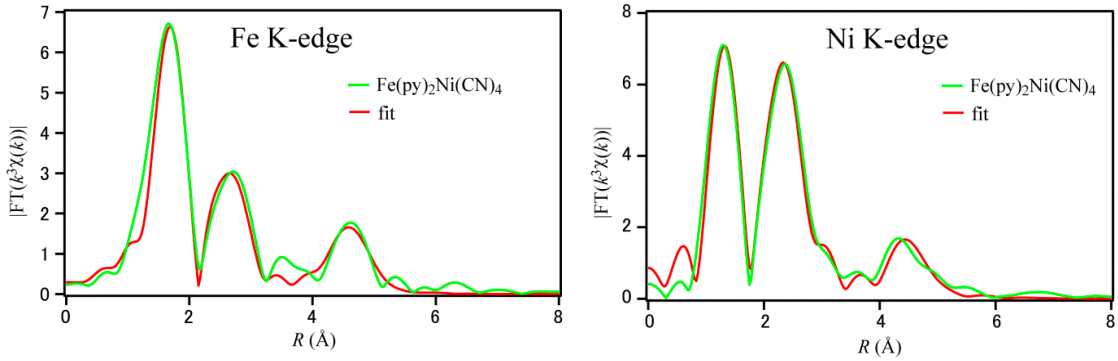

Figure S4. Fitting results of Extended X-ray Absorption Fine Structure (EXAFS) spectra for Fe(py)$_2$Ni(CN)$_4$.

Table S1. Extended X-ray Absorption Fine Structure (EXAFS) parameters used in the fitting shown in Figure S4.

Fe K-edge					
Path	**C.N.**	S_0^2	**σ² (Å²)**	E_0	**R (Å)**
Fe-N1	4.0	1.0	0.00704	3.87235	2.15105
Fe-N2	2.0	1.0	0.00704	3.87235	2.20445
Fe-C1	4.0	1.0	0.00855	3.87235	3.30683
Fe-C1-N1	8.0	1.0	0.00855	3.87235	3.31773
Fe-N1-C1-N1	4.0	1.0	0.00855	3.87235	3.32853
Fe-Ni	4.0	1.0	0.01873	3.87235	5.20465

Fe-Ni-C1	8.0	1.0	0.01873	3.87235	5.21774
Fe-Ni-N1	8.0	1.0	0.01873	3.87235	5.22795
Fe-Ni-C1-N1	8.0	1.0	0.01873	3.87235	5.22855
Fe-C1-Ni-C1	4.0	1.0	0.01873	3.87235	5.23074
Fe-C1-Ni-N1	8.0	1.0	0.01873	3.87235	5.24104
Ni K-edge					
Path	**C.N.**	**S_0^2**	**σ^2 (Å^2)**	**E_0**	**R (Å)**
Ni-C	4.0	1.0	0.00298	0.39879	1.84799
Ni-N	4.0	1.0	0.00609	0.39879	3.00953
Ni-N-C	8.0	1.0	0.00609	0.39879	3.01013
Ni-C-N-C	4.0	1.0	0.00609	0.39879	3.01063
Ni-Fe	4.0	1.0	0.01925	0.39879	5.17782
Ni-Fe-C	8.0	1.0	0.01925	0.39879	5.19092
Ni-Fe-N	8.0	1.0	0.01925	0.39879	5.20112
Ni-Fe-N-C	8.0	1.0	0.01925	0.39879	5.20172
Ni-C-Fe-C	4.0	1.0	0.01925	0.39879	5.20392
Ni-N-Fe-C	8.0	1.0	0.01925	0.39879	5.21422

path: scattering path; C.N.: degeneracy of path (coordination number); S_0^2: passive electron reduction factor; σ^2: mean square displacement (Debye-Waller factor); E_0: shift of energy origin; R: path length.