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Supporting Information

Changes in Magnetic Order Through Two Consecutive Dehydration Steps of Metal-Phosphonate Diamond Chains

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Table S1. Selected bond lengths (Å) for **Co-10H$_2$O** and **Ni-10H$_2$O**.

	Co-10H$_2$O	**Ni-10H$_2$O**
M1-O3	2.084(2)	2.043(4)
M1-O1W	2.167(3)	2.090(5)
M1-O5	2.097(2)	2.068(4)
M1-O1WA	2.167(3)	2.090(5)
M1-O3A	2.084(2)	2.043(4)
M1-O5A	2.097(2)	2.068(4)
M2-O1	2.202(2)	2.104(4)
M2-O2W	2.101(3)	2.046(4)
M2-O3W	2.205(3)	2.115(5)
M2-O4	2.112(2)	2.086(4)
M2-O6	2.029(2)	2.021(4)
M2-O2B	2.013(2)	2.001(4)
P1-O2	1.532(19)	1.516(4)
P1-O3	1.520(2)	1.510(4)
P1-O4	1.538(2)	1.532(4)
P2-O5	1.527(2)	1.523(4)
P2-O6	1.543(2)	1.537(4)
P2-O7	1.507(2)	1.494(4)

Symmetry code: A: 2-x, 1-y, 1-z; B: 2-x, 2-y, 2-z

Table S2. Selected bond angles (°) for **Co-10H$_2$O** and **Ni-10H$_2$O**

	Co-10H$_2$O	**Ni-10H$_2$O**
O1W-M1-O3	91.01(9)	90.93(15)
O1W-M1-O5	92.46(9)	92.98(16)
O1W-M1-O3A	88.99(9)	89.07(15)
O1W-M1-O5A	87.43(7)	87.02(16)
O3-M1-O5	88.43(7)	89.11(14)
O3-M1-O5A	91.57(7)	90.89(14)
O1-M2-O2W	172.01(10)	172.90(19)
O1-M2-O3W	88.87(9)	90.25(17)
O1-M2-O4	79.91(7)	81.06(15)
O1-M2-O6	82.41(7)	84.18(15)
O1-M2-O2B	94.79(7)	94.42(15)
O2W-M2-O3W	96.61(11)	95.1(2)
O2W-M2-O4	94.89(10)	93.82(19)
O2W-M2-O6	91.65(9)	90.97(17)
O2B-M2-O2W	91.56(9)	90.73(17)
O3W-M2-O4	168.31(9)	170.80(16)
O3W-M2-O6	91.01(9)	91.85(17)
O2B-M2-O3W	84.21(9)	84.79(17)
O4-M2-O6	90.78(8)	90.25(15)

Symmetry code: A: 2-x, 1-y, 1-z; B: 2-x, 2-y, 2-z

Table S3. Hydrogen bonds for **Co-10H$_2$O** [length Å and angles °]

D-H…A	d(D-H)	d(H...A)	d(D-A)	∠(DHA)
N1-H1A…O5W	0.89	1.98	2.849(4)	166
N1-H1B…O5	0.89	1.93	2.763(3)	155
O1W-H1WB…O3W	0.85	2.24	3.023(4)	153
O1W-H1WA…O4	0.85	2.32	3.083(3)	149
O2W-H2WB…O6	0.85	1.86	2.676(3)	160
O3W-H3WB…O4W	0.85	2.24	2.889(5)	133
O3W-H3WA…O5W	0.85	2.23	2.986(4)	149
O4W-H4WA…O7	0.90	1.97	2.852(4)	165
O4W-H4WB…O7	0.90	1.91	2.716(4)	148
O5W-H5WA…O2	0.90	1.99	2.883(4)	169
O5W-H5WB…O3	0.90	2.03	2.898(4)	163

Table S4. Hydrogen bonds for **Ni-10H$_2$O** [length /Å and angles°]

D-H…A	d(D-H)	d(H...A)	d(D-A)	∠(DHA)
N1-H1A…O5	0.89	1.91	2.742(6)	155
N1-H1B…O5W	0.89	1.96	2.835(6)	167
O1W-H1WB…O3W	0.84	2.25	3.025(6)	153
O1W-H1WA…O4	0.84	2.28	3.045(5)	151
O2W-H2WB…O6	0.84	1.87	2.675(6)	161
O3W-H3WB…O4W	0.84	2.19	2.839(8)	134
O3W-H3WA…O5W	0.84	2.21	2.975(6)	150
O4W-H4WA…O7	0.89	1.96	2.838(7)	167
O4W-H4WB…O7	0.90	1.87	2.694(7)	152
O5W-H5WA…O2	0.89	2.00	2.880(6)	169
O5W-H5WB…O3	0.90	2.02	2.888(6)	163

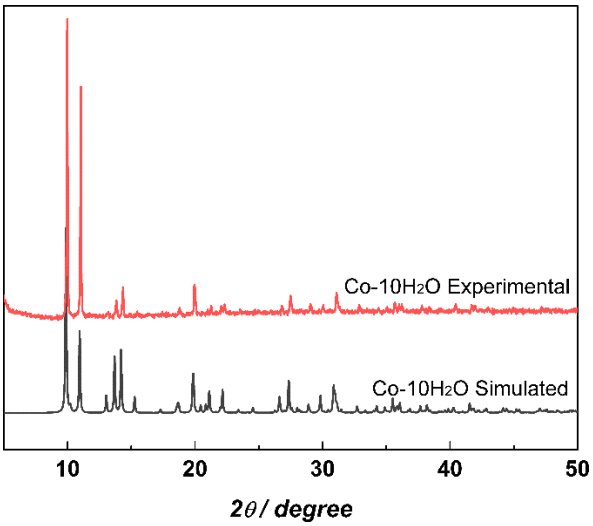

Figure S1. The comparison between experimental and calculated PXRD patterns for **Co-10H$_2$O**.

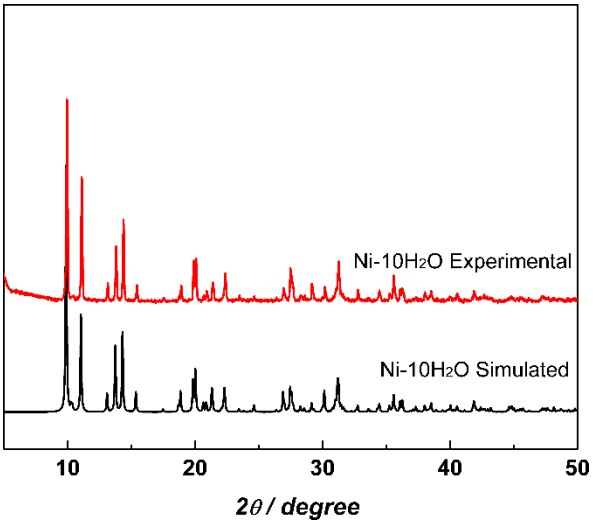

Figure S2. The comparison between experimental and calculated PXRD patterns for **Ni-10H$_2$O**.

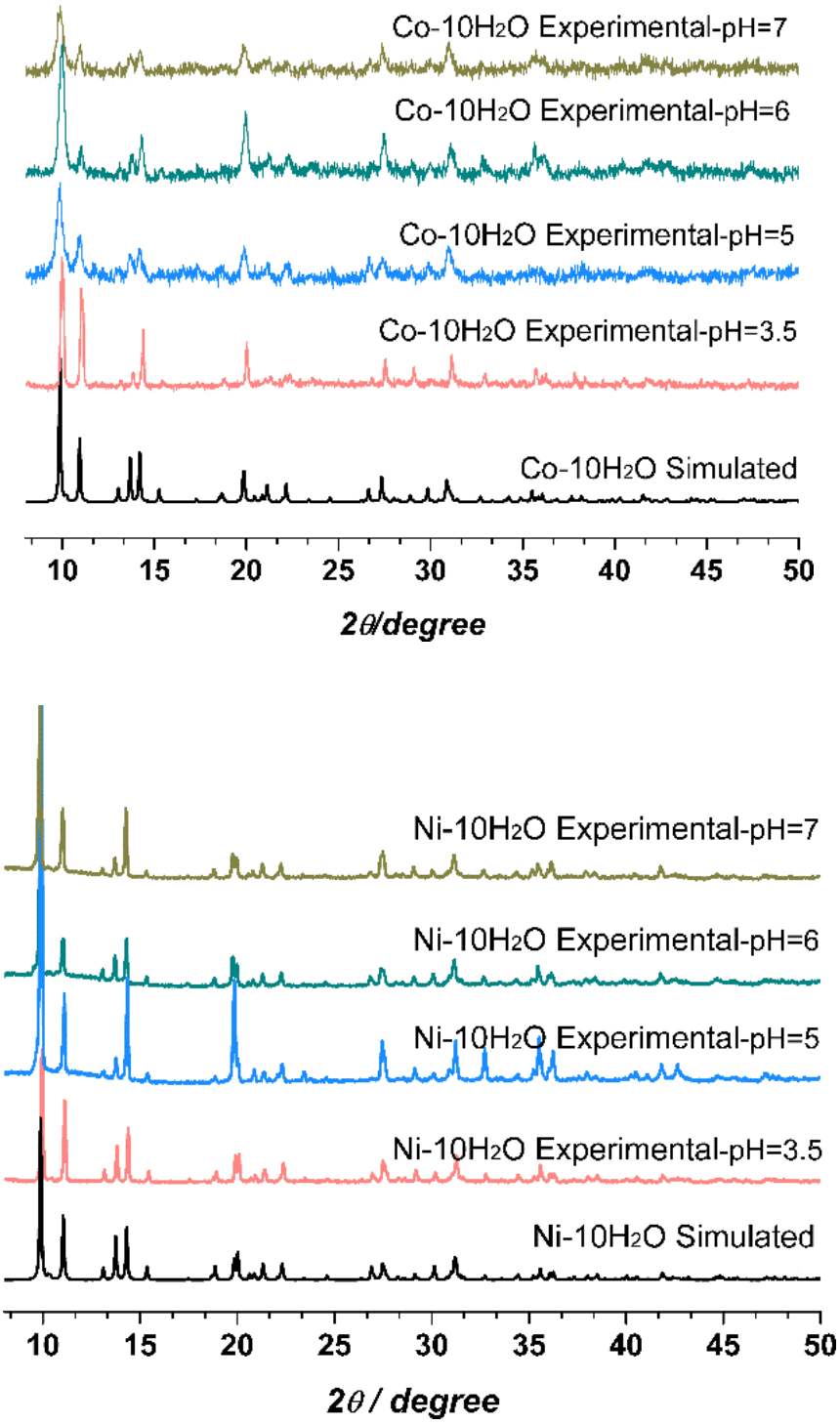

Figure S3. The PXRD patterns of the Co products (top) and Ni products (bottom) synthesized in different pH conditions.

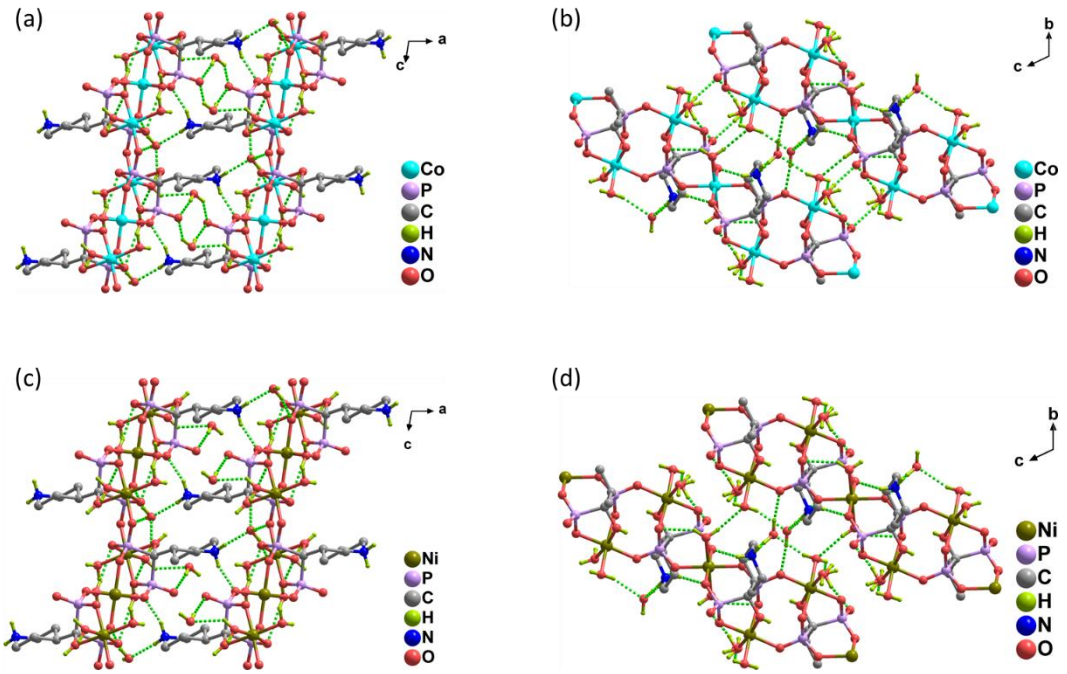

Figure S4. The hydrogen bond network in **Co-10H$_2$O** along *a* axis (a) and *c* axis (b); **Ni-10H$_2$O** along *a* axis (c) and *c* axis (d).

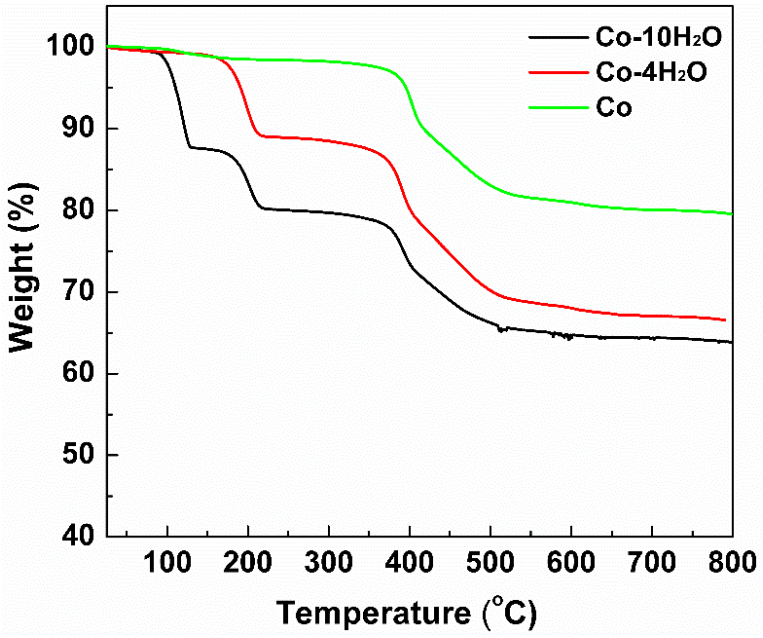

Figure S5. TG curves for compounds **Co-10H$_2$O**, **Co-4H$_2$O**, **Co**.

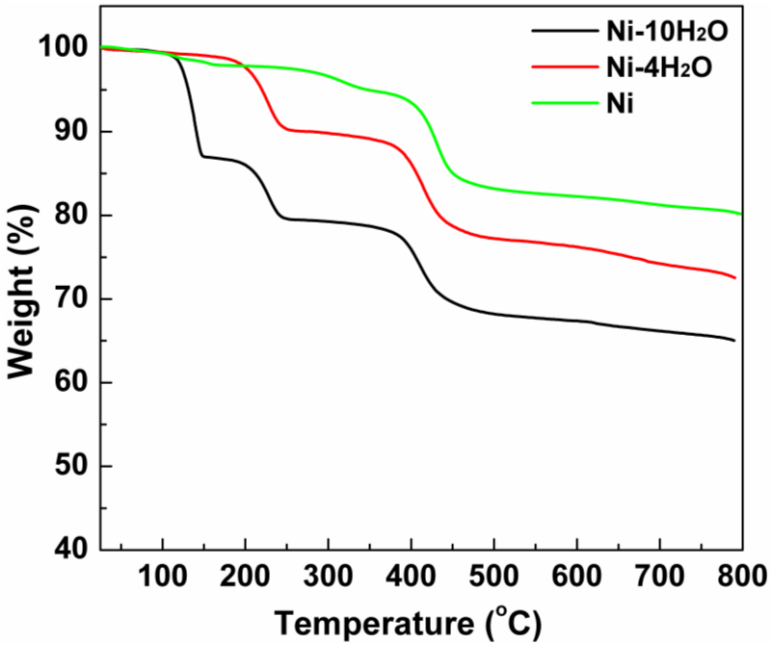

Figure S6. TG curves for compounds **Ni-10H$_2$O**, **Ni-4H$_2$O**, **Ni**.

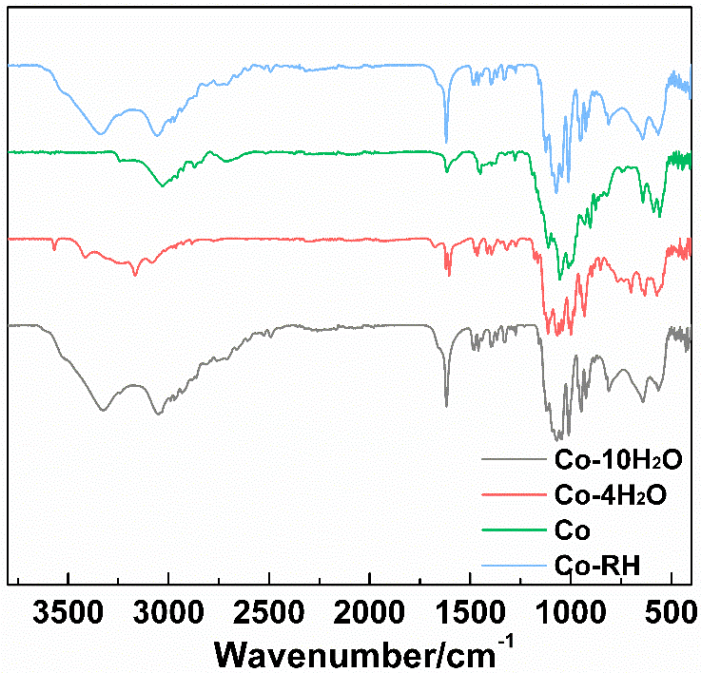

Figure S7. IR spectra for compounds **Co-10H$_2$O**, **Co-4H$_2$O**, **Co** and **Co-RH.**

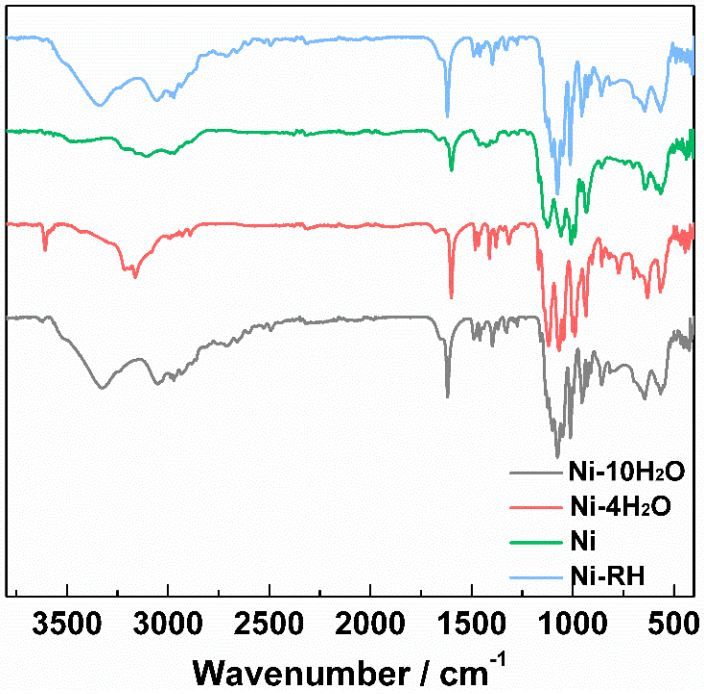

Figure S8. IR spectra for compounds **Ni-10H$_2$O**, **Ni-4H$_2$O**, **Ni** and **Ni -RH.**

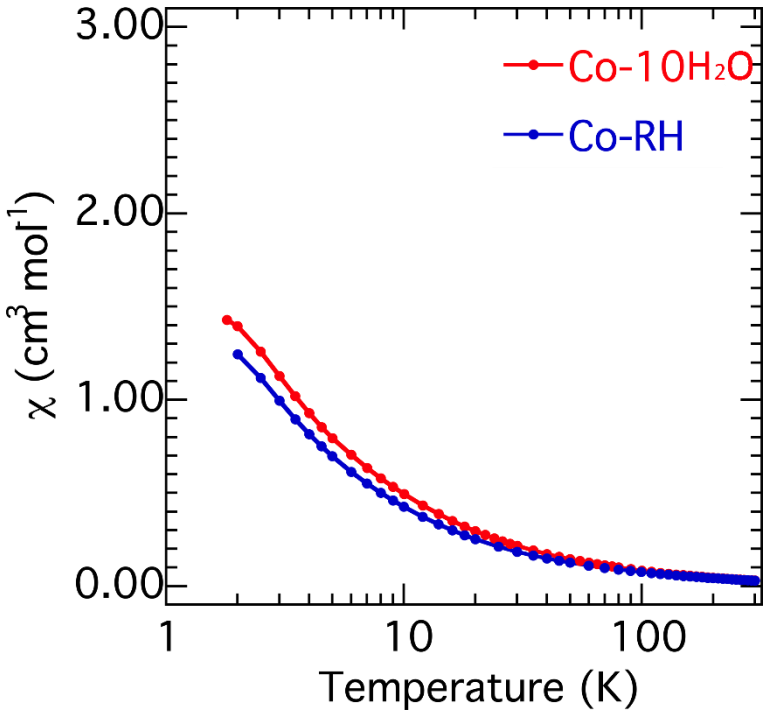

Figure S9. Temperature dependence of the dc-magnetic susceptibilities for **Co-10H$_2$O** and **Co-RH**.

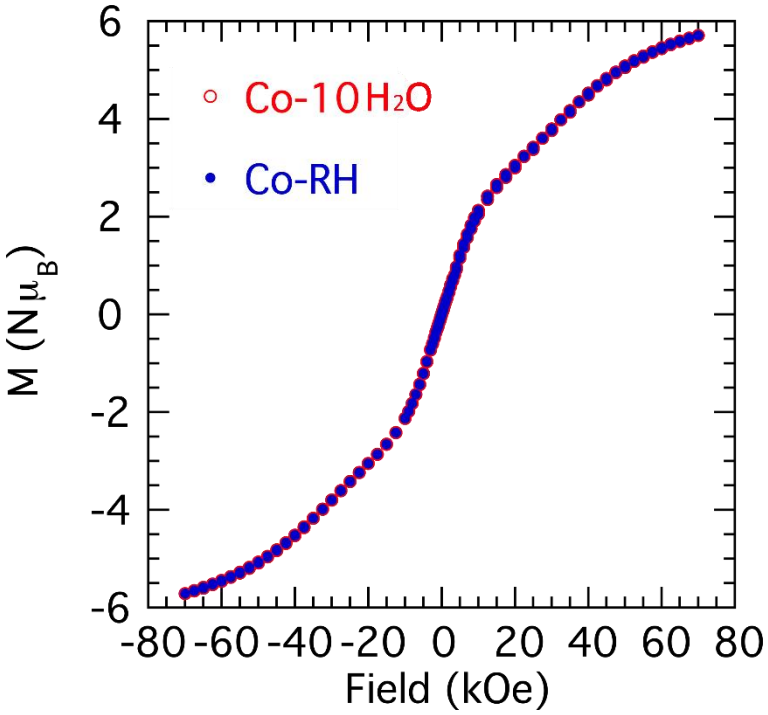

Figure S10. Isothermal magnetization at 2 K for **Co-10H$_2$O** and **Co-RH**.

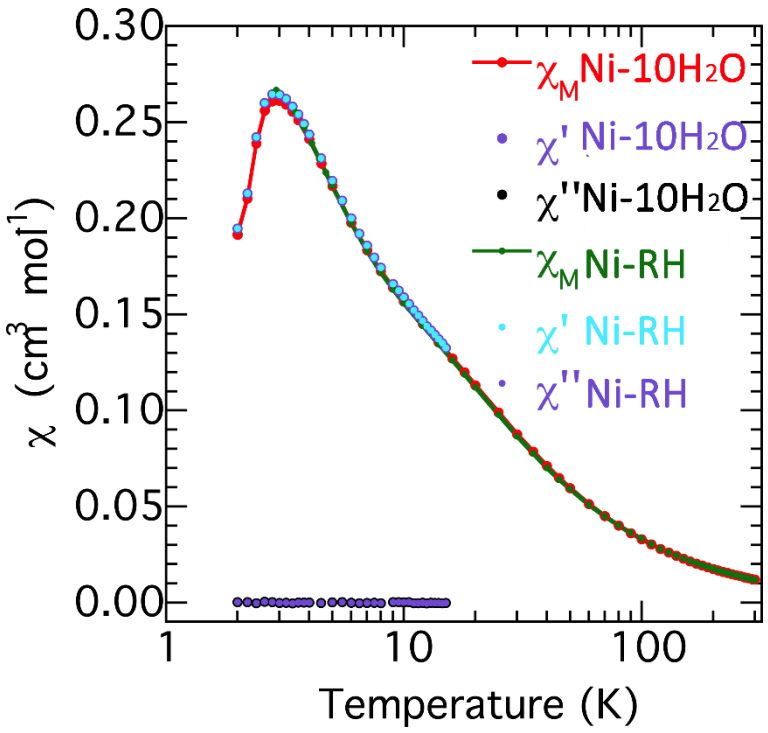

Figure S11. Temperature dependence of the dc- and ac- magnetic susceptibilities for **Ni-10H$_2$O** and **Ni-RH**.

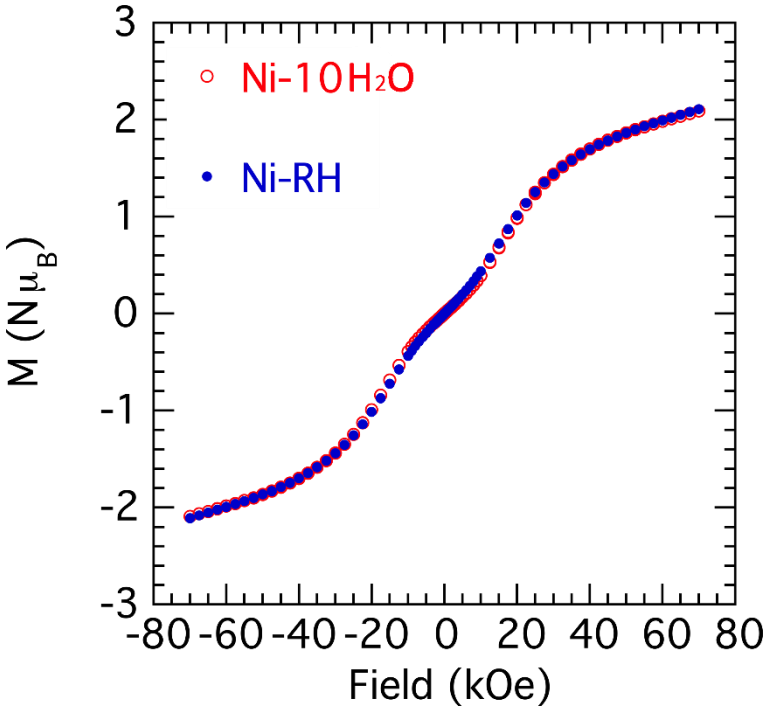

Figure S12. Isothermal magnetization at 2 K for **Ni-10H$_2$O** and **Ni-RH**.