

Electronic supplementary information (ESI)

Synthesis and characterisation of cobalt(II) phosphonate cage complexes utilizing carboxylates and pyridonates as co-ligands.**

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Table S1. Bond valence sum calculations for **1** (representative of the family of compounds **1** - **3**, **13** and **14**). The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	2.00	1.87
Co2	1.91	1.73
Co3	1.86	1.76
Co4	1.97	1.73
Co5	1.81	1.68

Table S2. Bond valence sum calculations for **4** (representative of compounds **4** - **9**). The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	1.91	1.85
Co2	1.99	1.86
Co3	1.92	1.79
Co4	1.93	1.71
Co5	1.98	1.76

Table S3. Bond valence sum calculations for **10**. The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	1.96	1.68
Co2	1.93	1.67
Co3	1.99	1.70
Co4	1.82	1.55
Co5	1.91	1.77
Co6	1.99	1.74
Co7	1.96	1.72
Co8	2.05	1.80
Co9	1.93	1.69
Co10	1.70	1.76

BVS calculations for the O atoms O3, O13 and O30 of 0.82, 1.15 and 1.19 respectively confirm that these are hydroxide ions. (The BVS values for O atoms of O²⁻, OH⁻, and H₂O groups are typically 1.8-2.0, 1.0-1.2, and 0.2-0.4, respectively).

Table S4. Bond valence sum calculations for **11**. The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	1.89	1.79
Co2	1.86	1.73
Co3	1.90	1.79
Co4	1.88	1.74
Co5	1.88	1.77
Co6	1.87	1.75
Co7	1.81	1.66
Co8	1.80	1.65
Co9	1.81	1.66

BVS calculation for the O atom O25 of 0.99 confirms that this is a hydroxide ion. (The BVS values for O atoms of O^{2-} , OH^- , and H_2O groups are typically 1.8-2.0, 1.0-1.2, and 0.2-0.4, respectively).

Table S5. Bond valence sum calculations for **12**. The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	1.88	1.85
Co2	1.80	1.70
Co3	1.88	1.65
Co4	1.95	1.71
Co5	2.00	1.76
Co6	1.63	1.72
Co7	2.04	1.80
Co8	2.05	1.80
Co9	1.79	1.70

BVS calculation for the O atom O28 of 1.01 confirms that this is a hydroxide ion. (The BVS values for O atoms of O^{2-} , OH^- , and H_2O groups are typically 1.8-2.0, 1.0-1.2, and 0.2-0.4, respectively).

Table S6. Bond valence sum calculations for **15**. The oxidation state for each metal is the whole number closest to the value in bold.

Atoms	Co(II)	Co(III)
Co1	1.91	1.78
Co2	1.92	1.80
Co3	1.88	1.72
Co4	2.00	1.78
Co5	1.91	1.82
Co6	1.90	1.78

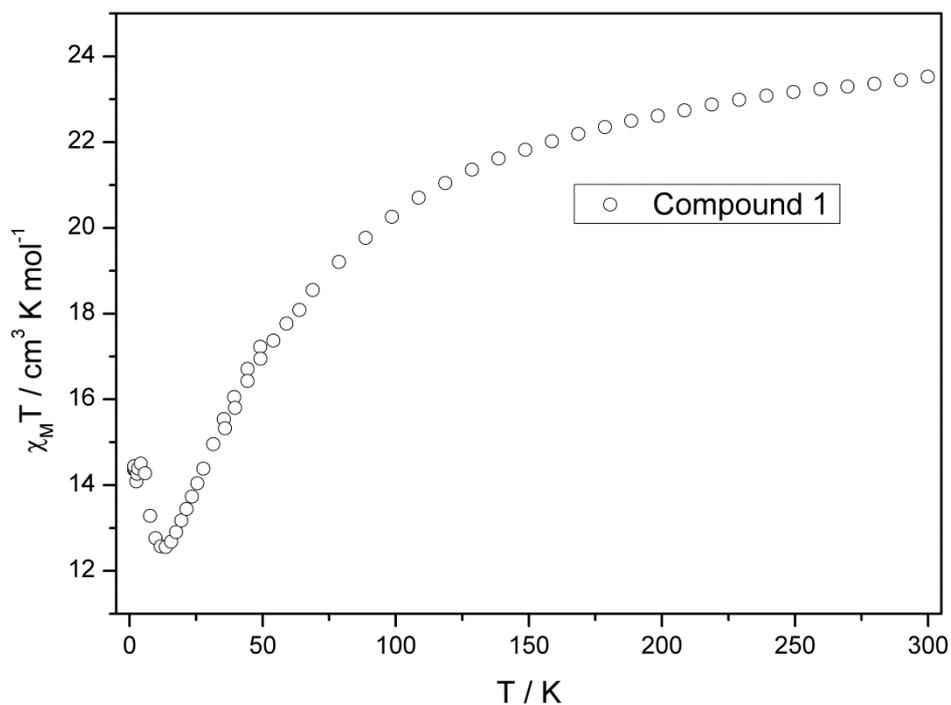


Figure S1. Plot of $\chi_M T$ vs T for compound 1.

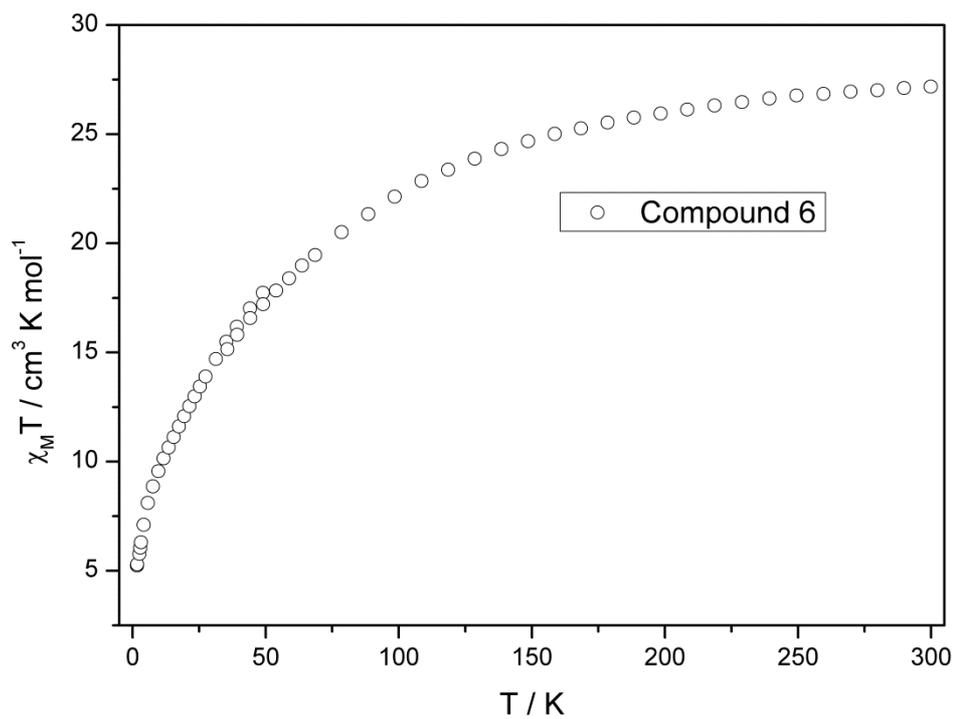


Figure S2. Plot of $\chi_M T$ vs T for compound 6.

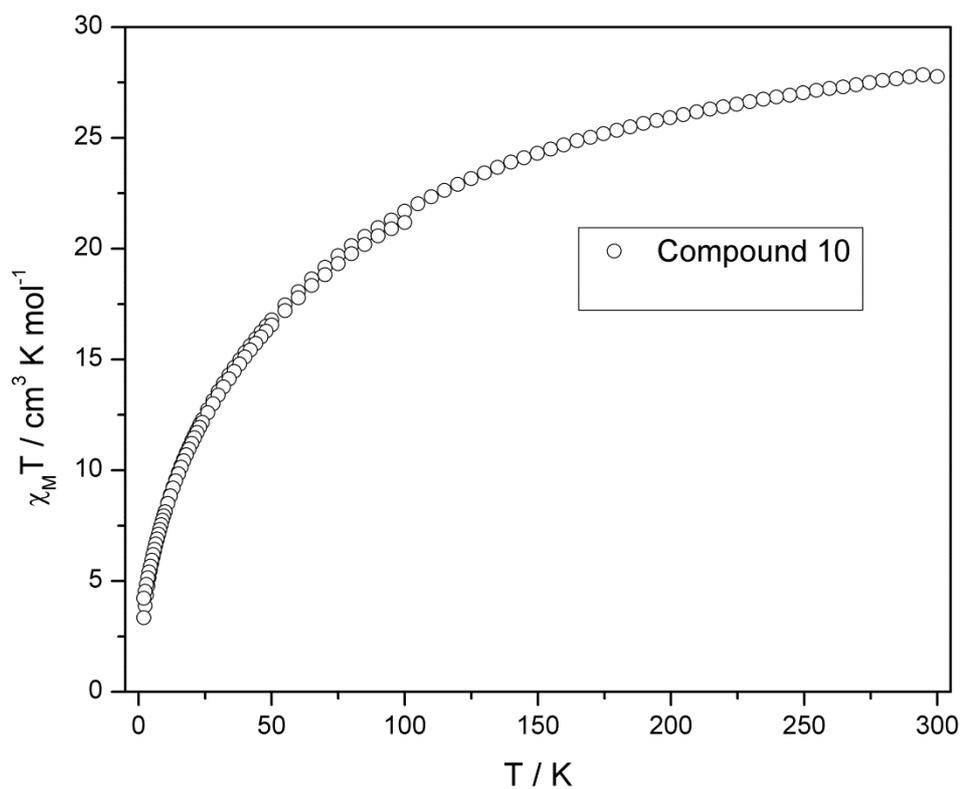


Figure S3. Plot of $\chi_M T$ vs T for compound 10.

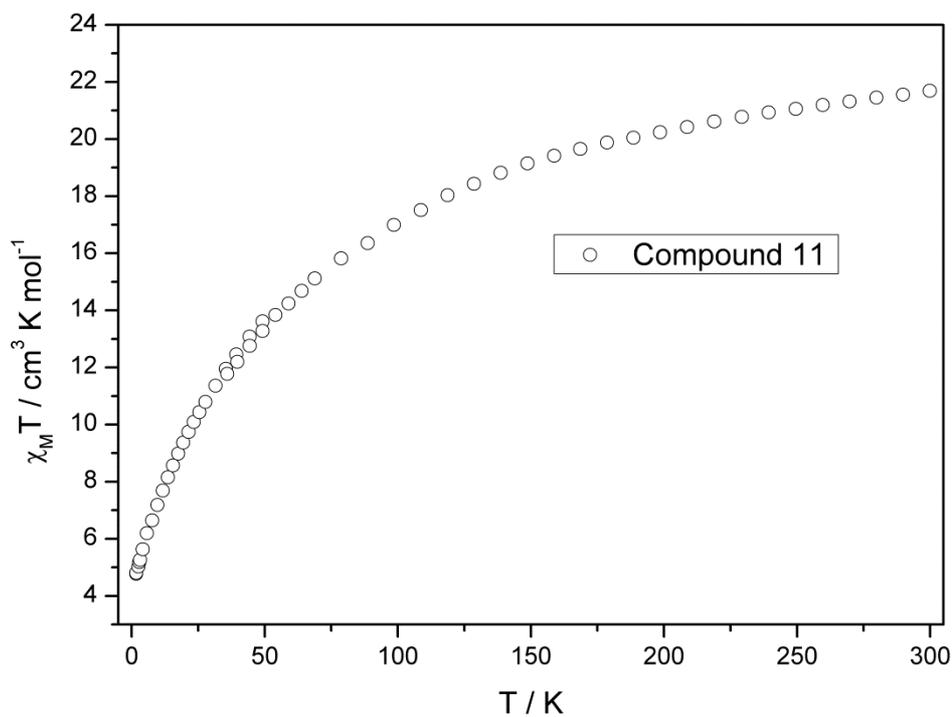


Figure S4. Plot of $\chi_M T$ vs T for compound 11.

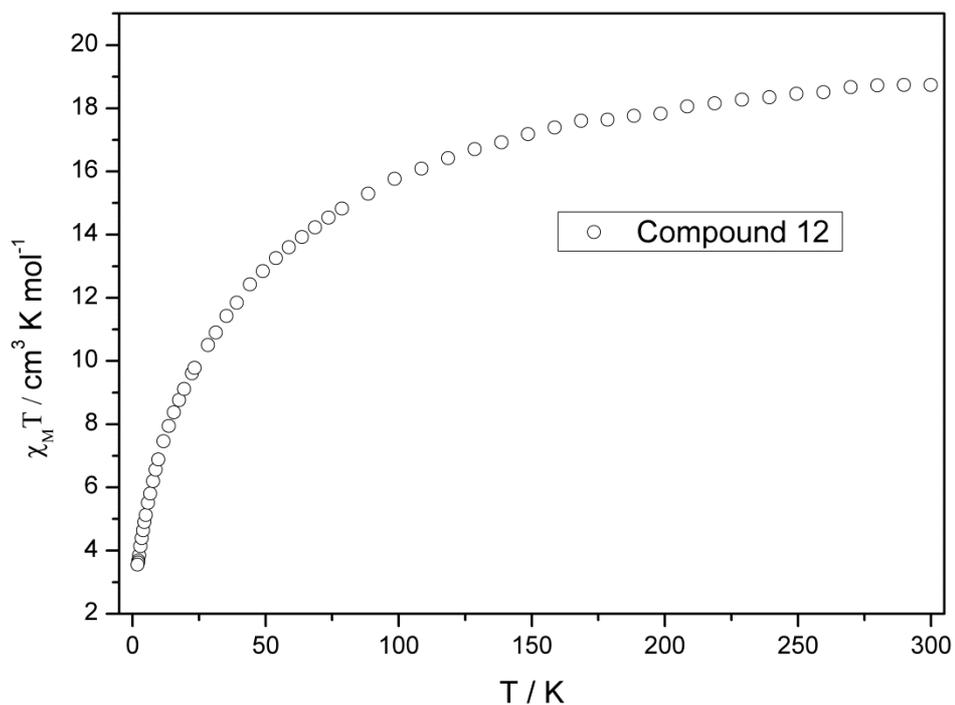


Figure S5. Plot of $\chi_M T$ vs T for compound 12.

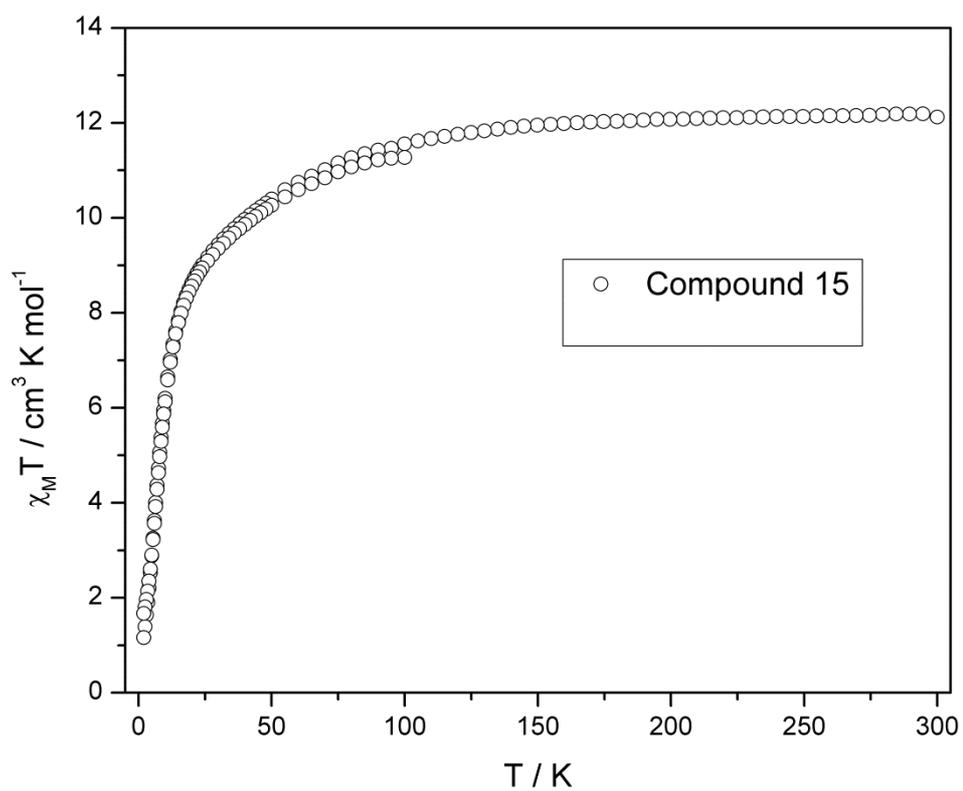


Figure S6. Plot of $\chi_M T$ vs T for compound 15.