Supplementary material to ”Temperature-dependent analysis of thermal motion, disorder and structures of tris(ethylenediamine)zinc(II) sulfate and tris(ethylenediamine)copper(II) sulfate”

Figure S1: Temperature evolution of the isotropic ADPs ($U_{eq}$) of the Zn, N and C atoms of 1.

Figure S2: Temperature evolution of the isotropic ADPs ($U_{eq}$) of the Cu, N and C atoms of 2.
Figure S3: Temperature evolution of the eigenvalues of the ADPs of the N1 atom of 1. $\lambda_1$ has a slope of 0.000096 Å$^2$/K of 0.0132 Å$^2$ at T=0 K, $\lambda_2$ has 0.000099 Å$^2$/K and 0.0050 Å$^2$ and $\lambda_3$ has 0.000070 Å$^2$/K and 0.0039 Å$^2$. 
Figure S4: Temperature evolution of the eigenvalues of the translation (left axis, Å²) and libration (right axis, rad²) tensors for 1, as calculated with THMA11 [2]. At T=0 K the standard uncertainties of the intercepts of the four interpolations are drawn.
Table S1: Translational (T; Å²), librational (L; rad²) and screw-coupling (S; Å rad) tensor components of the rigid body motion at 140-290 K for 1 as calculated using THMA11 [2]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

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Table S2: Translational (T; Å²), librational (L; rad²) and screw-coupling (S; Å rad) tensor components of the rigid body motion at 190-270 K for 2 as calculated using THMA11 [2]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

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Table S3: Translational (T; Å$^2$), librational (L; rad$^2$) and screw-coupling (S; Å·rad) tensor components of the rigid body motion at 140-290 K for 1 as calculated using NKA [1]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

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Table S4: Translational (T; Å$^2$), librational (L; rad$^2$) and screw-coupling (S; Å·rad) tensor components of the rigid body motion at 190-270 K for 2 as calculated using NKA [1]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

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