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**.

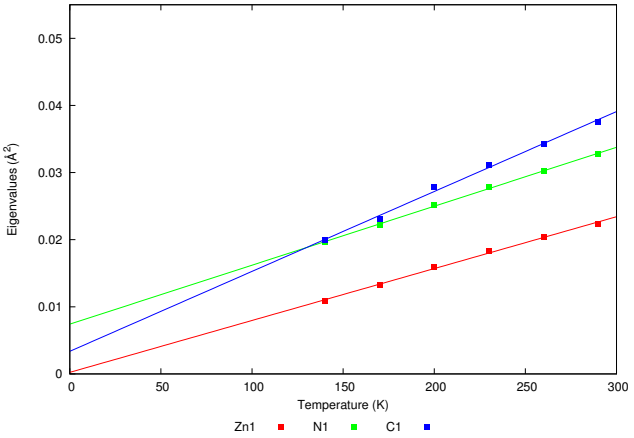

Figure S2: Temperature evolution of the isotropic ADPs (U_{eq}) of the Cu, N and C atoms of **2**.

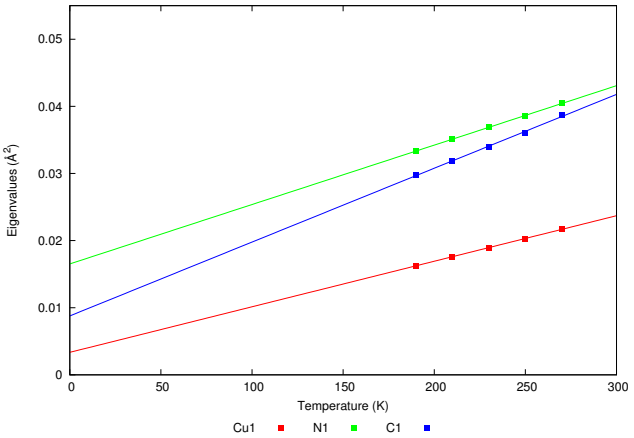

Figure S3: Temperature evolution of the eigenvalues of the ADPs of the N1 atom of **1**. λ_1 has a slope of 0.000096 Å^2/K of 0.0132 Å^2 at T=0 K, λ_2 has 0.000099 Å^2/K and 0.0050 Å^2 and λ_3 has 0.000070 Å^2/K and 0.0039 Å^2.

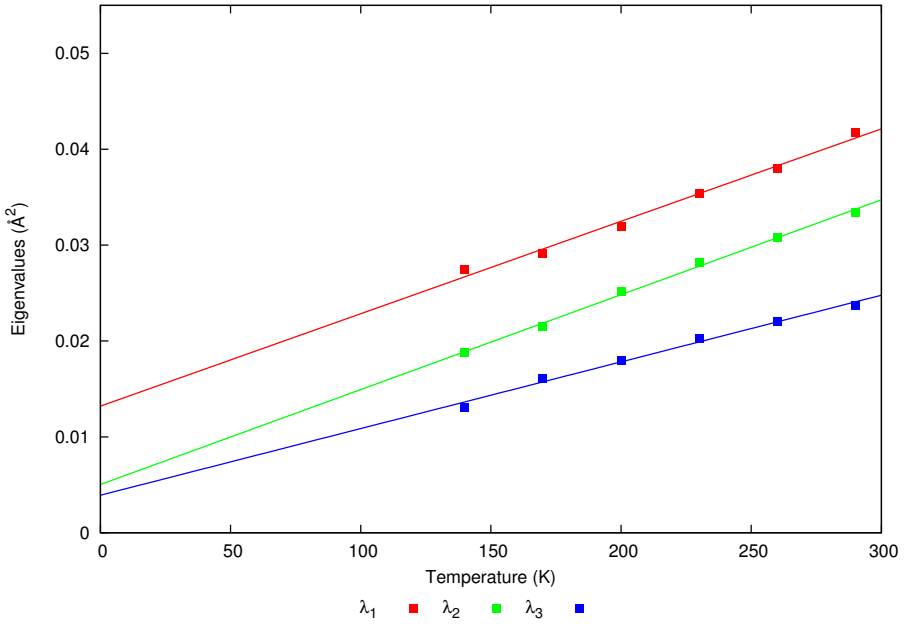

Figure S4: Temperature evolution of the eigenvalues of the translation (left axis, $Å^2$) and libration (right axis, rad^2) tensors for **1**, as calculated with THMA11 [2]. At T=0 K the standard uncertainties of the intercepts of the four interpolations are drawn.

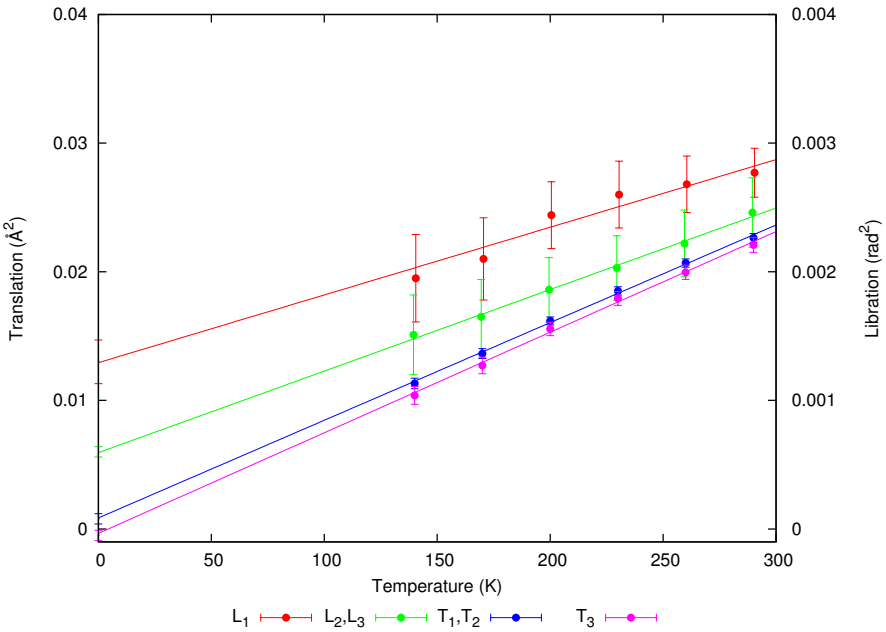

Table S1: Translational (T; Å^2), librational (L; rad^2) and screw-coupling (S; Å rad) tensor components of the rigid body motion at 140-290 K for **1** as calculated using THMA11 [2]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

T(K)	T_{11}	T_{22}	T_{33}
140	0.0113(4)	0.0113(4)	0.0104(6)
170	0.0136(3)	0.0136(3)	0.0127(6)
200	0.0162(3)	0.0162(3)	0.0156(5)
230	0.0185(3)	0.0185(3)	0.0179(5)
260	0.0207(3)	0.0207(3)	0.0200(5)
290	0.0226(3)	0.0226(3)	0.0221(5)

T(K)	L_{11}	L_{22}	L_{33}
140	0.0015(3)	0.0015(3)	0.0019(3)
170	0.0016(2)	0.0016(2)	0.0021(3)
200	0.0019(2)	0.0019(2)	0.0024(2)
230	0.0020(2)	0.0020(2)	0.0026(2)
260	0.0022(2)	0.0022(2)	0.0027(2)
290	0.0025(2)	0.0025(2)	0.00277(19)

T(K)	S_{11}	S_{22}	S_{33}
140	0.0002(2)	0.0002(2)	-0.0005(4)
170	0.0001(2)	0.0001(2)	-0.0003(4)
200	0.00005(18)	0.00005(18)	-0.0001(3)
230	-0.00001(19)	-0.00001(19)	0.0000(3)
260	0.00002(19)	0.00002(19)	-0.0001(3)
290	-0.0001(2)	-0.0001(2)	0.0001(3)

Table S2: 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 THMA11 [2]. Off-diagonal values have been omitted, because they equal 0 due to symmetry.

T(K)	T_{11}	T_{22}	T_{33}
190	0.0181(9)	0.0181(9)	0.0138(15)
210	0.0193(9)	0.0193(9)	0.0152(15)
230	0.0207(9)	0.0207(9)	0.0164(15)
250	0.0220(8)	0.0220(8)	0.0178(15)
270	0.0236(8)	0.0236(8)	0.0190(15)

T(K)	L_{11}	L_{22}	L_{33}
190	0.0021(7)	0.0021(7)	0.0025(8)
210	0.0022(7)	0.0022(7)	0.0025(8)
230	0.0023(7)	0.0023(7)	0.0027(8)
250	0.0025(7)	0.0025(7)	0.0027(7)
270	0.0027(7)	0.0027(7)	0.0029(7)

T(K)	S_{11}	S_{22}	S_{33}
190	-0.0001(5)	-0.0001(5)	0.0001(11)
210	-0.0000(5)	-0.0000(5)	0.0001(11)
230	-0.0000(5)	-0.0000(5)	0.0001(11)
250	-0.0001(5)	-0.0001(5)	0.0001(11)
270	-0.0000(5)	-0.0000(5)	0.0001(11)

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.

T(K)	T_{11}	T_{22}	T_{33}
140	0.01080(10)	0.01080(10)	0.01090(14)
170	0.01307(12)	0.01307(12)	0.01319(19)
200	0.01535(14)	0.01535(14)	0.0155(2)
230	0.01763(17)	0.01763(17)	0.0178(3)
260	0.01991(19)	0.01991(19)	0.0201(4)
290	0.0222(2)	0.0222(2)	0.0224(5)

T(K)	L_{11}	L_{22}	L_{33}
140	0.00094(4)	0.00094(4)	0.00097(4)
170	0.00112(4)	0.00112(4)	0.00117(5)
200	0.00131(5)	0.00131(5)	0.00137(7)
230	0.00150(6)	0.00150(6)	0.00157(9)
260	0.00169(7)	0.00169(7)	0.00177(11)
290	0.00188(7)	0.00188(7)	0.00197(12)

T(K)	S_{11}	S22	S_{33}
140	0.0000(4)	-0.0000(4)	0.0010(4)
170	0.0000(4)	-0.0000(4)	0.0012(5)
200	0.0000(4)	-0.0000(4)	0.0014(5)
230	0.0000(4)	-0.0000(4)	0.0016(5)
260	0.0000(4)	-0.0000(4)	0.0019(5)
290	0.0000(4)	-0.0000(4)	0.0021(6)

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.

T(K)	T_{11}	T_{22}	T_{33}
190	0.01353(16)	0.01353(16)	0.0119(2)
210	0.01494(18)	0.01494(18)	0.0132(3)
230	0.01635(19)	0.01635(19)	0.0144(3)
250	0.0178(2)	0.0178(2)	0.0156(3)
270	0.0192(2)	0.0192(2)	0.0169(3)

T(K)	L_{11}	L_{22}	L_{33}
190	0.00167(6)	0.00167(6)	0.00098(7)
210	0.00184(7)	0.00184(6)	0.00107(7)
230	0.00201(7)	0.00201(7)	0.00117(8)
250	0.00218(8)	0.00218(8)	0.00127(9)
270	0.00235(8)	0.00235(8)	0.00137(10)

T(K)	S_{11}	S_{22}	S_{33}
190	0.0000(5)	0.0000(5)	-0.0000(6)
210	0.0000(5)	0.0000(5)	-0.0000(6)
230	0.0000(5)	0.0000(5)	-0.0000(6)
250	0.0000(5)	0.0000(5)	-0.0000(6)
270	0.0000(5)	0.0000(5)	-0.0000(6)

References

[1] H. B. Bürgi and S. C. Capelli. Dynamics of molecules in crystals from multi-temperature anisotropic displacement parameters. i. theory. *Acta Crystallographica Section A*, 56(5):403–412, Sep 2000.

[2] V. Schomaker and K. N. Trueblood. Correlation of Internal Torsional Motion with Overall Molecular Motion in Crystals. *Acta Crystallographica Section B*, 54(5):507–514, Oct 1998.