Electronic Supplementary Material (ESI) for Dalton Transactions.

Compositional dependence of anomalous thermal expansion in perovskite-like ABX_3 formates

SUPPLEMENTARY INFORMATION

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1 Gua-Cd single-crystal X-ray diffraction

Single-crystal X-ray diffraction data were collected on Gua-Cd using a Nonius KappaCCD diffractometer ($\lambda = 0.71073\,\text{Å}$) fitted with an Oxford CryoSystems 600 series CryoStream open flow cooling device. The Gua-Cd crystal was mounted on a glass fibre and fixed using araldite and placed in the cold stream at 150 K. Diffraction data were measured at temperatures of 150 K and 250 K. A second crystal was similarly mounted on a Rigaku Oxford Diffraction (Agilent) SuperNova diffractometer ($\lambda = 0.71073\,\text{Å}$) fitted with an Oxford CryoSystems 700+ CryoStream open flow cooling device. Diffraction data were measured at temperatures of 300 K and 450 K. On completion, this crystal was heated up to 500 K, but as the crystallinity of the sample was greatly reduced only the unit cell was determined at this temperature.

In each case, the raw frame data were reduced using the appropriate software, DENZO/SCALEPACK[S1] or CrysAlisPro, including unit cell refinement and inter-frame scaling. *Ab initio* structure solution was carried out with SIR92[S2] using the data collected at 150K [Table S1; for the crystallographic details on the other temperatures see supplementary CIFs]. All non-hydrogen atoms were refined with anisotropic displacement parameters. In general, hydrogen atoms were visible in the difference Fourier map and were treated in the usual manner: *i.e.* positioned geometrically and then refined with soft restraints on the bond lengths, angles and temperature factors, after which a riding model was used.[S3] The structures were refined against $|F|^2$ using CRYSTALS.[S4] The 150 K structural model was used as a starting model for refinements against the 250 K, 300 K and 400 K datasets and a similar procedure was followed in each case.

Table S1: Crystallographic details of Gua-Cd

Crystal data	
Chemical formula	C4 H9 Cd1 N3 O6
M_r ($g\,mol^{-1}$)	307.53
crystal system, space group	trigonal, $R\bar{3}c$
Temperature (K)	150
a,b,c (Å)	9.2335(6), 9.2335(6), 19.2916(10)
V (Å^3)	1424.40(15)
Z	6
Radiation type	Mo Kα, $\lambda = 0.71073$ Å
μ (mm^{-1})	2.311
Crystal size (mm^3)	0.2, 0.2, 0.2
Data collection	
Diffractometer	Nonius KappaCCD diffractometer
Absorption correction	multi-scan
T_{min}, T_{max}	0.972, 1
No. of measured, independent and observed [I>2σ(I)] reflections	3262, 1129, 295
R_{int}	0.044
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2)$	0.0298, 0.0726
No. of reflections	295
No. of parameters	24
H-atom treatment	Located in the difference map, then a riding model was applied
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e/Å^3)	−0.92, 0.54

2 Rietveld fits for [A][M(HCOO)$_3$] compounds

For all Rietveld or Pawley fits, experimental data are given as points, the fitted profile as a solid red line, and the difference (data−fit) as a blue line. The pink *hkl* tick marks represent the [A][M(HCOO)$_3$] phase and green *hkl* tick marks indicate an impurity of metal formate dihydrate which formed in certain cases.

Phase transitions were observed upon cooling for $MeNH_3$-Cd, Me_2NH_2-Mn, Me_2NH_2-Co, Me_2NH_2-Zn, and Aze-Mn. For the Me_2NH_2-M family, the phase transition has already been characterised,[S5–7] and the low-temperature (LT) phase could be refined with the Cc model from Ref. S6 for Me_2NH_2-M structures, where M = Mn, Co and Zn. While hysteresis has been shown to be present in the phase transition temperature of Me_2NH_2-Mn,[S7] here we observe much greater hysteresis and moreover, even at the lowest temperatures of this study (110 K), there is a coexistence of the $R\bar{3}c$ (ambient phase) and Cc (LT-phase). For Me_2NH_2-Mn, the LT-phase is observed in the temperature range of 159–119 K upon cooling and 111–175 K upon heating. In the case of Me_2NH_2-Co and Me_2NH_2-Zn, the LT-phase is observed in the temperature range of 111–149 K for the heating run only. We suggest that because our diffraction patterns were measured relatively fast, there was not sufficient time for the HT-phase to completely convert to the LT-phase.

The Aze-Mn ferroelastic phase transition ($Pnma$ to $P2_1/n$) was observed at ∼250 K, and has been described in detail by Ref. S8.

The phase transition observed at low temperatures for $MeNH_3$-Cd could not be solved due to the coexistence of the ambient and LT phases.

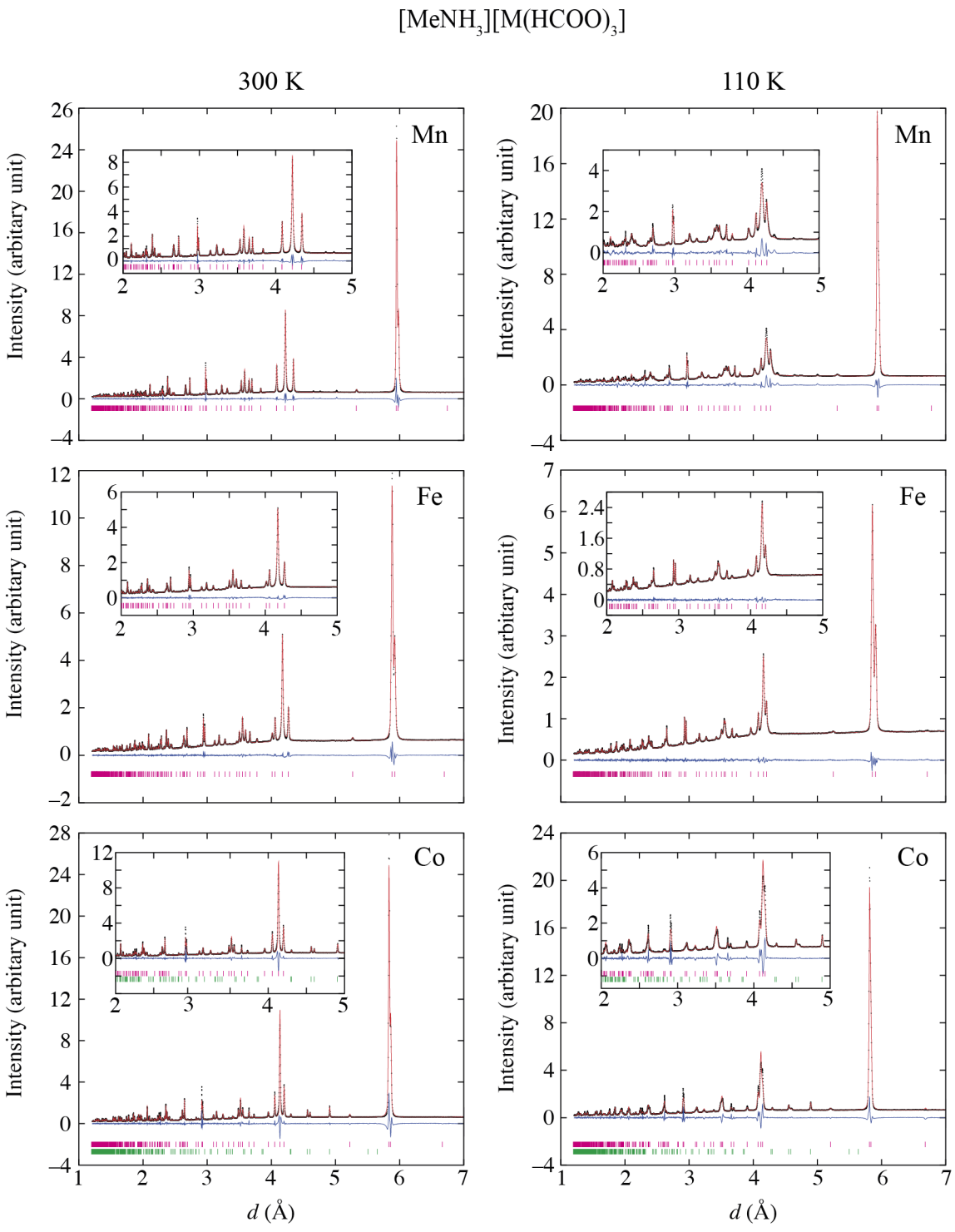

Figure S1: Rietveld fits for $[CH_3NH_3][M(HCOO)_3]$ with M = Mn, Fe, and Co at 300 K (left) and 110 K (right).

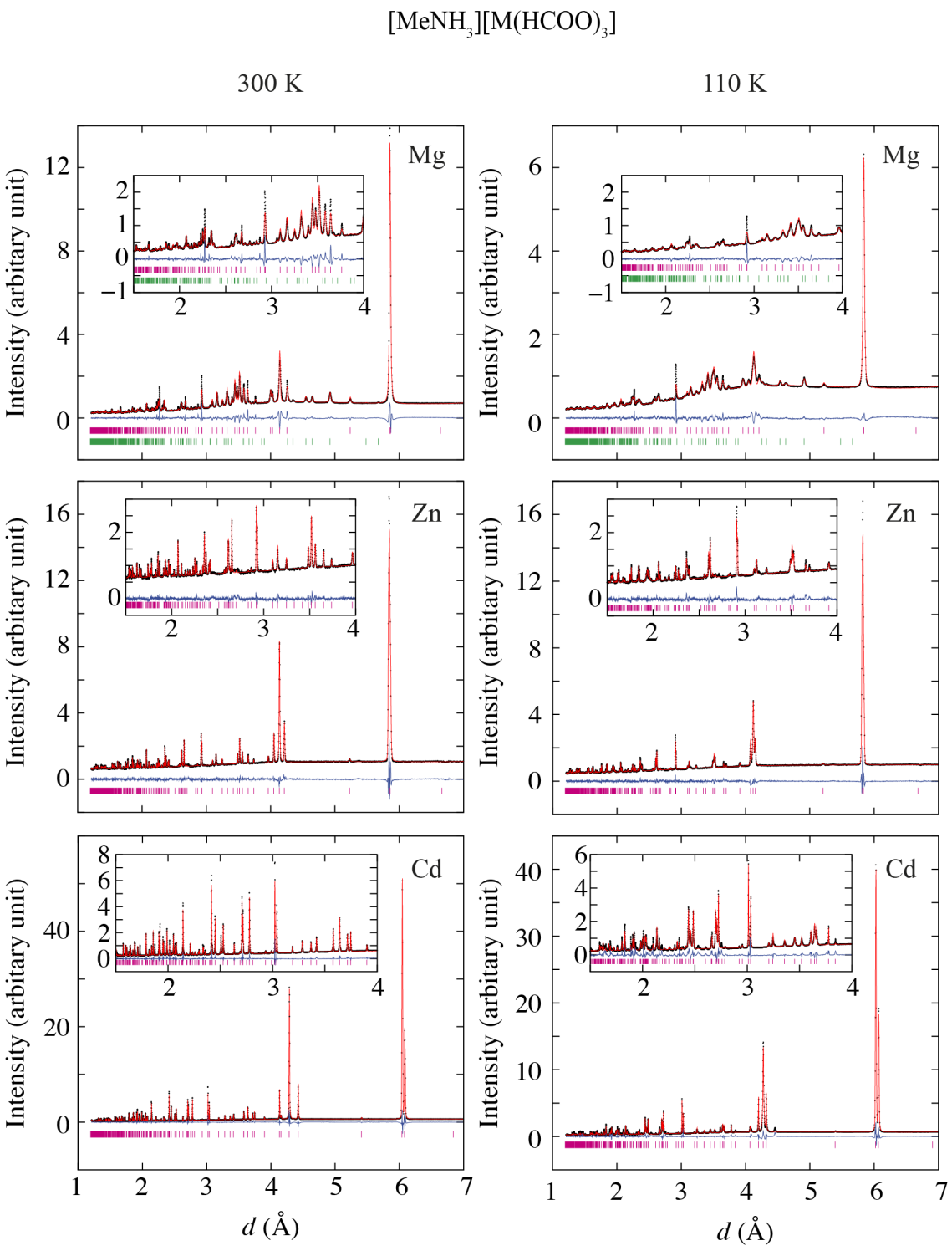

Figure S2: Rietveld fits for $[CH_3NH_3][M(HCOO)_3]$ with M = Mg, Zn, and Cd at 300 K (left) and 110 K (right).

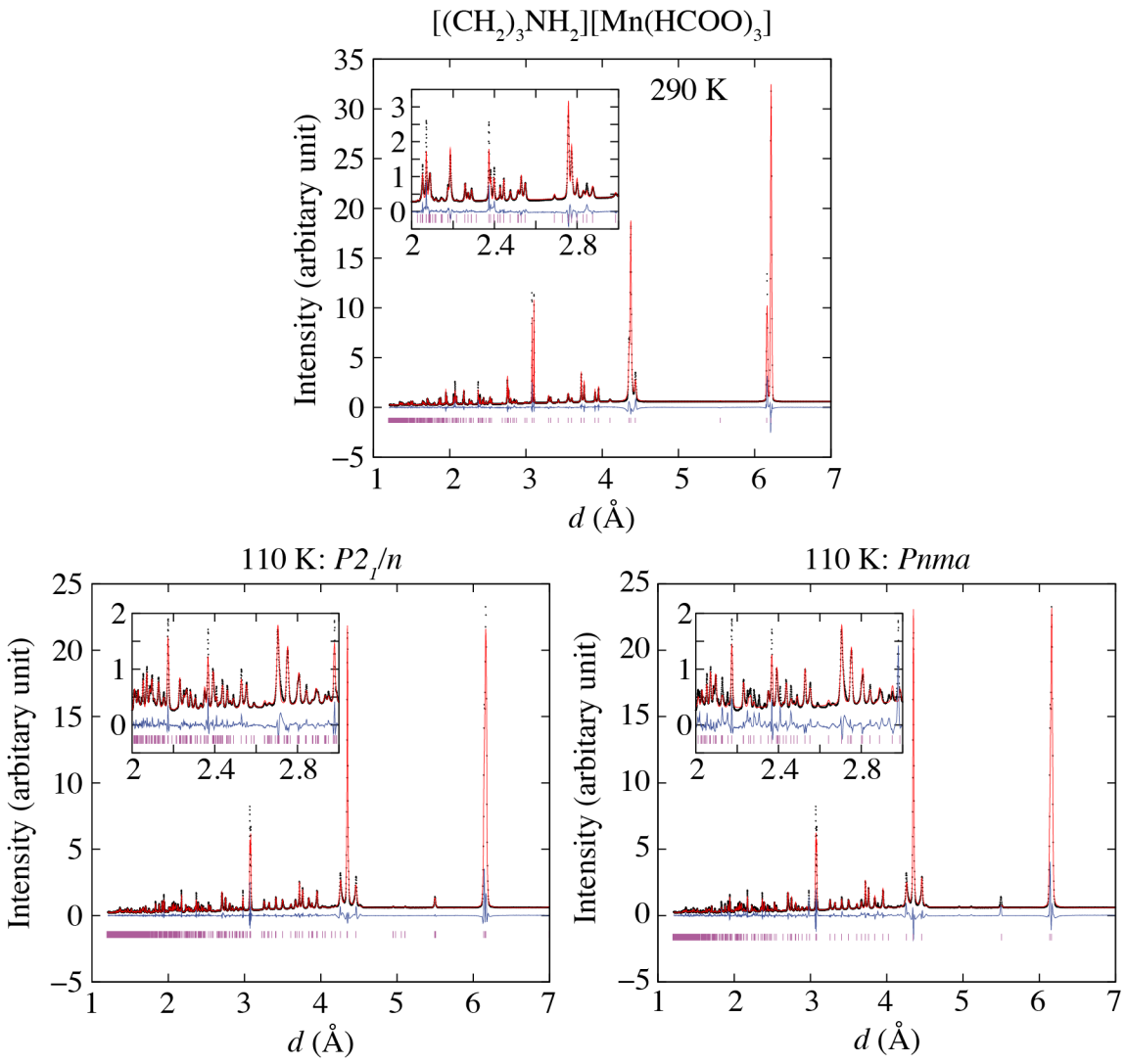

Figure S3: Rietveld fits for $[(CH_2)_3NH_2][Mn(HCOO)_3]$ at 290 and 110 K. The low-temperature diffraction is shown fitted with the monoclinic phase ($P2_1/n$) and the ambient phase ($Pnma$).

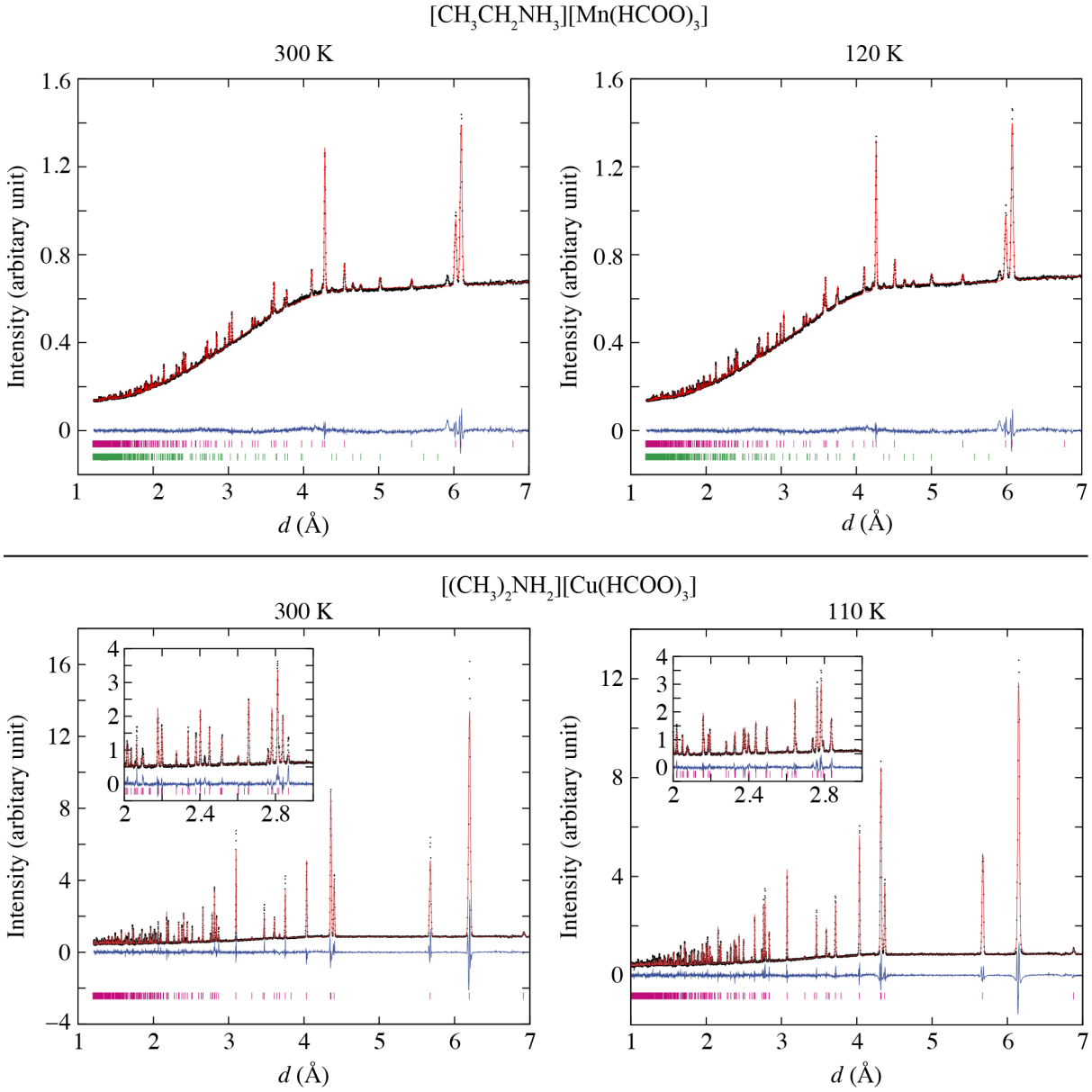

Figure S4: (*Top*) Rietveld fits for $[CH_3CH_2NH_3][Mn(HCOO)_3]$ at 300 and 120 K. The high background is due to the low sample content in the capillary. (*Bottom*) Rietveld fits for $[(CH_3)_2NH_2][Cu(HCOO)_3]$ at 300 and 100 K, both refined in the monoclinic $C2/c$ symmetry.

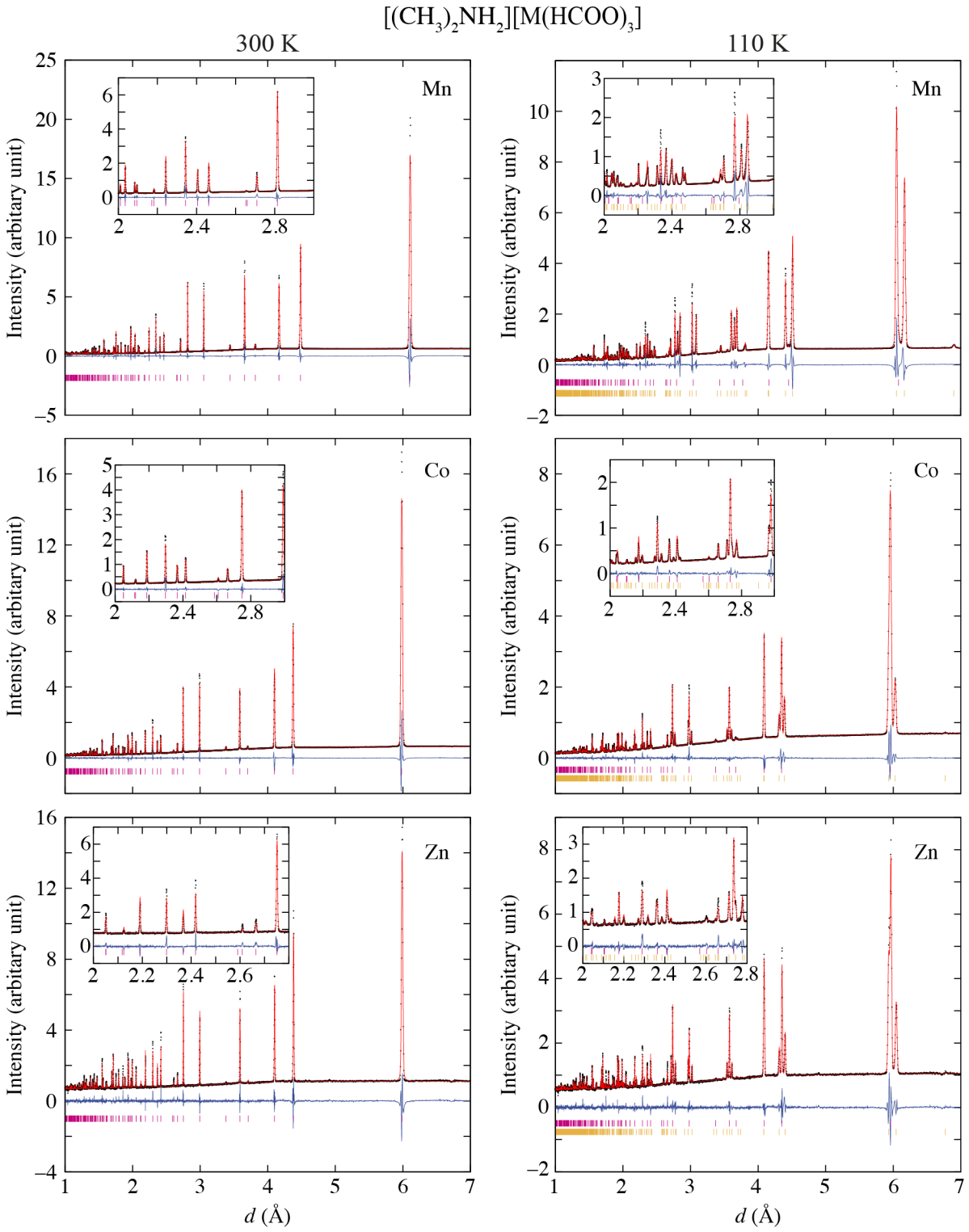

Figure S5: Rietveld fits for $[(CH_3)_2NH_2][M(HCOO)_3]$ with M = Mn, Co, Zn at 300 and 110 K. The ambient phase is indicated by pink *hkl* tick marks, while the LT phase is represented by orange *hkl* tick marks.

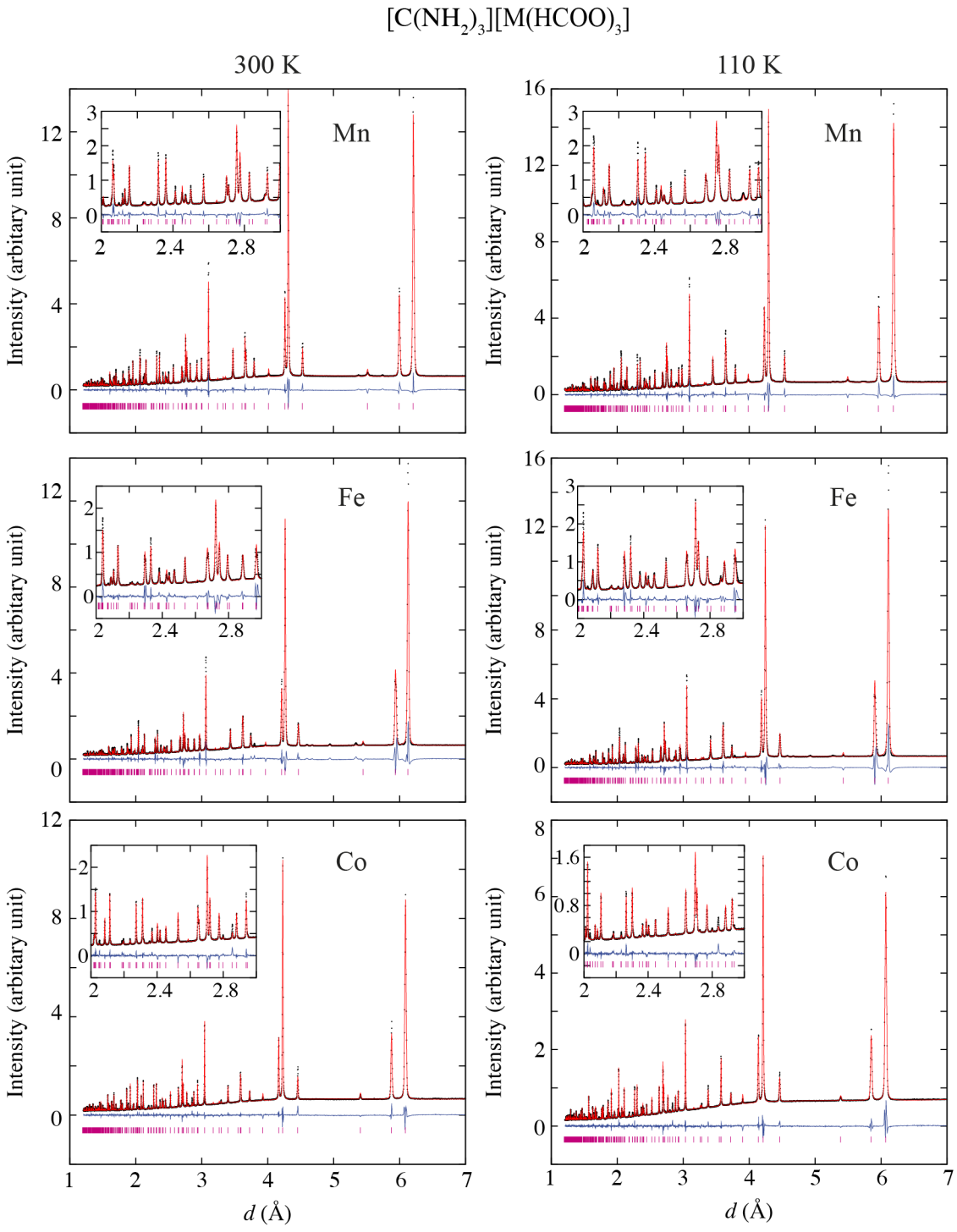

Figure S6: Rietveld fits for $[C(NH_2)_3][M(HCOO)_3]$ with M = Mn, Fe, Co at 300 K (left) and 110 K (right).

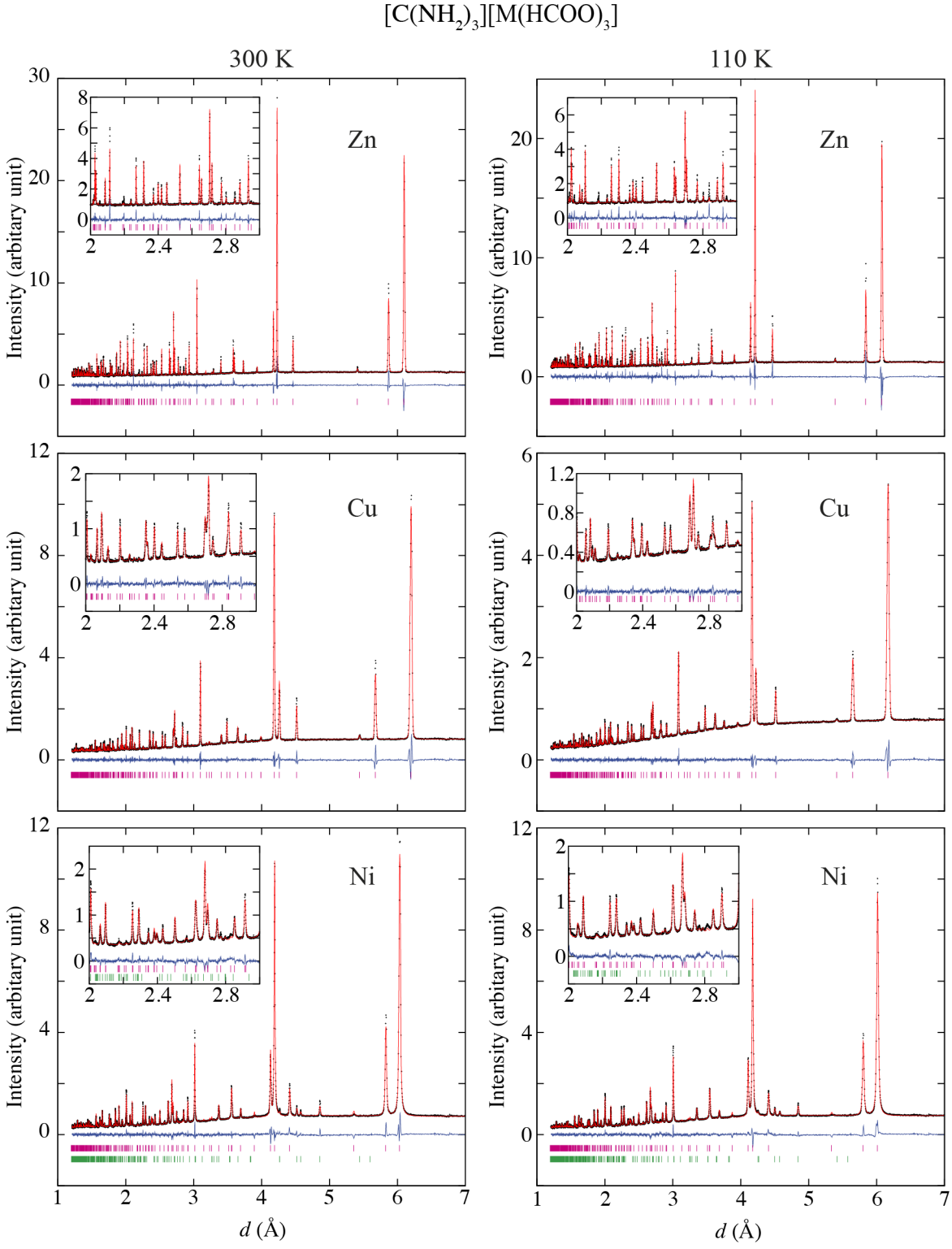

Figure S7: Rietveld fits for $[C(NH_2)_3][M(HCOO)_3]$ with M = Ni, Cu, Zn at 300 K (left) and 110 K (right).

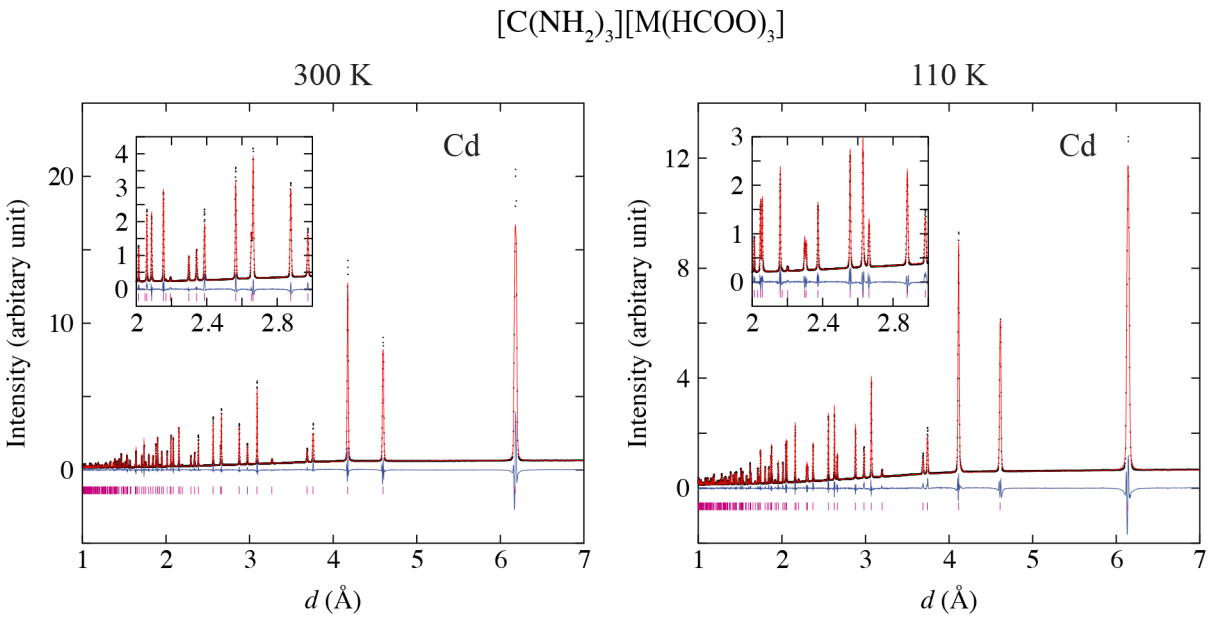

Figure S8: Rietveld fits for $[C(NH_2)_3][Cd(HCOO)_3]$ at 300 K and 110 K.

3 Lattice parameter evolutions for [A][M(HCOO)$_3$]

The lattice parameter evolutions as a function of temperature (110–300 K) for the [A][M(HCOO)$_3$] compounds investigated are found in Figures S9–S12. In all figures, the cooling data are indicated by the blue circles, and the heating data by red circles. The black dotted lines indicate the linear fits used to calculate the coefficients of thermal expansion (CTEs); the error on each of the CTEs is then calculated based upon the discrepancy between the linear fit and the data. Table S2 gives the CTEs for the monoclinic and orthorhombic phases of [$(CH_2)_3NH_2$][Mn(HCOO)$_3$]. These CTEs show that there is no great difference in the mechanical properties of the two phases.

Deviations from the straight line fits are observed in the cases where (*i*) phase transitions occur, *e.g.* $MeNH_3$-Cd and Aze-Mn, and where (*ii*) there are small changes in the lattice parameters coupled with anisotropic peak broadening, *e.g.* the *c*-lattice parameter in Gua-Fe and Gua-Cu.

Table S2: Calculated linear expansivities for the orthorhombic phase of Aze-Mn (*Pnna* symmetry), and the monoclinic phase arising below ∼250 K. In the orthorhombic phase, the $\mathbf{x}_1$, $\mathbf{x}_2$, and $\mathbf{x}_3$ directions correspond to **a**, **b**, and **c** lattice vectors, respectively, while for the monoclinic phase: $\mathbf{x}_1 = -0.6793\mathbf{a} + 0.7339\mathbf{c}$, $\mathbf{x}_2 = \mathbf{b}$, and $\mathbf{x}_3 = 0.7326\mathbf{a} + 0.6807\mathbf{c}$.[S9]

Symmetry	T range (K)	α (MK^{-1})		
		$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
Pnna	110–300	104(8)	15.3(1.2)	−21(6)
$P2_1/n$	110–260	109(11)	11.5(16)	−27(8)

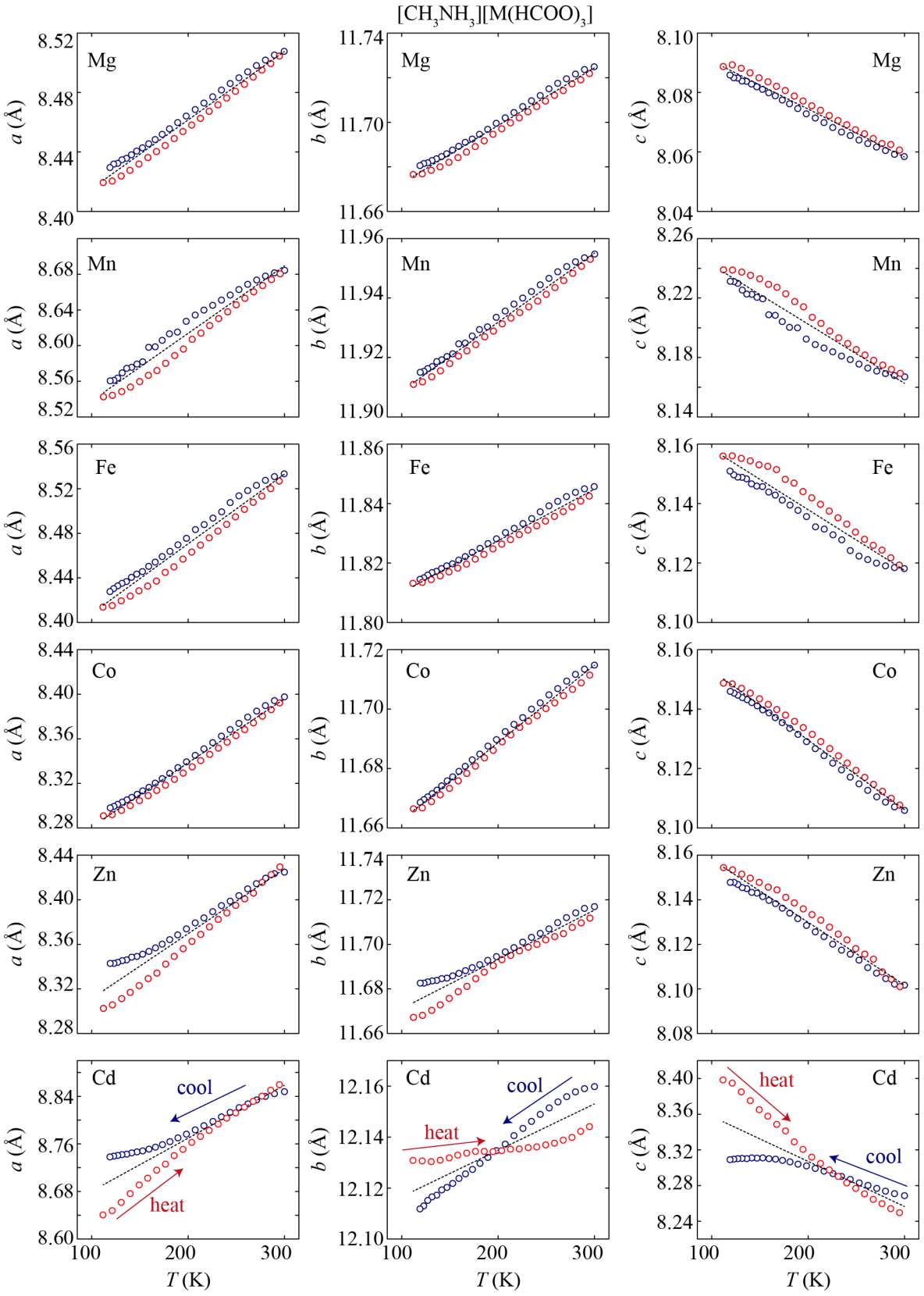

Figure S9: Lattice parameter evolutions as a function of temperature for the $[CH_3NH_3][M(HCOO)_3]$ family.

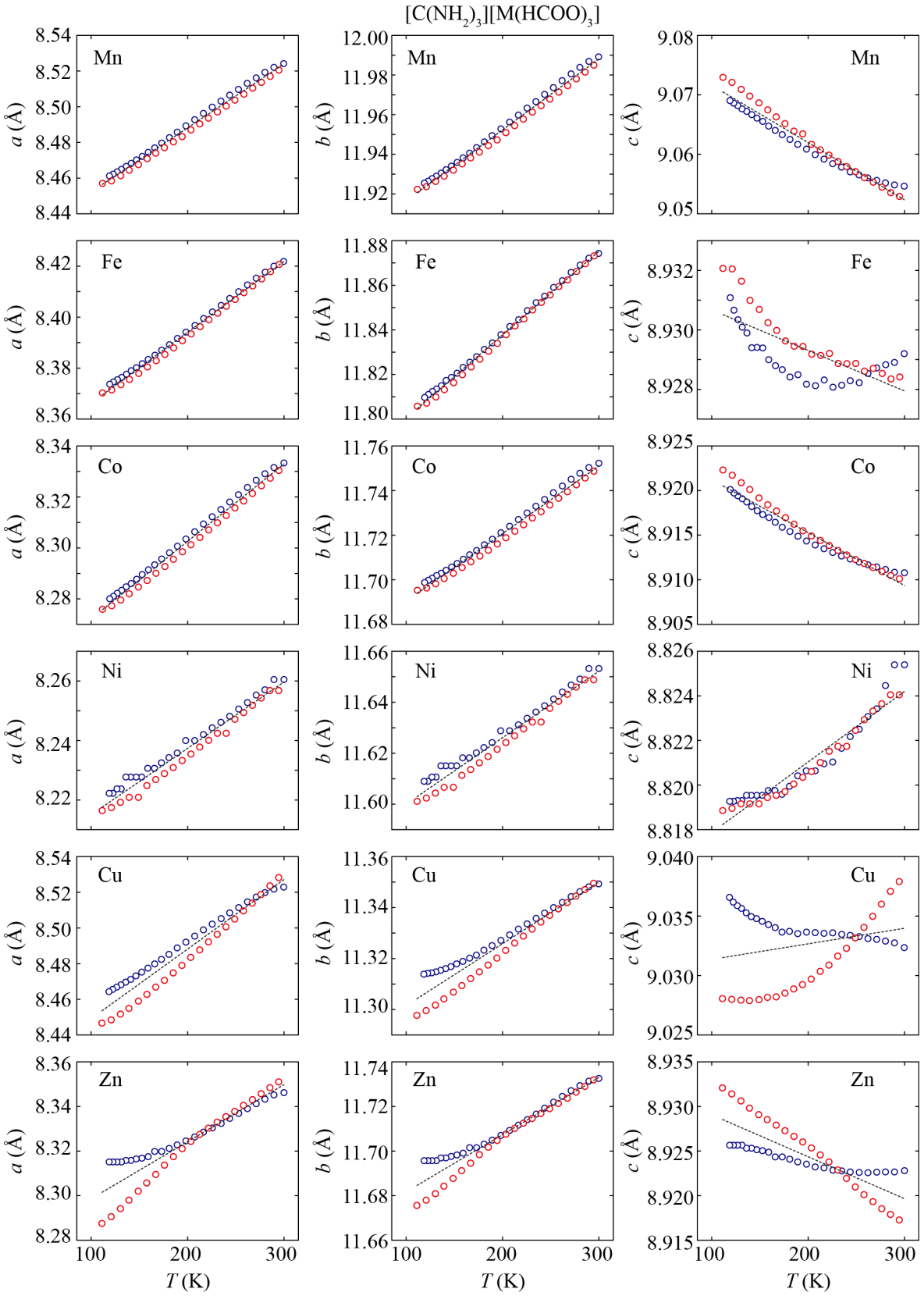

Figure S10: Lattice parameter evolutions as a function of temperature for the $[C(NH_2)_3][M(HCOO)_3]$ family.

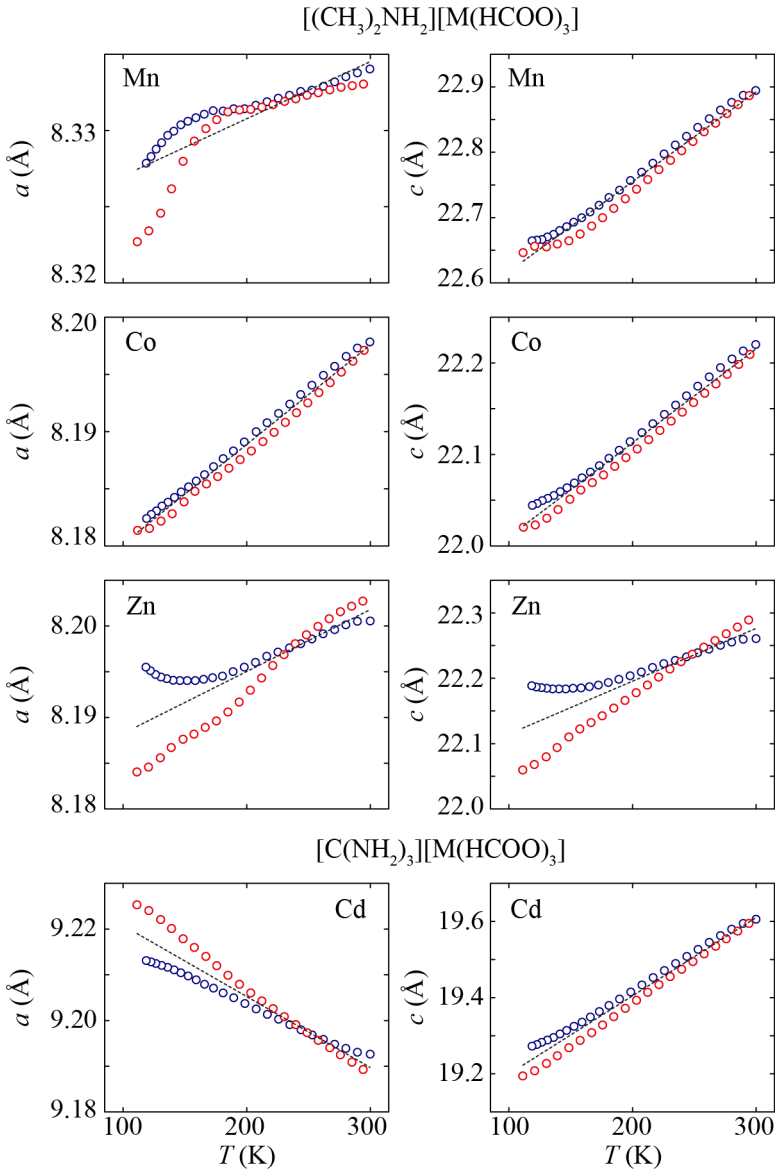

Figure S11: Lattice parameter evolutions as a function of temperature for the $[(CH_3)_2NH_2][M(HCOO)_3]$ family and $[C(NH_2)_3][Cd(HCOO)_3]$.

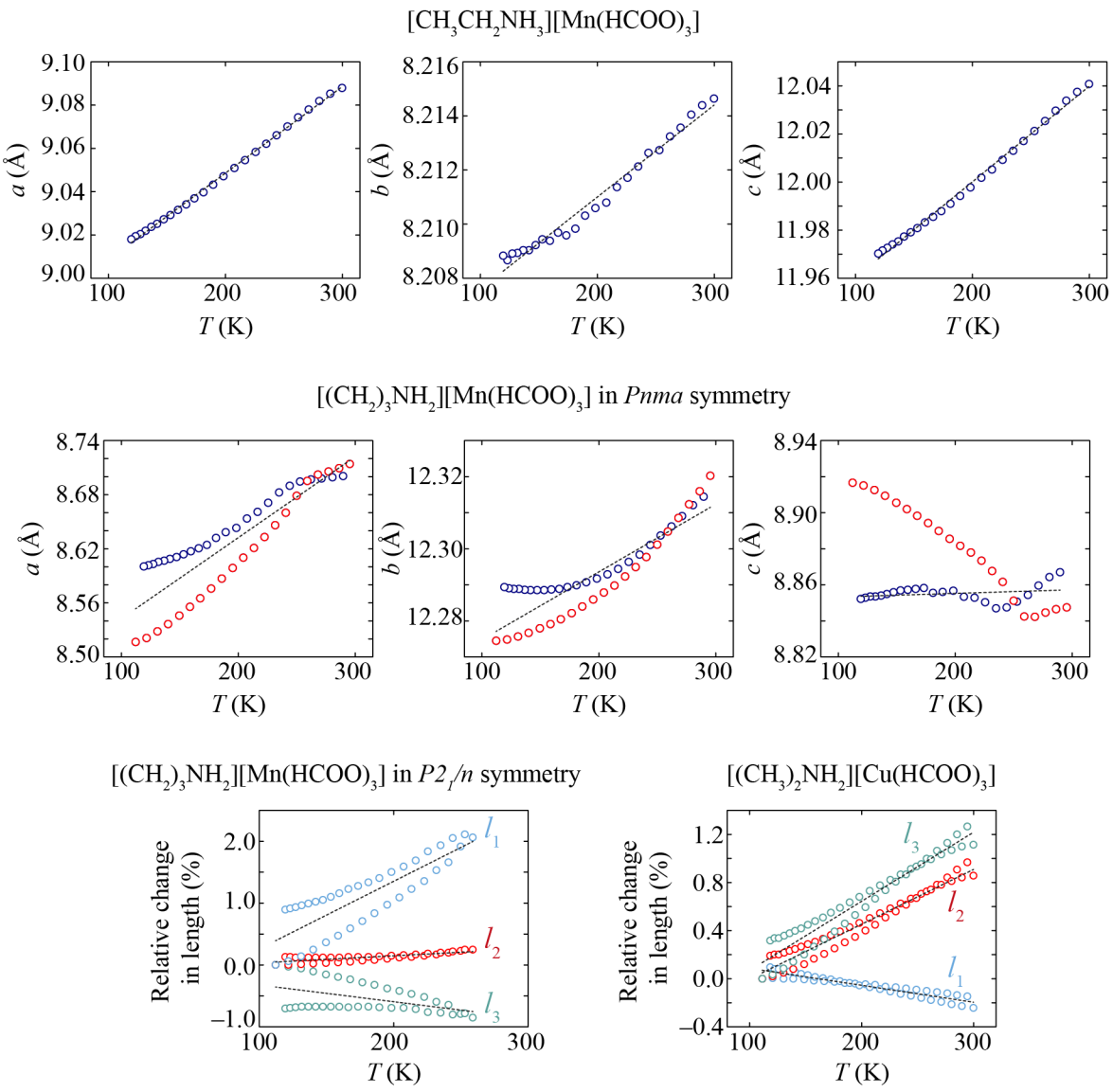

Figure S12: (*Top*) Lattice parameter evolutions as a function of temperature for $[CH_3CH_2NH_3][Mn(HCOO)_3]$, and $[(CH_2)_3NH_2][Mn(HCOO)_3]$ refined in orthorhombic *Pnma* symmetry. (*Bottom*) The relative changes in principal axes for the monoclinic structures: LT $[(CH_2)_3NH_2][Mn(HCOO)_3]$ and $[(CH_3)_2NH_2][Cu(HCOO)_3]$.

4 Variable-temperature lattice parameters for [A][M(HCOO)$_3$]

Table S3: Variable-temperature lattice parameter data for $MeNH_3$-Mg.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.78	8.5078	0.0002	11.7248	0.0002	8.0585	0.0002	803.85	0.03
289.54	8.5052	0.0002	11.7236	0.0002	8.0592	0.0002	803.60	0.03
280.22	8.5019	0.0002	11.7217	0.0003	8.0605	0.0002	803.28	0.03
271.06	8.4980	0.0002	11.7195	0.0003	8.0617	0.0002	802.88	0.03
261.98	8.4940	0.0002	11.7174	0.0003	8.0629	0.0002	802.47	0.03
252.84	8.4898	0.0002	11.7150	0.0003	8.0640	0.0002	802.03	0.04
243.73	8.4859	0.0002	11.7119	0.0003	8.0655	0.0002	801.60	0.04
234.62	8.4816	0.0002	11.7097	0.0003	8.0667	0.0002	801.16	0.04
225.50	8.4772	0.0002	11.7071	0.0003	8.0682	0.0002	800.72	0.04
216.37	8.4729	0.0003	11.7043	0.0003	8.0699	0.0002	800.29	0.04
207.31	8.4686	0.0003	11.7020	0.0003	8.0714	0.0002	799.87	0.04
198.19	8.4641	0.0003	11.6996	0.0003	8.0729	0.0003	799.43	0.04
189.15	8.4598	0.0003	11.6969	0.0003	8.0746	0.0003	799.00	0.04
180.80	8.4557	0.0003	11.6946	0.0003	8.0762	0.0003	798.62	0.04
173.09	8.4519	0.0003	11.6925	0.0004	8.0775	0.0003	798.25	0.04
165.97	8.4484	0.0003	11.6910	0.0004	8.0789	0.0003	797.95	0.05
159.24	8.4456	0.0003	11.6892	0.0004	8.0799	0.0003	797.66	0.05
152.75	8.4429	0.0003	11.6875	0.0004	8.0811	0.0003	797.41	0.05
146.83	8.4405	0.0003	11.6859	0.0004	8.0819	0.0003	797.16	0.05

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Table S3 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
141.30	8.4381	0.0004	11.6847	0.0004	8.0829	0.0003	796.94	0.06
136.12	8.4357	0.0004	11.6836	0.0005	8.0838	0.0004	796.73	0.06
131.42	8.4348	0.0004	11.6828	0.0005	8.0838	0.0004	796.59	0.06
126.90	8.4324	0.0004	11.6818	0.0005	8.0849	0.0004	796.41	0.06
122.82	8.4319	0.0004	11.6815	0.0005	8.0849	0.0004	796.34	0.06
119.04	8.4295	0.0004	11.6806	0.0006	8.0859	0.0004	796.15	0.07
111.88	8.4194	0.0005	11.6766	0.0006	8.0887	0.0004	795.20	0.07
121.21	8.4204	0.0004	11.6768	0.0006	8.0893	0.0004	795.38	0.07
130.70	8.4238	0.0004	11.6784	0.0005	8.0881	0.0004	795.68	0.07
139.72	8.4277	0.0004	11.6800	0.0005	8.0867	0.0004	796.01	0.06
149.06	8.4319	0.0004	11.6821	0.0004	8.0850	0.0004	796.38	0.06
158.26	8.4362	0.0003	11.6842	0.0004	8.0836	0.0004	796.80	0.05
167.26	8.4403	0.0003	11.6866	0.0004	8.0821	0.0003	797.21	0.05
176.34	8.4444	0.0003	11.6891	0.0004	8.0806	0.0003	797.61	0.05
185.58	8.4491	0.0003	11.6917	0.0003	8.0788	0.0003	798.06	0.05
194.63	8.4537	0.0003	11.6946	0.0003	8.0771	0.0003	798.52	0.04
203.66	8.4581	0.0003	11.6971	0.0003	8.0755	0.0003	798.95	0.04
212.77	8.4626	0.0003	11.6997	0.0003	8.0741	0.0003	799.41	0.04
221.93	8.4673	0.0003	11.7021	0.0003	8.0723	0.0003	799.83	0.04
231.01	8.4718	0.0003	11.7047	0.0003	8.0705	0.0002	800.27	0.04
240.17	8.4763	0.0002	11.7071	0.0003	8.0691	0.0002	800.72	0.04

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Table S3 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
249.21	8.4808	0.0002	11.7095	0.0003	8.0675	0.0002	801.15	0.04
258.35	8.4855	0.0002	11.7121	0.0003	8.0661	0.0002	801.63	0.04
267.48	8.4904	0.0002	11.7143	0.0002	8.0645	0.0002	802.08	0.03
276.57	8.4950	0.0002	11.7172	0.0002	8.0628	0.0002	802.55	0.03
285.70	8.4995	0.0002	11.7190	0.0002	8.0625	0.0002	803.07	0.03
294.80	8.5045	0.0002	11.7219	0.0002	8.0606	0.0002	803.55	0.03

Table S4: Variable-temperature lattice parameter data for $MeNH_3$-Mn.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
300.09	8.68444	0.00006	11.95480	0.00008	8.16700	0.00006	847.904	0.010
289.63	8.68145	0.00006	11.95352	0.00007	8.16793	0.00005	847.618	0.009
280.31	8.67778	0.00006	11.95217	0.00007	8.16929	0.00006	847.305	0.010
271.08	8.67350	0.00007	11.95061	0.00008	8.17090	0.00006	846.943	0.011
261.94	8.66872	0.00007	11.94877	0.00009	8.17290	0.00007	846.554	0.012
252.83	8.66289	0.00008	11.94659	0.00009	8.17555	0.00007	846.104	0.012
243.73	8.65677	0.00008	11.94445	0.00009	8.17853	0.00007	845.662	0.013
234.60	8.65120	0.00009	11.94216	0.00009	8.18094	0.00008	845.206	0.014
225.60	8.64514	0.00011	11.93995	0.00010	8.18389	0.00009	844.762	0.016
216.41	8.63978	0.00013	11.93796	0.00011	8.18636	0.00011	844.352	0.019
207.29	8.63416	0.00015	11.93558	0.00012	8.18871	0.00013	843.876	0.022

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Table S4 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
198.11	8.62721	0.00017	11.93348	0.00013	8.19242	0.00015	843.432	0.025
189.12	8.61525	0.00016	11.93034	0.00012	8.19997	0.00014	842.816	0.023
180.70	8.61332	0.00020	11.92940	0.00014	8.20032	0.00018	842.596	0.029
173.11	8.60601	0.00021	11.92717	0.00014	8.20418	0.00018	842.120	0.030
165.95	8.59875	0.00020	11.92485	0.00015	8.20842	0.00018	841.682	0.029
159.28	8.59800	0.00023	11.92458	0.00017	8.20876	0.00021	841.624	0.034
152.92	8.58187	0.00018	11.92122	0.00012	8.21951	0.00016	840.908	0.025
147.04	8.57932	0.00019	11.92026	0.00013	8.22050	0.00017	840.692	0.027
141.54	8.57561	0.00019	11.91921	0.00014	8.22247	0.00017	840.455	0.027
136.38	8.57446	0.00021	11.91867	0.00015	8.22267	0.00019	840.325	0.030
131.63	8.56958	0.00020	11.91694	0.00015	8.22534	0.00018	839.999	0.029
127.09	8.56355	0.00019	11.91626	0.00015	8.22984	0.00017	839.818	0.027
122.98	8.56114	0.00019	11.91531	0.00015	8.23112	0.00017	839.645	0.028
119.24	8.56053	0.00020	11.91504	0.00016	8.23121	0.00018	839.576	0.029
112.11	8.54250	0.00025	11.91097	0.00026	8.23898	0.00024	838.311	0.040
121.64	8.54413	0.00023	11.91179	0.00023	8.23875	0.00022	838.506	0.036
131.22	8.54840	0.00021	11.91353	0.00020	8.23746	0.00020	838.916	0.032
140.25	8.55356	0.00018	11.91551	0.00017	8.23523	0.00017	839.335	0.028
149.74	8.55957	0.00016	11.91796	0.00015	8.23287	0.00015	839.856	0.024
158.81	8.56678	0.00014	11.92049	0.00013	8.22931	0.00013	840.380	0.021
167.71	8.57197	0.00014	11.92223	0.00013	8.22715	0.00013	840.789	0.021

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Table S4 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
176.87	8.58002	0.00013	11.92439	0.00013	8.22288	0.00012	841.295	0.020
186.12	8.58891	0.00013	11.92694	0.00012	8.21768	0.00012	841.814	0.020
195.22	8.59619	0.00012	11.92893	0.00011	8.21404	0.00011	842.295	0.018
204.30	8.60698	0.00012	11.93136	0.00011	8.20699	0.00010	842.800	0.018
213.41	8.61401	0.00010	11.93329	0.00010	8.20295	0.00010	843.210	0.016
222.51	8.62245	0.00010	11.93513	0.00010	8.19780	0.00009	843.637	0.015
231.69	8.63037	0.00009	11.93701	0.00009	8.19328	0.00008	844.079	0.014
240.92	8.63778	0.00008	11.93900	0.00009	8.18936	0.00007	844.540	0.013
250.00	8.64558	0.00007	11.94124	0.00008	8.18533	0.00007	845.045	0.012
259.10	8.65289	0.00007	11.94350	0.00008	8.18171	0.00006	845.546	0.011
268.18	8.66022	0.00007	11.94586	0.00008	8.17815	0.00006	846.060	0.010
277.31	8.66737	0.00006	11.94826	0.00008	8.17488	0.00006	846.590	0.011
286.39	8.67403	0.00006	11.95067	0.00008	8.17204	0.00006	847.118	0.010
295.47	8.68057	0.00006	11.95299	0.00008	8.16941	0.00006	847.649	0.010

Table S5: Variable-temperature lattice parameter data for $MeNH_3$-Fe.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.79	8.53325	0.00006	11.84574	0.00006	8.11808	0.00006	820.597	0.009
289.50	8.53084	0.00006	11.84493	0.00006	8.11847	0.00005	820.348	0.009
280.22	8.52754	0.00006	11.84376	0.00006	8.11902	0.00006	820.006	0.009

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Table S5 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
271.07	8.52312	0.00006	11.84232	0.00007	8.12000	0.00006	819.580	0.010
261.94	8.51823	0.00007	11.84075	0.00007	8.12114	0.00007	819.117	0.011
252.85	8.51346	0.00007	11.83923	0.00008	8.12231	0.00007	818.671	0.011
243.71	8.50747	0.00008	11.83724	0.00008	8.12417	0.00008	818.144	0.012
234.74	8.49925	0.00007	11.83497	0.00007	8.12782	0.00006	817.564	0.010
225.66	8.49361	0.00007	11.83328	0.00006	8.12949	0.00007	817.072	0.010
216.56	8.48774	0.00006	11.83162	0.00006	8.13138	0.00006	816.583	0.010
207.51	8.48335	0.00008	11.83021	0.00007	8.13222	0.00007	816.148	0.011
198.41	8.47548	0.00007	11.82815	0.00007	8.13559	0.00007	815.587	0.011
189.44	8.46955	0.00008	11.82648	0.00007	8.13768	0.00007	815.111	0.011
181.14	8.46395	0.00008	11.82491	0.00007	8.13947	0.00008	814.643	0.012
173.31	8.45902	0.00008	11.82358	0.00007	8.14119	0.00008	814.248	0.013
166.02	8.45413	0.00009	11.82215	0.00008	8.14285	0.00009	813.844	0.013
159.29	8.45040	0.00009	11.82098	0.00008	8.14386	0.00009	813.506	0.014
152.70	8.44566	0.00010	11.81975	0.00008	8.14571	0.00009	813.151	0.014
146.78	8.44350	0.00010	11.81902	0.00009	8.14584	0.00010	812.905	0.015
141.24	8.44054	0.00011	11.81812	0.00009	8.14667	0.00010	812.641	0.016
136.09	8.43655	0.00011	11.81716	0.00009	8.14832	0.00010	812.355	0.016
131.30	8.43505	0.00011	11.81678	0.00010	8.14881	0.00011	812.234	0.017
126.83	8.43288	0.00012	11.81592	0.00010	8.14893	0.00011	811.977	0.017
122.77	8.43036	0.00012	11.81504	0.00010	8.14963	0.00012	811.745	0.018

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Table S5 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
118.83	8.42760	0.00012	11.81453	0.00010	8.15091	0.00012	811.570	0.018
111.79	8.41374	0.00010	11.81313	0.00009	8.15595	0.00010	810.641	0.015
121.25	8.41512	0.00010	11.81350	0.00009	8.15608	0.00010	810.813	0.015
130.67	8.41931	0.00009	11.81441	0.00008	8.15518	0.00009	811.189	0.013
139.84	8.42363	0.00008	11.81572	0.00008	8.15432	0.00008	811.610	0.013
149.11	8.42846	0.00008	11.81698	0.00007	8.15302	0.00008	812.032	0.012
158.11	8.43265	0.00008	11.81833	0.00007	8.15248	0.00008	812.475	0.012
167.24	8.43723	0.00008	11.81967	0.00007	8.15143	0.00008	812.904	0.012
176.26	8.44487	0.00007	11.82135	0.00007	8.14810	0.00007	813.423	0.011
185.37	8.44983	0.00007	11.82294	0.00007	8.14692	0.00007	813.892	0.011
194.61	8.45693	0.00007	11.82475	0.00007	8.14405	0.00007	814.413	0.011
203.65	8.46305	0.00007	11.82634	0.00007	8.14187	0.00007	814.895	0.011
212.76	8.46941	0.00007	11.82785	0.00007	8.13972	0.00007	815.396	0.011
221.90	8.47583	0.00007	11.82955	0.00006	8.13750	0.00007	815.909	0.010
231.02	8.48202	0.00007	11.83103	0.00006	8.13517	0.00007	816.373	0.010
240.08	8.48796	0.00007	11.83248	0.00007	8.13309	0.00007	816.835	0.010
249.20	8.49481	0.00007	11.83408	0.00006	8.13040	0.00006	817.335	0.010
258.39	8.50139	0.00006	11.83572	0.00006	8.12797	0.00006	817.837	0.010
267.48	8.50763	0.00007	11.83734	0.00007	8.12592	0.00007	818.342	0.011
276.61	8.51336	0.00006	11.83887	0.00007	8.12435	0.00006	818.841	0.010
285.70	8.52013	0.00008	11.84079	0.00008	8.12178	0.00007	819.366	0.011

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Table S5 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
294.63	8.52688	0.00006	11.84251	0.00006	8.11931	0.00006	819.885	0.009

Table S6: Variable-temperature lattice parameter data for $MeNH_3$-Co.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.87	8.39751	0.00009	11.71476	0.00010	8.10591	0.00009	797.417	0.014
289.68	8.39429	0.00009	11.71346	0.00010	8.10716	0.00009	797.146	0.014
280.32	8.38972	0.00009	11.71165	0.00010	8.10869	0.00009	796.740	0.014
271.19	8.38478	0.00009	11.70937	0.00011	8.11049	0.00009	796.293	0.015
261.95	8.37945	0.00010	11.70687	0.00011	8.11268	0.00009	795.831	0.015
252.85	8.37383	0.00010	11.70480	0.00011	8.11483	0.00010	795.367	0.015
243.73	8.36817	0.00010	11.70206	0.00011	8.11712	0.00010	794.868	0.015
234.62	8.36254	0.00010	11.70000	0.00011	8.11955	0.00010	794.431	0.016
225.57	8.35670	0.00011	11.69717	0.00011	8.12186	0.00010	793.910	0.016
216.46	8.35098	0.00011	11.69486	0.00011	8.12431	0.00011	793.449	0.017
207.39	8.34523	0.00011	11.69238	0.00012	8.12672	0.00011	792.970	0.017
198.30	8.33938	0.00011	11.68976	0.00012	8.12906	0.00011	792.465	0.018
189.36	8.33423	0.00012	11.68753	0.00013	8.13147	0.00012	792.059	0.018
180.96	8.32902	0.00012	11.68484	0.00013	8.13347	0.00012	791.576	0.019
173.19	8.32430	0.00013	11.68294	0.00013	8.13542	0.00013	791.189	0.020
166.04	8.32031	0.00013	11.68076	0.00014	8.13708	0.00013	790.823	0.020

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Table S6 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
159.36	8.31649	0.00014	11.67903	0.00014	8.13873	0.00014	790.503	0.021
153.03	8.31336	0.00014	11.67723	0.00014	8.13972	0.00014	790.180	0.022
147.13	8.31020	0.00015	11.67586	0.00015	8.14108	0.00015	789.919	0.023
141.55	8.30754	0.00016	11.67414	0.00016	8.14217	0.00015	789.655	0.023
136.42	8.30515	0.00016	11.67273	0.00016	8.14315	0.00016	789.428	0.024
131.65	8.30328	0.00017	11.67155	0.00016	8.14383	0.00016	789.236	0.025
127.07	8.30121	0.00018	11.67050	0.00017	8.14470	0.00017	789.053	0.026
122.97	8.29954	0.00019	11.66954	0.00018	8.14537	0.00017	788.894	0.027
119.13	8.29807	0.00019	11.66857	0.00019	8.14598	0.00018	788.748	0.028
112.13	8.29096	0.00026	11.66642	0.00023	8.14876	0.00025	788.195	0.038
121.35	8.29193	0.00025	11.66676	0.00023	8.14843	0.00023	788.279	0.036
130.93	8.29580	0.00022	11.66886	0.00021	8.14698	0.00020	788.648	0.032
140.03	8.30000	0.00019	11.67116	0.00018	8.14537	0.00018	789.047	0.028
149.39	8.30464	0.00018	11.67336	0.00018	8.14345	0.00017	789.451	0.026
158.55	8.30895	0.00016	11.67586	0.00016	8.14162	0.00015	789.853	0.024
167.49	8.31367	0.00015	11.67838	0.00015	8.13983	0.00014	790.298	0.023
176.65	8.31849	0.00014	11.68081	0.00015	8.13795	0.00014	790.737	0.021
185.81	8.32370	0.00013	11.68356	0.00014	8.13586	0.00013	791.216	0.020
195.00	8.32925	0.00013	11.68609	0.00014	8.13376	0.00012	791.711	0.020
204.13	8.33486	0.00012	11.68897	0.00013	8.13144	0.00012	792.213	0.019
213.14	8.34038	0.00012	11.69133	0.00013	8.12906	0.00012	792.665	0.018

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Table S6 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
222.32	8.34602	0.00011	11.69385	0.00012	8.12673	0.00011	793.146	0.017
231.42	8.35158	0.00011	11.69593	0.00012	8.12428	0.00011	793.576	0.017
240.50	8.35706	0.00011	11.69780	0.00012	8.12182	0.00011	793.984	0.017
249.63	8.36285	0.00011	11.70018	0.00011	8.11942	0.00010	794.459	0.016
258.66	8.36834	0.00010	11.70208	0.00011	8.11705	0.00010	794.878	0.016
267.83	8.37429	0.00010	11.70450	0.00011	8.11467	0.00010	795.375	0.015
277.03	8.38026	0.00010	11.70663	0.00011	8.11233	0.00009	795.856	0.015
286.08	8.38622	0.00010	11.70887	0.00011	8.10994	0.00009	796.341	0.015
295.17	8.39236	0.00009	11.71141	0.00010	8.10770	0.00009	796.877	0.015

Table S7: Variable-temperature lattice parameter data for $MeNH_3$-Zn.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.87	8.42480	0.00007	11.71688	0.00008	8.10176	0.00007	799.744	0.011
289.67	8.42354	0.00007	11.71617	0.00009	8.10221	0.00007	799.621	0.012
280.36	8.41940	0.00007	11.71413	0.00009	8.10456	0.00008	799.320	0.012
271.07	8.41443	0.00008	11.71197	0.00009	8.10714	0.00008	798.955	0.013
261.94	8.40974	0.00008	11.70975	0.00009	8.10951	0.00008	798.592	0.013
252.83	8.40365	0.00008	11.70691	0.00010	8.11291	0.00008	798.155	0.013
243.75	8.39875	0.00008	11.70484	0.00011	8.11565	0.00009	797.817	0.014
234.62	8.39467	0.00008	11.70306	0.00010	8.11737	0.00008	797.478	0.013

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Table S7 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
225.60	8.38944	0.00008	11.70093	0.00010	8.12013	0.00008	797.107	0.013
216.46	8.38367	0.00008	11.69846	0.00010	8.12338	0.00008	796.709	0.013
207.38	8.37928	0.00008	11.69663	0.00010	8.12558	0.00008	796.383	0.013
198.30	8.37391	0.00008	11.69446	0.00011	8.12849	0.00008	796.009	0.013
189.34	8.36846	0.00008	11.69278	0.00010	8.13151	0.00008	795.673	0.013
181.00	8.36420	0.00009	11.69087	0.00010	8.13396	0.00008	795.378	0.013
173.26	8.36021	0.00009	11.68949	0.00010	8.13621	0.00008	795.124	0.014
166.22	8.35675	0.00009	11.68816	0.00011	8.13824	0.00009	794.903	0.014
159.50	8.35376	0.00009	11.68700	0.00011	8.13976	0.00008	794.688	0.014
153.05	8.35121	0.00009	11.68588	0.00011	8.14140	0.00009	794.530	0.015
147.05	8.34918	0.00010	11.68479	0.00012	8.14301	0.00009	794.419	0.015
141.53	8.34858	0.00010	11.68466	0.00012	8.14332	0.00009	794.384	0.016
136.38	8.34602	0.00010	11.68386	0.00012	8.14496	0.00009	794.245	0.016
131.63	8.34535	0.00011	11.68359	0.00013	8.14539	0.00009	794.205	0.016
127.10	8.34370	0.00011	11.68309	0.00013	8.14694	0.00010	794.166	0.017
122.98	8.34289	0.00012	11.68263	0.00013	8.14785	0.00010	794.146	0.017
119.29	8.34289	0.00012	11.68263	0.00013	8.14785	0.00010	794.146	0.017
112.15	8.30243	0.00010	11.66721	0.00013	8.15441	0.00010	789.887	0.016
121.48	8.30574	0.00009	11.66813	0.00012	8.15340	0.00009	790.166	0.015
131.05	8.31120	0.00009	11.67040	0.00011	8.15145	0.00009	790.650	0.014
140.07	8.31685	0.00008	11.67280	0.00011	8.14963	0.00009	791.174	0.014

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Table S7 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
149.37	8.32291	0.00008	11.67575	0.00011	8.14776	0.00009	791.769	0.014
158.56	8.32917	0.00008	11.67884	0.00011	8.14567	0.00009	792.370	0.014
167.63	8.33424	0.00008	11.68113	0.00011	8.14442	0.00009	792.886	0.014
176.70	8.34214	0.00008	11.68462	0.00011	8.14109	0.00009	793.551	0.014
185.76	8.34910	0.00008	11.68758	0.00011	8.13857	0.00009	794.167	0.014
194.87	8.35608	0.00009	11.69047	0.00011	8.13588	0.00009	794.765	0.014
203.99	8.36272	0.00009	11.69318	0.00012	8.13331	0.00009	795.330	0.015
213.17	8.36886	0.00011	11.69503	0.00014	8.13088	0.00011	795.802	0.018
222.21	8.37567	0.00010	11.69711	0.00014	8.12769	0.00010	796.279	0.017
231.28	8.38233	0.00010	11.69874	0.00015	8.12454	0.00010	796.714	0.017
240.41	8.38808	0.00010	11.69994	0.00015	8.12198	0.00011	797.091	0.018
249.49	8.39499	0.00010	11.70198	0.00014	8.11801	0.00010	797.497	0.017
258.72	8.40073	0.00010	11.70338	0.00015	8.11559	0.00011	797.900	0.017
267.79	8.40602	0.00011	11.70477	0.00016	8.11332	0.00012	798.274	0.019
276.98	8.41544	0.00010	11.70757	0.00014	8.10768	0.00011	798.803	0.017
286.09	8.42250	0.00009	11.70961	0.00014	8.10436	0.00010	799.286	0.017
295.23	8.42945	0.00009	11.71180	0.00014	8.10107	0.00011	799.770	0.017

Table S8: Variable-temperature lattice parameter data for $MeNH_3$-Cd.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.88	8.84786	0.00003	12.15981	0.00004	8.26861	0.00003	889.606	0.006
289.65	8.84468	0.00003	12.15904	0.00004	8.27077	0.00003	889.463	0.006
280.33	8.83981	0.00004	12.15771	0.00004	8.27360	0.00003	889.179	0.006
271.17	8.83394	0.00004	12.15585	0.00004	8.27676	0.00003	888.792	0.006
262.02	8.82727	0.00004	12.15384	0.00004	8.28016	0.00004	888.339	0.006
252.94	8.82082	0.00005	12.15143	0.00005	8.28307	0.00004	887.826	0.007
243.85	8.81290	0.00005	12.14894	0.00005	8.28691	0.00004	887.258	0.008
234.69	8.80533	0.00005	12.14617	0.00005	8.29022	0.00005	886.648	0.008
225.69	8.79800	0.00005	12.14339	0.00005	8.29331	0.00005	886.036	0.008
216.48	8.79083	0.00006	12.14058	0.00005	8.29618	0.00005	885.417	0.009
207.38	8.78339	0.00007	12.13721	0.00006	8.29914	0.00006	884.737	0.011
198.32	8.77628	0.00007	12.13466	0.00006	8.30201	0.00007	884.140	0.011
189.35	8.77034	0.00008	12.13200	0.00006	8.30391	0.00007	883.551	0.012
181.09	8.76399	0.00008	12.12964	0.00006	8.30659	0.00008	883.024	0.013
173.37	8.75886	0.00009	12.12734	0.00007	8.30821	0.00008	882.512	0.013
166.22	8.75469	0.00009	12.12553	0.00007	8.30946	0.00009	882.093	0.014
159.34	8.75104	0.00011	12.12379	0.00007	8.31026	0.00011	881.683	0.017
152.89	8.74829	0.00010	12.12180	0.00007	8.31082	0.00010	881.321	0.015
146.88	8.74637	0.00010	12.12021	0.00007	8.31063	0.00009	880.991	0.015
141.38	8.74498	0.00011	12.11932	0.00008	8.31099	0.00010	880.826	0.017

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Table S8 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
136.23	8.74283	0.00010	12.11720	0.00007	8.31030	0.00010	880.381	0.016
131.38	8.74190	0.00011	12.11651	0.00008	8.31053	0.00011	880.262	0.017
126.87	8.74075	0.00011	12.11519	0.00008	8.31002	0.00010	879.996	0.016
122.77	8.73931	0.00011	12.11302	0.00007	8.30945	0.00010	879.634	0.016
119.00	8.73829	0.00010	12.11182	0.00007	8.30888	0.00010	879.383	0.015
111.83	8.64059	0.00011	12.13085	0.00012	8.39835	0.00011	880.296	0.019
121.30	8.64754	0.00011	12.13064	0.00011	8.39469	0.00010	880.604	0.018
130.61	8.66147	0.00008	12.13037	0.00008	8.38490	0.00007	880.975	0.012
139.81	8.67624	0.00006	12.13098	0.00005	8.37524	0.00006	881.505	0.009
149.23	8.69090	0.00007	12.13186	0.00006	8.36523	0.00006	882.003	0.010
158.23	8.70264	0.00008	12.13291	0.00006	8.35766	0.00007	882.473	0.011
167.35	8.71584	0.00009	12.13376	0.00007	8.34840	0.00008	882.892	0.013
176.54	8.72591	0.00012	12.13440	0.00010	8.34120	0.00011	883.196	0.018
185.55	8.74029	0.00008	12.13436	0.00007	8.32891	0.00008	883.347	0.013
194.67	8.75089	0.00008	12.13427	0.00007	8.32059	0.00007	883.527	0.012
203.77	8.76255	0.00007	12.13465	0.00006	8.31190	0.00007	883.808	0.011
212.89	8.77263	0.00009	12.13525	0.00008	8.30463	0.00008	884.095	0.014
221.99	8.78272	0.00010	12.13537	0.00009	8.29757	0.00009	884.368	0.015
231.12	8.79323	0.00008	12.13580	0.00007	8.29015	0.00007	884.666	0.012
240.16	8.80349	0.00007	12.13613	0.00007	8.28291	0.00007	884.948	0.011
249.30	8.81232	0.00009	12.13693	0.00008	8.27674	0.00008	885.235	0.013

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Table S8 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
258.41	8.82187	0.00007	12.13765	0.00007	8.27045	0.00007	885.573	0.012
267.60	8.83143	0.00007	12.13882	0.00007	8.26442	0.00007	885.972	0.011
276.69	8.84030	0.00007	12.13989	0.00007	8.25956	0.00007	886.419	0.011
285.77	8.85018	0.00007	12.14219	0.00007	8.25404	0.00006	886.983	0.011
294.90	8.85968	0.00007	12.14411	0.00007	8.24962	0.00007	887.601	0.011

Table S9: Variable-temperature lattice parameter data for $EtNH_3$-Mn.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.83	9.08800	0.00014	12.04075	0.00013	8.21464	0.00011	898.90	0.02
289.63	9.08523	0.00014	12.03751	0.00012	8.21440	0.00011	898.36	0.02
280.35	9.08187	0.00014	12.03384	0.00013	8.21405	0.00011	897.71	0.02
271.17	9.07808	0.00014	12.02974	0.00012	8.21357	0.00011	896.98	0.02
262.03	9.07428	0.00014	12.02541	0.00013	8.21324	0.00011	896.25	0.02
252.95	9.07018	0.00013	12.02117	0.00012	8.21274	0.00011	895.47	0.02
243.86	9.06611	0.00013	12.01707	0.00012	8.21264	0.00011	894.75	0.02
234.71	9.06218	0.00013	12.01301	0.00012	8.21213	0.00011	894.01	0.02
225.83	9.05834	0.00013	12.00925	0.00012	8.21172	0.00011	893.30	0.02
216.66	9.05460	0.00014	12.00517	0.00013	8.21137	0.00011	892.59	0.02
207.61	9.05092	0.00014	12.00178	0.00012	8.21080	0.00011	891.92	0.02
198.41	9.04718	0.00014	11.99780	0.00013	8.21060	0.00011	891.23	0.02

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Table S9 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
189.42	9.04330	0.00014	11.99427	0.00013	8.21031	0.00012	890.55	0.02
181.24	9.03972	0.00014	11.99091	0.00013	8.20983	0.00012	889.90	0.02
173.50	9.03698	0.00015	11.98788	0.00014	8.20958	0.00012	889.38	0.02
166.30	9.03419	0.00013	11.98548	0.00012	8.20968	0.00011	888.94	0.02
159.47	9.03156	0.00013	11.98326	0.00012	8.20939	0.00011	888.48	0.02
153.04	9.02919	0.00013	11.98092	0.00012	8.20944	0.00011	888.08	0.02
147.13	9.02722	0.00013	11.97908	0.00013	8.20923	0.00011	887.73	0.02
141.64	9.02520	0.00013	11.97732	0.00013	8.20904	0.00011	887.38	0.02
136.42	9.02368	0.00013	11.97540	0.00012	8.20904	0.00011	887.09	0.02
131.69	9.02199	0.00013	11.97407	0.00013	8.20894	0.00011	886.81	0.02
127.21	9.02047	0.00013	11.97271	0.00013	8.20891	0.00011	886.56	0.02
123.08	9.01940	0.00013	11.97149	0.00013	8.20867	0.00011	886.34	0.02
119.33	9.01808	0.00013	11.97025	0.00012	8.20884	0.00011	886.13	0.02

Table S10: Variable-temperature lattice parameter data for Me_2NH_2-Mn in the ambient phase.

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
299.86	8.33404	0.00002	22.89428	0.00012	1377.111	0.011
289.65	8.33378	0.00002	22.88712	0.00012	1376.593	0.011
280.31	8.33352	0.00002	22.87639	0.00012	1375.864	0.011
271.17	8.33319	0.00002	22.86443	0.00011	1375.035	0.010

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Table S10 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
262.03	8.33289	0.00002	22.85158	0.00012	1374.162	0.011
252.84	8.33264	0.00003	22.83830	0.00012	1373.280	0.011
243.74	8.33256	0.00003	22.82432	0.00013	1372.414	0.012
234.63	8.33230	0.00003	22.81104	0.00014	1371.531	0.012
225.58	8.33211	0.00003	22.79748	0.00013	1370.651	0.012
216.46	8.33188	0.00003	22.78321	0.00012	1369.719	0.011
207.39	8.33167	0.00002	22.76939	0.00011	1368.821	0.010
198.32	8.33144	0.00002	22.75660	0.00011	1367.974	0.010
189.35	8.33143	0.00003	22.74225	0.00012	1367.108	0.011
180.88	8.33127	0.00002	22.73057	0.00010	1366.356	0.010
172.96	8.33130	0.00002	22.71896	0.00012	1365.667	0.011
165.55	8.33106	0.00003	22.70887	0.00012	1364.983	0.011
158.81	8.33083	0.00002	22.69991	0.00010	1364.367	0.010
152.47	8.33060	0.00003	22.69271	0.00011	1363.860	0.011
146.56	8.33037	0.00003	22.68620	0.00014	1363.394	0.013
141.04	8.32995	0.00004	22.67998	0.00016	1362.882	0.015
135.95	8.32968	0.00005	22.67426	0.00020	1362.451	0.019
131.06	8.32920	0.00005	22.67021	0.00022	1362.051	0.022
126.62	8.32878	0.00006	22.66667	0.00027	1361.700	0.026
122.52	8.32830	0.00007	22.66545	0.00029	1361.468	0.029
118.77	8.32785	0.00008	22.66447	0.00033	1361.263	0.033

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Table S10 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
111.39	8.32270	0.00192	22.64630	0.00740	1358.491	0.768
120.70	8.32341	0.00216	22.65601	0.00808	1359.304	0.855
130.23	8.32457	0.00121	22.65498	0.00465	1359.621	0.483
139.21	8.32617	0.00051	22.65936	0.00199	1360.407	0.204
148.53	8.32798	0.00019	22.66463	0.00080	1361.313	0.080
157.71	8.32930	0.00009	22.67456	0.00038	1362.342	0.037
166.86	8.33013	0.00005	22.68690	0.00023	1363.355	0.022
175.81	8.33072	0.00004	22.69987	0.00017	1364.330	0.016
184.90	8.33121	0.00003	22.71423	0.00014	1365.354	0.013
194.09	8.33133	0.00003	22.72880	0.00014	1366.266	0.013
203.28	8.33138	0.00003	22.74336	0.00014	1367.161	0.013
212.41	8.33152	0.00003	22.75824	0.00014	1368.099	0.013
221.50	8.33171	0.00003	22.77322	0.00014	1369.063	0.013
230.62	8.33191	0.00003	22.78781	0.00014	1370.006	0.013
239.81	8.33208	0.00003	22.80234	0.00015	1370.937	0.013
248.94	8.33232	0.00003	22.81680	0.00015	1371.882	0.014
258.03	8.33249	0.00003	22.83107	0.00015	1372.799	0.014
267.19	8.33266	0.00003	22.84480	0.00015	1373.679	0.014
276.28	8.33284	0.00003	22.85909	0.00015	1374.598	0.013
285.51	8.33295	0.00003	22.87292	0.00015	1375.467	0.014
294.60	8.33305	0.00003	22.88654	0.00015	1376.319	0.014

Table S11: Variable-temperature lattice parameter data for Me_2NH_2-Mn in the low-temperature phase.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
158.81	14.37968	0.00094	8.32364	0.00061	8.89348	0.00054	120.907	0.005	913.32	0.11
152.47	14.37883	0.00032	8.32238	0.00022	8.89280	0.00019	120.962	0.002	912.53	0.04
146.56	14.37781	0.00024	8.32325	0.00015	8.89136	0.00013	120.986	0.001	912.19	0.03
141.04	14.37763	0.00019	8.32302	0.00012	8.89084	0.00010	121.004	0.001	911.92	0.02
135.95	14.37863	0.00019	8.32345	0.00012	8.88962	0.00010	121.014	0.001	911.82	0.02
131.06	14.37739	0.00019	8.32347	0.00012	8.88825	0.00010	121.019	0.001	911.55	0.02
126.62	14.37706	0.00020	8.32321	0.00012	8.88732	0.00011	121.024	0.001	911.35	0.02
122.52	14.37711	0.00020	8.32284	0.00012	8.88668	0.00011	121.031	0.001	911.19	0.02
118.77	14.37814	0.00021	8.32332	0.00013	8.88585	0.00011	121.045	0.001	911.09	0.02
111.39	14.36615	0.00019	8.31776	0.00011	8.87629	0.00010	120.868	0.001	910.42	0.02
120.70	14.36844	0.00020	8.31813	0.00011	8.87772	0.00011	120.886	0.001	910.58	0.02
130.23	14.36955	0.00020	8.31862	0.00012	8.88042	0.00011	120.892	0.001	910.93	0.02
139.21	14.37066	0.00020	8.31927	0.00012	8.88331	0.00011	120.892	0.001	911.37	0.02
148.53	14.37127	0.00019	8.31985	0.00011	8.88581	0.00010	120.883	0.001	911.81	0.02
157.71	14.37192	0.00017	8.32032	0.00010	8.88848	0.00009	120.868	0.001	912.32	0.02
166.86	14.37273	0.00017	8.32085	0.00011	8.89114	0.00009	120.856	0.001	912.82	0.02
175.81	14.37326	0.00024	8.32180	0.00016	8.89369	0.00013	120.848	0.001	913.29	0.03

Table S12: Variable-temperature lattice parameter data for Me_2NH_2-Co in the ambient phase.

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
299.86	8.19785	0.00003	22.22016	0.00013	1293.235	0.011
289.63	8.19731	0.00003	22.21308	0.00013	1292.653	0.012
280.37	8.19657	0.00003	22.20445	0.00013	1291.918	0.012
271.17	8.19572	0.00003	22.19514	0.00013	1291.109	0.011
262.04	8.19492	0.00003	22.18484	0.00013	1290.257	0.011
252.93	8.19405	0.00003	22.17458	0.00013	1289.386	0.011
243.83	8.19323	0.00003	22.16422	0.00013	1288.527	0.011
234.74	8.19241	0.00003	22.15399	0.00013	1287.673	0.011
225.69	8.19159	0.00003	22.14384	0.00013	1286.828	0.011
216.54	8.19078	0.00003	22.13369	0.00013	1285.982	0.012
207.52	8.18998	0.00003	22.12384	0.00013	1285.158	0.012
198.19	8.18911	0.00003	22.11407	0.00014	1284.319	0.012
189.22	8.18832	0.00003	22.10465	0.00014	1283.523	0.012
180.89	8.18764	0.00003	22.09581	0.00014	1282.796	0.012
173.09	8.18694	0.00003	22.08773	0.00014	1282.108	0.012
165.89	8.18625	0.00003	22.08089	0.00014	1281.497	0.012
159.11	8.18569	0.00003	22.07439	0.00014	1280.944	0.012
152.77	8.18517	0.00003	22.06899	0.00014	1280.466	0.012
146.89	8.18472	0.00003	22.06370	0.00014	1280.020	0.012
141.40	8.18425	0.00003	22.05951	0.00014	1279.629	0.013

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Table S12 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
136.24	8.18383	0.00003	22.05524	0.00014	1279.249	0.013
131.50	8.18349	0.00003	22.05204	0.00014	1278.958	0.013
126.98	8.18308	0.00003	22.04938	0.00014	1278.677	0.013
122.87	8.18276	0.00003	22.04641	0.00014	1278.405	0.013
119.10	8.18240	0.00003	22.04433	0.00015	1278.170	0.013
111.78	8.18136	0.00006	22.02038	0.00023	1276.458	0.022
121.28	8.18154	0.00006	22.02280	0.00023	1276.654	0.022
130.65	8.18216	0.00005	22.03028	0.00022	1277.281	0.021
139.70	8.18281	0.00005	22.03967	0.00020	1278.027	0.019
149.20	8.18386	0.00004	22.05105	0.00019	1279.019	0.018
158.15	8.18479	0.00003	22.06112	0.00014	1279.892	0.012
167.36	8.18542	0.00003	22.06912	0.00014	1280.553	0.013
176.45	8.18606	0.00003	22.07757	0.00014	1281.244	0.012
185.60	8.18679	0.00003	22.08712	0.00014	1282.026	0.013
194.62	8.18754	0.00003	22.09637	0.00014	1282.799	0.012
203.84	8.18832	0.00003	22.10617	0.00014	1283.611	0.013
213.09	8.18913	0.00003	22.11618	0.00014	1284.447	0.013
222.14	8.18995	0.00003	22.12619	0.00014	1285.286	0.013
231.20	8.19080	0.00003	22.13629	0.00014	1286.140	0.013
240.27	8.19165	0.00003	22.14625	0.00014	1286.987	0.013
249.44	8.19252	0.00003	22.15664	0.00014	1287.863	0.013

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Table S12 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
258.50	8.19342	0.00003	22.16707	0.00014	1288.753	0.013
267.69	8.19427	0.00003	22.17725	0.00014	1289.612	0.013
276.77	8.19520	0.00003	22.18774	0.00014	1290.513	0.013
285.89	8.19617	0.00003	22.19841	0.00015	1291.440	0.013
294.98	8.19710	0.00003	22.20928	0.00015	1292.366	0.013

Table S13: Variable-temperature lattice parameter data for Me_2NH_2-Co in the low-temperature phase.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
111.78	14.1448	0.0003	8.1775	0.0002	8.67243	0.00015	121.541	0.001	854.93	0.03
121.28	14.1463	0.0003	8.1777	0.0002	8.67393	0.00016	121.559	0.001	855.03	0.03
130.65	14.1482	0.0003	8.1784	0.0002	8.67568	0.00018	121.567	0.002	855.31	0.04
139.70	14.1485	0.0005	8.1801	0.0003	8.67739	0.00025	121.557	0.002	855.77	0.05
149.20	14.1432	0.0011	8.1837	0.0007	8.67871	0.00062	121.530	0.005	856.20	0.13

Table S14: Variable-temperature lattice parameter data for Me_2NH_2-Cu.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
299.87	13.67232	0.00013	8.72425	0.00008	8.85366	0.00007	123.8649	0.0006	876.913	0.02
289.63	13.67451	0.00014	8.72283	0.00008	8.85342	0.00008	123.8769	0.0007	876.764	0.02

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Table S14 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
280.33	13.67674	0.00014	8.72017	0.00008	8.85210	0.00008	123.8911	0.0007	876.363	0.02
271.17	13.67946	0.00014	8.71730	0.00009	8.85058	0.00008	123.9075	0.0007	875.930	0.02
262.03	13.68198	0.00014	8.71411	0.00009	8.84861	0.00008	123.9233	0.0007	875.413	0.02
252.95	13.68450	0.00015	8.71083	0.00009	8.84657	0.00009	123.9393	0.0007	874.878	0.02
243.98	13.68690	0.00015	8.70742	0.00009	8.84435	0.00009	123.9541	0.0008	874.318	0.02
234.73	13.68935	0.00016	8.70397	0.00010	8.84211	0.00009	123.9688	0.0008	873.756	0.02
225.65	13.69181	0.00016	8.70049	0.00010	8.83963	0.00010	123.9826	0.0008	873.177	0.02
216.34	13.69426	0.00016	8.69689	0.00010	8.83697	0.00010	123.9965	0.0008	872.566	0.02
207.30	13.69673	0.00017	8.69339	0.00011	8.83422	0.00010	124.0108	0.0009	871.954	0.02
198.16	13.69904	0.00017	8.69013	0.00011	8.83138	0.00010	124.0230	0.0009	871.367	0.02
189.18	13.70112	0.00017	8.68698	0.00011	8.82844	0.00011	124.0340	0.0009	870.781	0.02
180.62	13.70311	0.00018	8.68390	0.00011	8.82563	0.00011	124.0440	0.0009	870.219	0.02
172.66	13.70516	0.00018	8.68116	0.00012	8.82323	0.00011	124.0534	0.0009	869.742	0.02
165.26	13.70642	0.00019	8.67863	0.00012	8.82041	0.00011	124.0593	0.0009	869.230	0.02
158.53	13.70798	0.00019	8.67665	0.00012	8.81841	0.00012	124.0655	0.0009	868.870	0.02
152.13	13.70958	0.00019	8.67483	0.00012	8.81661	0.00012	124.0714	0.0010	868.551	0.02
146.23	13.71115	0.00020	8.67299	0.00012	8.81454	0.00012	124.0791	0.0010	868.184	0.02
140.70	13.71283	0.00020	8.67136	0.00013	8.81306	0.00012	124.0822	0.0010	867.949	0.02
135.45	13.71366	0.00021	8.67003	0.00013	8.81179	0.00013	124.0846	0.0010	867.718	0.02
130.66	13.71493	0.00021	8.66878	0.00014	8.81030	0.00013	124.0873	0.0011	867.500	0.03
126.24	13.71562	0.00022	8.66756	0.00014	8.80881	0.00014	124.0877	0.0011	867.270	0.03

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Table S14 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
122.17	13.71562	0.00022	8.66756	0.00014	8.80881	0.00013	124.0877	0.0011	867.271	0.03
118.45	13.71769	0.00022	8.66632	0.00014	8.80727	0.00014	124.0872	0.0011	867.130	0.03
111.13	13.70281	0.00014	8.64908	0.00009	8.78271	0.00008	124.1231	0.0007	861.692	0.02
120.66	13.70329	0.00014	8.65080	0.00009	8.78500	0.00008	124.1156	0.0007	862.194	0.02
130.09	13.70300	0.00014	8.65340	0.00009	8.78845	0.00008	124.1048	0.0007	862.884	0.02
139.09	13.70293	0.00015	8.65633	0.00009	8.79234	0.00009	124.0956	0.0007	863.646	0.02
148.57	13.70220	0.00015	8.65973	0.00009	8.79658	0.00009	124.0840	0.0007	864.476	0.02
157.52	13.70134	0.00015	8.66335	0.00009	8.80097	0.00009	124.0749	0.0007	865.306	0.02
166.64	13.70066	0.00016	8.66704	0.00010	8.80537	0.00009	124.0655	0.0008	866.162	0.02
175.87	13.69972	0.00016	8.67115	0.00010	8.81000	0.00010	124.0540	0.0008	867.087	0.02
184.86	13.69908	0.00016	8.67519	0.00010	8.81449	0.00010	124.0433	0.0008	868.001	0.02
194.04	13.69846	0.00017	8.67951	0.00010	8.81907	0.00010	124.0314	0.0008	868.968	0.02
203.15	13.69783	0.00017	8.68387	0.00010	8.82380	0.00010	124.0197	0.0008	869.949	0.02
212.24	13.69685	0.00017	8.68828	0.00011	8.82844	0.00010	124.0073	0.0009	870.914	0.02
221.33	13.69569	0.00017	8.69307	0.00011	8.83308	0.00011	123.9943	0.0009	871.912	0.02
230.49	13.69472	0.00017	8.69772	0.00011	8.83775	0.00011	123.9826	0.0009	872.897	0.02
239.58	13.69360	0.00017	8.70250	0.00011	8.84205	0.00011	123.9717	0.0009	873.844	0.02
248.73	13.69234	0.00018	8.70746	0.00011	8.84655	0.00011	123.9604	0.0009	874.822	0.02
257.99	13.69090	0.00018	8.71233	0.00011	8.85100	0.00011	123.9483	0.0009	875.783	0.02
267.10	13.68961	0.00019	8.71724	0.00012	8.85544	0.00011	123.9363	0.0009	876.759	0.02
276.21	13.68833	0.00019	8.72240	0.00012	8.86016	0.00011	123.9248	0.0010	877.781	0.02

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Table S14 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
285.18	13.68670	0.00020	8.72777	0.00013	8.86440	0.00012	123.9128	0.0010	878.761	0.02
294.32	13.68510	0.00020	8.73330	0.00013	8.86861	0.00012	123.8991	0.0010	879.774	0.02

Table S15: Variable-temperature lattice parameter data for Me_2NH_2-Zn in the ambient phase.

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
299.91	8.20056	0.00003	22.26072	0.00015	1296.453	0.013
289.62	8.20051	0.00003	22.25963	0.00016	1296.373	0.014
280.23	8.20013	0.00003	22.25556	0.00016	1296.015	0.014
271.09	8.19962	0.00004	22.25047	0.00017	1295.561	0.015
261.96	8.19914	0.00004	22.24478	0.00017	1295.077	0.016
252.83	8.19859	0.00004	22.23921	0.00018	1294.579	0.016
243.72	8.19806	0.00004	22.23299	0.00018	1294.050	0.016
234.55	8.19762	0.00004	22.22759	0.00019	1293.596	0.017
225.38	8.19713	0.00004	22.22242	0.00020	1293.139	0.018
216.28	8.19668	0.00004	22.21645	0.00020	1292.650	0.018
207.13	8.19603	0.00004	22.20961	0.00020	1292.047	0.018
197.95	8.19551	0.00004	22.20367	0.00020	1291.539	0.018
189.01	8.19503	0.00005	22.19830	0.00021	1291.073	0.019
180.42	8.19451	0.00005	22.19340	0.00021	1290.626	0.019
172.42	8.19434	0.00005	22.18974	0.00022	1290.358	0.020

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Table S15 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
165.17	8.19418	0.00005	22.18724	0.00022	1290.165	0.020
158.28	8.19402	0.00005	22.18528	0.00023	1289.999	0.021
151.96	8.19404	0.00005	22.18448	0.00024	1289.959	0.021
145.96	8.19401	0.00005	22.18380	0.00025	1289.912	0.022
140.47	8.19407	0.00005	22.18352	0.00025	1289.913	0.023
135.31	8.19425	0.00006	22.18386	0.00026	1289.990	0.023
130.55	8.19442	0.00006	22.18466	0.00026	1290.090	0.024
126.09	8.19472	0.00006	22.18585	0.00027	1290.254	0.024
121.99	8.19513	0.00006	22.18693	0.00028	1290.445	0.025
118.29	8.19550	0.00006	22.18864	0.00029	1290.662	0.026
111.01	8.18406	0.00006	22.05950	0.00024	1279.570	0.023
120.46	8.18456	0.00006	22.06776	0.00025	1280.204	0.024
130.03	8.18558	0.00006	22.07974	0.00024	1281.218	0.023
138.95	8.18673	0.00005	22.09414	0.00023	1282.414	0.021
148.48	8.18763	0.00005	22.11035	0.00022	1283.637	0.020
157.46	8.18817	0.00004	22.12228	0.00018	1284.499	0.016
166.54	8.18890	0.00004	22.13243	0.00018	1285.317	0.016
175.62	8.18963	0.00004	22.14243	0.00018	1286.130	0.016
184.80	8.19059	0.00004	22.15424	0.00019	1287.116	0.017
193.93	8.19168	0.00004	22.16607	0.00019	1288.148	0.017
202.92	8.19298	0.00004	22.17782	0.00020	1289.238	0.018

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Table S15 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
211.98	8.19433	0.00004	22.18953	0.00021	1290.344	0.018
221.19	8.19568	0.00004	22.20176	0.00021	1291.480	0.019
230.18	8.19687	0.00005	22.21395	0.00022	1292.565	0.019
239.27	8.19805	0.00005	22.22561	0.00022	1293.615	0.019
248.40	8.19905	0.00005	22.23655	0.00022	1294.569	0.020
257.59	8.19995	0.00005	22.24735	0.00023	1295.482	0.020
266.78	8.20079	0.00005	22.25767	0.00023	1296.348	0.020
275.90	8.20157	0.00005	22.26831	0.00023	1297.213	0.020
285.00	8.20215	0.00005	22.27867	0.00023	1298.001	0.020
294.11	8.20271	0.00005	22.28892	0.00023	1298.776	0.020

Table S16: Variable-temperature lattice parameter data for Me_2NH_2-Zn in the low-temperature phase.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
111.01	14.1504	0.0003	8.1717	0.0002	8.6753	0.0002	121.349	0.002	856.70	0.03
120.46	14.1532	0.0003	8.1733	0.0002	8.6789	0.0002	121.396	0.002	856.98	0.04
130.03	14.1570	0.0004	8.1750	0.0002	8.6829	0.0002	121.439	0.002	857.37	0.04
138.95	14.1592	0.0005	8.1770	0.0003	8.6863	0.0003	121.475	0.003	857.73	0.06
148.48	14.1564	0.0014	8.1797	0.0008	8.6876	0.0007	121.466	0.007	858.05	0.15

Table S17: Variable-temperature lattice parameter data for Aze-Mn in the ambient phase.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
289.72	8.70053	0.00010	12.31449	0.00007	8.86705	0.00011	950.04	0.02
280.43	8.69920	0.00010	12.31209	0.00007	8.86424	0.00011	949.41	0.02
271.15	8.69790	0.00011	12.30909	0.00008	8.85965	0.00012	948.54	0.02
262.03	8.69699	0.00009	12.30625	0.00007	8.85436	0.00010	947.66	0.02
252.93	8.69469	0.00011	12.30369	0.00008	8.85064	0.00011	946.81	0.02
243.87	8.68985	0.00012	12.30105	0.00008	8.84752	0.00013	945.75	0.02
234.70	8.68243	0.00016	12.29840	0.00008	8.84709	0.00016	944.69	0.03
225.57	8.67106	0.00018	12.29633	0.00008	8.85032	0.00019	943.64	0.03
216.46	8.66089	0.00019	12.29444	0.00009	8.85290	0.00019	942.66	0.03
207.41	8.65346	0.00019	12.29291	0.00008	8.85337	0.00019	941.79	0.03
198.26	8.64321	0.00019	12.29171	0.00009	8.85679	0.00020	940.94	0.03
189.15	8.63831	0.00020	12.29071	0.00009	8.85602	0.00021	940.25	0.03
180.94	8.63212	0.00021	12.28986	0.00010	8.85556	0.00022	939.47	0.03
173.31	8.62417	0.00021	12.28939	0.00010	8.85830	0.00021	938.85	0.03
166.18	8.62059	0.00021	12.28891	0.00009	8.85771	0.00021	938.37	0.03
159.42	8.61710	0.00022	12.28869	0.00010	8.85717	0.00022	937.91	0.03
153.10	8.61372	0.00022	12.28856	0.00010	8.85689	0.00023	937.50	0.04
147.15	8.61088	0.00023	12.28853	0.00011	8.85583	0.00024	937.08	0.04
141.68	8.60892	0.00024	12.28857	0.00011	8.85494	0.00024	936.78	0.04
136.54	8.60695	0.00024	12.28866	0.00011	8.85408	0.00025	936.48	0.04

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Table S17 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
131.70	8.60556	0.00025	12.28884	0.00011	8.85349	0.00026	936.28	0.04
127.21	8.60302	0.00026	12.28891	0.00011	8.85354	0.00027	936.01	0.04
123.06	8.60166	0.00027	12.28909	0.00011	8.85291	0.00028	935.81	0.04
119.29	8.60040	0.00027	12.28934	0.00011	8.85230	0.00028	935.63	0.04
112.15	8.51664	0.00023	12.27451	0.00015	8.91653	0.00025	932.11	0.04
121.49	8.52122	0.00021	12.27485	0.00013	8.91509	0.00022	932.49	0.03
130.94	8.52837	0.00020	12.27568	0.00013	8.91254	0.00022	933.07	0.03
139.92	8.53635	0.00019	12.27666	0.00012	8.90934	0.00021	933.68	0.03
149.44	8.54603	0.00019	12.27795	0.00011	8.90552	0.00020	934.44	0.03
158.48	8.55547	0.00018	12.27912	0.00011	8.90193	0.00020	935.18	0.03
167.49	8.56510	0.00018	12.28049	0.00010	8.89832	0.00019	935.96	0.03
176.76	8.57571	0.00018	12.28214	0.00010	8.89421	0.00019	936.81	0.03
185.81	8.58697	0.00017	12.28402	0.00010	8.88997	0.00018	937.74	0.03
195.14	8.59880	0.00016	12.28589	0.00009	8.88556	0.00017	938.70	0.03
204.26	8.61016	0.00016	12.28786	0.00010	8.88159	0.00017	939.68	0.03
213.35	8.62086	0.00016	12.28984	0.00010	8.87798	0.00017	940.61	0.03
222.52	8.63289	0.00016	12.29234	0.00009	8.87349	0.00016	941.64	0.03
231.59	8.64623	0.00016	12.29495	0.00008	8.86772	0.00017	942.68	0.03
240.67	8.65992	0.00019	12.29773	0.00009	8.86158	0.00019	943.73	0.03
249.79	8.67877	0.00019	12.30113	0.00009	8.85117	0.00019	944.94	0.03
258.89	8.69529	0.00017	12.30481	0.00009	8.84252	0.00017	946.10	0.03

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Table S17 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
268.00	8.70231	0.00012	12.30860	0.00008	8.84219	0.00013	947.12	0.02
277.06	8.70582	0.00011	12.31232	0.00007	8.84469	0.00012	948.05	0.02
286.19	8.70943	0.00012	12.31595	0.00008	8.84644	0.00013	948.91	0.02
295.42	8.71412	0.00011	12.32024	0.00007	8.84753	0.00012	949.87	0.02

Table S18: Variable-temperature lattice parameter data for Aze-Mn in the low-temperature phase.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
112.15	12.3215	0.0003	12.27396	0.00012	12.3377	0.0003	92.648	0.002	1863.88	0.07
121.49	12.3234	0.0003	12.27490	0.00010	12.3391	0.0003	92.605	0.002	1864.59	0.06
130.94	12.3262	0.0003	12.27583	0.00009	12.3424	0.0002	92.537	0.001	1865.75	0.05
139.92	12.3306	0.0003	12.27665	0.00010	12.3446	0.0003	92.468	0.002	1866.97	0.06
149.44	12.3351	0.0003	12.27807	0.00008	12.3482	0.0002	92.360	0.001	1868.57	0.05
158.48	12.3398	0.0003	12.27928	0.00010	12.3513	0.0003	92.278	0.002	1870.05	0.07
167.49	12.3440	0.0003	12.28077	0.00007	12.3558	0.0002	92.185	0.001	1871.70	0.05
176.76	12.3487	0.0003	12.28246	0.00008	12.3596	0.0002	92.098	0.001	1873.35	0.06
185.81	12.3533	0.0002	12.28432	0.00006	12.3644	0.0002	91.992	0.001	1875.19	0.04
195.14	12.3580	0.0003	12.28606	0.00008	12.3686	0.0002	91.905	0.002	1876.90	0.05
204.26	12.3630	0.0003	12.28801	0.00009	12.3729	0.0003	91.807	0.002	1878.72	0.06
213.35	12.3698	0.0002	12.29027	0.00006	12.3776	0.0002	91.678	0.001	1880.94	0.04
222.52	12.3743	0.0003	12.29253	0.00008	12.3823	0.0002	91.583	0.002	1882.77	0.06

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Table S18 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	β (°)	σ_β	V (Å^3)	σ_V
231.59	12.3797	0.0003	12.29501	0.00008	12.3875	0.0002	91.471	0.002	1884.84	0.05
240.67	12.3848	0.0003	12.29816	0.00008	12.3926	0.0002	91.294	0.002	1887.04	0.05
249.79	12.3899	0.0003	12.30154	0.00008	12.3983	0.0002	91.113	0.003	1889.33	0.05
258.89	12.3982	0.0003	12.30516	0.00008	12.4027	0.0002	90.970	0.002	1891.91	0.05

Table S19: Variable-temperature lattice parameter data for Gua-Mn.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.81	8.52412	0.00006	11.98914	0.00007	9.05465	0.00008	925.356	0.012
289.51	8.52204	0.00006	11.98680	0.00007	9.05487	0.00008	924.973	0.012
280.22	8.51928	0.00006	11.98387	0.00007	9.05519	0.00008	924.480	0.012
271.08	8.51621	0.00006	11.98056	0.00007	9.05560	0.00008	923.933	0.012
261.96	8.51307	0.00006	11.97711	0.00007	9.05604	0.00008	923.372	0.012
252.84	8.50972	0.00006	11.97361	0.00007	9.05655	0.00008	922.790	0.012
243.76	8.50647	0.00006	11.97020	0.00007	9.05705	0.00008	922.226	0.012
234.60	8.50305	0.00006	11.96663	0.00007	9.05784	0.00008	921.662	0.012
225.58	8.49977	0.00006	11.96326	0.00007	9.05844	0.00008	921.107	0.012
216.50	8.49625	0.00006	11.95975	0.00007	9.05918	0.00008	920.531	0.012
207.42	8.49283	0.00006	11.95624	0.00007	9.05994	0.00008	919.968	0.012
198.31	8.48927	0.00006	11.95276	0.00008	9.06086	0.00008	919.406	0.012
189.34	8.48581	0.00006	11.94943	0.00008	9.06166	0.00008	918.857	0.012

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Table S19 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
181.07	8.48271	0.00006	11.94622	0.00008	9.06250	0.00008	918.360	0.013
173.25	8.47965	0.00006	11.94333	0.00008	9.06331	0.00009	917.889	0.013
166.04	8.47696	0.00007	11.94056	0.00008	9.06402	0.00009	917.458	0.013
159.25	8.47439	0.00007	11.93819	0.00008	9.06476	0.00009	917.072	0.013
152.89	8.47222	0.00007	11.93595	0.00008	9.06552	0.00009	916.742	0.013
146.92	8.47016	0.00007	11.93400	0.00008	9.06609	0.00009	916.427	0.013
141.39	8.46820	0.00007	11.93219	0.00008	9.06668	0.00009	916.135	0.013
136.23	8.46656	0.00007	11.93053	0.00008	9.06722	0.00009	915.884	0.013
131.37	8.46487	0.00007	11.92901	0.00008	9.06765	0.00009	915.629	0.013
126.82	8.46348	0.00007	11.92767	0.00008	9.06817	0.00009	915.428	0.013
122.71	8.46221	0.00007	11.92649	0.00008	9.06860	0.00009	915.243	0.013
118.92	8.46119	0.00007	11.92545	0.00008	9.06903	0.00009	915.098	0.014
111.53	8.45699	0.00007	11.92226	0.00009	9.07292	0.00009	914.791	0.014
120.99	8.45842	0.00007	11.92367	0.00009	9.07208	0.00009	914.969	0.014
130.55	8.46132	0.00007	11.92637	0.00009	9.07092	0.00009	915.372	0.014
139.29	8.46443	0.00007	11.92904	0.00009	9.06980	0.00009	915.800	0.014
148.93	8.46753	0.00007	11.93206	0.00008	9.06867	0.00009	916.254	0.014
158.09	8.47096	0.00007	11.93517	0.00008	9.06748	0.00009	916.744	0.013
167.07	8.47394	0.00007	11.93816	0.00008	9.06629	0.00009	917.176	0.013
176.14	8.47706	0.00007	11.94108	0.00008	9.06514	0.00009	917.621	0.013
185.29	8.48031	0.00007	11.94436	0.00008	9.06389	0.00009	918.099	0.013

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Table S19 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
194.45	8.48318	0.00007	11.94734	0.00008	9.06344	0.00009	918.593	0.013
203.48	8.48703	0.00006	11.95099	0.00008	9.06168	0.00008	919.112	0.013
212.63	8.49035	0.00006	11.95447	0.00008	9.06076	0.00008	919.645	0.012
221.65	8.49368	0.00006	11.95776	0.00008	9.05984	0.00008	920.167	0.012
230.94	8.49707	0.00006	11.96125	0.00007	9.05881	0.00008	920.697	0.012
240.00	8.50041	0.00006	11.96457	0.00007	9.05793	0.00008	921.225	0.012
249.13	8.50371	0.00006	11.96787	0.00007	9.05707	0.00008	921.749	0.012
258.33	8.50705	0.00006	11.97131	0.00007	9.05609	0.00008	922.276	0.012
267.40	8.51037	0.00006	11.97462	0.00007	9.05532	0.00008	922.814	0.011
276.61	8.51366	0.00006	11.97799	0.00007	9.05447	0.00008	923.344	0.011
285.72	8.51703	0.00006	11.98148	0.00007	9.05358	0.00008	923.888	0.011
294.84	8.52047	0.00006	11.98495	0.00007	9.05290	0.00007	924.459	0.011

Table S20: Variable-temperature lattice parameter data for Gua-Fe.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.86	8.42185	0.00012	11.87427	0.00013	8.92920	0.00015	892.95	0.02
289.64	8.41999	0.00011	11.87212	0.00013	8.92890	0.00014	892.56	0.02
280.36	8.41767	0.00011	11.86901	0.00013	8.92883	0.00014	892.07	0.02
271.18	8.41523	0.00011	11.86575	0.00013	8.92872	0.00014	891.56	0.02
262.04	8.41262	0.00011	11.86203	0.00013	8.92854	0.00014	890.99	0.02

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Table S20 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
252.94	8.40997	0.00011	11.85900	0.00013	8.92822	0.00014	890.44	0.02
243.81	8.40731	0.00011	11.85512	0.00013	8.92829	0.00014	889.88	0.02
234.71	8.40463	0.00011	11.85214	0.00013	8.92814	0.00014	889.36	0.02
225.67	8.40203	0.00011	11.84860	0.00013	8.92807	0.00014	888.81	0.02
216.65	8.39946	0.00011	11.84453	0.00013	8.92832	0.00014	888.26	0.02
207.60	8.39676	0.00011	11.84154	0.00013	8.92812	0.00014	887.73	0.02
198.38	8.39412	0.00011	11.83783	0.00013	8.92817	0.00014	887.18	0.02
189.42	8.39166	0.00011	11.83418	0.00013	8.92849	0.00014	886.67	0.02
181.06	8.38916	0.00011	11.83119	0.00013	8.92842	0.00014	886.18	0.02
173.24	8.38702	0.00011	11.82797	0.00013	8.92866	0.00014	885.74	0.02
166.09	8.38508	0.00011	11.82546	0.00013	8.92879	0.00014	885.35	0.02
159.26	8.38341	0.00011	11.82316	0.00013	8.92900	0.00015	885.03	0.02
152.93	8.38171	0.00011	11.82058	0.00013	8.92939	0.00015	884.69	0.02
147.03	8.38017	0.00011	11.81864	0.00013	8.92941	0.00015	884.39	0.02
141.59	8.37904	0.00012	11.81735	0.00013	8.92940	0.00015	884.17	0.02
136.42	8.37759	0.00012	11.81501	0.00013	8.92990	0.00015	883.89	0.02
131.64	8.37636	0.00012	11.81351	0.00013	8.93009	0.00015	883.67	0.02
127.15	8.37548	0.00012	11.81237	0.00013	8.93034	0.00015	883.52	0.02
123.01	8.37458	0.00012	11.81106	0.00013	8.93066	0.00015	883.36	0.02
119.25	8.37367	0.00012	11.80965	0.00013	8.93108	0.00015	883.20	0.02
111.81	8.37027	0.00011	11.80576	0.00013	8.93207	0.00015	882.64	0.02

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Table S20 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
121.23	8.37143	0.00011	11.80714	0.00013	8.93205	0.00015	882.87	0.02
130.85	8.37353	0.00011	11.80994	0.00013	8.93164	0.00015	883.26	0.02
139.58	8.37552	0.00011	11.81316	0.00013	8.93099	0.00014	883.64	0.02
149.21	8.37793	0.00011	11.81627	0.00013	8.93069	0.00014	884.10	0.02
158.34	8.38050	0.00011	11.81987	0.00013	8.93024	0.00014	884.60	0.02
167.43	8.38292	0.00011	11.82333	0.00013	8.92998	0.00014	885.09	0.02
176.41	8.38541	0.00011	11.82683	0.00013	8.92963	0.00014	885.58	0.02
185.57	8.38791	0.00011	11.83045	0.00013	8.92945	0.00014	886.09	0.02
194.72	8.39080	0.00011	11.83397	0.00013	8.92944	0.00014	886.66	0.02
203.84	8.39338	0.00011	11.83784	0.00013	8.92918	0.00014	887.20	0.02
213.06	8.39622	0.00011	11.84172	0.00013	8.92914	0.00014	887.79	0.02
222.09	8.39896	0.00011	11.84492	0.00013	8.92921	0.00014	888.32	0.02
231.22	8.40153	0.00011	11.84895	0.00013	8.92887	0.00014	888.86	0.02
240.29	8.40426	0.00011	11.85230	0.00013	8.92886	0.00014	889.40	0.02
249.39	8.40697	0.00011	11.85560	0.00013	8.92887	0.00014	889.94	0.02
258.49	8.40960	0.00011	11.85949	0.00013	8.92861	0.00014	890.48	0.02
267.68	8.41229	0.00011	11.86240	0.00013	8.92870	0.00014	890.99	0.02
276.78	8.41502	0.00011	11.86623	0.00013	8.92853	0.00014	891.55	0.02
285.89	8.41780	0.00011	11.86970	0.00013	8.92835	0.00014	892.09	0.02
294.98	8.42071	0.00011	11.87318	0.00013	8.92842	0.00014	892.67	0.02

Table S21: Variable-temperature lattice parameter data for Gua-Co.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.93	8.33334	0.00004	11.75230	0.00005	8.91080	0.00005	872.687	0.008
289.62	8.33160	0.00004	11.75040	0.00005	8.91083	0.00005	872.367	0.008
280.35	8.32917	0.00004	11.74780	0.00005	8.91115	0.00005	871.950	0.008
271.17	8.32650	0.00004	11.74505	0.00005	8.91143	0.00005	871.495	0.008
262.04	8.32368	0.00004	11.74202	0.00005	8.91169	0.00005	871.000	0.008
252.92	8.32087	0.00004	11.73909	0.00005	8.91200	0.00005	870.519	0.008
243.76	8.31802	0.00004	11.73604	0.00005	8.91234	0.00005	870.028	0.008
234.60	8.31511	0.00004	11.73301	0.00005	8.91267	0.00005	869.532	0.008
225.58	8.31221	0.00004	11.73002	0.00005	8.91305	0.00005	869.043	0.008
216.46	8.30937	0.00004	11.72707	0.00005	8.91348	0.00005	868.570	0.008
207.38	8.30635	0.00004	11.72400	0.00006	8.91390	0.00005	868.068	0.008
198.27	8.30351	0.00005	11.72113	0.00006	8.91436	0.00005	867.603	0.008
189.35	8.30068	0.00005	11.71818	0.00006	8.91487	0.00005	867.140	0.008
181.09	8.29806	0.00004	11.71567	0.00005	8.91541	0.00005	866.733	0.008
173.19	8.29567	0.00005	11.71319	0.00005	8.91589	0.00005	866.346	0.008
165.95	8.29340	0.00005	11.71117	0.00005	8.91644	0.00005	866.013	0.008
159.30	8.29144	0.00004	11.70919	0.00005	8.91698	0.00005	865.715	0.008
152.92	8.28957	0.00005	11.70732	0.00005	8.91733	0.00005	865.415	0.008
147.07	8.28772	0.00005	11.70573	0.00006	8.91775	0.00005	865.145	0.008
141.56	8.28609	0.00005	11.70425	0.00006	8.91822	0.00005	864.911	0.008

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Table S21 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
136.39	8.28472	0.00004	11.70298	0.00005	8.91871	0.00005	864.722	0.008
131.60	8.28340	0.00004	11.70188	0.00005	8.91910	0.00005	864.540	0.008
127.10	8.28220	0.00004	11.70074	0.00005	8.91942	0.00005	864.363	0.008
122.94	8.28105	0.00004	11.69972	0.00005	8.91972	0.00005	864.196	0.008
119.16	8.28003	0.00004	11.69880	0.00005	8.92011	0.00005	864.059	0.008
111.65	8.27596	0.00005	11.69529	0.00006	8.92231	0.00006	863.588	0.009
121.12	8.27729	0.00005	11.69638	0.00006	8.92173	0.00006	863.752	0.009
130.60	8.27953	0.00005	11.69824	0.00006	8.92089	0.00006	864.041	0.009
139.48	8.28199	0.00005	11.70056	0.00006	8.92011	0.00006	864.393	0.009
148.97	8.28469	0.00005	11.70299	0.00006	8.91918	0.00006	864.765	0.009
158.01	8.28724	0.00005	11.70546	0.00006	8.91841	0.00006	865.138	0.009
167.24	8.29005	0.00005	11.70802	0.00006	8.91772	0.00006	865.554	0.009
176.40	8.29274	0.00005	11.71062	0.00006	8.91696	0.00006	865.953	0.009
185.44	8.29557	0.00005	11.71328	0.00006	8.91623	0.00006	866.375	0.009
194.54	8.29850	0.00005	11.71612	0.00006	8.91549	0.00006	866.820	0.009
203.57	8.30129	0.00005	11.71890	0.00006	8.91491	0.00006	867.260	0.009
212.77	8.30408	0.00005	11.72179	0.00006	8.91440	0.00006	867.716	0.009
221.98	8.30703	0.00005	11.72470	0.00006	8.91384	0.00006	868.184	0.009
230.99	8.30988	0.00005	11.72766	0.00006	8.91329	0.00006	868.649	0.009
239.97	8.31270	0.00005	11.73055	0.00006	8.91278	0.00006	869.107	0.009
249.10	8.31561	0.00005	11.73352	0.00006	8.91228	0.00006	869.583	0.009

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Table S21 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
258.19	8.31846	0.00005	11.73653	0.00006	8.91183	0.00006	870.060	0.009
267.29	8.32136	0.00005	11.73951	0.00006	8.91137	0.00006	870.541	0.009
276.50	8.32441	0.00005	11.74260	0.00006	8.91093	0.00006	871.045	0.008
285.60	8.32731	0.00005	11.74562	0.00006	8.91047	0.00006	871.528	0.008
294.71	8.33035	0.00005	11.74866	0.00006	8.91010	0.00006	872.035	0.008

Table S22: Variable-temperature lattice parameter data for Gua-Ni.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.89	8.26049	0.00009	11.65324	0.00010	8.82540	0.00011	849.546	0.016
289.63	8.26049	0.00012	11.65324	0.00013	8.82540	0.00015	849.546	0.021
280.35	8.25700	0.00009	11.64913	0.00010	8.82446	0.00012	848.797	0.016
271.20	8.25526	0.00009	11.64670	0.00010	8.82342	0.00012	848.341	0.016
262.06	8.25272	0.00009	11.64400	0.00010	8.82308	0.00011	847.852	0.016
252.95	8.25053	0.00009	11.64130	0.00010	8.82250	0.00011	847.373	0.016
243.71	8.24813	0.00009	11.63859	0.00009	8.82217	0.00011	846.898	0.015
234.63	8.24610	0.00009	11.63614	0.00010	8.82165	0.00011	846.461	0.015
225.56	8.24428	0.00009	11.63375	0.00010	8.82103	0.00011	846.042	0.016
216.51	8.24202	0.00009	11.63113	0.00010	8.82095	0.00011	845.612	0.015
207.40	8.23994	0.00009	11.62878	0.00010	8.82064	0.00011	845.198	0.015
198.17	8.23994	0.00010	11.62878	0.00011	8.82064	0.00012	845.198	0.017

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Table S22 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
189.19	8.23582	0.00009	11.62424	0.00010	8.82042	0.00011	844.424	0.015
180.66	8.23426	0.00009	11.62219	0.00009	8.81995	0.00011	844.070	0.015
172.83	8.23254	0.00009	11.62021	0.00009	8.81958	0.00011	843.715	0.015
165.59	8.23065	0.00008	11.61815	0.00009	8.81975	0.00011	843.388	0.015
158.71	8.23065	0.00009	11.61815	0.00010	8.81975	0.00011	843.388	0.016
152.50	8.22775	0.00009	11.61508	0.00010	8.81954	0.00011	842.847	0.015
146.69	8.22775	0.00009	11.61508	0.00010	8.81954	0.00011	842.848	0.016
141.14	8.22775	0.00010	11.61508	0.00012	8.81954	0.00013	842.848	0.019
135.95	8.22775	0.00011	11.61508	0.00013	8.81954	0.00014	842.848	0.020
131.19	8.22371	0.00009	11.61065	0.00010	8.81931	0.00011	842.091	0.016
126.72	8.22371	0.00009	11.61065	0.00010	8.81931	0.00012	842.091	0.016
122.57	8.22219	0.00009	11.60894	0.00010	8.81927	0.00011	841.808	0.016
118.75	8.22219	0.00009	11.60894	0.00010	8.81927	0.00012	841.807	0.016
111.32	8.21641	0.00009	11.60110	0.00010	8.81886	0.00012	840.608	0.016
120.98	8.21743	0.00009	11.60238	0.00010	8.81896	0.00012	840.815	0.016
130.45	8.21919	0.00009	11.60434	0.00010	8.81916	0.00011	841.156	0.016
139.37	8.22091	0.00009	11.60658	0.00010	8.81916	0.00011	841.495	0.016
149.04	8.22091	0.00010	11.60658	0.00012	8.81916	0.00013	841.495	0.018
157.92	8.22479	0.00009	11.61132	0.00010	8.81944	0.00011	842.262	0.016
166.89	8.22687	0.00009	11.61358	0.00010	8.81954	0.00011	842.649	0.016
176.12	8.22890	0.00009	11.61627	0.00010	8.81971	0.00011	843.069	0.016

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Table S22 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
185.18	8.23094	0.00009	11.61870	0.00010	8.82004	0.00011	843.485	0.016
194.35	8.23321	0.00009	11.62153	0.00010	8.82035	0.00011	843.953	0.016
203.47	8.23546	0.00008	11.62413	0.00009	8.82061	0.00011	844.397	0.015
212.60	8.23782	0.00009	11.62682	0.00010	8.82101	0.00011	844.873	0.015
221.74	8.24009	0.00009	11.62960	0.00010	8.82151	0.00011	845.355	0.016
230.90	8.24243	0.00009	11.63225	0.00010	8.82174	0.00011	845.812	0.015
240.03	8.24243	0.00010	11.63225	0.00011	8.82174	0.00013	845.811	0.018
249.09	8.24709	0.00009	11.63765	0.00010	8.82246	0.00011	846.750	0.016
258.22	8.24938	0.00009	11.64040	0.00010	8.82293	0.00011	847.232	0.016
267.31	8.25185	0.00009	11.64307	0.00010	8.82332	0.00011	847.717	0.016
276.37	8.25432	0.00009	11.64593	0.00010	8.82365	0.00011	848.211	0.016
285.47	8.25678	0.00009	11.64881	0.00010	8.82405	0.00012	848.712	0.016
294.58	8.25678	0.00011	11.64881	0.00012	8.82405	0.00014	848.712	0.019

Table S23: Variable-temperature lattice parameter data for Gua-Cu.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.86	8.52285	0.00008	11.34927	0.00009	9.03234	0.00010	873.681	0.015
289.63	8.52184	0.00008	11.34810	0.00009	9.03275	0.00010	873.527	0.014
280.31	8.51978	0.00008	11.34628	0.00009	9.03290	0.00010	873.190	0.014
271.19	8.51731	0.00008	11.34432	0.00009	9.03305	0.00010	872.802	0.014

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Table S23 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
262.02	8.51463	0.00008	11.34208	0.00009	9.03310	0.00010	872.359	0.014
252.94	8.51148	0.00008	11.34000	0.00009	9.03328	0.00010	871.894	0.014
243.82	8.50847	0.00008	11.33782	0.00009	9.03338	0.00010	871.428	0.014
234.78	8.50531	0.00008	11.33573	0.00009	9.03347	0.00009	870.952	0.014
225.59	8.50221	0.00008	11.33358	0.00008	9.03360	0.00009	870.483	0.014
216.45	8.49889	0.00008	11.33154	0.00009	9.03354	0.00009	869.980	0.014
207.38	8.49539	0.00008	11.32927	0.00008	9.03361	0.00009	869.454	0.014
198.32	8.49204	0.00008	11.32716	0.00008	9.03364	0.00009	868.952	0.014
189.29	8.48882	0.00007	11.32505	0.00008	9.03352	0.00009	868.449	0.013
180.69	8.48526	0.00008	11.32326	0.00008	9.03371	0.00009	867.967	0.013
172.86	8.48246	0.00007	11.32136	0.00008	9.03366	0.00009	867.529	0.013
165.75	8.47995	0.00007	11.32015	0.00008	9.03403	0.00009	867.216	0.013
158.92	8.47756	0.00007	11.31891	0.00008	9.03428	0.00009	866.900	0.013
152.41	8.47524	0.00007	11.31791	0.00008	9.03455	0.00009	866.613	0.013
146.52	8.47314	0.00007	11.31682	0.00008	9.03478	0.00009	866.336	0.013
140.99	8.47124	0.00007	11.31604	0.00008	9.03496	0.00009	866.099	0.013
135.80	8.46971	0.00007	11.31537	0.00008	9.03527	0.00009	865.922	0.013
131.01	8.46817	0.00007	11.31471	0.00008	9.03565	0.00009	865.750	0.013
126.55	8.46680	0.00007	11.31442	0.00008	9.03587	0.00009	865.609	0.013
122.38	8.46552	0.00007	11.31416	0.00008	9.03617	0.00009	865.487	0.013
118.54	8.46437	0.00007	11.31391	0.00008	9.03657	0.00009	865.388	0.013

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Table S23 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
111.15	8.44664	0.00008	11.29768	0.00009	9.02806	0.00010	861.525	0.015
120.80	8.44850	0.00008	11.29959	0.00009	9.02799	0.00010	861.854	0.014
130.30	8.45167	0.00008	11.30177	0.00009	9.02794	0.00010	862.338	0.014
139.17	8.45488	0.00008	11.30417	0.00009	9.02789	0.00010	862.844	0.014
148.91	8.45895	0.00008	11.30685	0.00009	9.02797	0.00010	863.472	0.014
157.90	8.46274	0.00008	11.30941	0.00009	9.02817	0.00010	864.074	0.014
166.93	8.46679	0.00008	11.31213	0.00009	9.02821	0.00010	864.698	0.014
176.07	8.47067	0.00008	11.31472	0.00009	9.02852	0.00010	865.323	0.014
185.20	8.47489	0.00008	11.31745	0.00009	9.02889	0.00010	865.998	0.014
194.22	8.47909	0.00008	11.32014	0.00009	9.02923	0.00010	866.666	0.014
203.34	8.48348	0.00008	11.32319	0.00009	9.02970	0.00010	867.394	0.014
212.50	8.48776	0.00008	11.32605	0.00009	9.03035	0.00010	868.112	0.014
221.59	8.49211	0.00008	11.32886	0.00009	9.03088	0.00009	868.824	0.014
230.70	8.49645	0.00008	11.33152	0.00009	9.03162	0.00010	869.543	0.014
239.80	8.50071	0.00008	11.33431	0.00009	9.03229	0.00010	870.258	0.014
248.95	8.50504	0.00008	11.33691	0.00009	9.03316	0.00010	870.985	0.014
258.01	8.50950	0.00008	11.33954	0.00009	9.03405	0.00010	871.730	0.014
267.11	8.51393	0.00008	11.34199	0.00009	9.03498	0.00010	872.462	0.014
276.20	8.51863	0.00008	11.34452	0.00009	9.03600	0.00010	873.237	0.014
285.42	8.52352	0.00008	11.34703	0.00009	9.03708	0.00010	874.035	0.014
294.49	8.52826	0.00008	11.34955	0.00009	9.03789	0.00010	874.794	0.015

Table S24: Variable-temperature lattice parameter data for Gua-Zn.

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
299.88	8.34623	0.00004	11.73260	0.00005	8.92279	0.00005	873.746	0.007
289.66	8.34520	0.00004	11.73137	0.00005	8.92267	0.00005	873.535	0.007
280.33	8.34325	0.00004	11.72933	0.00005	8.92267	0.00005	873.180	0.007
271.21	8.34124	0.00004	11.72708	0.00005	8.92263	0.00005	872.797	0.007
262.03	8.33900	0.00004	11.72448	0.00005	8.92259	0.00005	872.365	0.008
252.94	8.33688	0.00004	11.72189	0.00005	8.92260	0.00005	871.953	0.008
243.82	8.33463	0.00004	11.71924	0.00005	8.92267	0.00005	871.527	0.008
234.75	8.33248	0.00004	11.71663	0.00005	8.92277	0.00005	871.118	0.008
225.65	8.33040	0.00004	11.71413	0.00005	8.92287	0.00005	870.724	0.008
216.47	8.32844	0.00005	11.71165	0.00006	8.92310	0.00006	870.356	0.008
207.42	8.32638	0.00005	11.70927	0.00006	8.92324	0.00006	869.978	0.009
198.27	8.32454	0.00005	11.70699	0.00006	8.92355	0.00006	869.648	0.009
189.30	8.32279	0.00005	11.70490	0.00007	8.92377	0.00007	869.331	0.010
180.97	8.32117	0.00005	11.70314	0.00007	8.92408	0.00007	869.061	0.010
173.19	8.31989	0.00006	11.70153	0.00007	8.92434	0.00007	868.834	0.011
165.85	8.31989	0.00006	11.70153	0.00008	8.92434	0.00008	868.833	0.011
159.04	8.31752	0.00006	11.69900	0.00008	8.92488	0.00008	868.451	0.012
152.74	8.31686	0.00006	11.69835	0.00008	8.92505	0.00008	868.349	0.012
146.80	8.31651	0.00007	11.69765	0.00009	8.92516	0.00009	868.272	0.013

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Table S24 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
141.26	8.31589	0.00007	11.69692	0.00009	8.92532	0.00009	868.169	0.013
136.14	8.31589	0.00007	11.69692	0.00009	8.92532	0.00009	868.169	0.013
131.31	8.31520	0.00008	11.69573	0.00010	8.92567	0.00010	868.043	0.014
126.76	8.31520	0.00008	11.69572	0.00010	8.92567	0.00010	868.041	0.014
122.62	8.31520	0.00008	11.69572	0.00010	8.92567	0.00010	868.042	0.015
118.77	8.31520	0.00008	11.69572	0.00010	8.92567	0.00010	868.041	0.015
111.23	8.28760	0.00005	11.67565	0.00006	8.93207	0.00006	864.294	0.009
120.90	8.29060	0.00005	11.67795	0.00006	8.93140	0.00006	864.713	0.009
130.22	8.29417	0.00005	11.68086	0.00006	8.93062	0.00006	865.227	0.009
139.17	8.29807	0.00005	11.68427	0.00006	8.92981	0.00006	865.806	0.009
148.78	8.30207	0.00005	11.68776	0.00007	8.92908	0.00006	866.412	0.010
157.70	8.30573	0.00005	11.69119	0.00007	8.92854	0.00006	866.996	0.010
166.88	8.30953	0.00006	11.69464	0.00007	8.92790	0.00007	867.585	0.010
176.13	8.31367	0.00006	11.69839	0.00007	8.92728	0.00007	868.237	0.010
185.24	8.31746	0.00006	11.70178	0.00007	8.92665	0.00007	868.823	0.011
194.40	8.32110	0.00006	11.70481	0.00008	8.92604	0.00008	869.368	0.012
203.39	8.32441	0.00007	11.70758	0.00008	8.92535	0.00008	869.853	0.012
212.52	8.32751	0.00007	11.71016	0.00008	8.92457	0.00008	870.292	0.012
221.61	8.33028	0.00007	11.71251	0.00008	8.92377	0.00008	870.679	0.012
230.70	8.33291	0.00006	11.71468	0.00008	8.92290	0.00008	871.030	0.012
239.81	8.33544	0.00006	11.71692	0.00007	8.92194	0.00008	871.367	0.011

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Table S24 – continued from previous page

T (K)	a (Å)	σ_a	b (Å)	σ_b	c (Å)	σ_c	V (Å^3)	σ_V
248.91	8.33783	0.00006	11.71902	0.00007	8.92099	0.00007	871.681	0.011
257.98	8.34045	0.00006	11.72140	0.00007	8.92011	0.00007	872.046	0.011
267.33	8.34309	0.00006	11.72374	0.00007	8.91933	0.00007	872.419	0.011
276.40	8.34580	0.00006	11.72642	0.00007	8.91856	0.00007	872.827	0.010
285.49	8.34841	0.00005	11.72902	0.00007	8.91791	0.00007	873.230	0.010
294.62	8.35107	0.00005	11.73187	0.00006	8.91729	0.00007	873.660	0.010

Table S25: Variable-temperature lattice parameter data for Gua-Cd.

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
299.88	9.19263	0.00003	19.60561	0.00008	1434.797	0.010
289.67	9.19308	0.00003	19.59469	0.00008	1434.140	0.010
280.35	9.19391	0.00003	19.57954	0.00008	1433.290	0.010
271.15	9.19485	0.00003	19.56297	0.00008	1432.369	0.010
262.18	9.19586	0.00003	19.54550	0.00008	1431.405	0.010
253.04	9.19686	0.00003	19.52717	0.00008	1430.372	0.010
243.95	9.19799	0.00003	19.50852	0.00009	1429.357	0.010
234.84	9.19910	0.00003	19.48975	0.00008	1428.327	0.010
225.78	9.20025	0.00003	19.47154	0.00008	1427.350	0.010
216.67	9.20137	0.00003	19.45253	0.00008	1426.305	0.010
207.61	9.20256	0.00003	19.43366	0.00008	1425.287	0.010

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Table S25 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
198.47	9.20371	0.00003	19.41477	0.00008	1424.259	0.010
189.42	9.20498	0.00003	19.39621	0.00009	1423.290	0.011
180.91	9.20605	0.00003	19.37926	0.00009	1422.377	0.011
173.19	9.20710	0.00003	19.36323	0.00009	1421.524	0.011
165.90	9.20793	0.00003	19.34972	0.00009	1420.787	0.011
159.15	9.20888	0.00003	19.33585	0.00009	1420.064	0.011
152.72	9.20971	0.00003	19.32457	0.00009	1419.491	0.011
146.71	9.21042	0.00003	19.31383	0.00009	1418.919	0.012
141.21	9.21108	0.00003	19.30450	0.00010	1418.439	0.012
136.01	9.21164	0.00003	19.29603	0.00010	1417.988	0.012
131.14	9.21208	0.00003	19.28918	0.00010	1417.621	0.013
126.60	9.21247	0.00003	19.28305	0.00011	1417.290	0.013
122.50	9.21285	0.00003	19.27738	0.00011	1416.990	0.013
118.69	9.21313	0.00004	19.27298	0.00011	1416.752	0.014
111.23	9.22534	0.00003	19.19467	0.00010	1414.739	0.012
120.67	9.22403	0.00003	19.20802	0.00010	1415.322	0.012
130.27	9.22208	0.00003	19.22734	0.00010	1416.146	0.013
139.11	9.22009	0.00003	19.24753	0.00010	1417.020	0.013
148.56	9.21785	0.00003	19.26895	0.00010	1417.907	0.013
157.68	9.21601	0.00003	19.28782	0.00010	1418.731	0.012
166.84	9.21399	0.00003	19.30808	0.00010	1419.599	0.013

Continued on next page

Table S25 – continued from previous page

T (K)	a (Å)	σ_a	c (Å)	σ_c	V (Å^3)	σ_V
175.74	9.21200	0.00003	19.32874	0.00011	1420.503	0.013
184.87	9.20988	0.00003	19.35026	0.00011	1421.429	0.013
194.03	9.20794	0.00003	19.37172	0.00011	1422.407	0.013
203.29	9.20602	0.00003	19.39310	0.00011	1423.384	0.013
212.28	9.20431	0.00003	19.41371	0.00011	1424.368	0.013
221.38	9.20263	0.00003	19.43419	0.00011	1425.349	0.013
230.51	9.20082	0.00003	19.45477	0.00011	1426.296	0.014
239.68	9.19911	0.00003	19.47490	0.00011	1427.241	0.013
248.79	9.19736	0.00003	19.49509	0.00011	1428.178	0.014
257.92	9.19568	0.00004	19.51519	0.00012	1429.129	0.014
267.18	9.19401	0.00003	19.53495	0.00011	1430.054	0.013
276.00	9.19247	0.00003	19.55473	0.00011	1431.023	0.013
285.11	9.19092	0.00003	19.57482	0.00011	1432.012	0.013
294.21	9.18928	0.00003	19.59520	0.00011	1432.992	0.013

5 XBU cells

Table S26: Equations used to calculate an average r and θ values using the lattice parameters a, b and c for each structure type studied here. Note that the EtNH3-Mn and Gua-Cu structures have been transformed from the standard $Pna2_1$ to $Pn2_1a$ in order to be comparable with the other structures.

structure type	s.g.	r	θ
$MeNH_3$-M	$Pnma$	$r = \frac{1}{3}\left[\frac{b}{2} + \sqrt{(a^2 + c^2)}\right]$	$\theta = 2\tan^{-1}\left(\frac{a}{c}\right)$
$EtNH_3$-Mn	$Pn2_1a$	$r = \frac{1}{3}\left[\frac{b}{2} + \sqrt{(a^2 + c^2)}\right]$	$\theta = 2\tan^{-1}\left(\frac{a}{c}\right)$
Me_2NH_2-M	$R\bar{3}c$	$r = \sqrt{(a^2/3 + c^2/36)}$	$\theta = \cos^{-1}\left\{-\frac{[(c^2/36)-(a^2/6)]}{r^2}\right\}$
Aze-Mn	$Pnma$	$r = \frac{1}{3}\left[\frac{b}{2} + \sqrt{(a^2 + c^2)}\right]$	$\theta = 2\tan^{-1}\left(\frac{c}{a}\right)$
Gua-M	$Pnna$	$r = \frac{1}{3}\left[\frac{b}{2} + \sqrt{(a^2 + c^2)}\right]$	$\theta = 2\tan^{-1}\left(\frac{c}{a}\right)$
Gua-Cu	$Pn2_1a$	$r = \frac{1}{3}\left[\frac{b}{2} + \sqrt{(a^2 + c^2)}\right]$	$\theta = 2\tan^{-1}\left(\frac{c}{a}\right)$
Me_2NH_2-Cd	$R\bar{3}c$	$r = \sqrt{(a^2/3 + c^2/36)}$	$\theta = \cos^{-1}\left\{\frac{[(c^2/36)-(a^2/6)]}{r^2}\right\}$

For the Me_2NH_2-Cu structure (s.g. $C2/c$), the lattice parameters a, b and c as well as the monoclinic angle β were used to calculate an average r and θ, shown in equations S1 and S2.

$$r = \frac{1}{3}\left\{\sqrt{(b^2 + c^2)} + \frac{1}{2}\sqrt{[c^2 + (a + c\cos\beta)^2]}\right\} \tag{S1}$$

$$\theta = \cos^{-1}\left\{\frac{(-a\cos\beta - c)c}{\sqrt{(b^2 + c^2)}\sqrt{[c^2 + (a + c\cos\beta)^2]}}\right\} \tag{S2}$$

6 A-site cation sizes

The volumes of the ellipsoids fitted to the A-site cations are given by $\frac{4}{3}\pi\sqrt{L_{\min}L_{\mathrm{med}}L_{\max}}$, and so for the $EtNH_3$ and Aze cations we calculate a volume of 5.44 Å^3 and 7.40 Å^3, respectively, giving a ∼25% difference between them.

Due to the anisotropic shapes of the A-site molecular cations, there are different ways to represent its size. In this work, we have calculated the principle axis lengths and directions of the A-site cation centroid using the program CRYSTALS. This creates an ellipsoid which envelopes the A-site cation (including the hydrogen atoms), and from this ellipsoid, we have calculated its minimum, medium and maximum components. In the work of Ref. S10, the size of the A-site cations were calculated using the following formula

$$r_{\mathrm{Aeff}} = r_{\mathrm{mass}} + r_{\mathrm{ion}}, \tag{S3}$$

where r_{mass} is the distance between the centre of mass of the A-site cation and the atom with the largest distance to the centre of mass (excluding hydrogen atoms), and r_{ion} is the corresponding ionic radius of this atom. As this method considers the largest distance from the centroid to the edge of the molecule, it is somewhat related to the $L_{\max}$ value we obtain by calculating the principal axes of the ellipsoid of the A-site cation. The tolerance factors calculated in reference S10 give similar ranges of values compared to the ones we calculate using $\sqrt{L_{\max}}$: in particular, 0.81–1.01 calculated from Ref. S10 and 0.86–1.18 from our calculations. Table S27 gives the sizes of the A-site cations calculated using these two methods.

Table S27: The A-site cation sizes calculated using the largest distance from the center of mass (named centroid method), and using an A-site cation ellipsoid (named principal axis ellipsoid method). For the centroid method, the A-site cation sizes are taken from Ref. S10 and calculated from the structures used here for comparison. The ellipsoid calculation shows the maximum effective length of the A-site cation ($L_{\max}$) and the calculated volumes of these ellispoids.

	centroid		principal axis ellipsoid	
A-site cation	L by Ref. S10 (Å)	L calc (Å)	$L_{\max}$ (Å^2)	calc. V (Å^3)
$MeNH_3$	2.17	2.19	1.88	3.21
Aze	2.50	2.52	1.98	7.40
Me_2NH_2	2.72	2.74	3.25	7.01
$EtNH_3$	2.74	2.71	2.95	5.42
Gua	2.78	2.79	2.52	7.11

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