Supporting Information

Topotactic structural conversion and hydration-dependent thermal expansion in robust $LnM^{III}(CN)_6 \cdot nH_2O$ and flexible $ALnFe^{II}(CN)_6 \cdot nH_2O$ frameworks (A = Li, Na, K; Ln = La-Lu, Y; M = Co, Fe; $0 \leq n \leq 5$)

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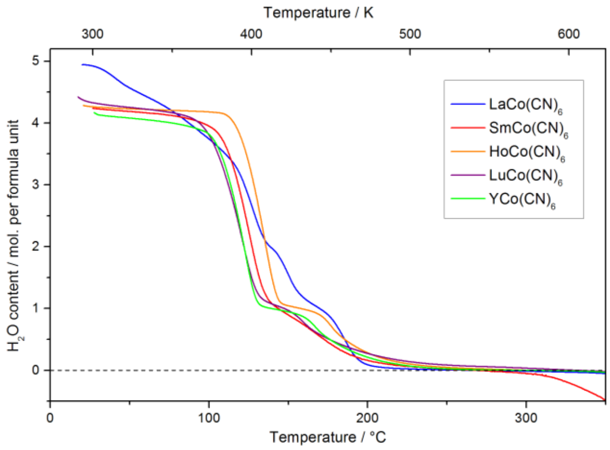

Figure S1 Thermogravimetrically-determined water content for a selection of $LnCo(CN)_6{\cdot}nH_2O$ compounds (Ln = La, Sm, Ho, Lu, Y).

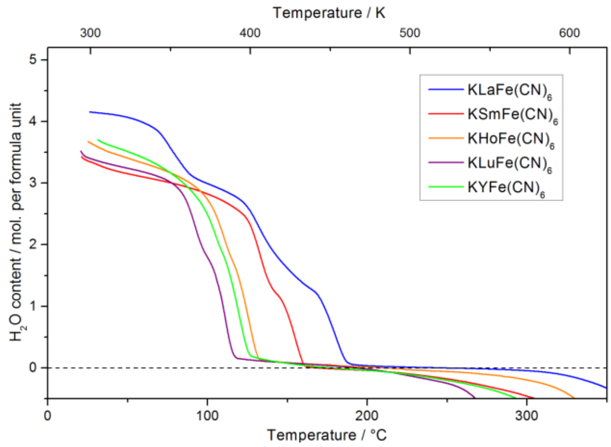

Figure S2 Thermogravimetrically-determined water content for a selection of $KLnFe(CN)_6{\cdot}nH_2O$ compounds (Ln = La, Sm, Ho, Lu, Y). Significant Ln-dependence is observed in the temperature required for full dehydration.

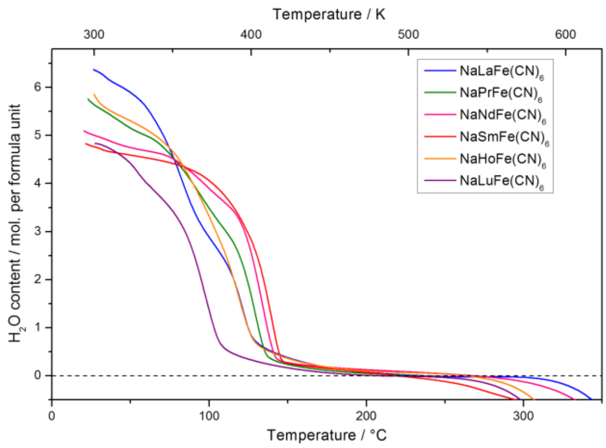

Figure S3 Thermogravimetrically-determined water content for a selection of $NaLnFe(CN)_6{\cdot}nH_2O$ compounds (Ln = La, Pr, Nd, Sm, Ho, Lu). The calculated water content is higher than expected based on the crystal structures (Figure S7), possibly due to incomplete drying of surface water from the sample prior to measurement.

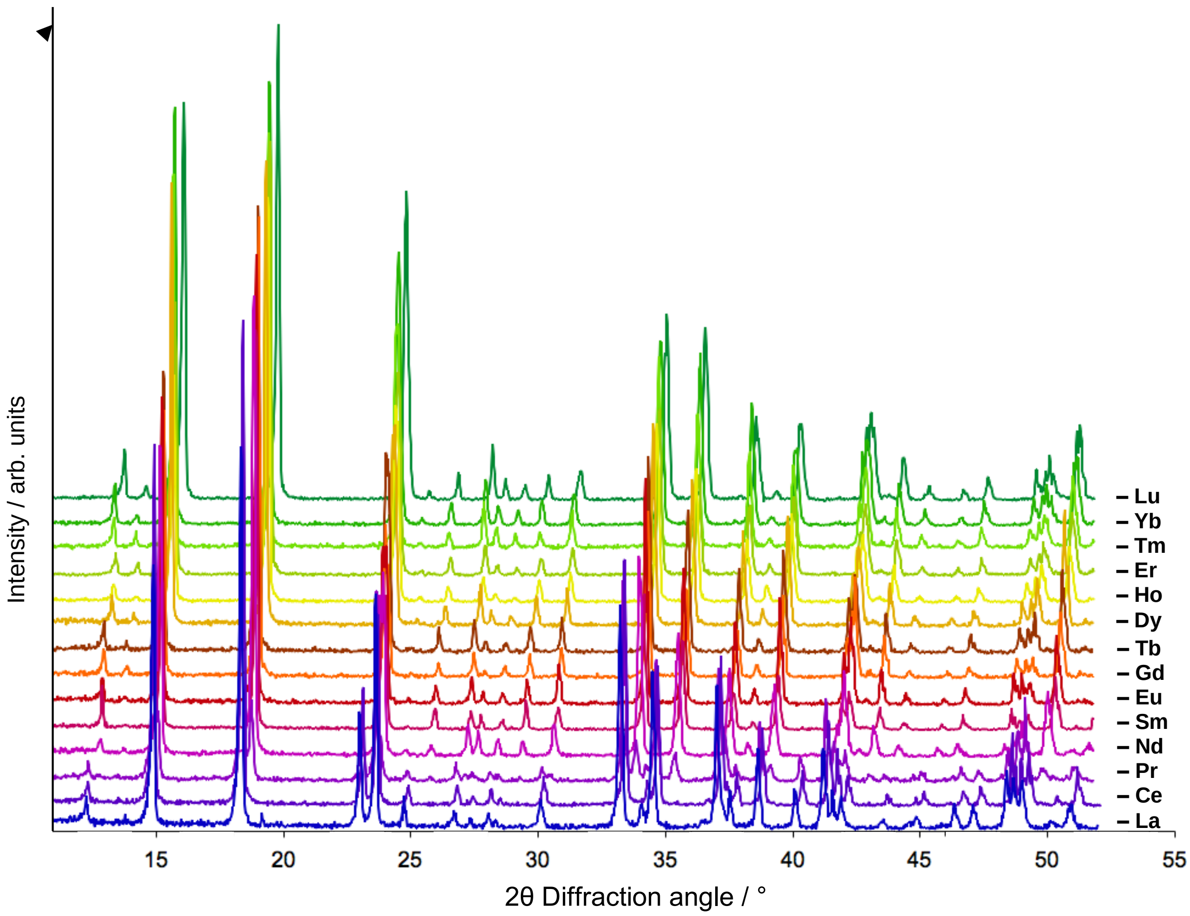

Figure S4 Laboratory X-ray powder diffraction patterns for the as-synthesised, hydrated $LnCo(CN)_6 \cdot nH_2O$ series. The transition from hexagonal pentahydrates to orthorhombic tetrahydrates is evident between Pr and Nd.

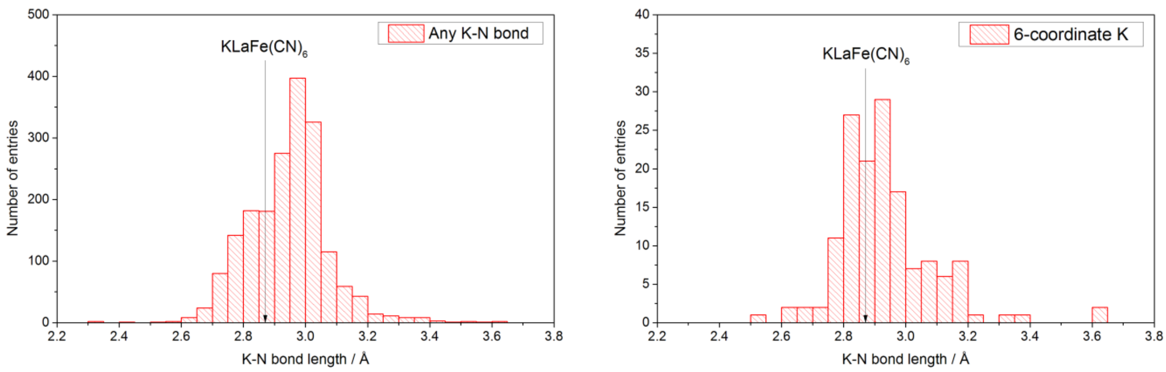

Figure S5 Average lengths of bonds in the Cambridge Structural Database for a) any K-N bond, and b) K-N bonds for 6-coordinate K. The observed K···N distance in $KLaFe(CN)_6$ (2.87 Å, indicated by the arrow) appears to be typical for K interacting with six N atoms, supporting the assertion that this type of interaction is present and is the cause of the structural transformation upon dehydration.

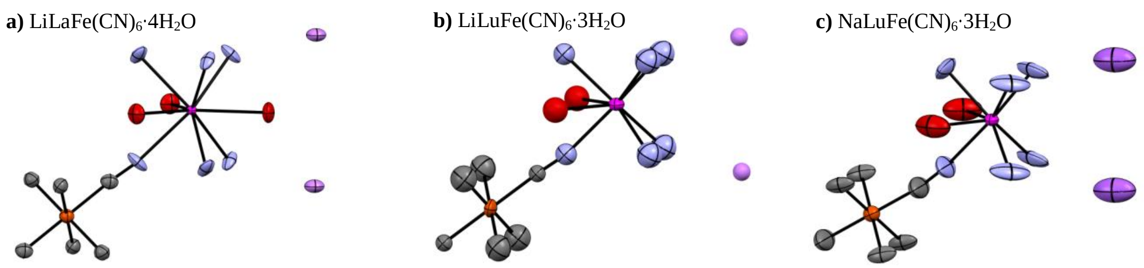

Figure S6 Structures of a) $LiLaFe(CN)_6{\cdot}4H_2O$, b) $LiLuFe(CN)_6{\cdot}3H_2O$, and c) $NaLuFe(CN)_6{\cdot}3H_2O$ determined from SCXRD data. The pink ellipsoids/spheres represent 50:50 A^+:O sites. The O atoms and Li+ ions in (b) are modelled isotropically.

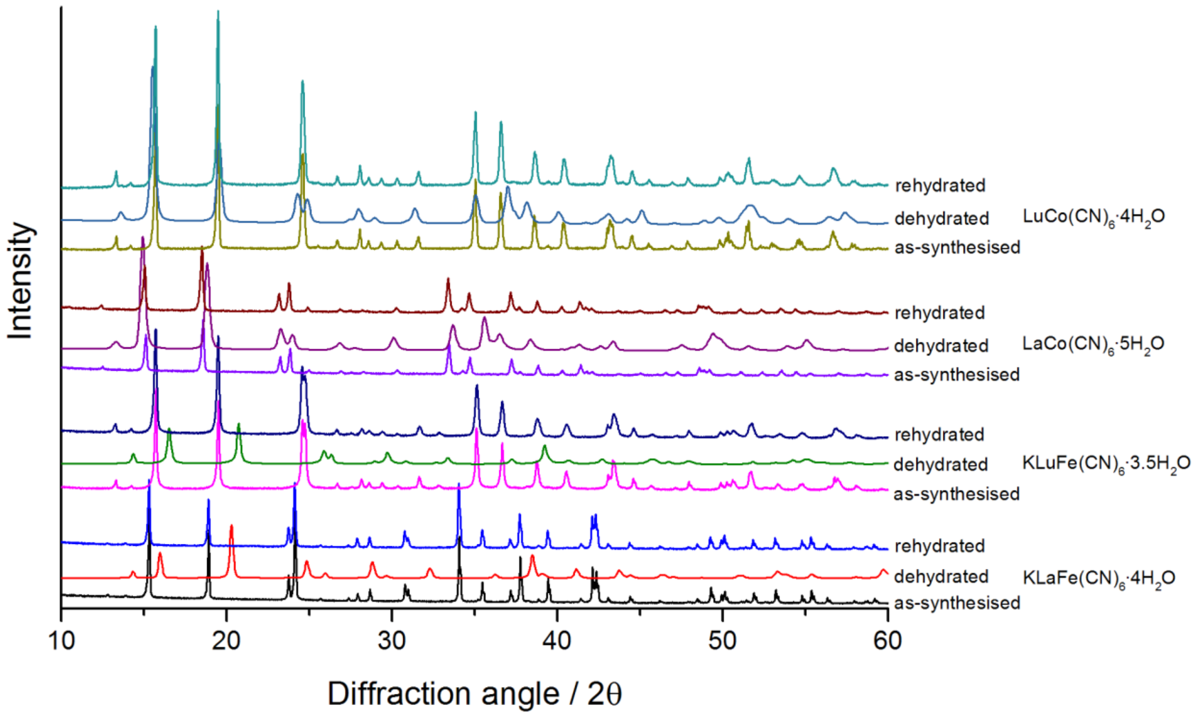

Figure S7 Laboratory XRPD data for $A_xLnM(CN)_6.nH_2O$ frameworks, with the close similarity of the as-synthesised and rehydrated patterns demonstrating the reversibility of the structural transformations that occur upon dehydration. Synchrotron data (with 2θ values rescaled to match the Cu Kα wavelength lab data) for the dehydrated materials are shown for comparison. The large shift of the peaks to higher angles upon dehydration of the $KLnFe(CN)_6.nH_2O$ materials is evident, corresponding to the large decrease in volume.

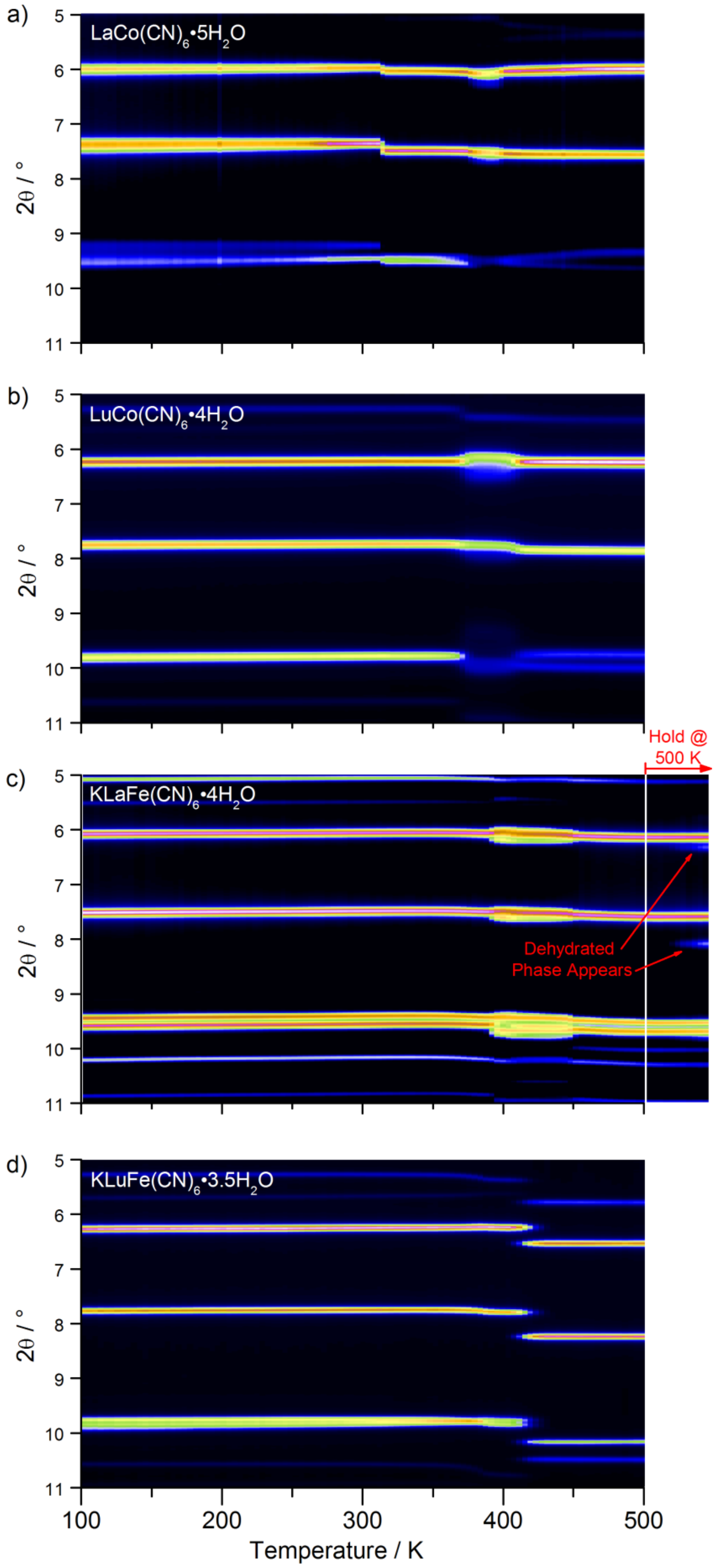

Figure S8 Selected 2θ range of the series of VT-XRPD patterns between 100-500 K for the dehydration of (a) $LaCo(CN)_6{\cdot}5H_2O$ showing two phase changes, (b) $LuCo(CN)_6{\cdot}4H_2O$ showing the symmetry change from orthorhombic to hexagonal via an un-indexed phase or phase mixture between 370-410 K, (c) $KLaFe(CN)_6{\cdot}4H_2O$ including data for temperature hold at 500 K, during which the fully dehydrated phase begins to appear, and (d) $KLuFe(CN)_6{\cdot}3.5H_2O$ with the dehydrated phase appearing in a similar manner at around 400 K. The X-ray wavelength used was 0.61951 Å for (a) & (b) and 0.61832 Å for (c) & (d).

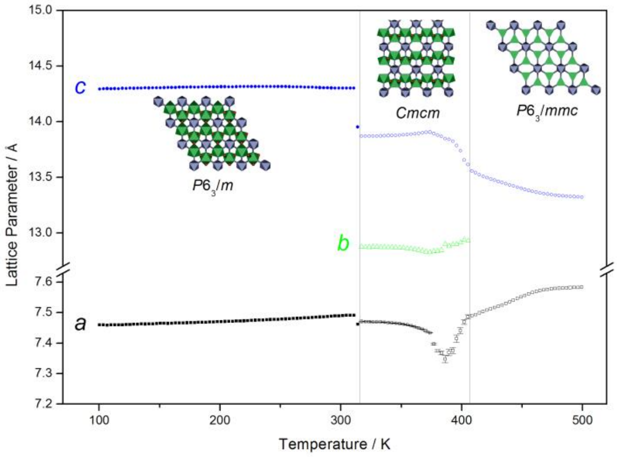

Figure S9 Unit cell *a*, *b*, and *c* parameters vs. temperature for $LaCo(CN)_6{\cdot}nH_2O$ during heating, from synchrotron XRPD data.

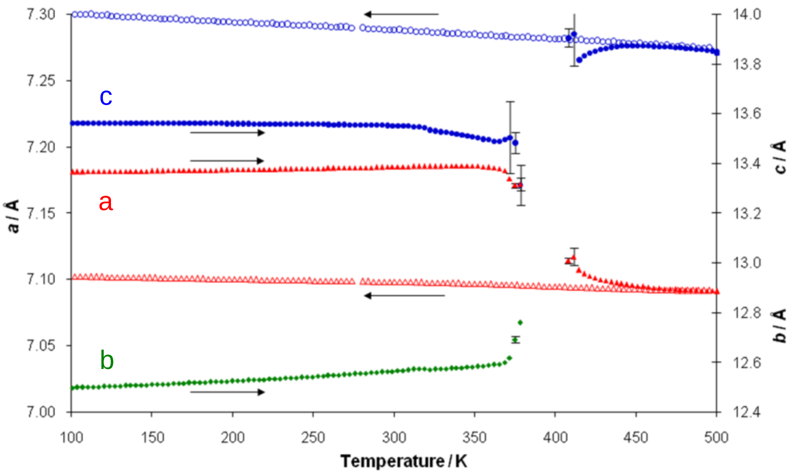

Figure S10 Unit cell *a*, *b*, and *c* parameters vs. temperature for $LuCo(CN)_6{\cdot}nH_2O$ from synchrotron XRPD data. Filled symbols represent the hydrated phase (*Cmcm*) during heating; open symbols represent the dehydrated phase ($P6_3/mmc$) during cooling.

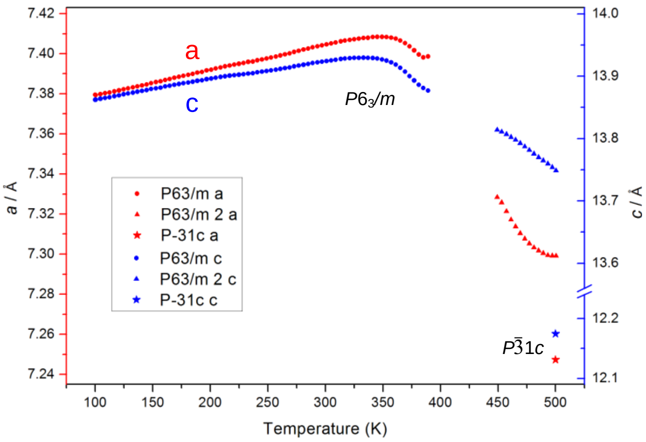

Figure S11 Unit cell parameters vs. temperature for $KLaFe(CN)_6{\cdot}4H_2O$ during thermal dehydration.

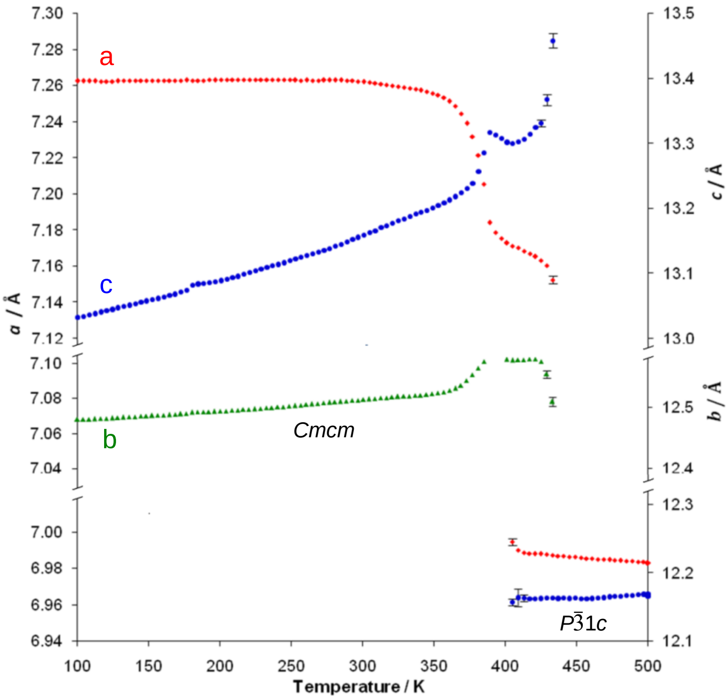

Figure S12 Unit cell *a*, *b*, and *c* parameters vs. temperature for $KLuFe(CN)_6{\cdot}3.5H_2O$ during thermal dehydration.

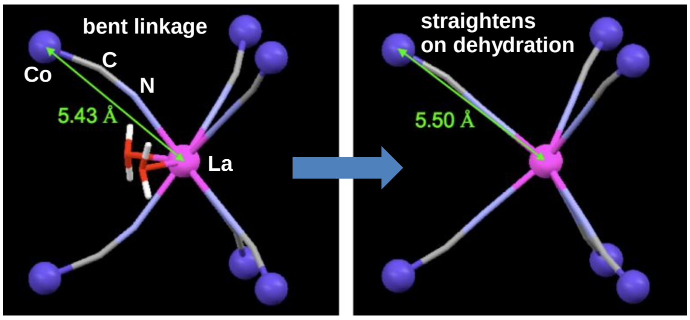

Figure S13 A portion of the structure from the Rietveld refinements for (a) $LaCo(CN)_6{\cdot}4H_2O$ with two coordinated water molecules, and (b) dehydrated $LaCo(CN)_6$, highlighting the effect of coordinated water on cyanide bending and Ln-M distance, which may explain in part the slight expansion of the material during the final stage of dehydration.

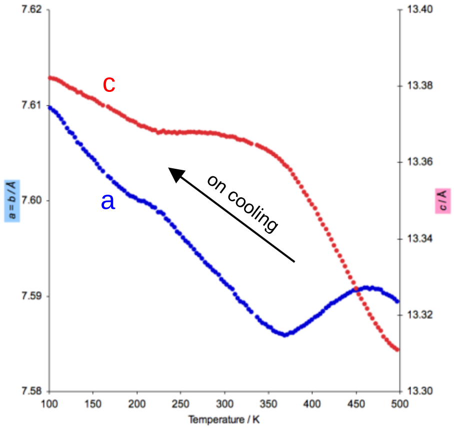

Figure S14 Unit cell *a* and *c* parameters for $LaCo(CN)_6$ on cooling. The non-linearities arise from undesired re-adsorption of residual water vapour into the extremely hygroscopic framework as the temperature is decreased.

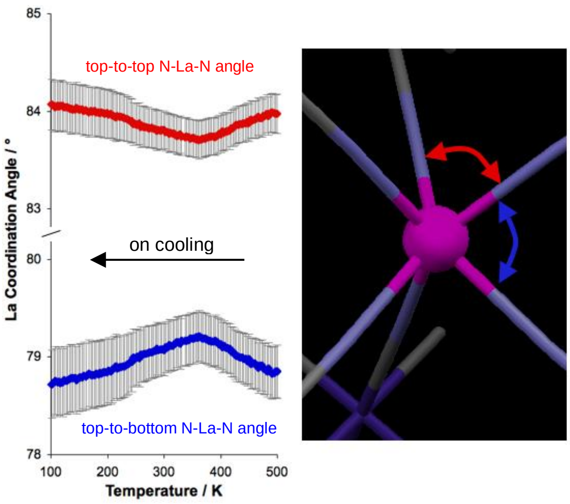

Figure S15 Coordination angles around the LaN_6 unit in $LaCo(CN)_6$ on cooling, determined by Rietveld refinement against the synchrotron XRPD data. 'Top-to-top' (red) and 'top-to-bottom' (blue) N-La-N angles are illustrated. The increase in the top-to-bottom angle on cooling from 500 K to 350 K (and concomitant decrease in the top-to-top angle) is a strong indication that water is coordinating at the equatorial coordination site during this period.

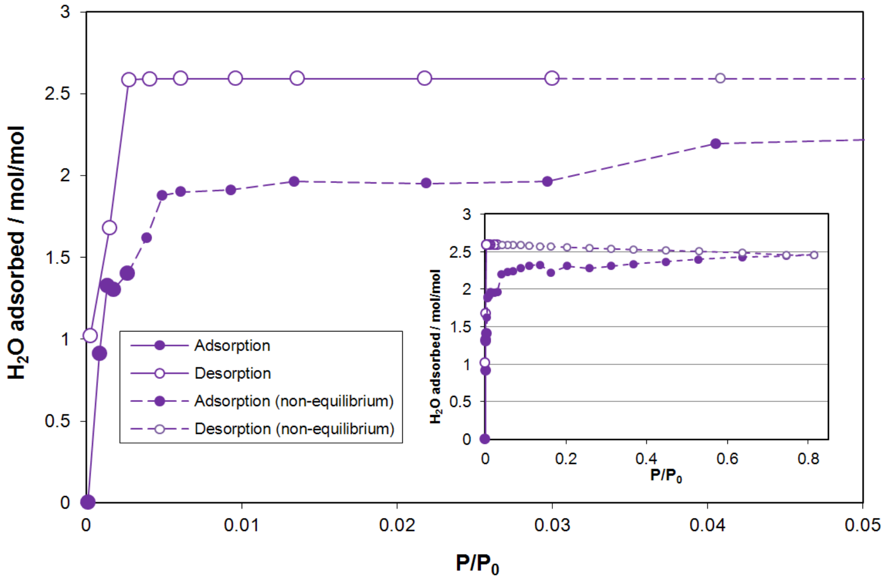

Figure S16 Low pressure portion of the gravimetric water adsorption (filled circles) and desorption (open circles) isotherms for $LuCo(CN)_6$ at 40 °C. The full isotherm is inset. The smaller symbols with dashed lines indicate non-equilibrium points. The kinetics of adsorption are very slow beyond the initial adsorption of the two coordinated water molecules. The sample continued to adsorb water vapour over several days even as the pressure was being decreased during the "desorption" phase of the measurement.

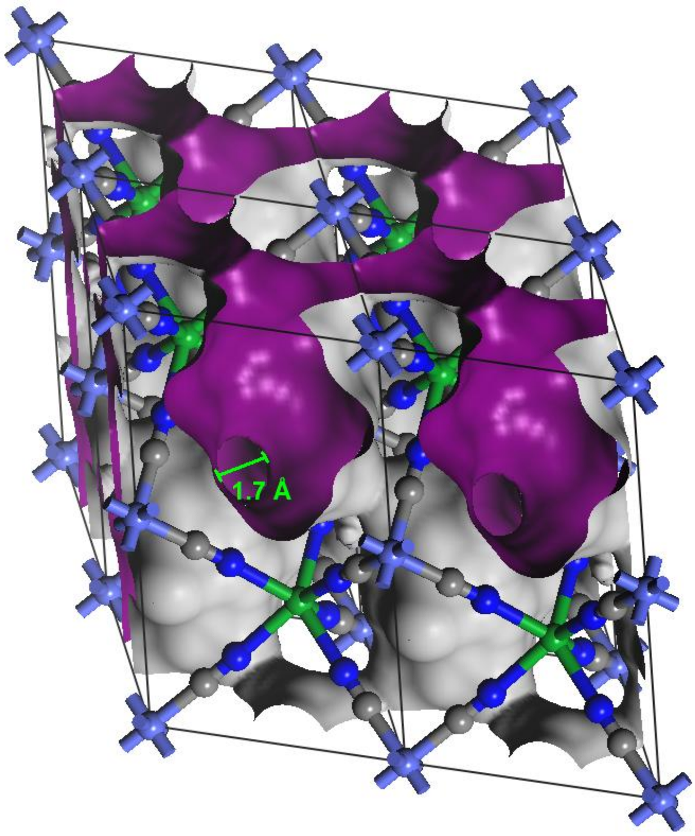

Figure S17 Pore structure in anhydrous $LuCo(CN)_6$, generated in Materials Studio using the Connolly method,[1] with a 1.1 Å probe radius. The narrow circular windows between the larger pore spaces are visible, with a diameter of only ~1.7 Å (or even less if a larger probe radius is used).

[1] M. Connolly, *Science*, 1983, **221**, 709-713.

Table S1 Lattice parameters and weighted profile R-factors from Rietveld refinement using XRPD data for dehydration of $LaCo(CN)_6 \cdot 5H_2O$ (12-BM, APS). No shading denotes refinements in *P*6_3/*m*. Light shading denotes refinements in *Cmcm*. Dark shading denotes refinements in *P*6_3/*mmc*.

T / K	*a* / Å	*b* / Å	*c* / Å	V / Å^3	wRp
100.4	7.4596(11)	*b* = *a*	14.293(4)	688.78(22)	0.0363
103.5	7.4597(11)	*b* = *a*	14.295(4)	688.88(22)	0.0366
106.6	7.4587(13)	*b* = *a*	14.297(4)	688.83(27)	0.0429
109.8	7.4593(12)	*b* = *a*	14.296(4)	688.87(24)	0.0386
112.9	7.4598(11)	*b* = *a*	14.297(4)	689.02(22)	0.0369
116.1	7.4601(11)	*b* = *a*	14.296(4)	689.04(23)	0.0370
119.2	7.4601(13)	*b* = *a*	14.300(4)	689.20(26)	0.0422
122.4	7.4613(11)	*b* = *a*	14.299(4)	689.38(23)	0.0378
125.5	7.4609(12)	*b* = *a*	14.301(4)	689.42(25)	0.0412
128.6	7.4619(11)	*b* = *a*	14.300(4)	689.57(22)	0.0369
131.8	7.4616(13)	*b* = *a*	14.302(4)	689.60(26)	0.0427
134.9	7.4630(11)	*b* = *a*	14.301(3)	689.78(22)	0.0365
138.0	7.4624(13)	*b* = *a*	14.304(4)	689.82(26)	0.0428
141.2	7.4632(11)	*b* = *a*	14.303(3)	689.93(22)	0.0367
144.3	7.4631(12)	*b* = *a*	14.305(4)	690.02(25)	0.0422
147.5	7.4639(11)	*b* = *a*	14.305(3)	690.15(21)	0.0365
150.6	7.4651(10)	*b* = *a*	14.305(3)	690.40(21)	0.0361
153.8	7.4647(10)	*b* = *a*	14.306(3)	690.35(21)	0.0359
156.9	7.4644(12)	*b* = *a*	14.307(4)	690.36(24)	0.0411
160.0	7.4650(10)	*b* = *a*	14.307(3)	690.45(21)	0.0359
163.2	7.4659(10)	*b* = *a*	14.307(3)	690.64(20)	0.0358
166.3	7.4656(11)	*b* = *a*	14.310(4)	690.71(23)	0.0404
169.5	7.4663(11)	*b* = *a*	14.310(4)	690.83(22)	0.0378
172.6	7.4665(11)	*b* = *a*	14.310(4)	690.91(22)	0.0380
175.8	7.4669(10)	*b* = *a*	14.311(3)	691.03(21)	0.0376
178.9	7.4671(10)	*b* = *a*	14.311(3)	691.05(20)	0.0352
182.0	7.4679(10)	*b* = *a*	14.311(3)	691.18(20)	0.0348
185.2	7.4682(9)	*b* = *a*	14.312(3)	691.29(19)	0.0346
188.3	7.4683(10)	*b* = *a*	14.313(4)	691.37(22)	0.0384
191.5	7.4689(9)	*b* = *a*	14.3127(30)	691.47(19)	0.0345
194.6	7.4694(9)	*b* = *a*	14.3125(30)	691.53(19)	0.0338
197.7	7.4700(9)	*b* = *a*	14.3135(29)	691.69(18)	0.0338
200.9	7.4701(9)	*b* = *a*	14.3139(29)	691.73(18)	0.0335
204.0	7.4707(9)	*b* = *a*	14.3141(28)	691.86(18)	0.0332
207.2	7.4711(8)	*b* = *a*	14.3135(28)	691.91(17)	0.0326
210.4	7.4717(8)	*b* = *a*	14.3137(28)	692.02(17)	0.0323
213.5	7.4721(8)	*b* = *a*	14.3143(27)	692.13(17)	0.0318
216.7	7.4724(8)	*b* = *a*	14.3147(27)	692.20(17)	0.0315
219.8	7.4729(8)	*b* = *a*	14.3148(26)	692.29(16)	0.0313
223.0	7.4737(8)	*b* = *a*	14.3147(25)	692.44(16)	0.0310
226.1	7.4742(7)	*b* = *a*	14.3152(25)	692.55(15)	0.0307
229.2	7.4749(7)	*b* = *a*	14.3159(24)	692.71(15)	0.0303
232.4	7.4753(7)	*b* = *a*	14.3159(24)	692.80(15)	0.0300
235.5	7.4759(7)	*b* = *a*	14.3165(23)	692.94(14)	0.0296
238.6	7.4764(7)	*b* = *a*	14.3167(23)	693.05(14)	0.0293
241.8	7.4769(6)	*b* = *a*	14.3160(22)	693.11(13)	0.0288
244.9	7.4776(6)	*b* = *a*	14.3160(21)	693.22(13)	0.0284
248.0	7.4780(6)	*b* = *a*	14.3161(21)	693.32(13)	0.0278
251.2	7.4786(6)	*b* = *a*	14.3162(20)	693.43(12)	0.0274
254.3	7.4792(5)	*b* = *a*	14.3153(19)	693.48(12)	0.0269
257.4	7.4798(5)	*b* = *a*	14.3140(18)	693.54(11)	0.0263

260.6	7.4804(5)	*b* = *a*	14.3136(17)	693.63(10)	0.0256
263.7	7.4812(4)	*b* = *a*	14.3133(16)	693.76(10)	0.0252
266.9	7.4818(4)	*b* = *a*	14.3126(15)	693.84(9)	0.0248
270.0	7.4825(4)	*b* = *a*	14.3112(14)	693.90(8)	0.0243
273.1	7.4832(35)	*b* = *a*	14.3102(13)	693.98(8)	0.0233
276.3	7.4841(32)	*b* = *a*	14.3091(12)	694.10(7)	0.0231
279.4	7.4845(29)	*b* = *a*	14.3074(11)	694.10(7)	0.0215
282.6	7.4854(26)	*b* = *a*	14.3056(10)	694.17(6)	0.0200
285.8	7.4861(23)	*b* = *a*	14.3046(9)	694.25(5)	0.0188
288.9	7.4869(21)	*b* = *a*	14.3034(7)	694.35(4)	0.0173
292.1	7.4880(18)	*b* = *a*	14.3026(6)	694.50(4)	0.0157
295.2	7.4888(16)	*b* = *a*	14.3019(5)	694.62(3)	0.0145
298.3	7.4896(14)	*b* = *a*	14.3018(5)	694.768(30)	0.0138
301.4	7.4905(13)	*b* = *a*	14.3015(4)	694.927(27)	0.0132
304.6	7.4911(13)	*b* = *a*	14.3011(4)	695.007(26)	0.0131
307.7	7.4916(12)	*b* = *a*	14.3008(4)	695.093(25)	0.0128
310.8	7.4917(12)	*b* = *a*	14.3007(4)	695.094(24)	0.0123
314.0	7.4620(15)	*b* = *a*	13.9520(8)	672.8(4)	0.0729
317.1	7.4708(7)	12.8749(11)	13.8707(6)	1334.15(18)	0.0166
320.3	7.4701(6)	12.8728(10)	13.8695(5)	1333.71(15)	0.0150
323.4	7.4701(5)	12.8711(9)	13.8699(5)	1333.57(14)	0.0141
326.6	7.4690(6)	12.8732(11)	13.8692(6)	1333.53(17)	0.0162
329.7	7.4690(6)	12.8732(11)	13.8692(6)	1333.53(17)	0.0162
332.9	7.4689(6)	12.8714(10)	13.8715(5)	1333.54(15)	0.0145
336.0	7.4683(6)	12.8708(10)	13.8728(6)	1333.49(16)	0.0154
339.2	7.4675(6)	12.8704(11)	13.8740(6)	1333.42(17)	0.0161
342.3	7.4661(6)	12.8703(11)	13.8747(5)	1333.24(16)	0.0156
345.4	7.4648(7)	12.8692(11)	13.8764(6)	1333.06(17)	0.0164
348.6	7.4639(7)	12.8667(11)	13.8789(6)	1332.87(18)	0.0165
351.7	7.4617(7)	12.8651(12)	13.8811(6)	1332.51(19)	0.0173
354.8	7.4597(7)	12.8614(12)	13.8842(6)	1332.08(19)	0.0176
358.0	7.4566(7)	12.8575(13)	13.8876(6)	1331.45(20)	0.0185
361.2	7.4534(8)	12.8520(13)	13.8911(7)	1330.65(20)	0.0191
364.3	7.4497(8)	12.8461(14)	13.8947(7)	1329.72(22)	0.0207
367.4	7.4451(9)	12.8391(15)	13.8995(8)	1328.63(23)	0.0220
370.6	7.4394(10)	12.8321(17)	13.9033(8)	1327.25(27)	0.0251
373.7	7.4335(11)	12.8264(18)	13.9057(9)	1325.84(28)	0.0260
376.9	7.3968(21)	12.834(4)	13.8926(18)	1318.9(6)	0.0403
380.0	7.374(4)	12.837(7)	13.878(3)	1313.6(11)	0.0480
383.2	7.368(5)	12.846(8)	13.867(4)	1312.5(12)	0.0468
386.3	7.348(12)	12.901(20)	13.846(10)	1312.5(32)	0.0732
389.5	7.369(11)	12.881(21)	13.841(9)	1313.7(30)	0.0700
392.6	7.376(10)	12.896(15)	13.823(8)	1314.8(24)	0.0618
395.7	7.415(12)	12.898(22)	13.786(11)	1318.4(32)	0.0944
398.9	7.441(10)	12.913(18)	13.737(7)	1319.9(26)	0.0753
402.0	7.4782(6)	*b* = *a*	13.5998(11)	659.70(11)	0.0276
405.2	7.4835(6)	*b* = *a*	13.5781(11)	658.54(9)	0.0273
408.3	7.4889(6)	*b* = *a*	13.5578(10)	658.50(9)	0.0255
411.4	7.4939(6)	*b* = *a*	13.5405(11)	658.54(9)	0.0261
414.6	7.4990(6)	*b* = *a*	13.5226(10)	658.56(9)	0.0236
417.7	7.5034(6)	*b* = *a*	13.5089(10)	658.66(9)	0.0233
420.9	7.5078(6)	*b* = *a*	13.4963(10)	658.82(9)	0.0230
424.0	7.5121(6)	*b* = *a*	13.4833(10)	658.94(9)	0.0227
427.1	7.5165(6)	*b* = *a*	13.4731(10)	659.22(9)	0.0230
430.3	7.5206(6)	*b* = *a*	13.4615(10)	659.37(9)	0.0221

433.4	7.5249(6)	*b* = *a*	13.4526(10)	659.69(9)	0.0227
436.5	7.5299(6)	*b* = *a*	13.4414(10)	660.02(9)	0.0217
439.7	7.5351(6)	*b* = *a*	13.4312(10)	660.42(9)	0.0216
442.8	7.5403(7)	*b* = *a*	13.4217(13)	660.87(11)	0.0271
445.9	7.5460(6)	*b* = *a*	13.4104(10)	661.31(9)	0.0214
449.1	7.5513(5)	*b* = *a*	13.4005(10)	661.75(8)	0.0212
452.2	7.5565(5)	*b* = *a*	13.3902(10)	662.15(8)	0.0212
455.3	7.5613(5)	*b* = *a*	13.3809(10)	662.54(8)	0.0210
458.5	7.5656(5)	*b* = *a*	13.3725(10)	662.88(8)	0.0213
461.6	7.5692(5)	*b* = *a*	13.3651(10)	663.13(8)	0.0212
464.7	7.5718(5)	*b* = *a*	13.3582(10)	663.25(8)	0.0208
467.9	7.5742(5)	*b* = *a*	13.3527(9)	663.40(8)	0.0208
471.0	7.5762(5)	*b* = *a*	13.3482(10)	663.52(7)	0.0209
474.2	7.5778(5)	*b* = *a*	13.3432(9)	663.55(7)	0.0208
477.3	7.5788(5)	*b* = *a*	13.3387(9)	663.51(7)	0.0208
480.5	7.5799(5)	*b* = *a*	13.3359(10)	663.57(7)	0.0212
483.6	7.5806(5)	*b* = *a*	13.3330(10)	663.54(7)	0.0213
486.8	7.5815(4)	*b* = *a*	13.3300(9)	663.54(7)	0.0210
489.9	7.5820(4)	*b* = *a*	13.3277(9)	663.51(7)	0.0212
493.0	7.5824(5)	*b* = *a*	13.3255(11)	663.48(8)	0.0228
496.2	7.5827(6)	*b* = *a*	13.3236(13)	663.44(9)	0.0254
499.3	7.5833(4)	*b* = *a*	13.3208(10)	663.40(7)	0.0216

Table S2 Lattice parameters and weighted profile R-factors from Rietveld refinement using XRPD data for dehydration of $LuCo(CN)_6{\cdot}4H_2O$ (12-BM, APS). No shading denotes refinements in *Cmcm*. Light shading denotes unsatisfactory refinements during the phase transition. Dark shading denotes refinements in $P6_3/mmc$.

T / K	*a* / Å	*b* / Å	*c* / Å	V / Å^3	wRp
100.3	7.21762(24)	12.4973(4)	13.36567(18)	1205.60(6)	0.0223
103.6	7.21767(24)	12.4981(5)	13.36596(18)	1205.70(6)	0.0225
106.9	7.21768(24)	12.4988(4)	13.36611(18)	1205.78(6)	0.0223
110.2	7.21772(24)	12.4997(5)	13.36648(18)	1205.92(6)	0.0225
113.5	7.21771(24)	12.5005(5)	13.36667(18)	1206.01(6)	0.0226
116.8	7.21774(24)	12.5012(5)	13.36681(18)	1206.10(6)	0.0226
120.1	7.21768(24)	12.5018(5)	13.36681(18)	1206.14(6)	0.0226
123.4	7.21782(24)	12.5030(5)	13.36738(18)	1206.33(6)	0.0227
126.7	7.21770(24)	12.5038(5)	13.36745(18)	1206.39(6)	0.0226
130.0	7.21781(24)	12.5048(5)	13.36791(18)	1206.55(6)	0.0227
133.3	7.21783(24)	12.5056(5)	13.36818(18)	1206.66(6)	0.0228
136.6	7.21773(24)	12.5063(5)	13.36817(18)	1206.70(6)	0.0227
139.9	7.21770(24)	12.5071(5)	13.36837(18)	1206.80(6)	0.0227
143.2	7.21771(24)	12.5079(5)	13.36855(18)	1206.89(6)	0.0226
146.5	7.21768(24)	12.5088(5)	13.36876(18)	1206.99(6)	0.0226
149.8	7.21774(24)	12.5099(5)	13.36922(18)	1207.15(6)	0.0227
153.1	7.21770(24)	12.5108(5)	13.36947(18)	1207.25(6)	0.0226
156.4	7.21772(24)	12.5117(5)	13.36971(18)	1207.37(6)	0.0226
159.7	7.21773(24)	12.5126(5)	13.36994(18)	1207.47(6)	0.0226
163.0	7.21768(24)	12.5136(5)	13.37021(18)	1207.58(6)	0.0225
166.3	7.21769(24)	12.5145(5)	13.37049(18)	1207.70(6)	0.0225
169.7	7.21777(24)	12.5156(5)	13.37098(18)	1207.86(6)	0.0226
173.0	7.21765(24)	12.5164(4)	13.37108(18)	1207.93(6)	0.0225
176.3	7.21763(23)	12.5174(4)	13.37137(18)	1208.05(6)	0.0222
179.6	7.21764(23)	12.5184(4)	13.37162(18)	1208.17(6)	0.0223
182.9	7.21766(23)	12.5196(4)	13.37213(18)	1208.33(6)	0.0223
186.3	7.21762(23)	12.5205(4)	13.37244(18)	1208.44(6)	0.0222
189.6	7.21754(23)	12.5214(4)	13.37256(18)	1208.53(6)	0.0221
192.9	7.21754(23)	12.5223(4)	13.37288(18)	1208.64(6)	0.0220
196.2	7.21750(23)	12.5233(4)	13.37309(17)	1208.76(6)	0.0218
199.5	7.21751(23)	12.5245(4)	13.37355(18)	1208.92(6)	0.0219
202.9	7.21749(22)	12.5256(4)	13.37391(18)	1209.05(6)	0.0218
206.2	7.21745(22)	12.5267(4)	13.37429(17)	1209.18(6)	0.0217
209.5	7.21739(22)	12.5278(4)	13.37456(17)	1209.30(6)	0.0216
212.8	7.21733(22)	12.5286(4)	13.37471(17)	1209.39(6)	0.0215
216.1	7.21726(21)	12.5298(4)	13.37506(17)	1209.52(6)	0.0213
219.4	7.21725(21)	12.5309(4)	13.37538(17)	1209.65(6)	0.0213
222.7	7.21728(21)	12.5321(4)	13.37584(17)	1209.82(5)	0.0213
226.0	7.21723(21)	12.5332(4)	13.37620(17)	1209.95(5)	0.0210
229.4	7.21722(21)	12.5344(4)	13.37663(17)	1210.10(5)	0.0211
232.7	7.21715(21)	12.5356(4)	13.37690(17)	1210.23(5)	0.0210
236.0	7.21703(20)	12.5365(4)	13.37707(17)	1210.31(5)	0.0208
239.3	7.21696(20)	12.5377(4)	13.37743(17)	1210.45(5)	0.0207
242.6	7.21700(20)	12.5391(4)	13.37796(17)	1210.63(5)	0.0207
245.9	7.21695(20)	12.5403(4)	13.37835(17)	1210.78(5)	0.0206
249.2	7.21689(19)	12.5417(4)	13.37878(17)	1210.94(5)	0.0205
252.5	7.21686(19)	12.5429(4)	13.37915(17)	1211.08(5)	0.0204
255.9	7.21685(19)	12.5441(4)	13.37958(17)	1211.24(5)	0.0203
259.2	7.21683(19)	12.5456(3)	13.37998(17)	1211.41(5)	0.0201
262.5	7.21667(18)	12.5467(3)	13.38018(17)	1211.52(5)	0.0200
265.7	7.21675(18)	12.5484(3)	13.38087(17)	1211.75(5)	0.0200

269.1	7.21670(18)	12.5498(3)	13.38133(17)	1211.93(5)	0.0199
272.4	7.21667(17)	12.5513(3)	13.38175(17)	1212.10(5)	0.0197
275.7	7.21664(17)	12.5529(3)	13.38224(17)	1212.29(4)	0.0198
279.0	7.21658(17)	12.5545(3)	13.38273(17)	1212.48(4)	0.0199
282.4	7.21661(17)	12.5563(3)	13.38330(17)	1212.71(4)	0.0198
285.6	7.21645(16)	12.5576(3)	13.38357(17)	1212.84(4)	0.0196
289.0	7.21634(16)	12.5592(3)	13.38405(17)	1213.02(4)	0.0196
292.3	7.21617(15)	12.5606(3)	13.38426(16)	1213.14(4)	0.0194
295.6	7.21613(15)	12.5622(3)	13.38488(16)	1213.35(4)	0.0194
298.9	7.21587(15)	12.5637(3)	13.38523(16)	1213.48(4)	0.0193
302.2	7.21587(14)	12.5655(3)	13.38591(16)	1213.71(4)	0.0193
305.5	7.21574(14)	12.5669(3)	13.38631(16)	1213.86(4)	0.0192
308.8	7.21550(14)	12.5683(3)	13.38661(16)	1213.99(4)	0.0191
312.1	7.21529(13)	12.5714(2)	13.38770(16)	1214.35(4)	0.0190
315.5	7.21513(13)	12.5729(2)	13.38816(16)	1214.51(4)	0.0190
318.8	7.21460(13)	12.5732(2)	13.38814(16)	1214.44(4)	0.0188
322.1	7.21262(14)	12.5705(3)	13.38737(17)	1213.78(4)	0.0184
325.4	7.21189(13)	12.5714(2)	13.38762(17)	1213.77(4)	0.0181
328.7	7.21133(14)	12.5727(2)	13.38798(17)	1213.83(4)	0.0183
332.0	7.21072(13)	12.5738(2)	13.38824(17)	1213.86(4)	0.0181
335.3	7.21021(13)	12.5752(2)	13.38863(17)	1213.94(4)	0.0180
338.6	7.20963(13)	12.5767(2)	13.38898(17)	1214.02(4)	0.0179
341.9	7.20899(13)	12.5781(2)	13.38927(17)	1214.08(4)	0.0180
345.2	7.20823(13)	12.5796(2)	13.38943(17)	1214.11(4)	0.0180
348.5	7.20750(13)	12.5812(2)	13.38931(18)	1214.13(4)	0.0180
351.8	7.20666(13)	12.5829(2)	13.38858(18)	1214.08(4)	0.0180
355.1	7.20581(14)	12.5850(2)	13.38691(19)	1213.99(4)	0.0189
358.4	7.20520(16)	12.5873(3)	13.38410(24)	1213.86(4)	0.0224
361.7	7.20428(23)	12.5898(4)	13.3821(3)	1213.77(6)	0.0297
365.0	7.2042(4)	12.5931(6)	13.3782(6)	1213.73(10)	0.0481
368.3	7.2052(7)	12.5989(11)	13.3718(12)	1213.86(19)	0.0766
371.6	7.207(27)	12.617(5)	13.339(4)	1212.9(8)	0.1602
374.9					
378.2					
381.6					
384.9					
388.2					
391.5					
394.8					
398.1					
401.4					
404.7					
408.0	7.282(7)	*b* = *a*	13.009(10)	597.4(9)	0.1734
411.3	7.285(24)	*b* = *a*	13.024(34)	599(3)	0.3257
414.6	7.2655(10)	*b* = *a*	12.9708(21)	592.96(15)	0.0897
417.9	7.2685(3)	*b* = *a*	12.9557(7)	592.75(5)	0.0414
421.2	7.27070(23)	*b* = *a*	12.9468(5)	592.72(4)	0.0333
424.5	7.27225(19)	*b* = *a*	12.9394(4)	592.627(30)	0.0297
427.8	7.27346(18)	*b* = *a*	12.9331(4)	592.537(28)	0.0279
431.1	7.27431(17)	*b* = *a*	12.9279(4)	592.437(26)	0.0269
434.4	7.27508(16)	*b* = *a*	12.9233(4)	592.353(25)	0.0262
437.7	7.27543(16)	*b* = *a*	12.9189(4)	592.207(25)	0.0258
441.0	7.27586(15)	*b* = *a*	12.9155(4)	592.119(24)	0.0254
444.3	7.27609(15)	*b* = *a*	12.9122(4)	592.006(24)	0.0252
447.6	7.27633(15)	*b* = *a*	12.9095(4)	591.922(24)	0.0251

451.0	7.27613(15)	*b* = *a*	12.9064(4)	591.747(24)	0.0250
454.3	7.27621(15)	*b* = *a*	12.9042(4)	591.662(24)	0.0250
457.6	7.27611(15)	*b* = *a*	12.9021(4)	591.550(24)	0.0249
460.9	7.27584(14)	*b* = *a*	12.8999(4)	591.402(23)	0.0247
464.2	7.27563(14)	*b* = *a*	12.8980(4)	591.282(23)	0.0245
467.5	7.27551(14)	*b* = *a*	12.8967(4)	591.204(23)	0.0245
470.8	7.27525(14)	*b* = *a*	12.8954(4)	591.101(23)	0.0243
474.1	7.27496(14)	*b* = *a*	12.8941(4)	590.992(23)	0.0241
477.4	7.27462(14)	*b* = *a*	12.8928(4)	590.877(23)	0.0240
480.7	7.27425(14)	*b* = *a*	12.8916(4)	590.762(23)	0.0239
484.0	7.27388(14)	*b* = *a*	12.8906(3)	590.659(23)	0.0237
487.3	7.27352(14)	*b* = *a*	12.8898(3)	590.564(22)	0.0235
490.6	7.27315(14)	*b* = *a*	12.8889(3)	590.459(22)	0.0233
493.9	7.27261(14)	*b* = *a*	12.8878(3)	590.325(22)	0.0232
497.2	7.27234(14)	*b* = *a*	12.8873(3)	590.257(22)	0.0230
500.6	7.27202(14)	*b* = *a*	12.8868(3)	590.182(22)	0.0229
500.0	7.27168(14)	*b* = *a*	12.8862(3)	590.099(22)	0.0227
500.0	7.27150(13)	*b* = *a*	12.8859(3)	590.054(22)	0.0226

Table S3 Lattice parameters and weighted profile R-factors from Rietveld refinement using XRPD data for dehydration of $KLaFe(CN)_6{\cdot}4H_2O$ (1-BM, APS). Light shading denotes unsatisfactory refinements during a phase transition.

***P*6₃/*m* hydrated phase**				
T / K	*a* / Å	*c* / Å	V / Å^3	wRp
100.0	7.37949(4)	13.86231(14)	653.761(8)	0.0585
100.4	7.37939(4)	13.86234(14)	653.744(8)	0.0587
104.6	7.37989(4)	13.86380(13)	653.902(8)	0.0583
108.6	7.38028(4)	13.86510(13)	654.033(8)	0.0584
112.7	7.38061(4)	13.86630(13)	654.148(8)	0.0583
116.7	7.38119(4)	13.86791(13)	654.326(8)	0.0580
120.7	7.38166(4)	13.86934(13)	654.476(8)	0.0579
124.7	7.38226(4)	13.87100(13)	654.663(8)	0.0578
128.7	7.38272(4)	13.87230(13)	654.805(8)	0.0580
132.7	7.38316(4)	13.87363(13)	654.945(8)	0.0578
136.8	7.38366(4)	13.87502(13)	655.100(8)	0.0573
140.7	7.38413(4)	13.87633(13)	655.246(8)	0.0572
144.8	7.38464(4)	13.87770(13)	655.400(8)	0.0572
148.8	7.38529(4)	13.87931(13)	655.593(8)	0.0572
152.8	7.38580(4)	13.88063(13)	655.744(8)	0.0571
156.8	7.38617(4)	13.88171(13)	655.862(8)	0.0569
160.8	7.38686(4)	13.88336(13)	656.062(8)	0.0571
164.8	7.38733(4)	13.88455(13)	656.201(8)	0.0569
168.8	7.38797(4)	13.88609(13)	656.389(8)	0.0573
172.8	7.38847(4)	13.88735(13)	656.536(8)	0.0570
176.8	7.38896(4)	13.88860(13)	656.684(8)	0.0572
180.8	7.38947(4)	13.88983(13)	656.833(8)	0.0577
184.8	7.38989(4)	13.89101(13)	656.961(8)	0.0564
188.8	7.39054(4)	13.89255(13)	657.151(8)	0.0568
192.8	7.39088(4)	13.89348(13)	657.254(8)	0.0563
196.8	7.39160(4)	13.89512(13)	657.460(8)	0.0566
200.8	7.39201(4)	13.89615(13)	657.582(8)	0.0562
204.8	7.39265(4)	13.89756(13)	657.764(8)	0.0565
208.9	7.39315(4)	13.89866(13)	657.904(8)	0.0564
212.9	7.39365(4)	13.89979(13)	658.047(8)	0.0564
216.9	7.39408(4)	13.90071(13)	658.167(8)	0.0561
220.9	7.39452(4)	13.90162(13)	658.288(8)	0.0561
224.9	7.39493(4)	13.90241(13)	658.399(8)	0.0558
228.9	7.39538(4)	13.90324(13)	658.518(8)	0.0557
232.9	7.39589(4)	13.90420(13)	658.654(8)	0.0563
236.9	7.39611(4)	13.90471(13)	658.718(8)	0.0552
240.9	7.39672(4)	13.90599(13)	658.887(8)	0.0559
244.9	7.39716(4)	13.90701(13)	659.013(8)	0.0554
248.9	7.39762(4)	13.90813(13)	659.150(8)	0.0554
252.9	7.39809(4)	13.90926(13)	659.286(8)	0.0548
256.9	7.39859(4)	13.91043(13)	659.431(8)	0.0547
260.9	7.39911(4)	13.91165(13)	659.581(8)	0.0546
264.9	7.39968(4)	13.91296(13)	659.746(8)	0.0545
269.0	7.40017(4)	13.91410(13)	659.886(8)	0.0536
272.9	7.40090(4)	13.91573(13)	660.094(8)	0.0548
276.9	7.40148(4)	13.91705(13)	660.260(8)	0.0551
281.0	7.40202(4)	13.91835(13)	660.418(8)	0.0548
285.0	7.40259(4)	13.91966(13)	660.581(8)	0.0552
289.0	7.40316(4)	13.92099(13)	660.748(8)	0.0553
293.0	7.40371(4)	13.92227(13)	660.906(8)	0.0559

297.0	7.40417(4)	13.92338(13)	661.040(8)	0.0562				
301.0	7.40464(4)	13.92443(13)	661.174(8)	0.0560				
305.0	7.40511(4)	13.92546(13)	661.308(8)	0.0561				
309.0	7.40557(4)	13.92645(14)	661.437(9)	0.0565				
313.5	7.40613(4)	13.92762(14)	661.591(9)	0.0567				
317.1	7.40659(5)	13.92845(14)	661.713(9)	0.0577				
321.1	7.40687(5)	13.92887(14)	661.784(9)	0.0580				
325.1	7.40721(5)	13.92929(14)	661.863(9)	0.0578				
329.1	7.40750(5)	13.92953(14)	661.928(9)	0.0583				
333.2	7.40781(5)	13.92966(14)	661.990(9)	0.0585				
337.1	7.40793(5)	13.92925(14)	661.991(9)	0.0578				
341.2	7.40828(5)	13.92909(14)	662.045(9)	0.0585				
345.2	7.40838(5)	13.92823(15)	662.024(9)	0.0586				
349.2	7.40840(5)	13.92691(15)	661.964(9)	0.0588				
353.1	7.40828(5)	13.92495(15)	661.849(9)	0.0589				
357.2	7.40802(5)	13.92229(15)	661.676(9)	0.0591				
361.2	7.40750(5)	13.91850(15)	661.403(9)	0.0590				
365.2	7.40659(5)	13.91339(15)	660.997(10)	0.0596				
369.2	7.40530(5)	13.90720(16)	660.474(10)	0.0606				
373.2	7.40361(5)	13.90017(16)	659.839(10)	0.0624				
377.2	7.40168(6)	13.89305(17)	659.156(11)	0.0645				
381.2	7.39961(6)	13.88617(18)	658.463(11)	0.0667				
385.2	7.39814(6)	13.88110(20)	657.960(12)	0.0708				
389.2	7.39867(17)	13.8770(6)	657.86(4)	0.1568				
393.2								
401.2								
409.2								
417.2								
425.2								
433.2								
441.2								
449.2	7.32838(8)	13.81403(26)	642.491(16)	0.0637				
453.2	7.32572(6)	13.81096(20)	641.882(12)	0.0561				
457.2	7.32141(6)	13.80714(20)	640.950(12)	0.0563				
461.2	7.31720(6)	13.80259(20)	640.001(12)	0.0563				
465.2	7.31375(6)	13.79792(20)	639.181(12)	0.0562				
469.2	7.31042(6)	13.79275(20)	638.361(12)	0.0562				
473.2	7.30774(6)	13.78727(20)	637.639(12)	0.0561				
477.2	7.30527(6)	13.78163(20)	636.949(12)	0.0559				
481.2	7.30329(6)	13.77581(20)	636.334(12)	0.0560				
485.3	7.30174(6)	13.77014(20)	635.802(12)	0.0555				
489.2	7.30045(6)	13.76478(20)	635.330(12)	0.0555				
493.2	7.29946(6)	13.75971(20)	634.922(12)	0.0551				
497.1	7.29917(6)	13.75413(20)	634.616(12)	0.0546				
500.3	7.29914(6)	13.74874(20)	634.361(12)	0.0546				
500.2	7.29848(6)	13.74522(19)	634.085(12)	0.0536				
500.0	7.29859(6)	13.74352(19)	634.026(12)	0.0527	**$P\bar{3}1c$ dehydrated phase**			
500.0	7.29876(6)	13.74320(19)	634.041(12)	0.0519	*a* / Å	*c* / Å	V / Å^3	wRp
500.0	7.29920(6)	13.74327(18)	634.120(11)	0.0486	7.2789(20)	12.103(7)	555.3(4)	0.0486
500.0	7.29958(6)	13.74367(18)	634.204(11)	0.0468	7.2722(16)	12.107(6)	554.47(31)	0.0468
500.0	7.30019(6)	13.74479(18)	634.362(11)	0.0457	7.2711(13)	12.113(5)	554.61(27)	0.0457
500.0	7.30031(6)	13.74513(18)	634.399(11)	0.0446	7.2615(12)	12.136(5)	554.17(25)	0.0446
500.0	7.30082(6)	13.74596(18)	634.525(11)	0.0435	7.2578(10)	12.146(4)	554.09(21)	0.0435
500.0	7.30082(6)	13.74635(18)	634.543(11)	0.0421	7.2524(9)	12.1613(32)	553.95(18)	0.0421
500.0	7.30102(6)	13.74712(19)	634.613(11)	0.0420	7.2474(9)	12.1748(28)	553.80(16)	0.0420

Table S4 Lattice parameters and weighted profile R-factors from Rietveld refinement using XRPD data for dehydration of $KLuFe(CN)_6{\cdot}3.5H_2O$ (1-BM, APS).

***Cmcm* hydrated phase**					
T / K	*a* / Å	*b* / Å	*c* / Å	V / Å^3	wRp
100.0	7.13181(16)	12.47974(25)	13.3958(3)	1192.27(4)	0.0590
100.1	7.13184(16)	12.47981(26)	13.3961(3)	1192.30(4)	0.0594
104.2	7.13236(16)	12.48001(25)	13.3959(3)	1192.40(4)	0.0590
108.3	7.13325(18)	12.48059(29)	13.3959(3)	1192.60(5)	0.0673
112.3	7.13387(16)	12.48089(25)	13.3958(3)	1192.72(4)	0.0588
116.3	7.13481(17)	12.48150(28)	13.3957(3)	1192.93(5)	0.0659
120.3	7.13541(16)	12.48180(25)	13.3957(3)	1193.06(4)	0.0586
124.3	7.13623(16)	12.48228(25)	13.3956(3)	1193.23(4)	0.0584
128.3	7.13714(15)	12.48303(25)	13.3960(3)	1193.49(4)	0.0585
132.3	7.13773(16)	12.48357(25)	13.3963(3)	1193.67(4)	0.0583
136.3	7.13852(18)	12.48406(28)	13.3964(3)	1193.85(5)	0.0666
140.3	7.13923(16)	12.48449(25)	13.39642(29)	1194.02(4)	0.0582
144.3	7.14011(15)	12.48513(25)	13.39636(29)	1194.22(4)	0.0577
148.3	7.14088(17)	12.48563(28)	13.3965(3)	1194.41(5)	0.0644
152.4	7.14153(15)	12.48613(25)	13.39656(29)	1194.57(4)	0.0572
156.3	7.14232(16)	12.48672(25)	13.39674(29)	1194.78(4)	0.0576
160.3	7.14309(16)	12.48720(25)	13.39684(29)	1194.96(4)	0.0576
164.4	7.14387(16)	12.48758(25)	13.39674(29)	1195.12(4)	0.0572
168.4	7.14466(16)	12.48829(25)	13.39695(29)	1195.34(4)	0.0572
172.4	7.14567(16)	12.48889(25)	13.39672(29)	1195.54(4)	0.0569
176.4	7.14668(15)	12.48971(25)	13.39704(28)	1195.82(4)	0.0566
180.4	7.14945(15)	12.49169(25)	13.39679(28)	1196.45(4)	0.0596
184.4	7.15033(17)	12.49233(27)	13.39684(32)	1196.66(5)	0.0625
188.4	7.15041(15)	12.49228(24)	13.39692(28)	1196.68(4)	0.0565
192.4	7.15085(18)	12.49275(29)	13.3975(3)	1196.85(5)	0.0658
196.5	7.15137(16)	12.49298(24)	13.39726(28)	1196.94(4)	0.0563
200.5	7.15218(16)	12.49367(25)	13.39771(28)	1197.18(4)	0.0564
204.5	7.15278(16)	12.49387(24)	13.39738(28)	1197.27(4)	0.0559
208.5	7.15386(15)	12.49466(24)	13.39748(28)	1197.53(4)	0.0558
212.5	7.15455(15)	12.49515(24)	13.39743(27)	1197.69(4)	0.0549
216.5	7.15561(17)	12.49599(27)	13.3978(3)	1197.99(5)	0.0617
220.5	7.15648(15)	12.49667(24)	13.39795(28)	1198.21(4)	0.0549
224.6	7.15745(15)	12.49712(24)	13.39762(28)	1198.38(4)	0.0550
228.6	7.15840(15)	12.49792(24)	13.39790(28)	1198.64(4)	0.0548
232.6	7.15932(15)	12.49866(24)	13.39788(27)	1198.87(4)	0.0544
236.6	7.16020(16)	12.49908(24)	13.39757(28)	1199.03(4)	0.0550
240.6	7.16109(15)	12.49990(24)	13.39763(27)	1199.26(4)	0.0540
244.6	7.16206(16)	12.50051(24)	13.39739(27)	1199.46(4)	0.0542
248.7	7.16305(16)	12.50150(24)	13.39744(27)	1199.72(4)	0.0542
252.7	7.16409(15)	12.50233(24)	13.39710(27)	1199.95(4)	0.0539
256.7	7.16499(16)	12.50316(25)	13.39700(28)	1200.17(4)	0.0545
260.7	7.16585(15)	12.50414(24)	13.39704(27)	1200.41(4)	0.0533
264.7	7.16679(15)	12.50494(24)	13.39680(27)	1200.63(4)	0.0531
268.7	7.16775(16)	12.50575(24)	13.39686(27)	1200.87(4)	0.0538
272.7	7.16874(27)	12.50660(40)	13.3972(5)	1201.15(7)	0.0909
276.7	7.16990(15)	12.50760(24)	13.39706(27)	1201.43(4)	0.0526
280.7	7.17103(15)	12.50840(24)	13.39709(27)	1201.69(4)	0.0525
284.7	7.17229(16)	12.50926(24)	13.39707(27)	1201.98(4)	0.0528
288.7	7.17357(15)	12.50995(24)	13.39663(27)	1202.23(4)	0.0524
292.7	7.17499(16)	12.51106(24)	13.39639(27)	1202.55(4)	0.0529
296.7	7.17609(16)	12.51160(24)	13.39538(26)	1202.70(4)	0.0524

300.6	7.17727(16)	12.51230(24)	13.39459(26)	1202.89(4)	0.0521				
304.6	7.17857(16)	12.51302(24)	13.39362(26)	1203.09(4)	0.0518				
308.6	7.17979(16)	12.51369(25)	13.39252(27)	1203.26(4)	0.0517				
312.7	7.18146(16)	12.51474(25)	13.39108(26)	1203.51(4)	0.0511				
316.7	7.18250(40)	12.5154(6)	13.38990(60)	1203.64(10)	0.1163				
320.7	7.18390(16)	12.51626(25)	13.38900(26)	1203.88(4)	0.0504				
324.8	7.18513(21)	12.5170(3)	13.3878(4)	1204.05(6)	0.0655				
328.9	7.18624(18)	12.51753(28)	13.3862(3)	1204.14(5)	0.0555				
332.9	7.18746(27)	12.5181(4)	13.3848(5)	1204.27(7)	0.0811				
337.0	7.18887(25)	12.5194(4)	13.3834(4)	1204.51(7)	0.0746				
340.8	7.18986(17)	12.51967(27)	13.38149(27)	1204.53(5)	0.0485				
344.8	7.19107(17)	12.52070(27)	13.37954(26)	1204.66(4)	0.0476				
348.8	7.19232(17)	12.52174(27)	13.37710(26)	1204.75(5)	0.0471				
352.8	7.19359(18)	12.52307(27)	13.37415(26)	1204.82(5)	0.0465				
356.8	7.19509(18)	12.52494(28)	13.37026(27)	1204.90(5)	0.0463				
360.9	7.19673(19)	12.52729(30)	13.36465(27)	1204.90(5)	0.0459				
364.9	7.19866(20)	12.5307(3)	13.35699(29)	1204.85(5)	0.0460				
368.9	7.20089(22)	12.5356(3)	13.3459(3)	1204.70(6)	0.0459				
372.9	7.20323(23)	12.5430(4)	13.3305(3)	1204.42(6)	0.0457				
376.9	7.20602(25)	12.5527(4)	13.3104(4)	1203.99(7)	0.0460				
380.9	7.21233(33)	12.5634(5)	13.2815(4)	1203.45(8)	0.0469				
384.9	7.2227(4)	12.5740(6)	13.2369(4)	1202.15(10)	0.0466				
388.9	7.23406(25)	12.5835(4)	13.17814(26)	1199.60(6)	0.0408				
392.9	7.23277(24)	12.5822(4)	13.16257(25)	1197.85(6)	0.0420				
396.9	7.23082(24)	12.5805(4)	13.15356(25)	1196.54(6)	0.0433	**$P\bar{3}1c$ dehydrated phase**			
401.0	7.22866(25)	12.5780(4)	13.14659(26)	1195.31(6)	0.0439	*a* / Å	*c* / Å	V / Å^3	wRp
405.0	7.22788(25)	12.5765(4)	13.14192(26)	1194.62(6)	0.0430	6.9615(18)	12.246(5)	513.95(29)	0.0430
409.0	7.22880(26)	12.5768(4)	13.13910(26)	1194.54(6)	0.0395	6.9640(50)	12.2334(13)	513.80(7)	0.0395
413.0	7.23032(29)	12.5768(5)	13.13426(27)	1194.36(7)	0.0363	6.9638(18)	12.2297(5)	513.623(29)	0.0363
417.0	7.2333(4)	12.5782(7)	13.1301(4)	1194.60(10)	0.0362	6.9634(10)	12.22858(28)	513.511(16)	0.0362
421.0	7.2368(7)	12.5787(12)	13.1257(6)	1194.82(18)	0.0382	6.96327(7)	12.22814(21)	513.472(12)	0.0382
425.0	7.2393(18)	12.575(3)	13.1195(11)	1194.3(4)	0.0425	6.96361(7)	12.22789(20)	513.512(11)	0.0425
429.0	7.252(3)	12.554(6)	13.1125(22)	1193.8(8)	0.0477	6.96388(7)	12.22709(21)	513.520(11)	0.0477
433.0	7.285(4)	12.509(7)	13.090(6)	1192.8(11)	0.0462	6.96390(6)	12.22628(19)	513.488(10)	0.0462
437.0						6.96357(6)	12.22522(19)	513.394(10)	0.0468
441.0						6.96369(6)	12.22480(19)	513.395(10)	0.0462
445.0						6.96363(6)	12.22402(19)	513.353(10)	0.0459
449.0						6.96374(6)	12.22329(19)	513.338(10)	0.0458
453.0						6.96350(6)	12.22218(18)	513.257(10)	0.0445
457.0						6.96344(6)	12.22143(18)	513.215(10)	0.0442
461.0						6.96364(6)	12.22088(18)	513.222(10)	0.0440
465.0						6.96388(6)	12.22033(18)	513.235(10)	0.0440
469.0						6.96409(6)	12.21980(18)	513.243(10)	0.0438
473.0						6.96447(6)	12.21950(18)	513.287(10)	0.0443
476.6						6.96461(6)	12.21877(18)	513.277(10)	0.0436
480.8						6.96489(6)	12.21824(18)	513.295(10)	0.0433
485.0						6.96512(6)	12.21768(18)	513.306(9)	0.0430
489.1						6.96538(6)	12.21729(18)	513.329(9)	0.0430
493.1						6.96561(6)	12.21675(18)	513.339(9)	0.0429
497.0						6.96585(6)	12.21621(18)	513.353(9)	0.0425
500.7						6.96612(6)	12.21574(18)	513.373(9)	0.0423
500.1						6.96611(6)	12.21553(18)	513.362(9)	0.0423
500.0						6.96616(6)	12.21556(18)	513.371(10)	0.0427