

Supplementary Material for

A cautionary tale on the use of GE-7031 varnish: Low temperature thermal expansion studies of ScF_3

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Table S1 Cubic lattice constants, unit cell volumes, and volumes normalized to 250 K, at various temperatures, of ScF₃. The lattice constants (a) were extracted during Rietveld analysis of the powder diffraction data. For the “No Varnish, He” sets, V₂₅₀ was linearly extrapolated from surrounding values (64.771); the same is true for both “Varnish” sets (64.748 was used for both). The V/V₂₅₀ data are plotted in Figure 1 of the main document.

T(K)	a (Å)	V (Å³)	V/V₂₅₀	Data set
10	4.02398	65.158	1.0079	Neutron ¹
60	4.02204	65.064	1.0065	Neutron ¹
110	4.01932	64.932	1.0044	Neutron ¹
180	4.01618	64.780	1.0021	Neutron ¹
250	4.01339	64.645	1.0000	Neutron ¹
6.6	4.025686(5)	65.241	1.0073	No Varnish, He (heat)
19.7	4.025338(5)	65.224	1.0070	No Varnish, He (heat)
33.75	4.024906(4)	65.203	1.0067	No Varnish, He (heat)
48.25	4.024422(4)	65.179	1.0063	No Varnish, He (heat)
62.15	4.023837(4)	65.151	1.0059	No Varnish, He (heat)
76.05	4.023215(4)	65.121	1.0054	No Varnish, He (heat)
90.1	4.022593(4)	65.091	1.0050	No Varnish, He (heat)
104	4.022058(4)	65.065	1.0046	No Varnish, He (heat)
118.05	4.021441(4)	65.035	1.0041	No Varnish, He (heat)
132.1	4.020798(4)	65.003	1.0036	No Varnish, He (heat)
146.2	4.020154(4)	64.972	1.0031	No Varnish, He (heat)
230.2	4.016597(4)	64.800	1.0005	No Varnish, He (heat)
298	4.014483(7)	64.698	0.9989	No Varnish, He (heat)
13	4.025749(5)	65.244	1.0073	No Varnish, He (cool)
27.1	4.025237(5)	65.219	1.0069	No Varnish, He (cool)
40.95	4.024803(5)	65.198	1.0066	No Varnish, He (cool)
55	4.024294(4)	65.173	1.0062	No Varnish, He (cool)
68.95	4.023705(4)	65.145	1.0058	No Varnish, He (cool)
82.95	4.023090(4)	65.115	1.0053	No Varnish, He (cool)
96.9	4.022463(4)	65.084	1.0048	No Varnish, He (cool)
111.05	4.021793(4)	65.052	1.0044	No Varnish, He (cool)
125.0 5	4.021125(4)	65.019	1.0038	No Varnish, He (cool)
139.1	4.020469(4)	64.988	1.0034	No Varnish, He (cool)
6.65	4.019261(23)	64.929	1.0026	Varnish, He
7.3	4.018627(25)	64.898	1.0021	Varnish, He
10	4.018734(24)	64.903	1.0022	Varnish, He
20	4.021092(22)	65.018	1.0040	Varnish, He
30.2	4.021388(22)	65.032	1.0042	Varnish, He
39.95	4.022528(17)	65.087	1.0051	Varnish, He
50.05	4.022403(15)	65.081	1.0050	Varnish, He
59.95	4.022300(11)	65.076	1.0049	Varnish, He
69.9	4.021892(10)	65.057	1.0046	Varnish, He

80	4.021618(8)	65.043	1.0044	Varnish, He
90	4.021167(8)	65.021	1.0040	Varnish, He
100.1 5	4.020867(8)	65.007	1.0038	Varnish, He
109.8 5	4.020480(7)	64.988	1.0035	Varnish, He
120	4.020113(7)	64.970	1.0033	Varnish, He
130	4.019731(6)	64.952	1.0030	Varnish, He
139.7	4.019424(6)	64.937	1.0027	Varnish, He
149.5 5	4.019009(6)	64.917	1.0024	Varnish, He
100.4	4.020846(8)	65.006	1.0038	Varnish, N ₂
110.15	4.020504(7)	64.989	1.0035	Varnish, N ₂
120.0 5	4.020102(7)	64.970	1.0033	Varnish, N ₂
130.1	4.019750(6)	64.953	1.0030	Varnish, N ₂
140.2 5	4.019399(6)	64.936	1.0027	Varnish, N ₂
150.1	4.019059(5)	64.919	1.0025	Varnish, N ₂
160.1	4.018699(5)	64.902	1.0022	Varnish, N ₂
180.1 5	4.018130(4)	64.874	1.0018	Varnish, N ₂
200.1 5	4.017473(4)	64.842	1.0013	Varnish, N ₂
220.1	4.016796(4)	64.810	1.0008	Varnish, N ₂
240.1 5	4.016085(4)	64.775	1.0002	Varnish, N ₂
260.1	4.015450(4)	64.744	0.9998	Varnish, N ₂
280.4	4.014883(4)	64.717	0.9993	Varnish, N ₂
300.1	4.014321(4)	64.690	0.9989	Varnish, N ₂

¹ Lattice constants taken from Greve *et al.* (2010). *J. Am. Chem. Soc.* **132**(44), 15496-15498.

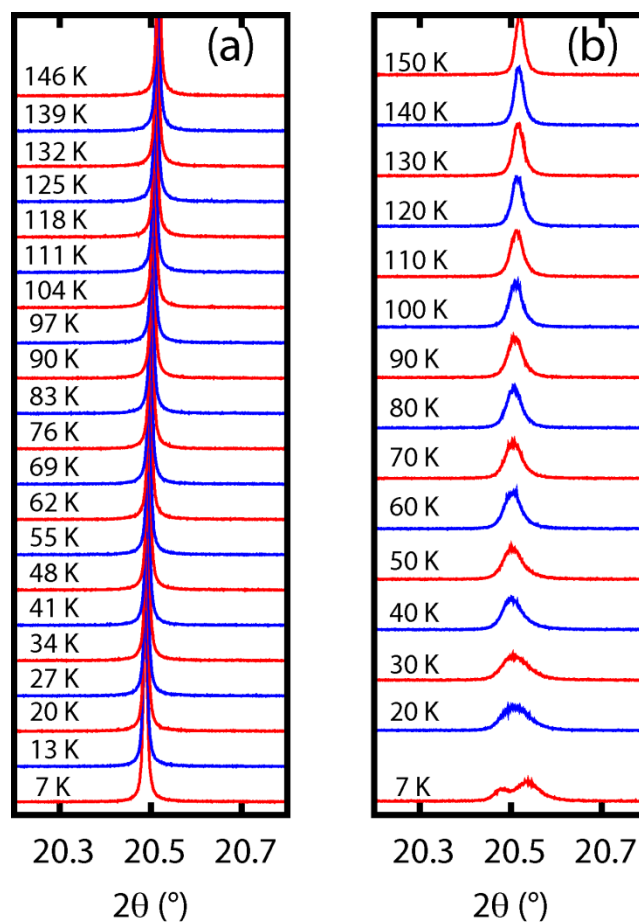


Figure S1 Variable temperature x-ray diffraction data of the (2 2 2) reflection in cubic ScF_3 , which splits into the (4 4 4) and (4 0 0) reflections after the cubic to rhombohedral phase transition. Panel (a) shows data for the “no varnish” sample, and the lack of peak splitting over this temperature range indicates the lack of a phase transition in this sample. Panel (b) shows data for the sample mixed in GE-7031 varnish; peak splitting is evident in patterns collected at the lowest temperatures.

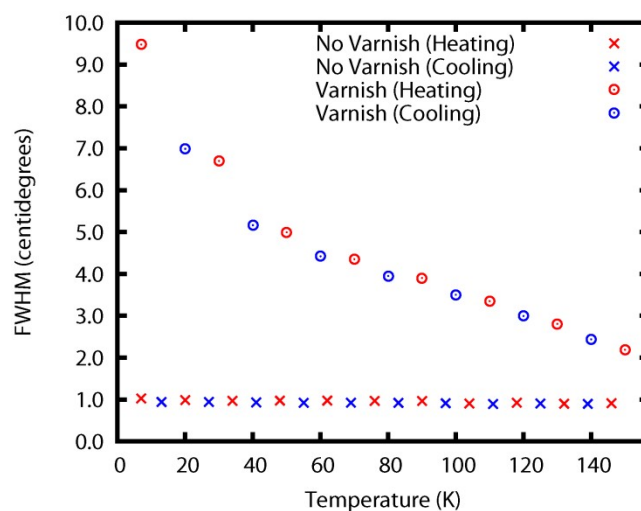


Figure S2 Temperature variation of the full width at half maximum (FWHM) of the (2 2 2) reflection in cubic ScF_3 , which splits into the (4 4 4) and (4 0 0) reflections after the cubic to rhombohedral phase transition. Peak broadening is evident in the varnish-mixed sample, indicative of a stress distribution in the ScF_3 /varnish composite. The peak width is fairly constant with temperature in the “no varnish” sample, at roughly the instrumental resolution of 0.01° . Peak widths were measured by fitting a pseudo-Voigt function to the data using *Fityk* [Wojdyc, M. (2010). *J. Appl. Cryst.* **43**, 1126-1128].