

A calorimetric and thermodynamic investigation of the synthetic analogue of mandarinoite, $\text{Fe}_2(\text{SeO}_3)_3 \cdot 5\text{H}_2\text{O}(\text{cr})$

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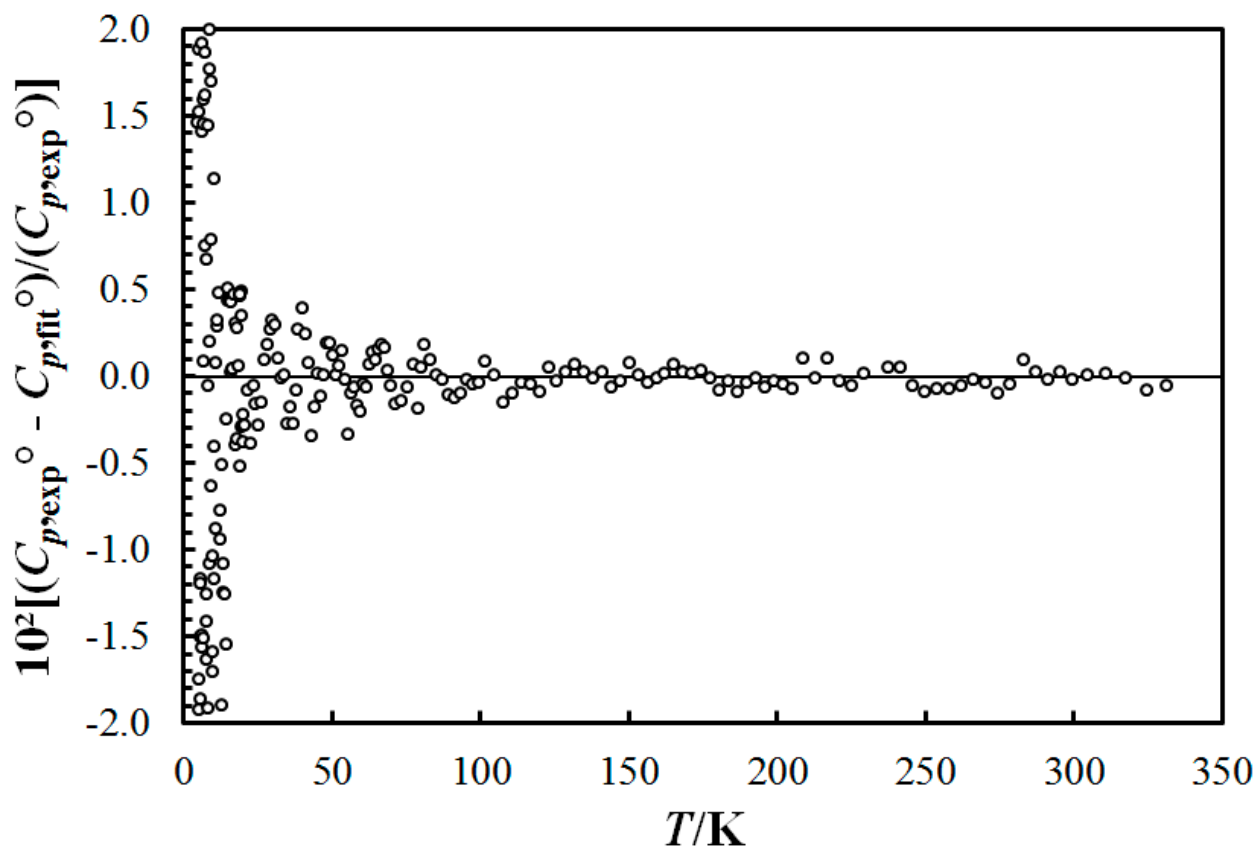


Fig. S1. Deviation of the $C_{p,m}^{\circ}(T)/J \cdot K^{-1} \cdot mol^{-1}$ values for benzoic acid from literature data presented in [1].

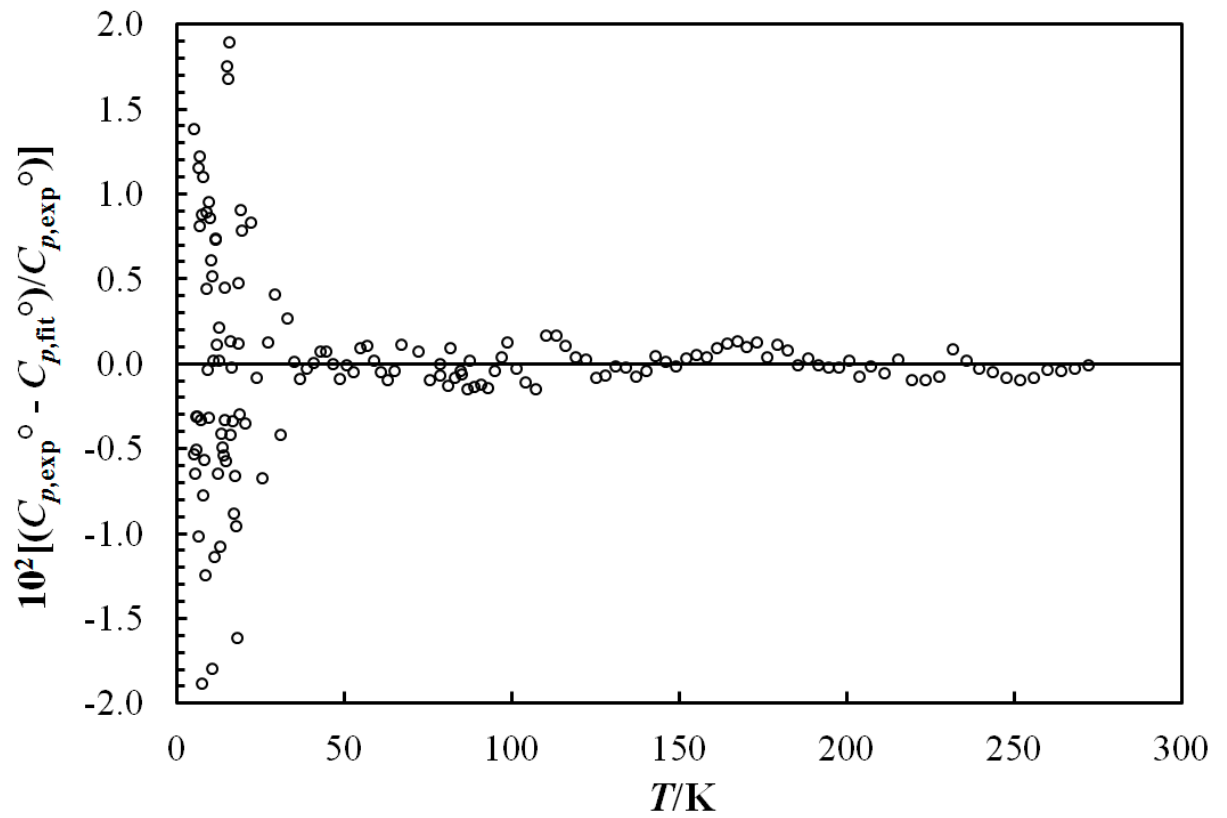


Fig. S2. Deviation of the $C_{p,m}^{\circ}(T)/J\cdot K^{-1}\cdot mol^{-1}$ values for synthetic sapphire from literature data presented in [2].

Table S3. Raw $C_{p,m}^{\circ}$ ($\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) data for the $\text{Fe}_2(\text{SeO}_3)_3 \cdot 5\text{H}_2\text{O}$ (cr, $M = 582.669 \text{ g}\cdot\text{mol}^{-1}$)at $p = 0.1 \text{ MPa}$.^a

T/K	$C_{p,m}^{\circ}$	T/K	$C_{p,m}^{\circ}$	T/K	$C_{p,m}^{\circ}$	T/K	$C_{p,m}^{\circ}$	T/K	$C_{p,m}^{\circ}$
Series 1		10.6	6.556	36.9	62.55	78.7	151.7	183.3	342.7
		10.9	7.171	38.1	63.12	81.1	158.0	186.4	347.2
5.3	0.375	11.3	7.956	39.3	64.34	83.1	162.7	189.4	351.7
5.6	0.401	11.7	8.722	40.5	65.83	85.1	167.8	192.5	356.2
5.8	0.419	12.1	9.501	41.6	67.71	87.1	172.5	195.6	360.2
6.0	0.444	12.4	10.20	42.8	69.47	89.1	177.9	198.6	364.5
6.1	0.471	12.8	10.99	44.0	71.21	91.1	181.9	201.7	368.7
6.2	0.497	13.2	11.78	45.2	73.77	93.1	186.1	204.7	373.2
6.4	0.520	13.6	12.41	46.4	76.71	95.1	190.1	208.3	378.8
6.5	0.544	14.0	13.16	47.6	79.43	97.1	194.2	212.4	383.6
6.6	0.569	14.4	13.98	48.8	82.36	99.1	198.1	216.5	390.2
6.7	0.600	14.8	14.74	50.0	85.00	101.5	203.8	220.6	396.0
6.8	0.644	15.2	15.49	51.2	87.84	104.5	209.4	224.7	402.1
6.9	0.687	15.6	16.25	52.4	90.15	107.5	215.3	228.8	407.6
7.0	0.746	16.0	17.02	53.6	92.88	110.5	221.0	232.9	413.0
7.1	0.820	16.4	17.86	54.9	95.81	113.5	225.6	237.0	417.9
7.2	0.903	16.8	18.93	56.1	98.69	116.5	231.5	241.1	422.9
7.3	0.988	17.3	19.81	57.3	101.7	119.5	237.1	245.2	427.6
7.4	1.081	17.7	20.71	59.0	105.6	122.5	242.7	249.3	432.8
7.5	1.180	18.1	21.74	60.9	110.4	125.5	248.1	253.4	438.2
7.6	1.299	18.5	22.66	62.3	114.1	128.6	253.6	257.5	443.7
7.7	1.447	18.9	23.67	63.6	116.8	131.6	259.3	261.6	448.7
7.8	1.574	19.4	24.67	64.8	119.9	134.6	264.3	265.7	454.2
8.0	1.761	19.8	25.59	66.0	122.8	137.6	269.7	269.8	459.2
8.1	1.976	20.5	27.24	67.2	125.4	140.6	275.2	273.9	464.6
8.2	2.186	21.6	29.43	68.5	127.8	143.7	280.4	278.0	469.7
8.4	2.388	22.7	31.71	69.7	131.1	146.7	285.5	282.2	475.1
8.5	2.555	23.7	34.28	71.3	134.5	149.8	290.5	286.3	480.2
8.6	2.818	24.9	37.62	73.3	139.2	152.8	295.6	290.3	485.6
8.8	3.011	26.6	43.22	75.3	143.9	155.8	300.3	294.4	490.4
8.9	3.214	27.7	47.26	77.4	148.9	158.9	305.6	298.5	496.1
9.1	3.590	28.9	51.02	79.4	153.9	161.9	310.2	303.3	502.6
9.2	3.926	30.0	55.29	81.4	158.4	165.0	315.6	308.7	510.1
9.4	4.297	31.1	59.16	83.4	162.8	168.1	319.6	314.1	517.2
9.6	4.623	32.3	63.64	85.4	168.3	171.1	324.2	319.5	524.6
9.8	4.960	33.4	66.27			174.2	329.0	324.8	532.4
10.0	5.316	34.6	65.15	Series 2		177.2	333.5		
10.2	5.820	35.8	62.63	78.7	151.7	180.3	337.9		

^a Standard uncertainties, u , are $u(T) = 0.05 \text{ K}$, $u(p) = 0.001 \text{ MPa}$. The combined expanded uncertainties, $U_{c,r}$ are $U_{c,r}(C_{p,m}^{\circ}(T)) = 0.02$ for $T < 15 \text{ K}$, 0.005 from $T = 15$ to 40 K , 0.002 between $T = 40 \text{ K}$ and $T = 330 \text{ K}$ (0.95 level of confidence).

Table S4. Best-fit coefficients for use in the $C_{p,m}^0(T)$ polynomial of Eq. (9) for $\text{Fe}_2(\text{SeO}_3)_3 \cdot 5\text{H}_2\text{O}(\text{cr})$ for the five temperature intervals.

T/K	k_0	k_1	k_2	k_3	k_4	k_5	k_6
5.3–9	36623	-164288	136415	66414.4	2955.08	169.638	-4.23233
10–21	9899.56	-387809	157908	25952.1	2241.47	27.3674	-0.142552
22–32	129107	-53317700	9956920	-502139	55.5848	0.125264	0.000140997
33–64	77223.1	146645000	16635100	-388694	801.495	5.91332	-0.0188656
65–325	-	-	-	-	-	-	-
	3585.18	174983000	-6925460	31337.5	14.5733	0.031968	0.0000314694

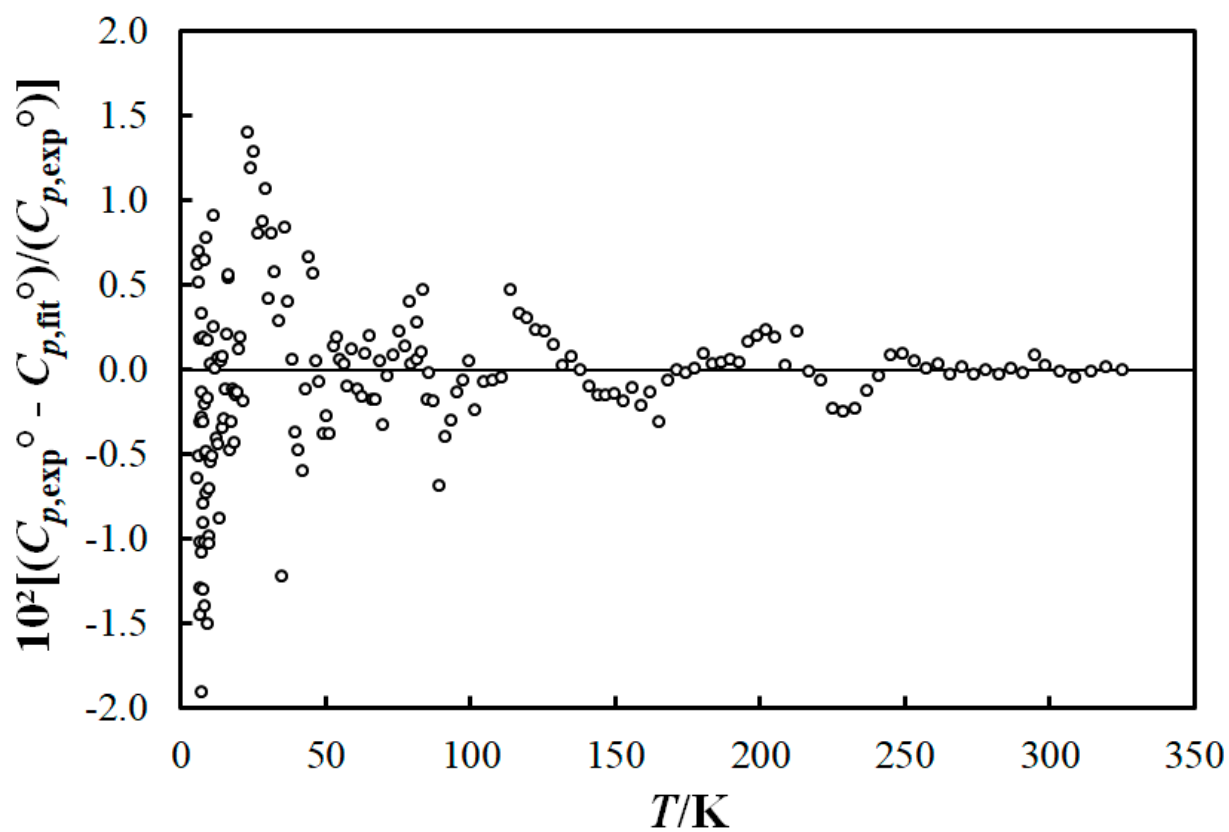


Fig. S5. Deviation of the raw experimental $C_{p,m}^{\circ}(T)$ data for $\text{Fe}_2(\text{SeO}_3)_3 \cdot 5\text{H}_2\text{O}(\text{cr})$ from the polynomial fit in % (Eq. 9 and Table S4).

References

- [1] G.T. Furukawa, R.E. Mccoskey, G.J. King, Journal of Research of the National Bureau of Standards 47 (1951) 256-261.
- [2] D.A. Ditmars, S. Ishihara, S.S. Chang, G. Bernstein, E.D. West, Journal of Research of the National Bureau of Standards 87 (1982) 159-163.