

**Table M15-i-001.** GeTe. Temperature variation of the rhombohedral unit cell parameters [87Cha].

$T$ [K]	$a$ [Å]	$\alpha$ [deg]	$V$ [Å <sup>3</sup> ]	$90 - \alpha$ [deg]
295	5.985(2)	88.17(3)	214.1(2)	1.83(3)
476	6.000(1)	88.56(2)	215.7(1)	1.44(2)
569	6.007(1)	88.73(1)	216.6(1)	1.27(1)
612	6.007(1)	88.82(1)	216.6(1)	1.18(1)
643	6.008(1)	88.91(1)	216.8(1)	1.09(1)
665	6.008(1)	88.98(1)	216.8(1)	1.02(1)
676	6.009(1)	88.04(1)	216.9(1)	0.96(1)
696	6.007(1)	89.29(1)	216.7(1)	0.71(1)
699	6.007(1)	89.34(1)	216.7(1)	0.66(1)
701	6.006(1)	89.40(1)	216.6(1)	0.60(1)
703	6.005(1)	89.46(1)	216.5(1)	0.54(1)
705	5.998(14)	89.80(2)	215.7(14)	0.20(2)
707	5.999(1)	89.97(2)	215.9(1)	0.04(2)
710	5.999(2)	89.98(2)	215.9(2)	0.02(2)
716	5.999(2)	89.97(2)	215.9(2)	0.03(2)

**Table M15-i-002.** GeTe. Temperature variation of the crystal structure [87Cha].  $u$ : fractional coordinates defined in the text.  $U_{ij}$ : anisotropic temperature parameters defined by Eq. (d) in Introduction.

$T$ [K]	Ge			Te		
	$u$	$U_{11}$ [Å <sup>2</sup> ]	$U_{12}$ [Å <sup>2</sup> ]	$u$	$U_{11}$ [Å <sup>2</sup> ]	$U_{12}$ [Å <sup>2</sup> ]
295	0.2376(1)	0.016(1)	0.0004(10)	-0.2376(1)	0.014(1)	-0.000(1)
421	0.2382(2)	0.027(2)	0.003(2)	-0.2382(2)	0.019(1)	-0.001(1)
476	0.2383(2)	0.026(1)	0.004(12)	-0.2383(2)	0.018(2)	-0.001(2)
535	0.2392(1)	0.034(1)	0.004(1)	-0.2392(1)	0.0237(9)	-0.0021(9)
645	0.2399(1)	0.0361(8)	0.0014(6)	-0.2399(4)	0.0224(4)	-0.0019(4)
655	0.2403(1)	0.037(1)	0.011(9)	-0.2403(1)	0.0231(8)	-0.0014(8)
688	0.2413(1)	0.0394(9)	0.0024(7)	-0.2413(1)	0.0241(5)	-0.0025(5)
716	0.2477(2)	0.037(2)	0.003(1)	-0.2477(2)	0.022(2)	-0.004(1)