

Table 4. Atomic positional parameters and isotropic thermal vibration parameters (\AA^2) at room temperature using SG $P2_1/a$ for $\text{CaTiO}(\text{Ge}_x\text{Si}_{1-x})\text{O}_4$.

Mol% Ge								
95	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	O3B
<i>x</i>	0.2368(5)	0.5035(4)	0.7450(3)	0.7342(5)	0.9300(1)	0.0955(5)	0.4058(2)	0.6179(2)
<i>y</i>	0.4201(1)	0.2378(4)	0.4324(6)	0.3203(9)	0.3003(9)	0.1923(5)	0.4539(1)	0.0357(3)
<i>z</i>	0.2419(9)	0.7480(6)	0.2560(9)	0.7473(3)	0.4558(6)	0.0838(3)	0.6402(8)	0.8670(7)
U_{iso} *	0.013(2)	0.014(1)	0.015(1)	0.007(1)	0.007(1)	0.007(1)	0.007(1)	0.007(1)
Occ	1.000	1.000	0.901(6)	1.000	1.000	1.000	1.000	1.000
			0.098(4)					
R_p 0.178								
$R(F^2)$ 0.105								

Mol% Ge								
90	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	O3B
<i>x</i>	0.2306(3)	0.5043(6)	0.7366(3)	0.7392(2)	0.9359(7)	0.0944(4)	0.4158(7)	0.6401(1)
<i>y</i>	0.4188(5)	0.2338(4)	0.4335(7)	0.3209(7)	0.3143(3)	0.2109(8)	0.4505(1)	0.0319(5)
<i>z</i>	0.2396(8)	0.7454(3)	0.2528(1)	0.7464(1)	0.4667(9)	0.0904(4)	0.6574(3)	0.8857(9)
U_{iso} *	0.003(2)	0.013(4)	0.008(3)	0.007(9)	0.007(9)	0.007(9)	0.007(9)	0.007(9)
Occ	1.000	1.000	0.871(4)	1.000	1.000	1.000	1.000	1.000
			0.128(6)					
R_p 0.203								
$R(F^2)$ 0.129								

Mol% Ge								
70	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	O3B
<i>x</i>	0.2479(3)	0.5078(1)	0.7491(8)	0.7399(6)	0.9252(2)	0.0927(7)	0.3920(7)	0.6140(4)
<i>y</i>	0.4193(2)	0.2433(9)	0.4331(5)	0.3257(8)	0.3083(5)	0.1942(6)	0.4616(2)	0.0378(8)
<i>z</i>	0.2424(5)	0.7420(1)	0.2557(7)	0.7611(9)	0.4453(3)	0.0741(9)	0.6538(3)	0.8689(8)
U_{iso} *	0.016(4)	0.021(4)	0.018(2)	0.010(5)	0.010(5)	0.010(5)	0.010(5)	0.010(5)
Occ	1.000	1.000	0.678(3)	1.000	1.000	1.000	1.000	1.000
			0.321(7)					
R_p 0.177								
$R(F^2)$ 0.141								

Mol% Ge								
50	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	O3B
<i>x</i>	0.2465(9)	0.5047(5)	0.7529(4)	0.7453(1)	0.9289(7)	0.1021(6)	0.4000(1)	0.6197(7)
<i>y</i>	0.4199(9)	0.2507(3)	0.4314(8)	0.3215(9)	0.3216(2)	0.2022(1)	0.4739(4)	0.0485(6)
<i>z</i>	0.2569(6)	0.7460(7)	0.2469(7)	0.7765(5)	0.4596(3)	0.0860(6)	0.6590(2)	0.8756(9)
<i>U</i> _{iso} *	0.019(5)	0.025(8)	0.019(1)	0.005(8)	0.005(8)	0.005(8)	0.005(8)	0.005(8)
Occ	1.000	1.000	0.490(0)	1.000	1.000	1.000	1.000	1.000
			0.510(0)					
<i>R</i> _p 0.178								
<i>R</i> (<i>F</i> ²) 0.120								

Mol% Ge								
30	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	O3B
<i>x</i>	0.2474(1)	0.5023(6)	0.7558(6)	0.7504(1)	0.9108(6)	0.0901(8)	0.3869(2)	0.6252(1)
<i>y</i>	0.4203(4)	0.2488(9)	0.4308(7)	0.3200(2)	0.2943(9)	0.1687(9)	0.4543(5)	0.0270(5)
<i>z</i>	0.2524(6)	0.7527(6)	0.2589(8)	0.7777(9)	0.4363(1)	0.0635(3)	0.6343(2)	0.8388(1)
<i>U</i> _{iso} *	0.026(6)	0.026(3)	0.006(2)	0.009(3)	0.009(3)	0.009(3)	0.009(3)	0.009(3)
Occ	1.000	1.000	0.336(3)	1.000	1.000	1.000	1.000	1.000
			0.663(7)					
<i>R</i> _p 0.169								
<i>R</i> (<i>F</i> ²) 0.124								

Mol% Ge								
20	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	03B
<i>x</i>	0.2315(1)	0.5062(2)	0.7460(1)	0.7490(6)	0.9007(9)	0.0840(9)	0.3824(1)	0.6381(7)
<i>y</i>	0.4175(2)	0.2530(1)	0.4316(4)	0.3174(2)	0.3160(6)	0.1929(6)	0.4736(6)	0.0462(6)
<i>z</i>	0.2476(6)	0.7404(4)	0.2577(6)	0.7673(8)	0.4501(8)	0.0714(9)	0.6462(2)	0.8449(3)
<i>U</i> _{iso} *	0.023(6)	0.020(3)	0.019(4)	0.009(2)	0.009(2)	0.009(2)	0.009(2)	0.009(2)
Occ	1.000	1.000	0.200(9)	1.000	1.000	1.000	1.000	1.000
			0.799(1)					
<i>R</i> _p 0.213								
<i>R</i> (<i>F</i> ²) 0.183								

Mol% Ge								
10	Ca	Ti	Ge,Si	O1	O2A	O2B	O3A	03B
<i>x</i>	0.2311(1)	0.5061(7)	0.7350(9)	0.7503(9)	0.8786(5)	0.0714(9)	0.3680(8)	0.5993(3)
<i>y</i>	0.4186(9)	0.2510(4)	0.4318(9)	0.3214(5)	0.3219(2)	0.2034(1)	0.4772(4)	0.0461(4)
<i>z</i>	0.2519(1)	0.7354(8)	0.2468(1)	0.7826(1)	0.4454(1)	0.0670(1)	0.6593(1)	0.8530(2)
<i>U</i> _{iso} *	0.026(9)	0.028(3)	0.016(2)	0.005(4)	0.005(4)	0.005(4)	0.005(4)	0.005(4)
Occ	1.000	1.000	0.096(7)	1.000	1.000	1.000	1.000	1.000
			0.903(3)					
<i>R</i> _p 0.201								
<i>R</i> (<i>F</i> ²) 0.187								

Table 8. $\text{CaTiO}(\text{Ge}_x\text{Si}_{1-x})\text{O}_4$. Lattice constants and volume for all intermediate samples as a function of temperature.

Mol% Ge						
95	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.1428(8)	8.8782(1)	6.6426(8)	113.776(1)	385.499(5)
	348	7.1464(8)	8.8833(7)	6.6455(6)	113.760(1)	386.132(7)
	373	7.1470(6)	8.8846(4)	6.6459(3)	113.754(1)	386.258(7)
	398	7.1473(8)	8.8867(6)	6.6469(4)	113.742(1)	386.462(4)
	423	7.1475(6)	8.8905(6)	6.6483(8)	113.736(1)	386.738(5)
	448	7.1476(7)	8.8917(3)	6.6493(9)	113.725(1)	386.886(5)
	473	7.1473(5)	8.8939(6)	6.6497(8)	113.718(1)	387.010(5)
	498	7.1471(2)	8.8946(1)	6.6509(2)	113.712(1)	387.109(6)
	523	7.1471(3)	8.8980(3)	6.6520(9)	113.698(1)	387.369(5)
	538	7.1469(6)	8.8986(3)	6.6526(4)	113.696(1)	387.424(8)
	553	7.1468(1)	8.8981(8)	6.6519(9)	113.688(1)	387.376(8)
	573	7.1469(4)	8.9014(8)	6.6538(8)	113.674(1)	387.685(5)
	598	7.1470(5)	8.9022(8)	6.6538(2)	113.671(1)	387.731(4)
	623	7.1481(3)	8.9045(6)	6.6555(6)	113.666(1)	388.005(5)
	648	7.1484(7)	8.9060(8)	6.6562(3)	113.658(1)	388.153(7)
	673	7.1492(4)	8.9086(4)	6.6578(3)	113.657(1)	388.401(5)
	723	7.1500(7)	8.9108(6)	6.6596(8)	113.650(1)	388.665(7)
	748	7.1507(7)	8.9134(1)	6.6607(8)	113.634(1)	388.929(7)
	773	7.1512(5)	8.9141(9)	6.6613(4)	113.634(1)	389.026(6)

Mol% Ge						
90	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.1346(4)	8.8734(6)	6.6388(7)	113.738(1)	384.738(7)
	348	7.1411(4)	8.8749(9)	6.6397(7)	113.749(1)	385.176(8)
	373	7.1413(3)	8.8784(2)	6.6420(5)	113.748(1)	385.471(7)
	398	7.1411(9)	8.8786(5)	6.6416(6)	113.730(1)	385.502(5)
	423	7.1415(3)	8.8802(4)	6.6421(5)	113.734(1)	385.608(6)
	448	7.1414(3)	8.8842(8)	6.6444(5)	113.714(1)	385.971(5)
	473	7.1415(6)	8.8864(3)	6.6445(4)	113.695(1)	386.130(5)
	498	7.1414(2)	8.8890(7)	6.6464(6)	113.697(1)	386.346(5)
	523	7.1414(5)	8.8906(7)	6.6475(6)	113.679(1)	386.530(6)
	538	7.1413(4)	8.8904(6)	6.6471(8)	113.678(1)	386.498(8)
	553	7.1415(8)	8.8932(2)	6.6483(5)	113.670(1)	386.724(4)
	573	7.1414(5)	8.8933(7)	6.6482(4)	113.666(1)	386.729(5)
	598	7.1421(6)	8.8947(7)	6.6501(3)	113.675(1)	386.909(5)
	623	7.1422(9)	8.8979(2)	6.6506(9)	113.660(1)	387.133(5)
	648	7.1425(6)	8.8999(4)	6.6522(9)	113.657(1)	387.337(5)
	673	7.1429(8)	8.9011(5)	6.6530(6)	113.648(1)	387.484(6)
	723	7.1443(1)	8.9037(2)	6.6551(4)	113.638(1)	387.820(5)
	748	7.1450(7)	8.9057(3)	6.6558(3)	113.642(1)	387.975(6)
	773	7.1452(2)	8.9071(3)	6.6564(6)	113.631(1)	388.113(5)

Mol% Ge						
70	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.1181(6)	8.8321(6)	6.6177(8)	113.767(1)	380.765(6)
	348	7.1238(1)	8.8390(3)	6.6213(7)	113.763(1)	381.584(6)
	373	7.1241(3)	8.8411(3)	6.6221(7)	113.744(1)	381.789(7)
	398	7.1242(2)	8.8420(1)	6.6216(5)	113.739(1)	381.821(5)
	423	7.1242(6)	8.8467(5)	6.6250(4)	113.746(1)	382.200(5)
	448	7.1243(7)	8.8469(3)	6.6242(7)	113.730(1)	382.212(6)
	473	7.1243(3)	8.8484(5)	6.6260(5)	113.726(1)	382.397(4)
	498	7.1241(6)	8.8511(6)	6.6281(7)	113.726(1)	382.627(5)
	523	7.1232(5)	8.8529(8)	6.6280(5)	113.716(1)	382.679(5)
	538	7.1222(7)	8.8500(4)	6.6268(9)	113.701(1)	382.477(7)
	553	7.1230(3)	8.8532(6)	6.6279(3)	113.704(1)	382.706(6)
	573	7.1242(7)	8.8544(1)	6.6294(6)	113.697(1)	382.933(5)
	598	7.1247(8)	8.8573(6)	6.6309(6)	113.702(1)	383.155(6)
	623	7.1252(7)	8.8599(6)	6.6322(5)	113.692(1)	383.399(6)
	648	7.1256(5)	8.8625(7)	6.6330(6)	113.686(1)	383.595(6)
	673	7.1261(6)	8.8637(8)	6.6332(1)	113.668(1)	383.743(4)
	723	7.1266(8)	8.8656(8)	6.6353(5)	113.663(1)	383.988(5)
	748	7.1272(5)	8.8680(3)	6.6359(3)	113.653(1)	384.184(6)
	773	7.1275(5)	8.8701(9)	6.6407(2)	113.663(1)	384.536(8)

Mol% Ge						
50	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.0953(4)	8.7917(3)	6.5962(8)	113.757(1)	376.606(6)
	348	7.0963(1)	8.7944(5)	6.5983(5)	113.743(1)	376.934(7)
	373	7.0965(3)	8.7970(4)	6.5974(7)	113.719(1)	377.076(7)
	398	7.0969(6)	8.7982(6)	6.6011(2)	113.732(1)	377.325(4)
	423	7.0968(4)	8.7998(5)	6.6013(5)	113.726(1)	377.415(4)
	448	7.0966(8)	8.8011(3)	6.6029(7)	113.720(1)	377.573(5)
	473	7.0965(2)	8.8035(2)	6.6025(3)	113.708(1)	377.677(4)
	498	7.0962(7)	8.8048(1)	6.6043(6)	113.701(1)	377.843(5)
	523	7.0959(5)	8.8054(4)	6.6045(2)	113.694(1)	377.884(2)
	538	7.0960(5)	8.8062(6)	6.6051(5)	113.688(1)	377.974(4)
	553	7.0963(6)	8.8071(9)	6.6047(3)	113.685(1)	378.016(7)
	573	7.0968(5)	8.8091(2)	6.6062(9)	113.686(1)	378.212(5)
	598	7.0972(8)	8.8103(8)	6.6071(6)	113.684(1)	378.346(4)
	623	7.0978(3)	8.8120(3)	6.6089(5)	113.675(1)	378.573(5)
	648	7.0987(6)	8.8129(3)	6.6096(8)	113.680(1)	378.691(5)
	673	7.0993(8)	8.8151(5)	6.6108(2)	113.675(1)	378.893(5)
	723	7.1000(2)	8.8190(7)	6.6130(5)	113.659(1)	379.276(6)
	748	7.1003(6)	8.8203(4)	6.6134(1)	113.655(1)	379.381(4)
	773	7.1011(2)	8.8216(9)	6.6141(5)	113.648(1)	379.541(4)
	823	7.1023(3)	8.8262(5)	6.6172(4)	113.648(1)	379.981(4)
	873	7.1040(8)	8.8305(1)	6.6195(7)	113.628(1)	380.450(4)
	923	7.1058(7)	8.8341(9)	6.6219(5)	113.637(1)	380.815(5)
	973	7.1080(2)	8.8367(6)	6.6236(3)	113.630(1)	381.158(5)
	1023	7.1100(5)	8.8397(2)	6.6265(8)	113.624(1)	381.581(5)
	1073	7.1112(5)	8.8425(6)	6.6291(6)	113.634(1)	381.888(5)

Mol% Ge						
30	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.0913(8)	8.7856(8)	6.5934(5)	113.766(1)	375.952(6)
	348	7.0954(3)	8.7894(9)	6.5962(2)	113.761(1)	376.504(6)
	373	7.0957(9)	8.7905(4)	6.5974(2)	113.757(1)	376.646(6)
	398	7.0962(3)	8.7928(4)	6.5983(4)	113.743(1)	376.861(5)
	423	7.0958(5)	8.7961(5)	6.5999(4)	113.737(1)	377.091(5)
	448	7.0958(2)	8.7972(2)	6.6002(4)	113.728(1)	377.181(4)
	473	7.0956(3)	8.7988(5)	6.6006(6)	113.727(1)	377.265(5)
	498	7.0953(4)	8.8003(4)	6.6019(2)	113.720(1)	377.406(4)
	523	7.0948(4)	8.7995(9)	6.6009(7)	113.704(1)	377.341(5)
	538	7.0954(5)	8.8020(3)	6.6022(3)	113.708(1)	377.540(7)
	553	7.0961(5)	8.8037(7)	6.6035(2)	113.705(1)	377.731(5)
	573	7.0967(9)	8.8053(4)	6.6047(6)	113.699(1)	377.923(4)
	598	7.0971(4)	8.8064(7)	6.6051(3)	113.691(1)	378.035(5)
	623	7.0981(3)	8.8084(9)	6.6061(5)	113.692(1)	378.226(5)
	648	7.0988(9)	8.8108(4)	6.6082(7)	113.686(1)	378.509(7)
	673	7.0994(3)	8.8128(9)	6.6088(3)	113.682(1)	378.669(5)
	723	7.1005(2)	8.8161(5)	6.6113(2)	113.676(1)	379.027(4)
	748	7.1011(6)	8.8186(4)	6.6122(5)	113.667(1)	379.248(5)
	773	7.1024(3)	8.8187(8)	6.6135(3)	113.669(1)	379.390(7)

Mol% Ge						
20	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.0718(3)	8.7437(2)	6.5730(5)	113.782(1)	371.925(4)
	348	7.0710(2)	8.7459(6)	6.5738(2)	113.762(1)	372.079(6)
	373	7.0710(6)	8.7478(9)	6.5743(3)	113.754(1)	372.216(6)
	398	7.0711(3)	8.7509(5)	6.5761(5)	113.737(1)	372.494(5)
	423	7.0709(4)	8.7515(6)	6.5766(3)	113.732(1)	372.556(5)
	448	7.0703(7)	8.7528(8)	6.5782(2)	113.726(1)	372.692(5)
	473	7.0698(7)	8.7543(5)	6.5788(4)	113.728(1)	372.757(5)
	498	7.0689(8)	8.7563(4)	6.5794(9)	113.713(1)	372.873(5)
	523	7.0704(3)	8.7579(5)	6.5803(6)	113.702(1)	373.100(4)
	538	7.0703(5)	8.7578(4)	6.5813(4)	113.702(1)	373.147(6)
	553	7.0707(8)	8.7590(6)	6.58149(6)	113.703(1)	373.228(5)
	573	7.0708(9)	8.7610(8)	6.5831(7)	113.697(1)	373.432(5)
	598	7.0718(6)	8.7631(6)	6.5838(8)	113.689(1)	373.636(4)
	623	7.0719(5)	8.7649(8)	6.5853(2)	113.688(1)	373.802(5)
	648	7.0727(3)	8.7657(3)	6.5861(8)	113.685(1)	373.932(4)
	673	7.0736(5)	8.7684(5)	6.5870(8)	113.680(1)	374.163(4)
	723	7.0745(9)	8.7707(3)	6.5889(5)	113.668(1)	374.448(5)
	748	7.0752(3)	8.7723(3)	6.5907(4)	113.674(1)	374.634(5)
	773	7.0756(1)	8.7732(1)	6.5916(9)	113.666(1)	374.766(7)

Mol% Ge						
10	T (K)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
	298	7.0658(3)	8.7305(7)	6.5662(7)	113.782(1)	370.688(5)
	348	7.0661(4)	8.7324(5)	6.5671(4)	113.785(1)	370.803(7)
	373	7.0663(9)	8.7344(5)	6.5690(3)	113.773(1)	371.042(8)
	398	7.0667(6)	8.7354(5)	6.5691(2)	113.762(1)	371.140(5)
	423	7.0665(5)	8.7373(6)	6.5702(4)	113.756(1)	371.288(5)
	448	7.0651(9)	8.7390(3)	6.5714(7)	113.736(1)	371.418(5)
	473	7.0641(8)	8.7406(9)	6.5732(8)	113.735(1)	371.541(6)
	498	7.0648(7)	8.7423(5)	6.5736(5)	113.726(1)	371.690(6)
	523	7.0651(6)	8.7445(3)	6.5753(4)	113.722(1)	371.909(5)
	538	7.0652(8)	8.7450(8)	6.5759(8)	113.720(1)	371.974(8)
	553	7.0653(2)	8.7463(8)	6.5762(9)	113.714(1)	372.074(5)
	573	7.0655(8)	8.7474(4)	6.5769(4)	113.711(1)	372.176(5)
	598	7.0663(3)	8.7491(8)	6.5779(9)	113.702(1)	372.376(6)
	623	7.0663(8)	8.7507(4)	6.5792(9)	113.698(1)	372.530(6)
	648	7.0667(5)	8.7520(8)	6.5805(2)	113.704(1)	372.660(5)
	673	7.0672(3)	8.7543(2)	6.5820(9)	113.701(1)	372.660(5)
	723	7.0685(8)	8.7575(4)	6.5832(6)	113.681(1)	373.209(6)
	748	7.0689(7)	8.7576(6)	6.5840(2)	113.683(1)	373.273(6)
	773	7.0701(7)	8.7587(5)	6.5844(6)	113.671(2)	373.438(7)