

Structure evolution of Ge-doped CaTiO₃ (CTG) at high pressure:

Search for the first 2:4 locked-tilt perovskite

by synchrotron X-ray diffraction and DFT calculations

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SUPPLEMENTARY MATERIAL

Figures

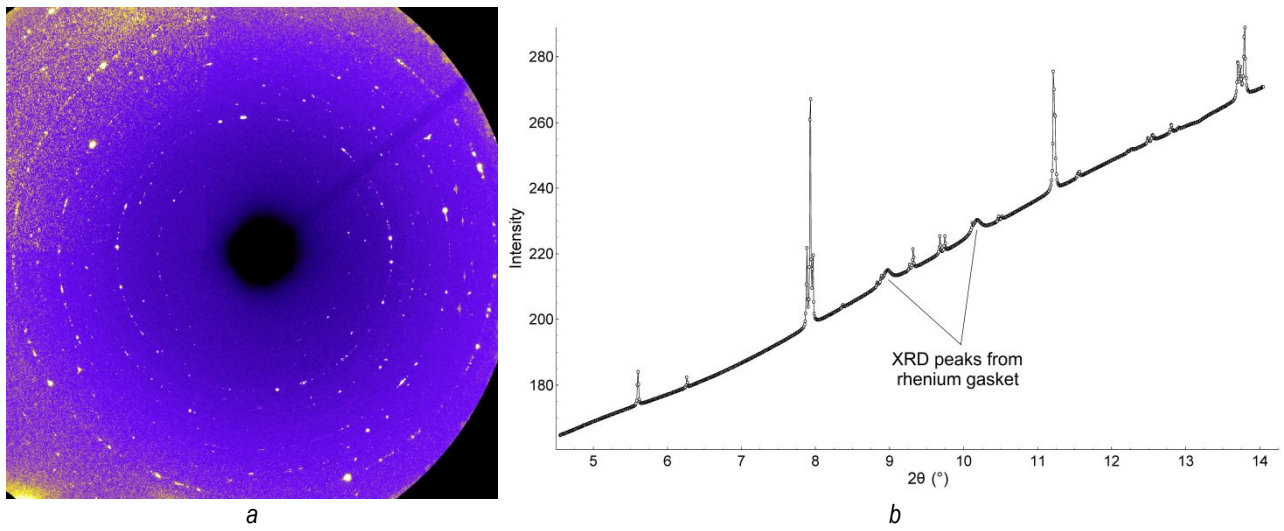


Figure S1. Debye-Scherrer rings collected with the MAR165 CCD detector at the ID27 beamline (ESRF) (*a*), and data reduction by the DIOPTAS program (*b*) of the CTG sample at 0.20 GPa.

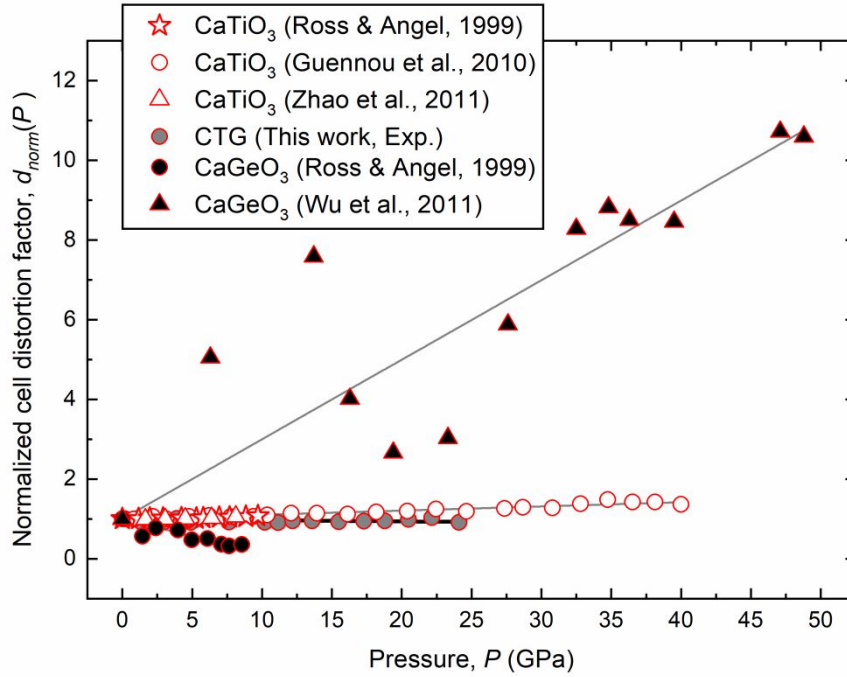


Figure S2. Normalized cell distortion factor with pressure, $d_{norm}(P)$, as a function of pressure for $\text{CaB}^{2+}\text{O}_3$ orthorhombic perovskites as derived from X-ray diffraction experiments. Solid lines are linear fits to the data. Data for the isotopic series $\text{CaB}^{2+}\text{O}_3$ ($B = \text{Ti}$ and Ge) are from ¹⁻⁴.

Figure S2 references

- (1) Guennou, M.; Bouvier, P.; Krikler, B.; Kreisel, J.; Haumont, R.; Garbarino, G. High-pressure investigation of CaTiO_3 up to 60 GPa using x-ray diffraction and Raman spectroscopy. *Phys. Rev. B* **2010**, *82*(13), 134101.
- (2) Ross, N. L.; Angel, R. J. Compression of CaTiO_3 and CaGeO_3 perovskites. *Am. Mineral.* **1999**, *84*(3), 277-281.
- (3) Wu, X.; Qin, S.; Gu, T. T.; Yang, J.; Manthilake, G. Structural and elastic properties of CaGeO_3 perovskite at high pressures. *Phys. Earth Planet. In.* **2011**, *189*(3-4), 151-156.
- (4) Zhao, J.; Ross, N. L.; Wang, D.; Angel, R. J. High-pressure crystal structure of elastically isotropic CaTiO_3 perovskite under hydrostatic and non-hydrostatic conditions. *J. Phys.-Condens. Mat.* **2011**, *23*(45), 455401.

Tables

Table S1. Unit-cell parameters (a , b , c , and V) of the CTG perovskite (s.g. $Pbnm$) up to 24 GPa derived from HP diffraction experiments and extracted by a whole powder pattern decomposition (WPPD) through a Pawley profile fit using TOPAS v. 5.0 software.

P (GPa)	a (Å)	b (Å)	c (Å)	V (Å ³)
0.20(5)	5.3758(7)	5.4330(6)	7.6293(6)	222.83(4)
1.35(8)	5.3670(4)	5.4216(4)	7.6143(4)	221.56(3)
1.90(5)	5.3617(4)	5.4164(4)	7.6059(4)	220.88(3)
2.55(8)	5.3556(5)	5.4103(5)	7.5988(5)	220.18(3)
3.00(5)	5.3507(5)	5.4051(5)	7.5905(5)	219.52(3)
3.90(10)	5.3419(6)	5.3994(5)	7.5842(5)	218.75(4)
4.90(5)	5.3346(7)	5.3883(7)	7.5665(7)	217.49(5)
7.65(8)	5.3120(7)	5.3659(7)	7.5360(7)	214.80(4)
10.20(5)	5.2901(8)	5.3437(8)	7.5055(8)	212.17(5)
11.15(7)	5.2808(7)	5.3337(7)	7.4896(7)	210.95(4)
12.20(10)	5.2735(7)	5.3281(7)	7.4825(7)	210.24(4)
13.60(10)	5.2626(7)	5.3172(6)	7.4677(7)	208.96(4)
15.50(10)	5.2479(6)	5.3014(6)	7.4446(6)	207.12(4)
17.30(10)	5.2359(7)	5.2899(6)	7.4293(7)	205.77(4)
18.80(10)	5.2249(8)	5.2792(7)	7.4149(8)	204.52(5)
20.50(10)	5.2133(7)	5.2687(6)	7.4003(6)	203.26(4)
22.15(13)	5.2017(6)	5.2584(5)	7.3859(6)	202.02(3)
24.10(5)	5.1893(5)	5.2419(5)	7.3628(6)	200.28(3)

Table S2. Pressure-volume-energy values and unit-cell parameters of the supercell model for the $\text{Ca}(\text{Ti}_{0.94}\text{Ge}_{0.06})\text{O}_3$ perovskite as obtained from DFT calculations up to 25 GPa.

P (GPa)	V (Å ³)	E (Ry)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
0.004	1757.16	-9513.18	10.6652	10.8597	15.1714	89.974	89.990	90.011
0.206	1755.25	-9513.18	10.6613	10.8558	15.1659	89.974	89.990	90.011
1.623	1742.20	-9513.17	10.6346	10.8291	15.1282	89.976	89.990	90.011
2.530	1734.12	-9513.16	10.6179	10.8126	15.1047	89.978	89.990	90.011
3.032	1729.73	-9513.16	10.6088	10.8036	15.0919	89.978	89.990	90.011
3.942	1721.93	-9513.14	10.5927	10.7874	15.0691	89.979	89.990	90.011
5.038	1712.77	-9513.12	10.5734	10.7689	15.0422	89.981	89.990	90.011
7.679	1691.87	-9513.06	10.5319	10.7225	14.9819	89.979	89.987	90.014
10.055	1673.84	-9512.99	10.4895	10.6900	14.9274	89.989	89.990	90.011
15.079	1638.95	-9512.78	10.4128	10.6183	14.8232	89.996	89.990	90.012
20.081	1607.49	-9512.53	10.3404	10.5542	14.7295	90.002	89.989	90.013
25.141	1578.41	-9512.22	10.2706	10.4948	14.6437	90.007	89.989	90.015

Table S13. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 0.004$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00489	0.02145	0.12512	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10406	-0.10424	0.22989
Ca2	Ca	-0.00443	0.02134	-0.37492	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10399	-0.10475	-0.26956
Ca3	Ca	-0.00469	-0.47713	0.12428	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10396	0.39576	0.22883
Ca4	Ca	-0.00415	-0.47805	-0.37536	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10408	0.39571	-0.27113
Ca5	Ca	0.49585	0.02203	0.12451	O65	O	0.04030	0.23965	0.12496	O125	O	0.39601	-0.10424	0.22881
Ca6	Ca	0.49538	0.02289	-0.37564	O66	O	0.03993	0.23990	-0.37501	O126	O	0.39611	-0.10419	-0.27104
Ca7	Ca	0.49552	-0.47862	0.12509	O67	O	0.03849	-0.25881	0.12258	O127	O	0.39600	0.39522	0.23038
Ca8	Ca	0.49515	-0.47838	-0.37481	O68	O	0.03849	-0.25946	-0.37458	O128	O	0.39602	0.39586	-0.27002
Ca9	Ca	0.00462	-0.02289	-0.12436	O69	O	-0.46145	0.24043	0.12538	O129	O	0.14292	-0.14730	-0.02023
Ca10	Ca	0.00415	-0.02202	0.37549	O70	O	-0.46158	0.24115	-0.37739	O130	O	0.14573	-0.14467	0.47978
Ca11	Ca	0.00485	0.47839	-0.12519	O71	O	-0.46006	-0.25999	0.12498	O131	O	0.14465	0.35599	-0.02125
Ca12	Ca	0.00448	0.47863	0.37491	O72	O	-0.45976	-0.26021	-0.37498	O132	O	0.14531	0.35496	0.47895
Ca13	Ca	-0.49557	-0.02133	-0.12508	O73	O	-0.03842	-0.24114	-0.12261	O133	O	-0.35475	-0.14495	-0.02217
Ca14	Ca	-0.49511	-0.02144	0.37488	O74	O	-0.03855	-0.24042	0.37462	O134	O	-0.35524	-0.14403	0.47884
Ca15	Ca	-0.49585	0.47805	-0.12464	O75	O	-0.04024	0.26022	-0.12502	O135	O	-0.35438	0.35540	-0.02037
Ca16	Ca	-0.49531	0.47714	0.37572	O76	O	-0.03994	0.26000	0.37502	O136	O	-0.35711	0.35273	0.47975
Ca17	Ca	0.24556	0.22775	-0.12469	O77	O	0.46006	-0.23990	-0.12499	O137	O	-0.14594	0.14563	0.22890
Ca18	Ca	0.24537	0.22812	0.37502	O78	O	0.45970	-0.23965	0.37504	O138	O	-0.14573	0.14541	-0.27108
Ca19	Ca	0.24491	-0.27127	-0.12490	O79	O	0.46151	0.25947	-0.12542	O139	O	-0.14605	-0.35420	0.22998
Ca20	Ca	0.24472	-0.27175	0.37505	O80	O	0.46151	0.25881	0.37742	O140	O	-0.14603	-0.35405	-0.26990
Ca21	Ca	-0.25519	0.22824	-0.12504	O81	O	-0.21077	0.01065	-0.12507	O141	O	0.35396	0.14595	0.23004
Ca22	Ca	-0.25507	0.22868	0.37518	O82	O	-0.21135	0.01102	0.37520	O142	O	0.35397	0.14577	-0.27000
Ca23	Ca	-0.25453	-0.27181	-0.12494	O83	O	-0.21041	-0.49086	-0.12502	O143	O	0.35437	-0.35464	0.22885
Ca24	Ca	-0.25449	-0.27220	0.37533	O84	O	-0.21118	-0.49179	0.37520	O144	O	0.35400	-0.35430	-0.27095
Ca25	Ca	-0.24493	-0.22867	0.12482	O85	O	0.28867	0.00820	-0.12480	O145	O	-0.10230	-0.10734	0.01999
Ca26	Ca	-0.24481	-0.22823	-0.37496	O86	O	0.28961	0.00912	0.37496	O146	O	-0.10516	-0.10459	-0.47968
Ca27	Ca	-0.24451	0.27220	0.12467	O87	O	0.28858	-0.48901	-0.12479	O147	O	-0.10497	0.39467	0.02118
Ca28	Ca	-0.24547	0.27181	-0.37506	O88	O	0.28931	-0.48936	0.37497	O148	O	-0.10523	0.39475	-0.47900
Ca29	Ca	0.25463	-0.22811	0.12498	O89	O	0.21039	-0.00911	0.12504	O149	O	0.39472	-0.10520	0.02097
Ca30	Ca	0.25444	-0.22774	-0.37531	O90	O	0.21133	-0.00819	-0.37520	O150	O	0.39523	-0.10518	-0.47884
Ca31	Ca	0.25528	0.27175	0.12495	O91	O	0.21068	0.48937	0.12503	O151	O	0.39480	0.39541	0.02024
Ca32	Ca	0.25508	0.27127	-0.37510	O92	O	0.21142	0.48901	-0.37521	O152	O	0.39779	0.39268	-0.47987
Ge33	Ge	0.00003	-0.25003	-0.00003	O93	O	-0.28865	-0.01102	0.12480	O153	O	0.10389	0.10420	-0.22896
Ti34	Ti	-0.00004	-0.25000	-0.49994	O94	O	-0.28923	-0.01064	-0.37493	O154	O	0.10399	0.10425	0.27119
Ti35	Ti	0.00002	0.24988	-0.00002	O95	O	-0.28882	0.49180	0.12480	O155	O	0.10398	-0.39586	-0.22998
Ti36	Ti	-0.00001	0.25006	-0.49996	O96	O	-0.28959	0.49087	-0.37498	O156	O	0.10400	-0.39521	0.26962
Ti37	Ti	-0.49999	-0.25006	-0.00004	O97	O	-0.14476	0.14404	0.02116	O157	O	-0.39601	0.10476	-0.23044
Ti38	Ti	-0.50002	-0.24988	-0.49998	O98	O	-0.14525	0.14496	-0.47883	O158	O	-0.39594	0.10425	0.27011
Ti39	Ti	-0.49996	0.25000	-0.00006	O99	O	-0.14289	-0.35272	0.02025	O159	O	-0.39592	-0.39570	-0.22887
Ge40	Ge	-0.50003	0.25004	-0.49997	O100	O	-0.14562	-0.35539	-0.47963	O160	O	-0.39604	-0.39575	0.27117
Ti41	Ti	0.00016	-0.25035	-0.24894	O101	O	0.35427	0.14467	0.02022					
Ti42	Ti	-0.00020	-0.24967	0.24895	O102	O	0.35708	0.14731	-0.47977					
Ti43	Ti	0.00003	0.24981	-0.24993	O103	O	0.35469	-0.35495	0.02105					
Ti44	Ti	-0.00004	0.25011	0.24991	O104	O	0.35535	-0.35598	-0.47875					
Ti45	Ti	-0.50003	-0.24981	-0.25007	O105	O	0.14603	-0.14577	-0.23000					
Ti46	Ti	-0.49996	-0.25011	0.25009	O106	O	0.14604	-0.14594	0.26996					
Ti47	Ti	-0.50016	0.25036	-0.25106	O107	O	0.14600	0.35431	-0.22905					
Ti48	Ti	-0.49981	0.24968	0.25105	O108	O	0.14563	0.35464	0.27115					
Ti49	Ti	-0.24898	-0.00126	-0.00024	O109	O	-0.35427	-0.14540	-0.22892					
Ti50	Ti	-0.25102	0.00126	-0.49976	O110	O	-0.35406	-0.14562	0.27110					
Ti51	Ti	-0.24869	-0.49905	-0.00024	O111	O	-0.35397	0.35406	-0.23010					
Ti52	Ti	-0.25131	-0.50094	-0.49976	O112	O	-0.35395	0.35421	0.27002					
Ti53	Ti	0.24872	-0.00104	0.00026	O113	O	0.10477	0.10519	-0.02116					
Ti54	Ti	0.25128	0.00105	-0.50026	O114	O	0.10528	0.10521	0.47903					
Ti55	Ti	0.24892	-0.49877	0.00022	O115	O	0.10221	-0.39267	-0.02013					
Ti56	Ti	0.25108	-0.50123	-0.50022	O116	O	0.10520	-0.39540	0.47976					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39484	0.10459	-0.02032					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39770	0.10735	0.48001					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39477	-0.39475	-0.02100					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39503	-0.39467	0.47881					

Table SI4. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 0.206$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00490	0.02147	0.12512	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10402	-0.10421	0.22987
Ca2	Ca	-0.00443	0.02135	-0.37492	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10395	-0.10472	-0.26957
Ca3	Ca	-0.00469	-0.47711	0.12429	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10393	0.39579	0.22881
Ca4	Ca	-0.00415	-0.47803	-0.37537	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10404	0.39574	-0.27116
Ca5	Ca	0.49585	0.02205	0.12451	O65	O	0.04035	0.23965	0.12496	O125	O	0.39605	-0.10421	0.22879
Ca6	Ca	0.49538	0.02291	-0.37564	O66	O	0.03998	0.23990	-0.37501	O126	O	0.39615	-0.10416	-0.27107
Ca7	Ca	0.49552	-0.47861	0.12509	O67	O	0.03852	-0.25880	0.12258	O127	O	0.39603	0.39525	0.23037
Ca8	Ca	0.49515	-0.47836	-0.37481	O68	O	0.03853	-0.25946	-0.37458	O128	O	0.39605	0.39590	-0.27004
Ca9	Ca	0.00462	-0.02290	-0.12436	O69	O	-0.46141	0.24043	0.12538	O129	O	0.14294	-0.14733	-0.02025
Ca10	Ca	0.00415	-0.02204	0.37549	O70	O	-0.46155	0.24115	-0.37739	O130	O	0.14576	-0.14469	0.47976
Ca11	Ca	0.00485	0.47836	-0.12519	O71	O	-0.46001	-0.25999	0.12498	O131	O	0.14468	0.35596	-0.02127
Ca12	Ca	0.00448	0.47861	0.37491	O72	O	-0.45971	-0.26021	-0.37498	O132	O	0.14535	0.35493	0.22893
Ca13	Ca	-0.49557	-0.02134	-0.12508	O73	O	-0.03845	-0.24115	-0.12261	O133	O	-0.35471	-0.14498	-0.02119
Ca14	Ca	-0.49510	-0.02146	0.37488	O74	O	-0.03859	-0.24042	0.37462	O134	O	-0.35522	-0.14405	0.47881
Ca15	Ca	-0.49585	0.47803	-0.12463	O75	O	-0.04029	0.26022	-0.12502	O135	O	-0.35435	0.35537	-0.02038
Ca16	Ca	-0.49531	0.47712	0.37571	O76	O	-0.03999	0.26000	0.37502	O136	O	-0.35709	0.35271	0.47974
Ca17	Ca	0.24557	0.22773	-0.12469	O77	O	0.46002	-0.23989	-0.12499	O137	O	-0.14598	0.14566	0.22887
Ca18	Ca	0.24537	0.22810	0.37502	O78	O	0.45965	-0.23964	0.37504	O138	O	-0.14576	0.14544	-0.27110
Ca19	Ca	0.24491	-0.27128	-0.12491	O79	O	0.46147	0.25947	-0.12542	O139	O	-0.14609	-0.35417	0.22996
Ca20	Ca	0.24471	-0.27177	0.37505	O80	O	0.46148	0.25881	0.37742	O140	O	-0.14607	-0.35401	-0.26992
Ca21	Ca	-0.25519	0.22822	-0.12504	O81	O	-0.21072	0.01065	-0.12507	O141	O	0.35393	0.14598	0.23002
Ca22	Ca	-0.25507	0.22866	0.37518	O82	O	-0.21131	0.01103	0.37520	O142	O	0.35394	0.14580	-0.27002
Ca23	Ca	-0.25453	-0.27183	-0.12495	O83	O	-0.21036	-0.49086	-0.12502	O143	O	0.35434	-0.35461	0.22883
Ca24	Ca	-0.25449	-0.27222	0.37534	O84	O	-0.21114	-0.49179	0.37520	O144	O	0.35396	-0.35427	-0.27097
Ca25	Ca	-0.24493	-0.22865	0.12482	O85	O	0.28872	0.00819	-0.12480	O145	O	-0.10227	-0.10732	0.02001
Ca26	Ca	-0.24481	-0.22821	-0.37496	O86	O	0.28965	0.00912	0.37496	O146	O	-0.10513	-0.10456	-0.47966
Ca27	Ca	-0.24551	0.27222	0.12466	O87	O	0.28862	-0.48900	-0.12479	O147	O	-0.10493	0.39470	0.02121
Ca28	Ca	-0.24547	0.27183	-0.37505	O88	O	0.28936	-0.48935	0.37497	O148	O	-0.10520	0.39478	-0.47898
Ca29	Ca	0.25463	-0.22809	0.12498	O89	O	0.21035	-0.00911	0.12504	O149	O	0.39475	-0.10518	0.02099
Ca30	Ca	0.25443	-0.22772	-0.37531	O90	O	0.21128	-0.00819	-0.37520	O150	O	0.39526	-0.10516	-0.47882
Ca31	Ca	0.25529	0.27177	0.12495	O91	O	0.21064	0.48936	0.12503	O151	O	0.39483	0.39544	0.02026
Ca32	Ca	0.25509	0.27129	-0.37509	O92	O	0.21138	0.48901	-0.37521	O152	O	0.39782	0.39270	-0.47986
Ge33	Ge	0.00003	-0.25003	-0.00003	O93	O	-0.28869	-0.01102	0.12480	O153	O	0.10386	0.10417	-0.22893
Ti34	Ti	-0.00004	-0.25000	-0.49994	O94	O	-0.28928	-0.01065	-0.37493	O154	O	0.10395	0.10421	0.27121
Ti35	Ti	0.00002	0.24989	-0.00001	O95	O	-0.28886	0.49180	0.12480	O155	O	0.10395	-0.39589	-0.22996
Ti36	Ti	-0.00000	0.25006	-0.49996	O96	O	-0.28964	0.49087	-0.37498	O156	O	0.10397	-0.39524	0.26963
Ti37	Ti	-0.50000	-0.25006	-0.00004	O97	O	-0.14479	0.14406	0.02119	O157	O	-0.39605	0.10473	-0.23043
Ti38	Ti	-0.50002	-0.24988	-0.49999	O98	O	-0.14529	0.14499	-0.47881	O158	O	-0.39598	0.10421	0.27013
Ti39	Ti	-0.49996	0.25000	-0.00006	O99	O	-0.14291	-0.35270	0.02026	O159	O	-0.39596	-0.39573	-0.22884
Ge40	Ge	-0.50003	0.25004	-0.49997	O100	O	-0.14566	-0.35537	-0.47962	O160	O	-0.39607	-0.39578	0.27119
Ti41	Ti	0.00016	-0.25035	-0.24894	O101	O	0.35424	0.14470	0.02024					
Ti42	Ti	-0.00019	-0.24967	0.24895	O102	O	0.35705	0.14734	-0.47975					
Ti43	Ti	0.00003	0.24981	-0.24993	O103	O	0.35465	-0.35492	0.02107					
Ti44	Ti	-0.00004	0.25011	0.24991	O104	O	0.35532	-0.35596	-0.47873					
Ti45	Ti	-0.50003	-0.24981	-0.25007	O105	O	0.14606	-0.14580	-0.22998					
Ti46	Ti	-0.49996	-0.25011	0.25009	O106	O	0.14607	-0.14597	0.26998					
Ti47	Ti	-0.50016	0.25036	-0.25106	O107	O	0.14604	0.35428	-0.22903					
Ti48	Ti	-0.49981	0.24968	0.25105	O108	O	0.14566	0.35461	0.27117					
Ti49	Ti	-0.24897	-0.00126	-0.00024	O109	O	-0.35424	-0.14543	-0.22890					
Ti50	Ti	-0.25103	0.00127	-0.49976	O110	O	-0.35402	-0.14565	0.27113					
Ti51	Ti	-0.24869	-0.49904	-0.00024	O111	O	-0.35394	0.35402	-0.23008					
Ti52	Ti	-0.25131	-0.50095	-0.49976	O112	O	-0.35391	0.35418	0.27004					
Ti53	Ti	0.24872	-0.00104	0.00026	O113	O	0.10474	0.10516	-0.02118					
Ti54	Ti	0.25128	0.00105	-0.50026	O114	O	0.10525	0.10518	0.47901					
Ti55	Ti	0.24891	-0.49876	0.00022	O115	O	0.10218	-0.39270	-0.02014					
Ti56	Ti	0.25109	-0.50123	-0.50022	O116	O	0.10517	-0.39543	0.47974					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39487	0.10457	-0.02034					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39773	0.10733	0.47999					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39480	-0.39477	-0.02102					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39507	-0.39470	0.47879					

Table S15. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 1.623$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00494	0.02161	0.12511	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10379	-0.10399	0.22973
Ca2	Ca	-0.00446	0.02145	-0.37493	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10371	-0.10451	-0.26971
Ca3	Ca	-0.00471	-0.47700	0.12433	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10369	0.39599	0.22865
Ca4	Ca	-0.00416	-0.47787	-0.37538	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10380	0.39595	-0.27132
Ca5	Ca	0.49583	0.02221	0.12449	O65	O	0.04069	0.23962	0.12496	O125	O	0.39630	-0.10399	0.22863
Ca6	Ca	0.49536	0.02302	-0.37561	O66	O	0.04029	0.23987	-0.37501	O126	O	0.39638	-0.10395	-0.27122
Ca7	Ca	0.49547	-0.47850	0.12507	O67	O	0.03874	-0.25877	0.12256	O127	O	0.39628	0.39546	0.23024
Ca8	Ca	0.49512	-0.47821	-0.37482	O68	O	0.03880	-0.25945	-0.37457	O128	O	0.39629	0.39612	-0.27017
Ca9	Ca	0.00464	-0.02301	-0.12439	O69	O	-0.46115	0.24044	0.12538	O129	O	0.14313	-0.14751	-0.02035
Ca10	Ca	0.00417	-0.02221	0.37551	O70	O	-0.46133	0.24119	-0.37741	O130	O	0.14598	-0.14487	0.47963
Ca11	Ca	0.00488	0.47821	-0.12518	O71	O	-0.45970	-0.26004	0.12498	O131	O	0.14490	0.35577	-0.02144
Ca12	Ca	0.00453	0.47850	0.37493	O72	O	-0.45939	-0.26023	-0.37499	O132	O	0.14557	0.35473	0.47877
Ca13	Ca	-0.49554	-0.02145	-0.12507	O73	O	-0.03867	-0.24119	-0.12259	O133	O	-0.35448	-0.14520	-0.02134
Ca14	Ca	-0.49506	-0.02161	0.37489	O74	O	-0.03885	-0.24044	0.37462	O134	O	-0.35500	-0.14424	0.47864
Ca15	Ca	-0.49584	0.47788	-0.12463	O75	O	-0.04061	0.26024	-0.12501	O135	O	-0.35411	0.35518	-0.02051
Ca16	Ca	-0.49529	0.47701	0.37567	O76	O	-0.04030	0.26004	0.37502	O136	O	-0.35692	0.35254	0.47964
Ca17	Ca	0.24557	0.22758	-0.12468	O77	O	0.45971	-0.23986	-0.12499	O137	O	-0.14622	0.14588	0.22871
Ca18	Ca	0.24536	0.22795	0.37499	O78	O	0.45931	-0.23961	0.37504	O138	O	-0.14599	0.14563	-0.27126
Ca19	Ca	0.24491	-0.27140	-0.12492	O79	O	0.46120	0.25945	-0.12543	O139	O	-0.14633	-0.35397	0.22982
Ca20	Ca	0.24466	-0.27191	0.37507	O80	O	0.46126	0.25877	0.37744	O140	O	-0.14632	-0.35379	-0.27005
Ca21	Ca	-0.25525	0.22808	-0.12501	O81	O	-0.21040	0.01069	-0.12508	O141	O	0.35367	0.14621	0.22989
Ca22	Ca	-0.25508	0.22854	0.37518	O82	O	-0.21100	0.01107	0.37520	O142	O	0.35370	0.14600	-0.27015
Ca23	Ca	-0.25455	-0.27198	-0.12497	O83	O	-0.21005	-0.49087	-0.12503	O143	O	0.35410	-0.35441	0.22868
Ca24	Ca	-0.25447	-0.27236	0.37535	O84	O	-0.21083	-0.49181	0.37521	O144	O	0.35371	-0.35405	-0.27112
Ca25	Ca	-0.24492	-0.22854	0.12483	O85	O	0.28903	0.00817	-0.12480	O145	O	-0.10206	-0.10717	0.02011
Ca26	Ca	-0.24476	-0.22808	-0.37499	O86	O	0.28996	0.00913	0.37495	O146	O	-0.10493	-0.10436	-0.47953
Ca27	Ca	-0.24553	0.27237	0.12465	O87	O	0.28893	-0.48897	-0.12479	O147	O	-0.10469	0.39488	0.02137
Ca28	Ca	-0.24545	0.27199	-0.37503	O88	O	0.28967	-0.48932	0.37496	O148	O	-0.10498	0.39499	-0.47882
Ca29	Ca	0.25464	-0.22794	0.12501	O89	O	0.21004	-0.00912	0.12505	O149	O	0.39499	-0.10498	0.02115
Ca30	Ca	0.25443	-0.22758	-0.37532	O90	O	0.21097	-0.00817	-0.37520	O150	O	0.39549	-0.10496	-0.47866
Ca31	Ca	0.25534	0.27191	0.12493	O91	O	0.21033	0.48932	0.12504	O151	O	0.39504	0.39563	0.02039
Ca32	Ca	0.25509	0.27140	-0.37508	O92	O	0.21107	0.48897	-0.37521	O152	O	0.39802	0.39285	-0.47975
Ge33	Ge	0.00003	-0.25003	-0.00003	O93	O	-0.28900	-0.01106	0.12480	O153	O	0.10362	0.10396	-0.22878
Ti34	Ti	-0.00003	-0.25001	-0.49994	O94	O	-0.28960	-0.01069	-0.37492	O154	O	0.10370	0.10400	0.27137
Ti35	Ti	-0.00000	0.24990	0.00001	O95	O	-0.28917	0.49182	0.12479	O155	O	0.10371	-0.39611	-0.22983
Ti36	Ti	0.00003	0.25004	-0.49995	O96	O	-0.28995	0.49087	-0.37497	O156	O	0.10372	-0.39546	0.26976
Ti37	Ti	-0.50003	-0.25004	-0.00005	O97	O	-0.14500	0.14424	0.02136	O157	O	-0.39629	0.10451	-0.23029
Ti38	Ti	-0.50000	-0.24990	-0.50001	O98	O	-0.14552	0.14521	-0.47866	O158	O	-0.39621	0.10400	0.27027
Ti39	Ti	-0.49997	0.25002	-0.00006	O99	O	-0.14308	-0.35253	0.02036	O159	O	-0.39620	-0.39594	-0.22868
Ge40	Ge	-0.50003	0.25003	-0.49997	O100	O	-0.14589	-0.35518	-0.47949	O160	O	-0.39631	-0.39599	0.27135
Ti41	Ti	0.00015	-0.25036	-0.24891	O101	O	0.35402	0.14488	0.02037					
Ti42	Ti	-0.00018	-0.24967	0.24893	O102	O	0.35687	0.14752	-0.47965					
Ti43	Ti	0.00002	0.24981	-0.24992	O103	O	0.35443	-0.35472	0.02123					
Ti44	Ti	-0.00005	0.25010	0.24992	O104	O	0.35510	-0.35577	-0.47856					
Ti45	Ti	-0.50002	-0.24981	-0.25009	O105	O	0.14630	-0.14600	-0.22985					
Ti46	Ti	-0.49995	-0.25010	0.25008	O106	O	0.14633	-0.14620	0.27011					
Ti47	Ti	-0.50015	0.25036	-0.25109	O107	O	0.14629	0.35405	-0.22888					
Ti48	Ti	-0.49982	0.24967	0.25107	O108	O	0.14589	0.35442	0.27132					
Ti49	Ti	-0.24895	-0.00129	-0.00024	O109	O	-0.35401	-0.14563	-0.22874					
Ti50	Ti	-0.25105	0.00130	-0.49976	O110	O	-0.35378	-0.14587	0.27129					
Ti51	Ti	-0.24869	-0.49899	-0.00023	O111	O	-0.35368	0.35380	-0.22995					
Ti52	Ti	-0.25131	-0.50100	-0.49977	O112	O	-0.35367	0.35398	0.27018					
Ti53	Ti	0.24868	-0.00106	0.00025	O113	O	0.10451	0.10497	-0.02134					
Ti54	Ti	0.25132	0.00107	-0.50025	O114	O	0.10501	0.10498	0.47885					
Ti55	Ti	0.24886	-0.49874	0.00021	O115	O	0.10198	-0.39285	-0.02025					
Ti56	Ti	0.25114	-0.50126	-0.50021	O116	O	0.10496	-0.39562	0.47961					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39507	0.10437	-0.02047					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39794	0.10718	0.47989					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39502	-0.39498	-0.02118					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39531	-0.39488	0.47863					

Table SI6. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 2.530$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00496	0.02171	0.12510	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10364	-0.10387	0.22965
Ca2	Ca	-0.00448	0.02153	-0.37493	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10356	-0.10438	-0.26979
Ca3	Ca	-0.00473	-0.47693	0.12435	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10355	0.39612	0.22855
Ca4	Ca	-0.00417	-0.47777	-0.37538	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10364	0.39608	-0.27142
Ca5	Ca	0.49582	0.02232	0.12449	O65	O	0.04090	0.23960	0.12496	O125	O	0.39645	-0.10387	0.22853
Ca6	Ca	0.49535	0.02309	-0.37559	O66	O	0.04048	0.23985	-0.37501	O126	O	0.39653	-0.10382	-0.27131
Ca7	Ca	0.49545	-0.47842	0.12506	O67	O	0.03889	-0.25875	0.12256	O127	O	0.39642	0.39559	0.23015
Ca8	Ca	0.49510	-0.47811	-0.37483	O68	O	0.03897	-0.25944	-0.37457	O128	O	0.39643	0.39625	-0.27025
Ca9	Ca	0.00465	-0.02309	-0.12441	O69	O	-0.46099	0.24046	0.12539	O129	O	0.14324	-0.14762	-0.02041
Ca10	Ca	0.00418	-0.02232	0.37551	O70	O	-0.46119	0.24122	-0.37741	O130	O	0.14612	-0.14499	0.47955
Ca11	Ca	0.00490	0.47811	-0.12517	O71	O	-0.45951	-0.26006	0.12499	O131	O	0.14505	0.35565	-0.02154
Ca12	Ca	0.00456	0.47842	0.37494	O72	O	-0.45919	-0.26025	-0.37499	O132	O	0.14571	0.35460	0.47868
Ca13	Ca	-0.49552	-0.02153	-0.12507	O73	O	-0.03881	-0.24121	-0.12259	O133	O	-0.35434	-0.14534	-0.02143
Ca14	Ca	-0.49504	-0.02170	0.37490	O74	O	-0.03901	-0.24045	0.37461	O134	O	-0.35486	-0.14435	0.47854
Ca15	Ca	-0.49583	0.47778	-0.12462	O75	O	-0.04081	0.26025	-0.12501	O135	O	-0.35397	0.35506	-0.02059
Ca16	Ca	-0.49527	0.47694	0.37565	O76	O	-0.04049	0.26007	0.37501	O136	O	-0.35681	0.35243	0.47958
Ca17	Ca	0.24557	0.22749	-0.12467	O77	O	0.45952	-0.23984	-0.12499	O137	O	-0.14637	0.14602	0.22862
Ca18	Ca	0.24536	0.22785	0.37498	O78	O	0.45910	-0.23959	0.37504	O138	O	-0.14614	0.14575	-0.27135
Ca19	Ca	0.24491	-0.27148	-0.12493	O79	O	0.46102	0.25945	-0.12543	O139	O	-0.14647	-0.35385	0.22974
Ca20	Ca	0.24463	-0.27201	0.37508	O80	O	0.46111	0.25875	0.37744	O140	O	-0.14648	-0.35365	-0.27014
Ca21	Ca	-0.25527	0.22799	-0.12499	O81	O	-0.21021	0.01072	-0.12508	O141	O	0.35352	0.14634	0.22980
Ca22	Ca	-0.25509	0.22846	0.37517	O82	O	-0.21081	0.01109	0.37520	O142	O	0.35355	0.14613	-0.27024
Ca23	Ca	-0.25456	-0.27209	-0.12499	O83	O	-0.20986	-0.49086	-0.12504	O143	O	0.35396	-0.35429	0.22860
Ca24	Ca	-0.25446	-0.27246	0.37536	O84	O	-0.21064	-0.49182	0.37521	O144	O	0.35356	-0.35391	-0.27121
Ca25	Ca	-0.24491	-0.22846	0.12483	O85	O	0.28922	0.00817	-0.12479	O145	O	-0.10193	-0.10707	0.02018
Ca26	Ca	-0.24473	-0.22798	-0.37501	O86	O	0.29015	0.00914	0.37495	O146	O	-0.10480	-0.10424	-0.47946
Ca27	Ca	-0.24555	0.27246	0.12464	O87	O	0.28912	-0.48895	-0.12479	O147	O	-0.10455	0.39500	0.02147
Ca28	Ca	-0.24544	0.27209	-0.37501	O88	O	0.28986	-0.48930	0.37496	O148	O	-0.10484	0.39512	-0.47873
Ca29	Ca	0.25464	-0.22785	0.12502	O89	O	0.20985	-0.00913	0.12505	O149	O	0.39514	-0.10485	0.02125
Ca30	Ca	0.25442	-0.22749	-0.37533	O90	O	0.21078	-0.00816	-0.37521	O150	O	0.39563	-0.10484	-0.47856
Ca31	Ca	0.25537	0.27201	0.12492	O91	O	0.21014	0.48931	0.12504	O151	O	0.39517	0.39575	0.02047
Ca32	Ca	0.25509	0.27149	-0.37507	O92	O	0.21088	0.48896	-0.37521	O152	O	0.39814	0.39295	-0.47969
Ge33	Ge	0.00003	-0.25003	-0.00003	O93	O	-0.28919	-0.01108	0.12480	O153	O	0.10347	0.10383	-0.22869
Ti34	Ti	-0.00002	-0.25002	-0.49994	O94	O	-0.28979	-0.01071	-0.37492	O154	O	0.10355	0.10387	0.27147
Ti35	Ti	-0.00001	0.24991	0.00002	O95	O	-0.28936	0.49182	0.12479	O155	O	0.10357	-0.39625	-0.22975
Ti36	Ti	0.00004	0.25004	-0.49995	O96	O	-0.29014	0.49087	-0.37496	O156	O	0.10358	-0.39559	0.26985
Ti37	Ti	-0.50004	-0.25003	-0.00005	O97	O	-0.14514	0.14436	0.02146	O157	O	-0.39644	0.10438	-0.23021
Ti38	Ti	-0.49999	-0.24990	-0.50002	O98	O	-0.14566	0.14534	-0.47856	O158	O	-0.39636	0.10387	0.27035
Ti39	Ti	-0.49998	0.25002	-0.00006	O99	O	-0.14319	-0.35242	0.02042	O159	O	-0.39636	-0.39607	-0.22858
Ge40	Ge	-0.50003	0.25003	-0.49997	O100	O	-0.14603	-0.35506	-0.47941	O160	O	-0.39645	-0.39611	0.27145
Ti41	Ti	0.00014	-0.25036	-0.24889	O101	O	0.35388	0.14499	0.02045					
Ti42	Ti	-0.00017	-0.24967	0.24892	O102	O	0.35676	0.14763	-0.47958					
Ti43	Ti	0.00002	0.24981	-0.24991	O103	O	0.35429	-0.35460	0.02132					
Ti44	Ti	-0.00005	0.25010	0.24993	O104	O	0.35495	-0.35564	-0.47846					
Ti45	Ti	-0.50002	-0.24981	-0.25009	O105	O	0.14645	-0.14612	-0.22976					
Ti46	Ti	-0.49995	-0.25010	0.25007	O106	O	0.14648	-0.14633	0.27020					
Ti47	Ti	-0.50014	0.25036	-0.25111	O107	O	0.14644	0.35392	-0.22879					
Ti48	Ti	-0.49983	0.24968	0.25109	O108	O	0.14604	0.35430	0.27140					
Ti49	Ti	-0.24894	-0.00131	-0.00024	O109	O	-0.35386	-0.14575	-0.22865					
Ti50	Ti	-0.25106	0.00131	-0.49976	O110	O	-0.35363	-0.14601	0.27138					
Ti51	Ti	-0.24869	-0.49897	-0.00023	O111	O	-0.35353	0.35366	-0.22986					
Ti52	Ti	-0.25131	-0.50102	-0.49977	O112	O	-0.35353	0.35386	0.27026					
Ti53	Ti	0.24867	-0.00107	0.00025	O113	O	0.10437	0.10484	-0.02144					
Ti54	Ti	0.25133	0.00108	-0.50025	O114	O	0.10486	0.10486	0.47876					
Ti55	Ti	0.24883	-0.49873	0.00021	O115	O	0.10186	-0.39295	-0.02031					
Ti56	Ti	0.25116	-0.50127	-0.50021	O116	O	0.10483	-0.39574	0.47954					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39520	0.10425	-0.02054					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39807	0.10708	0.47982					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39516	-0.39511	-0.02127					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39545	-0.39500	0.47853					

Table SI7. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 3.032$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00498	0.02177	0.12510	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10357	-0.10380	0.22961
Ca2	Ca	-0.00450	0.02158	-0.37493	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10348	-0.10431	-0.26984
Ca3	Ca	-0.00474	-0.47689	0.12437	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10348	0.39618	0.22850
Ca4	Ca	-0.00417	-0.47772	-0.37538	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10356	0.39614	-0.27147
Ca5	Ca	0.49581	0.02238	0.12448	O65	O	0.04102	0.23959	0.12497	O125	O	0.39653	-0.10380	0.22848
Ca6	Ca	0.49534	0.02313	-0.37558	O66	O	0.04058	0.23984	-0.37501	O126	O	0.39660	-0.10376	-0.27136
Ca7	Ca	0.49543	-0.47837	0.12506	O67	O	0.03896	-0.25874	0.12255	O127	O	0.39650	0.39567	0.23011
Ca8	Ca	0.49508	-0.47805	-0.37484	O68	O	0.03906	-0.25944	-0.37457	O128	O	0.39651	0.39633	-0.27029
Ca9	Ca	0.00466	-0.02313	-0.12442	O69	O	-0.46090	0.24047	0.12539	O129	O	0.14330	-0.14768	-0.02045
Ca10	Ca	0.00419	-0.02238	0.37552	O70	O	-0.46112	0.24123	-0.37742	O130	O	0.14620	-0.14505	0.47951
Ca11	Ca	0.00492	0.47805	-0.12516	O71	O	-0.45941	-0.26008	0.12499	O131	O	0.14512	0.35558	-0.02159
Ca12	Ca	0.00457	0.47837	0.37494	O72	O	-0.45908	-0.26025	-0.37499	O132	O	0.14578	0.35454	0.47863
Ca13	Ca	-0.49550	-0.02157	-0.12507	O73	O	-0.03888	-0.24122	-0.12258	O133	O	-0.35426	-0.14540	-0.02149
Ca14	Ca	-0.49502	-0.02176	0.37490	O74	O	-0.03910	-0.24046	0.37461	O134	O	-0.35478	-0.14442	0.47848
Ca15	Ca	-0.49583	0.47772	-0.12462	O75	O	-0.04092	0.26026	-0.12501	O135	O	-0.35389	0.35500	-0.02063
Ca16	Ca	-0.49526	0.47689	0.37563	O76	O	-0.04059	0.26009	0.37501	O136	O	-0.35675	0.35237	0.47954
Ca17	Ca	0.24557	0.22743	-0.12466	O77	O	0.45942	-0.23983	-0.12499	O137	O	-0.14645	0.14609	0.22857
Ca18	Ca	0.24535	0.22779	0.37497	O78	O	0.45898	-0.23958	0.37503	O138	O	-0.14621	0.14582	-0.27140
Ca19	Ca	0.24491	-0.27153	-0.12493	O79	O	0.46093	0.25944	-0.12543	O139	O	-0.14655	-0.35379	0.22969
Ca20	Ca	0.24462	-0.27207	0.37508	O80	O	0.46104	0.25874	0.37745	O140	O	-0.14656	-0.35358	-0.27019
Ca21	Ca	-0.25529	0.22793	-0.12499	O81	O	-0.21010	0.01073	-0.12508	O141	O	0.35344	0.14642	0.22975
Ca22	Ca	-0.25510	0.22842	0.37517	O82	O	-0.21070	0.01110	0.37520	O142	O	0.35347	0.14619	-0.27028
Ca23	Ca	-0.25456	-0.27215	-0.12500	O83	O	-0.20976	-0.49087	-0.12504	O143	O	0.35388	-0.35423	0.22855
Ca24	Ca	-0.25445	-0.27251	0.37536	O84	O	-0.21053	-0.49182	0.37521	O144	O	0.35348	-0.35384	-0.27126
Ca25	Ca	-0.24490	-0.22841	0.12483	O85	O	0.28933	0.00816	-0.12479	O145	O	-0.10186	-0.10702	0.02021
Ca26	Ca	-0.24471	-0.22793	-0.37501	O86	O	0.29025	0.00914	0.37494	O146	O	-0.10473	-0.10418	-0.47941
Ca27	Ca	-0.24555	0.27252	0.12464	O87	O	0.28922	-0.48894	-0.12479	O147	O	-0.10447	0.39506	0.02152
Ca28	Ca	-0.24544	0.27216	-0.37500	O88	O	0.28996	-0.48929	0.37496	O148	O	-0.10476	0.39519	-0.47868
Ca29	Ca	0.25464	-0.22779	0.12503	O89	O	0.20975	-0.00913	0.12506	O149	O	0.39522	-0.10478	0.02130
Ca30	Ca	0.25442	-0.22743	-0.37534	O90	O	0.21067	-0.00816	-0.37521	O150	O	0.39570	-0.10478	-0.47851
Ca31	Ca	0.25538	0.27207	0.12492	O91	O	0.21004	0.48929	0.12504	O151	O	0.39524	0.39581	0.02051
Ca32	Ca	0.25509	0.27153	-0.37507	O92	O	0.21078	0.48895	-0.37521	O152	O	0.39821	0.39300	-0.47966
Ge33	Ge	0.00003	-0.25003	-0.00002	O93	O	-0.28930	-0.01109	0.12480	O153	O	0.10340	0.10376	-0.22864
Ti34	Ti	-0.00002	-0.25002	-0.49994	O94	O	-0.28990	-0.01073	-0.37492	O154	O	0.10347	0.10381	0.27152
Ti35	Ti	-0.00001	0.24991	0.00002	O95	O	-0.28947	0.49183	0.12479	O155	O	0.10349	-0.39632	-0.22971
Ti36	Ti	0.00004	0.25003	-0.49995	O96	O	-0.29024	0.49087	-0.37496	O156	O	0.10350	-0.39566	0.26989
Ti37	Ti	-0.50004	-0.25003	-0.00005	O97	O	-0.14522	0.14443	0.02152	O157	O	-0.39652	0.10431	-0.23016
Ti38	Ti	-0.49999	-0.24991	-0.50002	O98	O	-0.14574	0.14541	-0.47851	O158	O	-0.39643	0.10380	0.27039
Ti39	Ti	-0.49998	0.25002	-0.00006	O99	O	-0.14325	-0.35237	0.02046	O159	O	-0.39644	-0.39614	-0.22853
Ge40	Ge	-0.50003	0.25003	-0.49997	O100	O	-0.14611	-0.35500	-0.47937	O160	O	-0.39653	-0.39618	0.27150
Ti41	Ti	0.00013	-0.25036	-0.24889	O101	O	0.35380	0.14505	0.02049					
Ti42	Ti	-0.00017	-0.24967	0.24891	O102	O	0.35670	0.14769	-0.47955					
Ti43	Ti	0.00002	0.24981	-0.24991	O103	O	0.35422	-0.35453	0.02138					
Ti44	Ti	-0.00005	0.25010	0.24993	O104	O	0.35488	-0.35558	-0.47841					
Ti45	Ti	-0.50002	-0.24981	-0.25009	O105	O	0.14653	-0.14619	-0.22972					
Ti46	Ti	-0.49995	-0.25010	0.25007	O106	O	0.14657	-0.14641	0.27025					
Ti47	Ti	-0.50013	0.25036	-0.25111	O107	O	0.14652	0.35384	-0.22874					
Ti48	Ti	-0.49984	0.24968	0.25109	O108	O	0.14612	0.35424	0.27145					
Ti49	Ti	-0.24894	-0.00131	-0.00024	O109	O	-0.35379	-0.14581	-0.22860					
Ti50	Ti	-0.25106	0.00132	-0.49976	O110	O	-0.35355	-0.14608	0.27143					
Ti51	Ti	-0.24869	-0.49896	-0.00022	O111	O	-0.35344	0.35358	-0.22981					
Ti52	Ti	-0.25131	-0.50104	-0.49977	O112	O	-0.35345	0.35380	0.27031					
Ti53	Ti	0.24866	-0.00108	0.00025	O113	O	0.10430	0.10478	-0.02149					
Ti54	Ti	0.25134	0.00108	-0.50025	O114	O	0.10478	0.10479	0.47870					
Ti55	Ti	0.24882	-0.49872	0.00020	O115	O	0.10179	-0.39300	-0.02034					
Ti56	Ti	0.25118	-0.50127	-0.50020	O116	O	0.10476	-0.39581	0.47949					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39527	0.10418	-0.02059					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39814	0.10703	0.47979					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39524	-0.39519	-0.02132					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39553	-0.39506	0.47848					

Table S18. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 3.942$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00500	0.02185	0.12510	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10344	-0.10371	0.22951
Ca2	Ca	-0.00452	0.02165	-0.37495	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10335	-0.10419	-0.26993
Ca3	Ca	-0.00474	-0.47682	0.12438	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10337	0.39628	0.22841
Ca4	Ca	-0.00419	-0.47761	-0.37538	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10343	0.39626	-0.27156
Ca5	Ca	0.49579	0.02250	0.12449	O65	O	0.04119	0.23957	0.12497	O125	O	0.39665	-0.10370	0.22839
Ca6	Ca	0.49532	0.02320	-0.37556	O66	O	0.04075	0.23983	-0.37501	O126	O	0.39674	-0.10364	-0.27144
Ca7	Ca	0.49540	-0.47830	0.12505	O67	O	0.03911	-0.25871	0.12255	O127	O	0.39661	0.39578	0.23003
Ca8	Ca	0.49507	-0.47796	-0.37485	O68	O	0.03925	-0.25943	-0.37458	O128	O	0.39664	0.39644	-0.27039
Ca9	Ca	0.00468	-0.02320	-0.12444	O69	O	-0.46073	0.24049	0.12539	O129	O	0.14342	-0.14779	-0.02051
Ca10	Ca	0.00421	-0.02250	0.37551	O70	O	-0.46097	0.24125	-0.37742	O130	O	0.14633	-0.14518	0.47941
Ca11	Ca	0.00493	0.47797	-0.12515	O71	O	-0.45924	-0.26010	0.12499	O131	O	0.14526	0.35546	-0.02166
Ca12	Ca	0.00460	0.47831	0.37495	O72	O	-0.45892	-0.26027	-0.37500	O132	O	0.14594	0.35440	0.47856
Ca13	Ca	-0.49548	-0.02165	-0.12505	O73	O	-0.03903	-0.24125	-0.12258	O133	O	-0.35411	-0.14555	-0.02156
Ca14	Ca	-0.49500	-0.02185	0.37490	O74	O	-0.03927	-0.24049	0.37461	O134	O	-0.35465	-0.14454	0.47839
Ca15	Ca	-0.49581	0.47762	-0.12462	O75	O	-0.04108	0.26027	-0.12500	O135	O	-0.35376	0.35488	-0.02071
Ca16	Ca	-0.49526	0.47683	0.37562	O76	O	-0.04076	0.26011	0.37501	O136	O	-0.35664	0.35227	0.47947
Ca17	Ca	0.24556	0.22736	-0.12465	O77	O	0.45925	-0.23983	-0.12499	O137	O	-0.14656	0.14620	0.22849
Ca18	Ca	0.24534	0.22772	0.37496	O78	O	0.45881	-0.23956	0.37503	O138	O	-0.14635	0.14594	-0.27148
Ca19	Ca	0.24490	-0.27162	-0.12493	O79	O	0.46075	0.25944	-0.12542	O139	O	-0.14667	-0.35369	0.22958
Ca20	Ca	0.24460	-0.27217	0.37509	O80	O	0.46089	0.25872	0.37745	O140	O	-0.14669	-0.35346	-0.27027
Ca21	Ca	-0.25530	0.22785	-0.12497	O81	O	-0.20990	0.01072	-0.12508	O141	O	0.35333	0.14651	0.22966
Ca22	Ca	-0.25509	0.22833	0.37516	O82	O	-0.21053	0.01109	0.37520	O142	O	0.35334	0.14630	-0.27038
Ca23	Ca	-0.25457	-0.27224	-0.12500	O83	O	-0.20957	-0.49085	-0.12504	O143	O	0.35375	-0.35413	0.22848
Ca24	Ca	-0.25444	-0.27259	0.37536	O84	O	-0.21035	-0.49181	0.37521	O144	O	0.35334	-0.35372	-0.27133
Ca25	Ca	-0.24491	-0.22833	0.12484	O85	O	0.28951	0.00818	-0.12479	O145	O	-0.10173	-0.10692	0.02029
Ca26	Ca	-0.24470	-0.22784	-0.37503	O86	O	0.29045	0.00917	0.37494	O146	O	-0.10459	-0.10407	-0.47934
Ca27	Ca	-0.24556	0.27259	0.12464	O87	O	0.28938	-0.48896	-0.12478	O147	O	-0.10432	0.39519	0.02161
Ca28	Ca	-0.24543	0.27225	-0.37500	O88	O	0.29014	-0.48932	0.37495	O148	O	-0.10463	0.39531	-0.47860
Ca29	Ca	0.25466	-0.22771	0.12504	O89	O	0.20955	-0.00916	0.12506	O149	O	0.39537	-0.10466	0.02138
Ca30	Ca	0.25444	-0.22736	-0.37535	O90	O	0.21049	-0.00817	-0.37521	O150	O	0.39585	-0.10464	-0.47843
Ca31	Ca	0.25540	0.27218	0.12491	O91	O	0.20986	0.48932	0.12505	O151	O	0.39538	0.39593	0.02058
Ca32	Ca	0.25510	0.27162	-0.37507	O92	O	0.21062	0.48896	-0.37522	O152	O	0.39833	0.39310	-0.47959
Ge33	Ge	0.00003	-0.25002	-0.00002	O93	O	-0.28947	-0.01108	0.12480	O153	O	0.10327	0.10365	-0.22856
Ti34	Ti	-0.00001	-0.25002	-0.49994	O94	O	-0.29010	-0.01072	-0.37492	O154	O	0.10335	0.10370	0.27161
Ti35	Ti	-0.00002	0.24991	0.00003	O95	O	-0.28965	0.49182	0.12479	O155	O	0.10335	-0.39644	-0.22961
Ti36	Ti	0.00004	0.25003	-0.49995	O96	O	-0.29043	0.49085	-0.37496	O156	O	0.10338	-0.39578	0.26997
Ti37	Ti	-0.50004	-0.25002	-0.00005	O97	O	-0.14535	0.14454	0.02161	O157	O	-0.39665	0.10420	-0.23007
Ti38	Ti	-0.49998	-0.24991	-0.50003	O98	O	-0.14589	0.14555	-0.47844	O158	O	-0.39656	0.10372	0.27049
Ti39	Ti	-0.49999	0.25002	-0.00006	O99	O	-0.14337	-0.35226	0.02053	O159	O	-0.39657	-0.39625	-0.22844
Ge40	Ge	-0.50003	0.25003	-0.49998	O100	O	-0.14624	-0.35487	-0.47929	O160	O	-0.39664	-0.39627	0.27159
Ti41	Ti	0.00013	-0.25036	-0.24888	O101	O	0.35367	0.14519	0.02059					
Ti42	Ti	-0.00014	-0.24969	0.24890	O102	O	0.35658	0.14779	-0.47949					
Ti43	Ti	0.00002	0.24982	-0.24991	O103	O	0.35406	-0.35439	0.02144					
Ti44	Ti	-0.00004	0.25011	0.24993	O104	O	0.35474	-0.35546	-0.47834					
Ti45	Ti	-0.50002	-0.24982	-0.25009	O105	O	0.14666	-0.14629	-0.22962					
Ti46	Ti	-0.49996	-0.25011	0.25007	O106	O	0.14667	-0.14651	0.27034					
Ti47	Ti	-0.50013	0.25036	-0.25111	O107	O	0.14666	0.35372	-0.22867					
Ti48	Ti	-0.49986	0.24970	0.25110	O108	O	0.14625	0.35413	0.27152					
Ti49	Ti	-0.24894	-0.00131	-0.00023	O109	O	-0.35365	-0.14593	-0.22852					
Ti50	Ti	-0.25106	0.00132	-0.49977	O110	O	-0.35344	-0.14620	0.27151					
Ti51	Ti	-0.24870	-0.49895	-0.00022	O111	O	-0.35331	0.35347	-0.22973					
Ti52	Ti	-0.25130	-0.50104	-0.49978	O112	O	-0.35333	0.35370	0.27042					
Ti53	Ti	0.24866	-0.00108	0.00024	O113	O	0.10415	0.10465	-0.02157					
Ti54	Ti	0.25134	0.00108	-0.50024	O114	O	0.10463	0.10466	0.47862					
Ti55	Ti	0.24881	-0.49872	0.00022	O115	O	0.10167	-0.39310	-0.02041					
Ti56	Ti	0.25118	-0.50128	-0.50022	O116	O	0.10462	-0.39592	0.47942					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39541	0.10408	-0.02066					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39827	0.10693	0.47971					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39537	-0.39531	-0.02140					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39568	-0.39518	0.47839					

Table SI12. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 15.079$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00543	0.02322	0.12501	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10195	-0.10234	0.22885
Ca2	Ca	-0.00491	0.02291	-0.37500	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10185	-0.10293	-0.27072
Ca3	Ca	-0.00501	-0.47553	0.12453	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10190	0.39750	0.22754
Ca4	Ca	-0.00441	-0.47620	-0.37540	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10187	0.39752	-0.27246
Ca5	Ca	0.49552	0.02391	0.12450	O65	O	0.04325	0.23949	0.12498	O125	O	0.39816	-0.10242	0.22748
Ca6	Ca	0.49506	0.02451	-0.37545	O66	O	0.04258	0.23967	-0.37500	O126	O	0.39817	-0.10241	-0.27234
Ca7	Ca	0.49496	-0.47702	0.12495	O67	O	0.04038	-0.25845	0.12246	O127	O	0.39816	0.39704	0.22925
Ca8	Ca	0.49462	-0.47658	-0.37497	O68	O	0.04081	-0.25927	-0.37448	O128	O	0.39816	0.39780	-0.27109
Ca9	Ca	0.00494	-0.02450	-0.12455	O69	O	-0.45925	0.24072	0.12548	O129	O	0.14455	-0.14892	-0.02112
Ca10	Ca	0.00448	-0.02391	0.37550	O70	O	-0.45972	0.24157	-0.37751	O130	O	0.14783	-0.14623	0.47869
Ca11	Ca	0.00538	0.47658	-0.12503	O71	O	-0.45745	-0.26032	0.12499	O131	O	0.14671	0.35425	-0.02264
Ca12	Ca	0.00504	0.47703	0.37505	O72	O	-0.45694	-0.26032	-0.37503	O132	O	0.14733	0.35320	0.47759
Ca13	Ca	-0.49509	-0.02291	-0.12500	O73	O	-0.04028	-0.24156	-0.12249	O133	O	-0.35272	-0.14680	-0.02248
Ca14	Ca	-0.49457	-0.02322	0.37499	O74	O	-0.04075	-0.24072	0.37452	O134	O	-0.35318	-0.14571	0.47736
Ca15	Ca	-0.49559	0.47621	-0.12460	O75	O	-0.04306	0.26033	-0.12497	O135	O	-0.35224	0.35380	-0.02141
Ca16	Ca	-0.49499	0.47553	0.37547	O76	O	-0.04255	0.26032	0.37501	O136	O	-0.35554	0.35119	0.47890
Ca17	Ca	0.24550	0.22590	-0.12461	O77	O	0.45742	-0.23966	-0.12500	O137	O	-0.14815	0.14750	0.22758
Ca18	Ca	0.24520	0.22630	0.37488	O78	O	0.45675	-0.23948	0.37502	O138	O	-0.14780	0.14711	-0.27237
Ca19	Ca	0.24463	-0.27283	-0.12494	O79	O	0.45919	0.25928	-0.12552	O139	O	-0.14814	-0.35249	0.22890
Ca20	Ca	0.24412	-0.27352	0.37519	O80	O	0.45962	0.25845	0.37754	O140	O	-0.14830	-0.35211	-0.27110
Ca21	Ca	-0.25579	0.22652	-0.12483	O81	O	-0.20807	0.01100	-0.12510	O141	O	0.35168	0.14791	0.22886
Ca22	Ca	-0.25544	0.22719	0.37515	O82	O	-0.20869	0.01130	0.37519	O142	O	0.35184	0.14755	-0.27105
Ca23	Ca	-0.25473	-0.27372	-0.12511	O83	O	-0.20772	-0.49098	-0.12509	O143	O	0.35230	-0.35291	0.22764
Ca24	Ca	-0.25445	-0.27407	0.37541	O84	O	-0.20850	-0.49201	0.37523	O144	O	0.35179	-0.35240	-0.27226
Ca25	Ca	-0.24456	-0.22718	0.12485	O85	O	0.29134	0.00798	-0.12476	O145	O	-0.10038	-0.10601	0.02087
Ca26	Ca	-0.24421	-0.22651	-0.37517	O86	O	0.29229	0.00908	0.37490	O146	O	-0.10336	-0.10283	-0.47863
Ca27	Ca	-0.24555	0.27407	0.12459	O87	O	0.29121	-0.48878	-0.12482	O147	O	-0.10290	0.39632	0.02259
Ca28	Ca	-0.24528	0.27373	-0.37489	O88	O	0.29196	-0.48907	0.37494	O148	O	-0.10315	0.39657	-0.47769
Ca29	Ca	0.25480	-0.22630	0.12512	O89	O	0.20771	-0.00907	0.12510	O149	O	0.39684	-0.10341	0.02229
Ca30	Ca	0.25450	-0.22590	-0.37539	O90	O	0.20865	-0.00797	-0.37524	O150	O	0.39722	-0.10352	-0.47745
Ca31	Ca	0.25588	0.27352	0.12481	O91	O	0.20804	0.48907	0.12506	O151	O	0.39660	0.39717	0.02132
Ca32	Ca	0.25537	0.27283	-0.37506	O92	O	0.20879	0.48878	-0.37518	O152	O	0.39967	0.39405	-0.47903
Ge33	Ge	0.00004	-0.25002	-0.00001	O93	O	-0.29131	-0.01130	0.12481	O153	O	0.10183	0.10242	-0.22766
Ti34	Ti	0.00003	-0.25003	-0.49995	O94	O	-0.29193	-0.01099	-0.37490	O154	O	0.10184	0.10242	0.27252
Ti35	Ti	-0.00002	0.24995	0.00006	O95	O	-0.29150	0.49202	0.12477	O155	O	0.10183	-0.39780	-0.22891
Ti36	Ti	0.00005	0.25000	-0.49997	O96	O	-0.29228	0.49098	-0.37491	O156	O	0.10184	-0.39704	0.27075
Ti37	Ti	-0.50005	-0.24999	-0.00003	O97	O	-0.14682	0.14572	0.02263	O157	O	-0.39815	0.10294	-0.22928
Ti38	Ti	-0.49998	-0.24994	-0.50006	O98	O	-0.14729	0.14680	-0.47752	O158	O	-0.39805	0.10234	0.27115
Ti39	Ti	-0.50003	0.25004	-0.00005	O99	O	-0.14446	-0.35118	0.02110	O159	O	-0.39813	-0.39751	-0.22754
Ge40	Ge	-0.50004	0.25002	-0.49999	O100	O	-0.14776	-0.35379	-0.47859	O160	O	-0.39810	-0.39749	0.27246
Ti41	Ti	-0.00001	-0.25039	-0.24872	O101	O	0.35217	0.14624	0.02131					
Ti42	Ti	-0.00001	-0.24962	0.24874	O102	O	0.35545	0.14892	-0.47888					
Ti43	Ti	0.00001	0.24986	-0.24989	O103	O	0.35267	-0.35320	0.02242					
Ti44	Ti	-0.00008	0.25003	0.24990	O104	O	0.35329	-0.35424	-0.47736					
Ti45	Ti	-0.50001	-0.24985	-0.25011	O105	O	0.14816	-0.14754	-0.22895					
Ti46	Ti	-0.49992	-0.25003	0.25010	O106	O	0.14832	-0.14790	0.27114					
Ti47	Ti	-0.49999	0.25040	-0.25128	O107	O	0.14821	0.35240	-0.22774					
Ti48	Ti	-0.49999	0.24962	0.25126	O108	O	0.14770	0.35291	0.27236					
Ti49	Ti	-0.24871	-0.00145	-0.00021	O109	O	-0.35220	-0.14710	-0.22763					
Ti50	Ti	-0.25129	0.00145	-0.49979	O110	O	-0.35185	-0.14749	0.27242					
Ti51	Ti	-0.24863	-0.49870	-0.00014	O111	O	-0.35171	0.35212	-0.22890					
Ti52	Ti	-0.25137	-0.50129	-0.49986	O112	O	-0.35186	0.35250	0.27110					
Ti53	Ti	0.24854	-0.00130	0.00016	O113	O	0.10278	0.10353	-0.02255					
Ti54	Ti	0.25145	0.00131	-0.50016	O114	O	0.10316	0.10342	0.47771					
Ti55	Ti	0.24859	-0.49858	0.00015	O115	O	0.10033	-0.39405	-0.02097					
Ti56	Ti	0.25141	-0.50142	-0.50015	O116	O	0.10340	-0.39717	0.47868					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39664	0.10284	-0.02137					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.39962	0.10602	0.47913					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39685	-0.39657	-0.02231					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39710	-0.39632	0.47741					

Table S114. Atomic coordinates obtained from the DFT calculation for the sample CTG at $P = 25.141$ GPa.

Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z	Atom label	Atom type	x	y	z
Ca1	Ca	-0.00594	0.02439	0.12494	Ti61	Ti	0.25000	0.00000	-0.25000	O121	O	-0.10060	-0.10117	0.22847
Ca2	Ca	-0.00549	0.02407	-0.37506	Ti62	Ti	0.25000	0.00000	0.25000	O122	O	-0.10062	-0.10195	-0.27120
Ca3	Ca	-0.00538	-0.47435	0.12455	Ti63	Ti	0.25000	-0.50000	-0.25000	O123	O	-0.10067	0.39846	0.22694
Ca4	Ca	-0.00484	-0.47487	-0.37538	Ti64	Ti	0.25000	-0.50000	0.25000	O124	O	-0.10060	0.39853	-0.27302
Ca5	Ca	0.49509	0.02519	0.12456	O65	O	0.04464	0.23951	0.12495	O125	O	0.39942	-0.10139	0.22693
Ca6	Ca	0.49465	0.02568	-0.37542	O66	O	0.04396	0.23972	-0.37499	O126	O	0.39939	-0.10142	-0.27299
Ca7	Ca	0.49440	-0.47586	0.12489	O67	O	0.04116	-0.25805	0.12241	O127	O	0.39942	0.39805	0.22879
Ca8	Ca	0.49408	-0.47545	-0.37504	O68	O	0.04188	-0.25905	-0.37443	O128	O	0.39952	0.39892	-0.27153
Ca9	Ca	0.00535	-0.02568	-0.12458	O69	O	-0.45822	0.24099	0.12554	O129	O	0.14555	-0.14985	-0.02145
Ca10	Ca	0.00491	-0.02519	0.37544	O70	O	-0.45890	0.24199	-0.37758	O130	O	0.14914	-0.14711	0.47819
Ca11	Ca	0.00592	0.47545	-0.12496	O71	O	-0.45603	-0.26026	0.12501	O131	O	0.14798	0.35327	-0.02335
Ca12	Ca	0.00560	0.47586	0.37511	O72	O	-0.45552	-0.26028	-0.37506	O132	O	0.14855	0.35219	0.47690
Ca13	Ca	-0.49451	-0.02407	-0.12494	O73	O	-0.04110	-0.24199	-0.12242	O133	O	-0.35149	-0.14782	-0.02315
Ca14	Ca	-0.49406	-0.02438	0.37506	O74	O	-0.04178	-0.24099	0.37446	O134	O	-0.35195	-0.14668	0.47662
Ca15	Ca	-0.49516	0.47488	-0.12462	O75	O	-0.04448	0.26028	-0.12494	O135	O	-0.35095	0.35290	-0.02187
Ca16	Ca	-0.49462	0.47435	0.37545	O76	O	-0.04397	0.26027	0.37499	O136	O	-0.35453	0.35027	0.47857
Ca17	Ca	0.24529	0.22454	-0.12460	O77	O	0.45604	-0.23971	-0.12501	O137	O	-0.14947	0.14850	0.22696
Ca18	Ca	0.24482	0.22508	0.37488	O78	O	0.45536	-0.23951	0.37505	O138	O	-0.14904	0.14811	-0.27298
Ca19	Ca	0.24411	-0.27385	-0.12498	O79	O	0.45812	0.25906	-0.12557	O139	O	-0.14940	-0.35145	0.22849
Ca20	Ca	0.24349	-0.27465	0.37533	O80	O	0.45884	0.25806	0.37759	O140	O	-0.14963	-0.35108	-0.27162
Ca21	Ca	-0.25643	0.22539	-0.12471	O81	O	-0.20671	0.01107	-0.12510	O141	O	0.35034	0.14896	0.22839
Ca22	Ca	-0.25592	0.22621	0.37508	O82	O	-0.20750	0.01149	0.37521	O142	O	0.35056	0.14861	-0.27145
Ca23	Ca	-0.25511	-0.27495	-0.12512	O83	O	-0.20633	-0.49121	-0.12510	O143	O	0.35104	-0.35187	0.22705
Ca24	Ca	-0.25459	-0.27544	0.37541	O84	O	-0.20724	-0.49241	0.37524	O144	O	0.35052	-0.35138	-0.27293
Ca25	Ca	-0.24408	-0.22621	0.12492	O85	O	0.29259	0.00758	-0.12476	O145	O	-0.09920	-0.10526	0.02125
Ca26	Ca	-0.24357	-0.22538	-0.37529	O86	O	0.29369	0.00886	0.37489	O146	O	-0.10223	-0.10179	-0.47820
Ca27	Ca	-0.24541	0.27545	0.12459	O87	O	0.29242	-0.48862	-0.12484	O147	O	-0.10164	0.39731	0.02330
Ca28	Ca	-0.24489	0.27495	-0.37488	O88	O	0.29331	-0.48899	0.37494	O148	O	-0.10193	0.39756	-0.47707
Ca29	Ca	0.25518	-0.22508	0.12512	O89	O	0.20631	-0.00885	0.12511	O149	O	0.39806	-0.10244	0.02291
Ca30	Ca	0.25471	-0.22454	-0.37540	O90	O	0.20741	-0.00757	-0.37524	O150	O	0.39846	-0.10254	-0.47674
Ca31	Ca	0.25651	0.27466	0.12467	O91	O	0.20668	0.48899	0.12506	O151	O	0.39772	0.39823	0.02178
Ca32	Ca	0.25589	0.27386	-0.37502	O92	O	0.20758	0.48862	-0.37516	O152	O	0.40085	0.39484	-0.47866
Ge33	Ge	0.00003	-0.25002	-0.00001	O93	O	-0.29250	-0.01149	0.12479	O153	O	0.10061	0.10143	-0.22701
Ti34	Ti	0.00004	-0.25002	-0.49997	O94	O	-0.29329	-0.01106	-0.37490	O154	O	0.10058	0.10140	0.27307
Ti35	Ti	-0.00002	0.24995	0.00005	O95	O	-0.29275	0.49242	0.12476	O155	O	0.10048	-0.39891	-0.22848
Ti36	Ti	0.00002	0.24999	-0.49999	O96	O	-0.29367	0.49122	-0.37490	O156	O	0.10058	-0.39805	0.27121
Ti37	Ti	-0.50002	-0.24998	-0.00001	O97	O	-0.14805	0.14669	0.02338	O157	O	-0.39938	0.10196	-0.22880
Ti38	Ti	-0.49998	-0.24994	-0.50005	O98	O	-0.14851	0.14783	-0.47685	O158	O	-0.39940	0.10117	0.27153
Ti39	Ti	-0.50004	0.25003	-0.00003	O99	O	-0.14548	-0.35026	0.02143	O159	O	-0.39940	-0.39853	-0.22698
Ge40	Ge	-0.50003	0.25002	-0.49999	O100	O	-0.14905	-0.35289	-0.47813	O160	O	-0.39934	-0.39846	0.27306
Ti41	Ti	-0.00020	-0.25045	-0.24859	O101	O	0.35086	0.14711	0.02181					
Ti42	Ti	0.00019	-0.24953	0.24859	O102	O	0.35445	0.14985	-0.47855					
Ti43	Ti	0.00003	0.24990	-0.24985	O103	O	0.35145	-0.35218	0.02310					
Ti44	Ti	-0.00011	0.24999	0.24984	O104	O	0.35202	-0.35326	-0.47665					
Ti45	Ti	-0.50003	-0.24990	-0.25015	O105	O	0.14944	-0.14861	-0.22855					
Ti46	Ti	-0.49989	-0.24998	0.25016	O106	O	0.14966	-0.14896	0.27161					
Ti47	Ti	-0.49980	0.25046	-0.25141	O107	O	0.14948	0.35139	-0.22707					
Ti48	Ti	-0.50019	0.24953	0.25141	O108	O	0.14896	0.35187	0.27295					
Ti49	Ti	-0.24852	-0.00151	-0.00016	O109	O	-0.35096	-0.14810	-0.22702					
Ti50	Ti	-0.25148	0.00152	-0.49984	O110	O	-0.35053	-0.14849	0.27304					
Ti51	Ti	-0.24854	-0.49850	-0.00007	O111	O	-0.35038	0.35109	-0.22838					
Ti52	Ti	-0.25146	-0.50149	-0.49993	O112	O	-0.35060	0.35146	0.27151					
Ti53	Ti	0.24848	-0.00152	0.00008	O113	O	0.10154	0.10255	-0.02326					
Ti54	Ti	0.25152	0.00152	-0.50008	O114	O	0.10194	0.10244	0.47710					
Ti55	Ti	0.24844	-0.49851	0.00010	O115	O	0.09915	-0.39483	-0.02134					
Ti56	Ti	0.25156	-0.50148	-0.50010	O116	O	0.10228	-0.39822	0.47822					
Ti57	Ti	-0.25000	0.00000	-0.25000	O117	O	-0.39777	0.10180	-0.02180					
Ti58	Ti	-0.25000	0.00000	0.25000	O118	O	-0.40080	0.10526	0.47875					
Ti59	Ti	-0.25000	-0.50000	-0.25000	O119	O	-0.39807	-0.39755	-0.02293					
Ti60	Ti	-0.25000	-0.50000	0.25000	O120	O	-0.39836	-0.39730	0.47669					

Table S15. Unit-cell parameters (a , b , c , and V) and selected bond lengths and angles at room conditions for CaTiO₃ orthorhombic perovskites from the literature and those for the CTG sample investigated here, derived from X-ray diffraction experiments.

a (Å)	b (Å)	c (Å)	V (Å ³)	$B-O1$ (Å)	$B-O2$ (Å)	$B-O2'$ (Å)	$\langle B-O \rangle$ (Å)	$V(BO_6)$ (Å ³)	ECoN	$B-O1-B$ (°)	$B-O2-B$ (°)	Reference
5.3829(3)	7.6453(4)	5.4458(3)	224.12(4)	1.952(2)	1.953(2)	1.963(2)	1.956(2)	9.98	5.999	156.3	155.8	5
5.3796(1)	5.4423(3)	7.6401(5)	223.68(1)	1.9503(3)	1.9551(8)	1.9587(8)	1.9547	9.96	5.999	156.67(8)	155.71(5)	6
5.3785(2)	5.4419(2)	7.6400(3)	223.62(3)	1.939(1)	1.950(1)	1.957(1)	1.952	9.86	5.997	156.8	158.2	7
5.380(1)	5.440(1)	7.639(1)	223.56(7)	1.950	1.957	1.957	1.955	9.95	5.999	156.8	155.6	8
5.378(1)	5.444(1)	7.637(3)	223.59	1.951	1.958	1.958	1.956	9.97	5.999	156.3	155.4	9
5.3814(1)	5.4418(1)	7.6409(2)	223.76	1.947	1.953	1.968	1.956	9.97	5.996	157.8	154.9	10
5.3827(5)	5.4537(5)	7.6551(9)	224.72	1.952	1.959	1.964	1.958	10.01	5.999	157.2	155.2	11
5.3799(5)	5.4411(5)	7.6411(8)	223.67	1.950	1.950	1.960	1.955	9.95	5.999	156.7	155.7	12
5.4043(8)	5.4224(7)	7.6510(12)	224.19	1.946(1)	1.951(3)	1.960(3)	1.952(2)	9.90(4)	5.998	158.7	156.3	13
5.378(7)	5.439(7)	7.638(1)	223.42	1.954	1.960	1.969	1.961	10.05	5.998	152.0	155.4	14
5.38052(7)	5.44251(6)	7.64096(9)	223.754(8)	1.951	1.954	1.958	1.954	9.95	6.000	156.7	156.0	15
5.38159(6)	5.44281(7)	7.64207(10)	223.843(5)	1.949(1)	1.953(3)	1.961(3)	1.954(2)	9.953(2)	5.999	157.1	155.8	16
5.3789(2)	5.4361(2)	7.6388(3)	223.36	1.951	1.953	1.961	1.955	9.96	5.999	156.0	155.6	17
5.3810(3)	5.4445(4)	7.6484(2)	224.07	1.952	1.956	1.961	1.953	9.98	5.999	156.9	155.5	18
5.38095(2)	5.43710(2)	7.64208(5)	223.58	1.951	1.956	1.958	1.955	9.96	6.000	156.5	155.6	19
5.3709(2)	5.4280(2)	7.6268(3)	222.35(2)	1.946	1.949	1.958	1.951	9.90	5.999	156.8	155.6	20
5.3828	5.4460	7.6391	223.94	1.950	1.956	1.960	1.955	9.97	5.999	156.7	155.7	21
5.3786(2)	5.4322(2)	7.6397(3)	223.21	1.948(1)	1.950(1)	1.964(3)	1.954	9.94	5.997	157.0(1)	155.3(3)	22
5.38176(22)	5.44403(21)	7.6425(7)	223.913(25)	1.9513(10)	1.9585(24)	1.9587(25)	1.957	9.981(19)	5.999	156.39(28)	155.32(26)	23
5.38079(12)	5.44273(12)	7.64138(16)	223.787(8)	1.948(3)	1.963(3)	1.9548(10)	1.955	9.96	5.998	155.5(2)	156.3(2)	24
5.38097(2)	5.43780(2)	7.64012(3)	223.555(1)	1.9494(4)	1.9517(11)	1.9556(11)	1.9522(9)	9.92	6.000	156.94(10)	156.44(7)	<i>This work</i>

Table S3 references

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