Supporting Information

Multiple Pathways in Pressure-Induced Phase Transition of Coesite

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Supplementary Figures. In this supplementary document, we have included 7 additional figures: (1) Calculated energy dispersive one-dimensional X-Ray Diffraction (XRD) of selected structures in Path I (**Figure S1**). For comparison, the experimental XRD of coesite at 14.4 GPa is also shown.[1] (2) Si-O-Si angle evolution along Path I (a), II (b) and III (c) at 300K (**Figure S2**). Here, we chose only the oxygen atom site (O1), where Si-O-Si angle is equal to 180° in coesite.[2] (3) Averaged shear stress along Path III at 300K from 28 to 54 GPa under constrained "diagonal" compression (**Figure S3**). (4) Oxygen polyhedral evolution along Path I (a), II (b) and III (c) at 300K (**Figure S4**). The oxygen sublattice was calculated by bond angle analysis as suggested by Ackland and Jones.[3] (5) Snapshots of the supercells at different pressures along Path III at 300K (**Figure S5**). (6) Relative enthalpy ΔH as function of pressure for $P2_1/c^{(I)}$ and $P\text{-}1^{(II\text{-}1)}$ phases in the pressure range of 20–32 GPa with *ab initio* calculations[4,5] (a) and in the pressure range of 24-26 GPa with Tangney-Scandolo (TS) potential[6] (b) (**Figure S6**). (7) Relative enthalpy ΔH as function of pressure for coesite ($C2/c$), new HPO ($P1^{(2)}$), and α-PbO_2 phases in the pressure range of 0–36 GPa with *ab initio* calculation (a) and with TS potential (b) (**Figure S7**). In case of TS potential, coesite changes into $P2_1/c^{(I)}$ or $P\text{-}1^{(II\text{-}1)}$ phase at 22 GPa. So, the EOS of coesite was extrapolated to higher pressure using the 3rd order Birch-Murnaghan equation[7], which, in turn, was used as reference state in Figure S6 and S7.

In addition, lattice parameters and fractional atomic coordinates of selected phases transformed from coesite under high pressure. (a) $P2_1/c^{(I)}$, (b) $P\text{-}1^{(I\text{-}1)}$, (c) $P2_1/c^{(II)}$, (d) $P\text{-}1^{(II\text{-}1)}$, (e) $P\text{-}1^{(II\text{-}2)}$, (f) $P\text{-}1^{(III)}$, (g) $P1^{(2)}$ were shown in **Table S1**.

***Ab initio* method for calculating enthalpies of selected phases.** First-principles calculations based on the Density Functional Theory (DFT) were performed by using the Vienna *ab initio* simulation package (VASP).[4,5] The interaction between ions and electrons is described by the projector augmented wave (PAW) method. Exchange correlation functions were taken in a form proposed by Ceperly and Alder (CA) parameterized by Perdew and Zunger within the local density approximation (LDA). An energy cutoff of 550 eV was used for the plane-wave expansion of wave functions and the tetrahedron method with Blöchl corrections was employed to set partial occupancies for each wave functions. Structural optimizations at each pressure were performed with variable shape, volume and atom positions using the conjugate gradient algorithm. The force convergence criterion was less than 0.005 eV/ Å in structure optimizations. Crystalline unit cells of these phases were employed in the calculations. For $P1^{(2)}$ phase, the Γ-centered 3×3×3 *k*-point mesh was adopted for Brillouin zone sampling according to Monkhorst-Pack scheme; for $P2_1/c^{(I)}$ phase, the Γ-centered 6×1×6 *k*-point mesh was adopted; for $C2/c$ and $P\text{-}1^{(II\text{-}1)}$ phases, the Γ-centered 6×3×6 *k*-point mesh was adopted; for α-PbO_2 type of silica, the Γ-centered 9×9×9 *k*-point mesh was adopted. The enthalpies were obtained by fitting the *ab initio* results of the total energy and volume to the 3rd order Birch-Murnaghan equation.[7] The transition pressure from coesite to α-PbO_2 phase is 1.87 GPa for *ab initio* calculation with LDA approximation. It seems that LDA tends to underestimate the transition pressure from low-pressure tetrahedral phases to high-pressure octahedral phases. For example, the phase transition from coesite to stishovite was reported to be at 1.6 GPa.[8]

References

(1) Hemley RJ, Jephcoat AP, Mao HK, Ming LC, Manghnani MH (1988) Pressure-induced amorphization of crystalline silica. *Nature* 334(7):52–54.

(2) Angel RJ, Shaw CSJ, Gibbs GV (2003) Compression mechanisms of coesite. *Phys Chem Minerals* 30(3):167–176.

(3) The oxygen sublattice was distinguished by the bond angle analysis method: Ackland GJ, Jones AP (2006) Applications of local crystal structure measures in experiment and simulation. *Phys Rev B* 73(5):054104.

(4) Kresse G, Hafner J (1993) Ab initio molecular dynamics for liquid metals. *Phys Rev B* 47(1):558-561.

(5) Kresse G, Furthmüller J (1996) Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys Rev B* 54(16):11169–11186.

(6) Tangney P, Scandolo S (2002) An *ab initio* parametrized interatomic force field for silica. *J Chem Phys* 117(19):8898-8904.

(7) Birch F (1947) Finite elastic strain of cubic crystals. *Phys Rev* 71(11):809–824.

(8) Demuth, T, Jeanvoine Y, Hafner J, Angyan JG (1999) Polymorphism in silica studied in the local density and generalized-gradient approximations. *J Phys Condensed Matter* 11: 3833–3874.

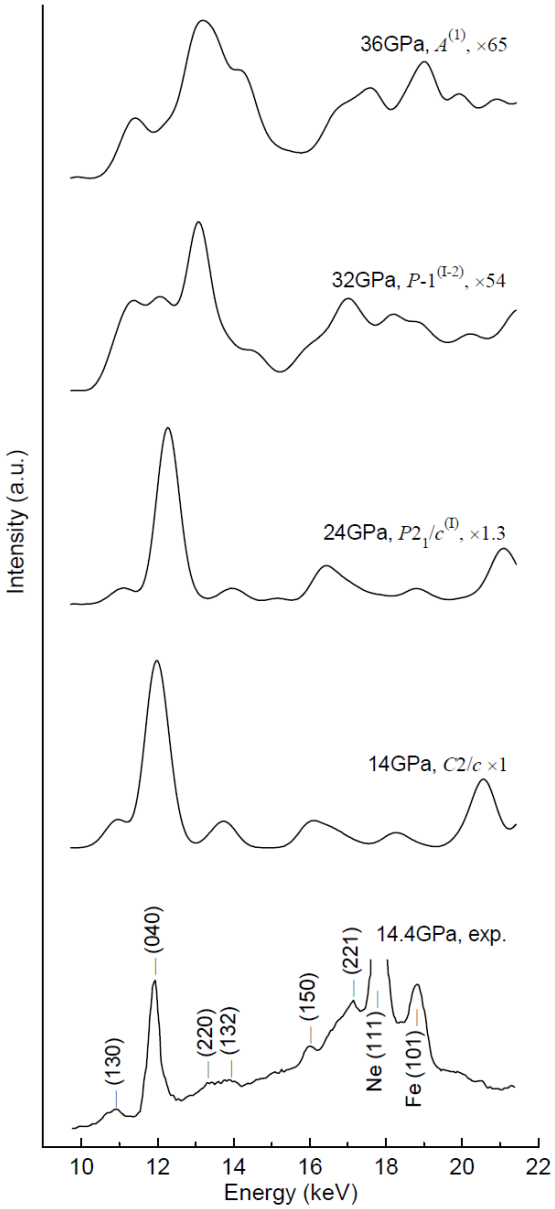

Figure S1: Calculated energy dispersive one-dimensional XRD of some phases in Path I. For the convenience of comparison, the experimental XRD of coesite at 14.4 GPa[1] is also shown. The displayed intensity of each calculated XRD is amplified by the number after the symbol "×".

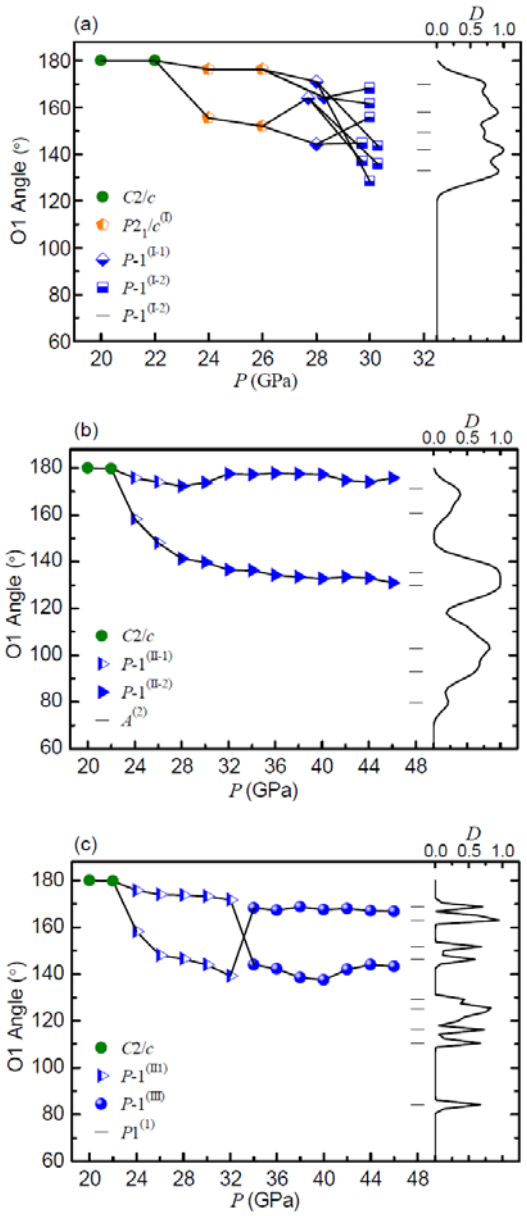

Figure S2: Si-O-Si angle evolution along Path I (a), II (b) and III (c) at 300K. The oxygen atom site (O1) was chosen, where Si-O-Si angle is equal to 180° in coesite.[2] Since the Si-O-Si angle values are dispersed in $P\text{-}1^{(I\text{-}2)}$ phase in Path I, $A^{(2)}$ phase in Path II, and $P1^{(1)}$ phase in Path III, distribution (D) curves are presented.

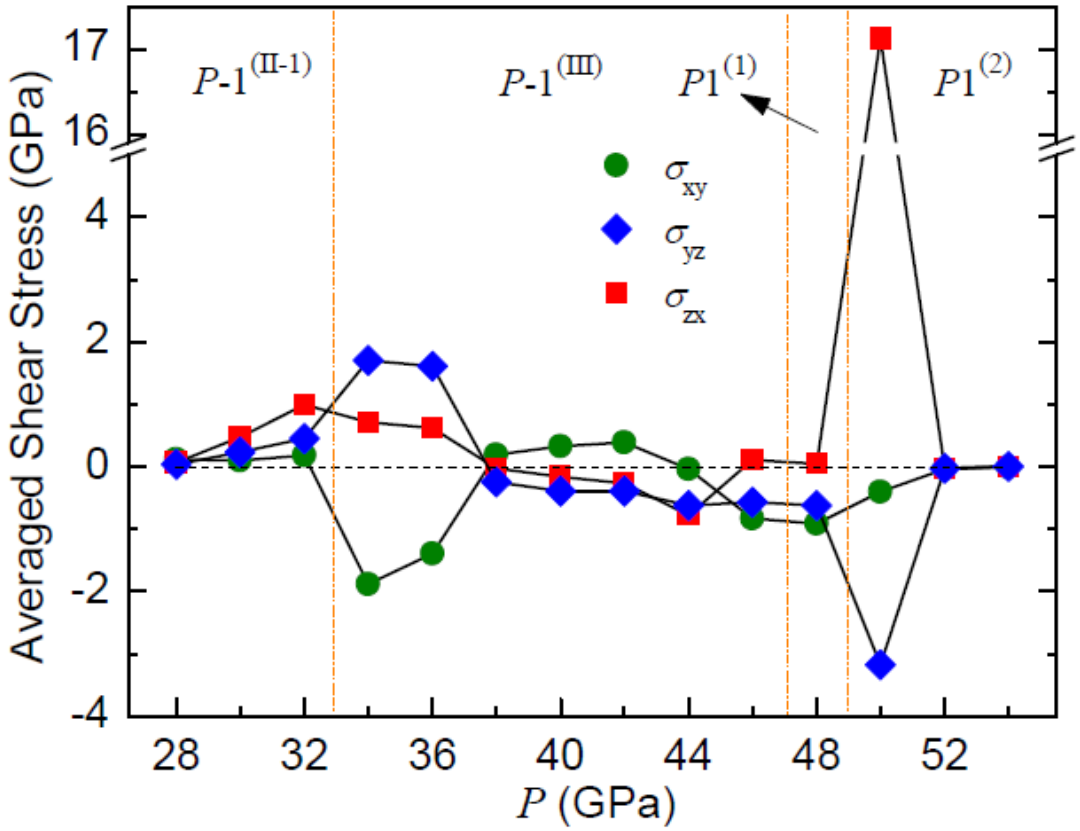

Figure S3: Averaged shear stress along Path III at 300K from 28 to 54 GPa under constrained "diagonal" compression. Vertical dash lines indicate the first-order transition pressures along Path III ($V^{(III)}$) as shown in Figure 1. Note we used the midpoint pressure to denote the transition point.

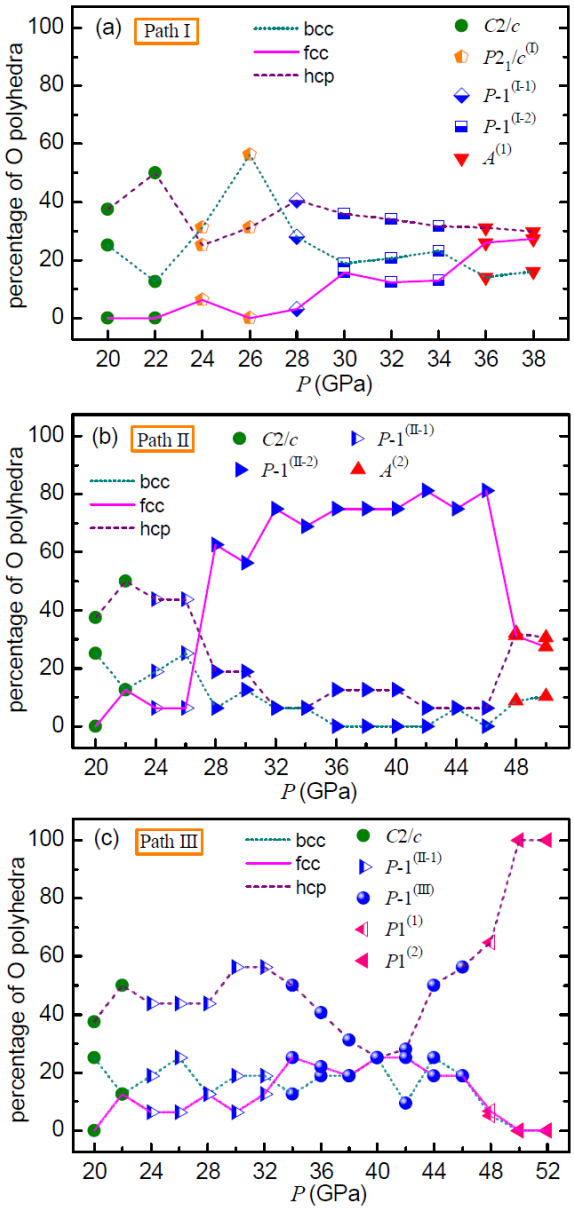

Figure S4: Oxygen polyhedral evolution along Path I (a), II (b) and III (c) at 300K. The oxygen sublattice is calculated by bond angle analysis.[3]

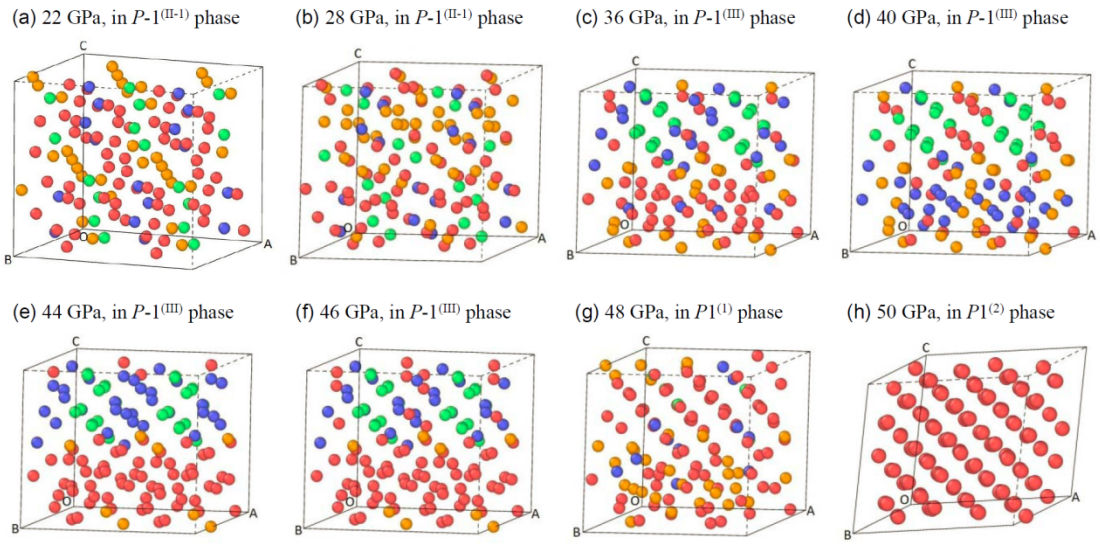

Figure S5: Snapshots of the supercells at different pressures along Path III at 300K. Only oxygen atoms are shown. Blue, green and red balls represent oxygen atoms in bcc, fcc and hcp sublattices, respectively. Orange balls represent oxygen atoms in none of the forementioned sublattices. The oxygen sublattice is defined by the bond angle analysis method.[3]

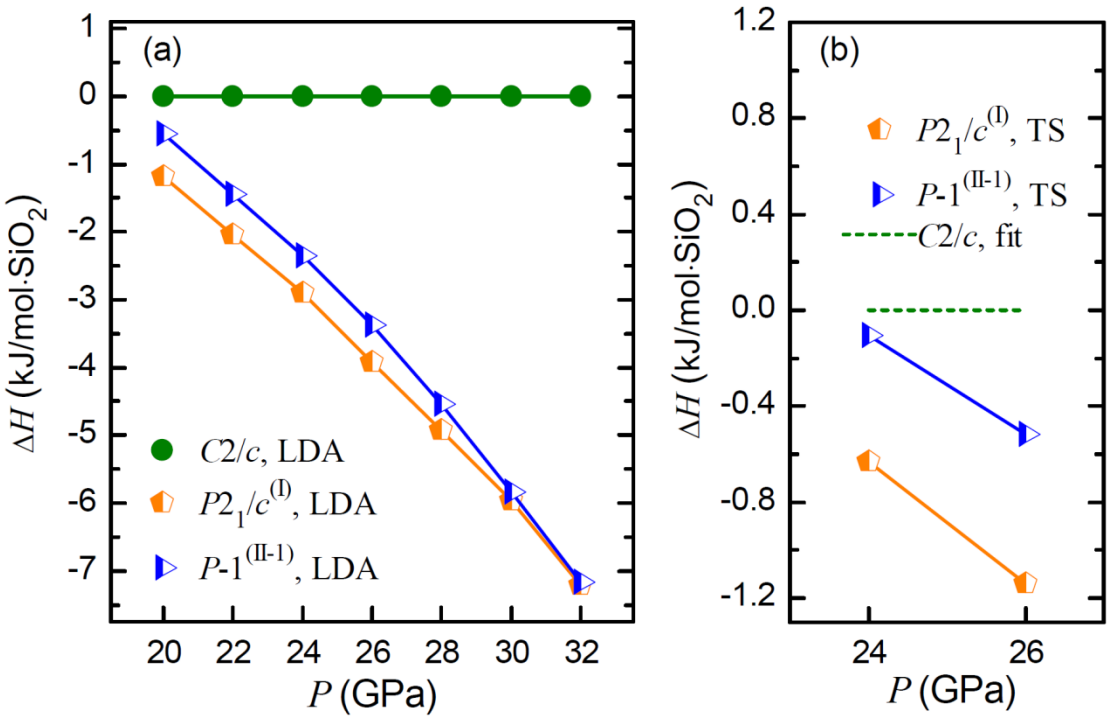

Figure S6: Relative enthalpy ΔH as function of pressure for $P2_1/c^{(I)}$ and $P\text{-}1^{(II\text{-}1)}$ phases in the pressure range of 20–32 GPa with *ab initio* calculation (a) and in the pressure range of 24-26 GPa with TS potential (b). Note: For ab initio calculations, the enthalpies in panel (a) were obtained by fitting the total energy and volume to the 3rd order Birch-Murnaghan equation.[7] In case of TS potential, both $P2_1/c^{(I)}$ and $P\text{-}1^{(II\text{-}1)}$ phases change into coesite phase when recover to 22 GPa, and coesite changes into $P2_1/c^{(I)}$ or $P\text{-}1^{(II\text{-}1)}$ phase (at ~22-24 GPa). The EOS of coesite is extrapolated to higher pressure using the 3rd order Birch-Murnaghan equation[7], which is used as reference state. Path I shows lower enthalpy in both methods as anticipated. The enthalpies of $P2_1/c^{(I)}$ and $P\text{-}1^{(II\text{-}1)}$ phases start to be lower than that of coesite at ~16.0 GPa, and ~18.0 GPa, respectively, according to *ab initio* calculations, which are in good agreement with predictions from TS potential (both at ~22-24 GPa).

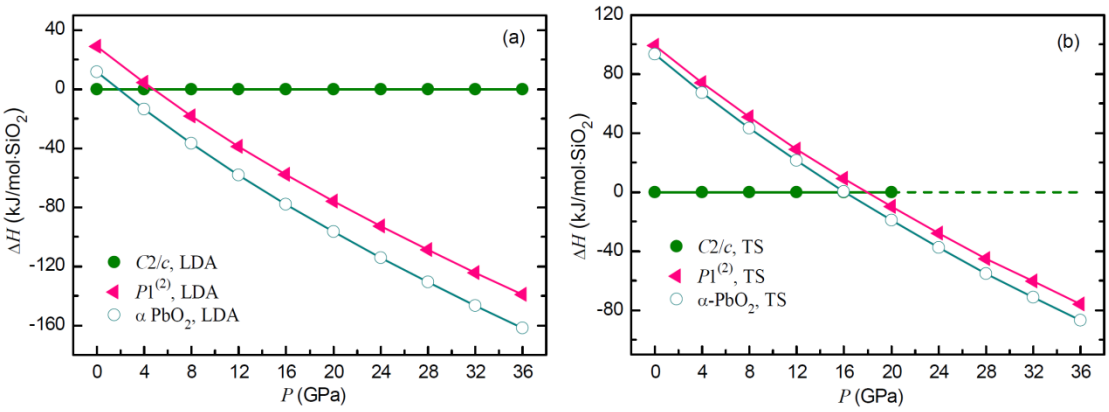

Figure S7: Relative enthalpy ΔH as function of pressure for coesite ($C2/c$), new HPO ($P1^{(2)}$), and α-PbO_2 phases in the pressure range of 0–36 GPa with *ab initio* calculation (a) and with TS potential (b). Note: Similar to Figure S6, we used 3rd order Birch-Murnaghan equation[7] for both Panels (a) and (b). α-PbO_2 and new HPO phases are stable at high pressure in comparison with coesite in both methods as anticipated.

Supplementary Table

Table S1: Lattice parameters and fractional atomic coordinates of selected phases transformed from coesite under high pressure. (a) $P2_1/c^{(I)}$, (b) $P\text{-}1^{(I\text{-}1)}$, (c) $P2_1/c^{(II)}$, (d) $P\text{-}1^{(II\text{-}1)}$, (e) $P\text{-}1^{(II\text{-}2)}$, (f) $P\text{-}1^{(III)}$, (g) $P1^{(2)}$.

(a) $P2_1/c^{(I)}$, 24 GPa

space group $P2_1/c$ No. 14					
a=6.7542 Å, b=23.3717 Å, c=6.6249 Å, β=119.3686°					
number	element	x	y	z	Wyckoff index
1	Si	0.344096	0.319744	0.335162	4e x, y, z
2	Si	0.179516	0.438935	0.128749	4e x, y, z
3	Si	0.809167	0.423465	0.395304	4e x, y, z
4	Si	0.706379	0.315248	0.087713	4e x, y, z
5	Si	0.232341	0.295913	0.710320	4e x, y, z
6	Si	0.278517	0.460614	0.728929	4e x, y, z
7	Si	0.708699	0.444748	0.768845	4e x, y, z
8	Si	0.817902	0.301276	0.705975	4e x, y, z
9	O	0.302523	0.380108	0.218916	4e x, y, z
10	O	0.761890	0.370214	0.238125	4e x, y, z
11	O	0.033192	0.171078	0.215171	4e x, y, z
12	O	0.512292	0.576396	0.233460	4e x, y, z
13	O	0.601071	0.300447	0.446719	4e x, y, z
14	O	0.914593	0.439426	0.032108	4e x, y, z
15	O	0.061776	0.443696	0.483618	4e x, y, z
16	O	0.443680	0.302464	0.970622	4e x, y, z
17	O	0.278485	0.327069	0.529621	4e x, y, z
18	O	0.193572	0.449031	0.902329	4e x, y, z
19	O	0.741775	0.408541	0.586561	4e x, y, z
20	O	0.767848	0.328520	0.892089	4e x, y, z
21	O	0.860886	0.265886	0.260808	4e x, y, z
22	O	0.644502	0.474158	0.240175	4e x, y, z
23	O	0.297960	0.489965	0.311241	4e x, y, z
24	O	0.190841	0.270922	0.155956	4e x, y, z

(b) $P\text{-}1^{(I\text{-}1)}$, 28 GPa

space group P-1 No. 2					
a=6.4552 Å, b=6.6057 Å, c=23.0028 Å, α=89.0231°, β=88.2520°, γ=64.2127°					
number	element	x	y	z	Wyckoff index
1	Si	0.865657	0.672180	0.814708	2i x, y, z
2	Si	0.685731	0.869689	0.938663	2i x, y, z
3	Si	0.323067	0.607977	0.923848	2i x, y, z
4	Si	0.234969	0.917724	0.815115	2i x, y, z

5	Si	0.300053	0.095790	0.581353	2i x, y, z
6	Si	0.682389	0.373748	0.558540	2i x, y, z
7	Si	0.757494	0.281770	0.794122	2i x, y, z
8	Si	0.786203	0.264940	0.961491	2i x, y, z
9	Si	0.213089	0.235578	0.943703	2i x, y, z
10	Si	0.337510	0.297627	0.802140	2i x, y, z
11	Si	0.207734	0.722862	0.558654	2i x, y, z
12	Si	0.771341	0.777819	0.535764	2i x, y, z
13	Si	0.804926	0.583578	0.311336	2i x, y, z
14	Si	0.158959	0.829305	0.323268	2i x, y, z
15	Si	0.685836	0.193861	0.305028	2i x, y, z
16	Si	0.278721	0.190007	0.297741	2i x, y, z
17	O	0.808245	0.768365	0.878557	2i x, y, z
18	O	0.314685	0.742930	0.867425	2i x, y, z
19	O	0.243409	0.272198	0.631669	2i x, y, z
20	O	0.809731	0.305968	0.617883	2i x, y, z
21	O	0.535001	0.794336	0.665244	2i x, y, z
22	O	0.007929	0.761357	0.078017	2i x, y, z
23	O	0.017312	0.283825	0.424831	2i x, y, z
24	O	0.129132	0.564909	0.797860	2i x, y, z
25	O	0.418195	0.969083	0.943104	2i x, y, z
26	O	0.571740	0.517599	0.947646	2i x, y, z
27	O	0.968124	0.027740	0.809006	2i x, y, z
28	O	0.551974	0.015041	0.557750	2i x, y, z
29	O	0.418362	0.464138	0.568059	2i x, y, z
30	O	0.809095	0.469044	0.818015	2i x, y, z
31	O	0.700207	0.098693	0.942983	2i x, y, z
32	O	0.246423	0.424778	0.909066	2i x, y, z
33	O	0.287609	0.114915	0.834177	2i x, y, z
34	O	0.223826	0.908925	0.598335	2i x, y, z
35	O	0.680588	0.603328	0.538915	2i x, y, z
36	O	0.390098	0.761195	0.762165	2i x, y, z
37	O	0.142469	0.779280	0.972096	2i x, y, z
38	O	0.809127	0.685528	0.989532	2i x, y, z
39	O	0.709503	0.873310	0.769691	2i x, y, z
40	O	0.786903	0.188182	0.506732	2i x, y, z
41	O	0.135280	0.243223	0.529298	2i x, y, z
42	O	0.448065	0.711690	0.169917	2i x, y, z
43	O	0.071824	0.459221	0.297941	2i x, y, z
44	O	0.910672	0.940398	0.297826	2i x, y, z
45	O	0.739059	0.389073	0.323219	2i x, y, z
46	O	0.226983	0.019712	0.335280	2i x, y, z
47	O	0.319424	0.664984	0.271764	2i x, y, z

48	O	0.643455	0.773604	0.265218	2i x, y, z

(c) $P2_1/c^{(II)}$, 24 GPa

space group $P2_1/c$ No. 14					
a=6.6143 Å, b=11.8496 Å, c=6.7583 Å, β=119.2974°					
number	element	x	y	z	Wyckoff index
1	Si	0.618415	0.865699	0.169386	4e x, y, z
2	Si	0.877596	0.636959	0.303999	4e x, y, z
3	Si	0.237275	0.902187	0.282204	4e x, y, z
4	Si	0.252914	0.589737	0.198000	4e x, y, z
5	O	0.728716	0.746153	0.208568	4e x, y, z
6	O	0.753347	0.153704	0.505447	4e x, y, z
7	O	0.516311	0.901114	0.912686	4e x, y, z
8	O	0.980018	0.615123	0.565306	4e x, y, z
9	O	0.426117	0.850018	0.237174	4e x, y, z
10	O	0.085405	0.654198	0.257534	4e x, y, z
11	O	0.713376	0.966704	0.665982	4e x, y, z
12	O	0.807852	0.542186	0.831258	4e x, y, z

(d) $P\text{-}1^{(II\text{-}1)}$, 26 GPa

space group P-1 No. 2					
a=6.4574 Å, b=6.5881 Å, c=11.7096 Å, α= 85.7954°, β= 89.7211°, γ= 64.3944°					
number	element	x	y	z	Wyckoff index
1	Si	0.819407	0.559694	0.870626	2i x, y, z
2	Si	0.706203	0.384905	0.654701	2i x, y, z
3	Si	0.328753	0.032806	0.622866	2i x, y, z
4	Si	0.180909	0.959383	0.859385	2i x, y, z
5	Si	0.705561	0.053139	0.905130	2i x, y, z
6	Si	0.800509	0.920241	0.609830	2i x, y, z
7	Si	0.229547	0.535974	0.576366	2i x, y, z
8	Si	0.295812	0.470280	0.900435	2i x, y, z
9	O	0.762525	0.482921	0.758826	2i x, y, z
10	O	0.210944	0.069097	0.741270	2i x, y, z
11	O	0.508165	0.735509	0.158857	2i x, y, z
12	O	0.976093	0.308660	0.348143	2i x, y, z
13	O	0.085393	0.414130	0.897842	2i x, y, z
14	O	0.450141	0.557344	0.613010	2i x, y, z
15	O	0.594546	0.861244	0.628047	2i x, y, z
16	O	0.925548	0.092430	0.898885	2i x, y, z
17	O	0.755893	0.822453	0.852274	2i x, y, z
18	O	0.778226	0.120286	0.683998	2i x, y, z

19	O	0.323916	0.270779	0.591492	2i x, y, z
20	O	0.250986	0.702971	0.833490	2i x, y, z
21	O	0.342265	0.958872	0.960460	2i x, y, z
22	O	0.206883	0.979415	0.520536	2i x, y, z
23	O	0.865319	0.389401	0.552600	2i x, y, z
24	O	0.670838	0.515575	0.966492	2i x, y, z

(e) $P\text{-}1^{(II\text{-}2)}$, 28 GPa

space group P-1 No. 2					
a=6.4571 Å, b=6.4882 Å, c=11.5646 Å, α=91.9300°, β=92.0764°, γ=119.8414°					
number	element	x	y	z	Wyckoff index
1	Si	0.627059	0.705777	0.868564	2i x, y, z
2	Si	0.489350	0.864040	0.633572	2i x, y, z
3	Si	0.109335	0.258634	0.665333	2i x, y, z
4	Si	0.948983	0.395821	0.889787	2i x, y, z
5	Si	0.096857	0.887927	0.935307	2i x, y, z
6	Si	0.981923	0.746391	0.599957	2i x, y, z
7	Si	0.564428	0.374106	0.587942	2i x, y, z
8	Si	0.472844	0.194558	0.892846	2i x, y, z
9	O	0.560681	0.801612	0.755342	2i x, y, z
10	O	0.078087	0.418998	0.770961	2i x, y, z
11	O	0.732156	0.024094	0.167491	2i x, y, z
12	O	0.203654	0.471996	0.347338	2i x, y, z
13	O	0.448195	0.453183	0.891872	2i x, y, z
14	O	0.619377	0.121473	0.590131	2i x, y, z
15	O	0.956943	0.979920	0.663544	2i x, y, z
16	O	0.160615	0.631646	0.967765	2i x, y, z
17	O	0.869547	0.688731	0.865694	2i x, y, z
18	O	0.230307	0.774114	0.623191	2i x, y, z
19	O	0.368199	0.304908	0.674709	2i x, y, z
20	O	0.699826	0.236391	0.835440	2i x, y, z
21	O	0.011274	0.137177	0.929838	2i x, y, z
22	O	0.067113	0.315391	0.535202	2i x, y, z
23	O	0.549587	0.677466	0.546520	2i x, y, z
24	O	0.620658	0.886389	0.976818	2i x, y, z

(f) $P\text{-}1^{(III)}$, 36 GPa

space group P-1 No. 2					
a=5.8261 Å, b=6.4775 Å, c=11.0111 Å, α=85.6411°, β=89.6391°, γ=67.0233°					
number	element	x	y	z	Wyckoff index
1	Si	0.882965	0.542524	0.855510	2i x, y, z

2	Si	0.802112	0.363738	0.626477	2i x, y, z
3	Si	0.395988	0.968024	0.631328	2i x, y, z
4	Si	0.240824	0.898727	0.893619	2i x, y, z
5	Si	0.739786	0.075173	0.830319	2i x, y, z
6	Si	0.919102	0.867137	0.586497	2i x, y, z
7	Si	0.317817	0.463664	0.658446	2i x, y, z
8	Si	0.369405	0.398353	0.940538	2i x, y, z
9	O	0.931399	0.422554	0.729392	2i x, y, z
10	O	0.338870	0.940680	0.768260	2i x, y, z
11	O	0.529317	0.682433	0.203189	2i x, y, z
12	O	0.899406	0.301721	0.298680	2i x, y, z
13	O	0.133044	0.353369	0.930644	2i x, y, z
14	O	0.516645	0.540011	0.615808	2i x, y, z
15	O	0.678515	0.828101	0.605101	2i x, y, z
16	O	0.959392	0.098957	0.887406	2i x, y, z
17	O	0.761408	0.823419	0.837721	2i x, y, z
18	O	0.816958	0.109618	0.675802	2i x, y, z
19	O	0.339610	0.235153	0.609571	2i x, y, z
20	O	0.205730	0.675317	0.904777	2i x, y, z
21	O	0.393605	0.877595	0.018065	2i x, y, z
22	O	0.193897	0.956247	0.544779	2i x, y, z
23	O	0.899674	0.367661	0.494836	2i x, y, z
24	O	0.638849	0.543578	0.911054	2i x, y, z

(g) $P1^{(2)}$, 50 GPa

space group $P1$ No. 1					
a=11.7093 Å, b=11.2923 Å, c=10.2365 Å, α=91.4108°, β=77.5664°, γ=87.5721°					
number	element	x	y	z	Wyckoff index
1	Si	0.028676	0.342618	0.133863	1a x, y, z
2	Si	0.583428	0.972276	0.874940	1a x, y, z
3	Si	0.729095	0.145669	0.837733	1a x, y, z
4	Si	0.795529	0.266682	0.084616	1a x, y, z
5	Si	0.041854	0.266669	0.585066	1a x, y, z
6	Si	0.355607	0.392129	0.336062	1a x, y, z
7	Si	0.092151	0.464286	0.382627	1a x, y, z
8	Si	0.402569	0.092031	0.633128	1a x, y, z
9	Si	0.915594	0.009596	0.086962	1a x, y, z
10	Si	0.602469	0.391349	0.832702	1a x, y, z
11	Si	0.967173	0.212806	0.884283	1a x, y, z
12	Si	0.480963	0.139219	0.336659	1a x, y, z
13	Si	0.279118	0.340830	0.633103	1a x, y, z
14	Si	0.218161	0.214951	0.383360	1a x, y, z

15	Si	0.151493	0.092155	0.133333	1a x, y, z
16	Si	0.417411	0.518219	0.582120	1a x, y, z
17	Si	0.693297	0.904868	0.036991	1a x, y, z
18	Si	0.844877	0.462353	0.882651	1a x, y, z
19	Si	0.981708	0.639751	0.836987	1a x, y, z
20	Si	0.522853	0.769682	0.079622	1a x, y, z
21	Si	0.802449	0.760688	0.591197	1a x, y, z
22	Si	0.696024	0.815630	0.430575	1a x, y, z
23	Si	0.845970	0.969632	0.379443	1a x, y, z
24	Si	0.655147	0.584869	0.626230	1a x, y, z
25	Si	0.163726	0.518583	0.084821	1a x, y, z
26	Si	0.349826	0.893234	0.837068	1a x, y, z
27	Si	0.215076	0.715424	0.885177	1a x, y, z
28	Si	0.227794	0.642369	0.335710	1a x, y, z
29	Si	0.033278	0.839580	0.632484	1a x, y, z
30	Si	0.460569	0.725997	0.388446	1a x, y, z
31	Si	0.896684	0.591224	0.142550	1a x, y, z
32	Si	0.166517	0.017604	0.585415	1a x, y, z
33	Si	0.526498	0.341301	0.133767	1a x, y, z
34	Si	0.090558	0.965193	0.885449	1a x, y, z
35	Si	0.228196	0.142900	0.835586	1a x, y, z
36	Si	0.289612	0.269208	0.086303	1a x, y, z
37	Si	0.540025	0.270291	0.582980	1a x, y, z
38	Si	0.854219	0.395367	0.335188	1a x, y, z
39	Si	0.596900	0.474575	0.383067	1a x, y, z
40	Si	0.903857	0.090256	0.633827	1a x, y, z
41	Si	0.409671	0.019374	0.088903	1a x, y, z
42	Si	0.104328	0.390731	0.835068	1a x, y, z
43	Si	0.464621	0.217398	0.883633	1a x, y, z
44	Si	0.979049	0.146011	0.334755	1a x, y, z
45	Si	0.779540	0.340142	0.633139	1a x, y, z
46	Si	0.715995	0.218092	0.386195	1a x, y, z
47	Si	0.651643	0.105075	0.145560	1a x, y, z
48	Si	0.917910	0.515426	0.584452	1a x, y, z
49	Si	0.273110	0.841262	0.135407	1a x, y, z
50	Si	0.340067	0.465479	0.882261	1a x, y, z
51	Si	0.477867	0.640738	0.830661	1a x, y, z
52	Si	0.036100	0.769724	0.085876	1a x, y, z
53	Si	0.289821	0.767417	0.586513	1a x, y, z
54	Si	0.102643	0.893384	0.335429	1a x, y, z
55	Si	0.341749	0.962893	0.383838	1a x, y, z
56	Si	0.154814	0.588676	0.633048	1a x, y, z
57	Si	0.668063	0.503753	0.075340	1a x, y, z

58	Si	0.860813	0.887951	0.828956	1a x, y, z
59	Si	0.721595	0.709245	0.879203	1a x, y, z
60	Si	0.659258	0.692244	0.206004	1a x, y, z
61	Si	0.523379	0.844376	0.638587	1a x, y, z
62	Si	0.965388	0.716275	0.382284	1a x, y, z
63	Si	0.402065	0.584484	0.132470	1a x, y, z
64	Si	0.664534	0.019744	0.583892	1a x, y, z
65	O	0.852994	0.321993	0.932732	1a x, y, z
66	O	0.709845	0.175167	0.001861	1a x, y, z
67	O	0.031222	0.406870	0.533886	1a x, y, z
68	O	0.171535	0.557228	0.467781	1a x, y, z
69	O	0.727167	0.077441	0.437270	1a x, y, z
70	O	0.836164	0.424334	0.502525	1a x, y, z
71	O	0.047234	0.307098	0.967656	1a x, y, z
72	O	0.407211	0.157291	0.034421	1a x, y, z
73	O	0.881348	0.340173	0.164138	1a x, y, z
74	O	0.583627	0.118724	0.850537	1a x, y, z
75	O	0.988468	0.488322	0.868901	1a x, y, z
76	O	0.417615	0.868614	0.120529	1a x, y, z
77	O	0.048879	0.114536	0.619627	1a x, y, z
78	O	0.504488	0.395002	0.302226	1a x, y, z
79	O	0.209988	0.367078	0.349645	1a x, y, z
80	O	0.395313	0.242890	0.599353	1a x, y, z
81	O	0.764411	0.998381	0.104646	1a x, y, z
82	O	0.692688	0.465764	0.910777	1a x, y, z
83	O	0.877211	0.137774	0.803935	1a x, y, z
84	O	0.536636	0.204529	0.183587	1a x, y, z
85	O	0.191488	0.265281	0.552853	1a x, y, z
86	O	0.363621	0.239831	0.369297	1a x, y, z
87	O	0.091513	0.034258	0.284250	1a x, y, z
88	O	0.505093	0.594466	0.665037	1a x, y, z
89	O	0.736197	0.188924	0.220119	1a x, y, z
90	O	0.718040	0.282047	0.783386	1a x, y, z
91	O	0.860896	0.431558	0.718004	1a x, y, z
92	O	0.572487	0.010241	0.054097	1a x, y, z
93	O	0.164836	0.448746	0.684125	1a x, y, z
94	O	0.397033	0.049920	0.250665	1a x, y, z
95	O	0.067801	0.216556	0.416672	1a x, y, z
96	O	0.522189	0.299116	0.749740	1a x, y, z
97	O	0.603377	0.829648	0.937736	1a x, y, z
98	O	0.961327	0.673207	0.000533	1a x, y, z
99	O	0.778331	0.903733	0.533665	1a x, y, z
100	O	0.921523	0.058897	0.468157	1a x, y, z

101	O	0.976091	0.575271	0.434927	1a x, y, z
102	O	0.588299	0.918057	0.503399	1a x, y, z
103	O	0.796505	0.808350	0.962900	1a x, y, z
104	O	0.656192	0.653623	0.035944	1a x, y, z
105	O	0.128057	0.841385	0.166081	1a x, y, z
106	O	0.332987	0.618124	0.849067	1a x, y, z
107	O	0.236047	0.991033	0.869481	1a x, y, z
108	O	0.174092	0.366324	0.118960	1a x, y, z
109	O	0.299766	0.614799	0.619436	1a x, y, z
110	O	0.250065	0.891617	0.303443	1a x, y, z
111	O	0.959911	0.868751	0.351385	1a x, y, z
112	O	0.146759	0.741146	0.600379	1a x, y, z
113	O	0.020875	0.493033	0.099437	1a x, y, z
114	O	0.439254	0.968714	0.918738	1a x, y, z
115	O	0.129760	0.639458	0.802701	1a x, y, z
116	O	0.293485	0.700027	0.184615	1a x, y, z
117	O	0.946654	0.764341	0.554128	1a x, y, z
118	O	0.611464	0.733264	0.364339	1a x, y, z
119	O	0.343755	0.533007	0.283740	1a x, y, z
120	O	0.253860	0.092633	0.666540	1a x, y, z
121	O	0.983403	0.683838	0.219404	1a x, y, z
122	O	0.468751	0.784413	0.787041	1a x, y, z
123	O	0.108640	0.933101	0.718984	1a x, y, z
124	O	0.314411	0.515666	0.051484	1a x, y, z
125	O	0.914082	0.948427	0.682430	1a x, y, z
126	O	0.648865	0.548251	0.237048	1a x, y, z
127	O	0.313640	0.716119	0.417843	1a x, y, z
128	O	0.273436	0.799411	0.751906	1a x, y, z
129	O	0.351931	0.325322	0.934951	1a x, y, z
130	O	0.211574	0.175763	0.000564	1a x, y, z
131	O	0.528753	0.409892	0.533772	1a x, y, z
132	O	0.670039	0.553053	0.471067	1a x, y, z
133	O	0.228026	0.074774	0.434831	1a x, y, z
134	O	0.335429	0.425234	0.500489	1a x, y, z
135	O	0.546614	0.308479	0.965891	1a x, y, z
136	O	0.905441	0.154238	0.033629	1a x, y, z
137	O	0.377904	0.343220	0.166179	1a x, y, z
138	O	0.083573	0.116987	0.848611	1a x, y, z
139	O	0.486311	0.490597	0.866626	1a x, y, z
140	O	0.931419	0.869816	0.117923	1a x, y, z
141	O	0.548165	0.114767	0.618802	1a x, y, z
142	O	0.005871	0.389215	0.303265	1a x, y, z
143	O	0.708324	0.369235	0.349191	1a x, y, z

144	O	0.895537	0.241040	0.600679	1a x, y, z
145	O	0.267020	0.994013	0.099824	1a x, y, z
146	O	0.191546	0.466791	0.915193	1a x, y, z
147	O	0.378222	0.141527	0.803283	1a x, y, z
148	O	0.040448	0.201515	0.184007	1a x, y, z
149	O	0.690169	0.266516	0.554408	1a x, y, z
150	O	0.861927	0.242671	0.371219	1a x, y, z
151	O	0.591480	0.041661	0.281767	1a x, y, z
152	O	0.005272	0.589895	0.666410	1a x, y, z
153	O	0.234967	0.183755	0.217628	1a x, y, z
154	O	0.218632	0.282907	0.784251	1a x, y, z
155	O	0.359754	0.434088	0.717131	1a x, y, z
156	O	0.066650	0.017599	0.050960	1a x, y, z
157	O	0.664000	0.448994	0.685102	1a x, y, z
158	O	0.898247	0.053835	0.249835	1a x, y, z
159	O	0.566494	0.219525	0.417239	1a x, y, z
160	O	0.023417	0.297588	0.750768	1a x, y, z
161	O	0.102890	0.824650	0.933089	1a x, y, z
162	O	0.459132	0.673129	0.998772	1a x, y, z
163	O	0.278558	0.907823	0.537316	1a x, y, z
164	O	0.422545	0.056436	0.469315	1a x, y, z
165	O	0.476735	0.579653	0.433198	1a x, y, z
166	O	0.086200	0.925072	0.501440	1a x, y, z
167	O	0.296351	0.808787	0.968831	1a x, y, z
168	O	0.155352	0.658664	0.035209	1a x, y, z
169	O	0.621430	0.829960	0.159565	1a x, y, z
170	O	0.835783	0.615535	0.848997	1a x, y, z
171	O	0.733722	0.983839	0.878058	1a x, y, z
172	O	0.674087	0.361288	0.116196	1a x, y, z
173	O	0.799106	0.613138	0.622069	1a x, y, z
174	O	0.758626	0.893259	0.311354	1a x, y, z
175	O	0.447804	0.864673	0.350680	1a x, y, z
176	O	0.648204	0.745557	0.590717	1a x, y, z
177	O	0.519607	0.489940	0.093956	1a x, y, z
178	O	0.940551	0.965397	0.914774	1a x, y, z
179	O	0.628327	0.644269	0.801695	1a x, y, z
180	O	0.794537	0.699578	0.178949	1a x, y, z
181	O	0.439391	0.767605	0.556091	1a x, y, z
182	O	0.111888	0.739671	0.368451	1a x, y, z
183	O	0.847469	0.526381	0.281594	1a x, y, z
184	O	0.753158	0.088237	0.670143	1a x, y, z
185	O	0.490750	0.682135	0.215946	1a x, y, z
186	O	0.970015	0.780535	0.783252	1a x, y, z

187	O	0.608960	0.933738	0.718304	1a x, y, z
188	O	0.816204	0.511562	0.049385	1a x, y, z
189	O	0.413166	0.951601	0.687605	1a x, y, z
190	O	0.148623	0.549926	0.250718	1a x, y, z
191	O	0.815701	0.721798	0.424020	1a x, y, z
192	O	0.773494	0.798121	0.749622	1a x, y, z