Supplementary Information for "Partially Diffusive Helium-Silica Compound under High Pressure"

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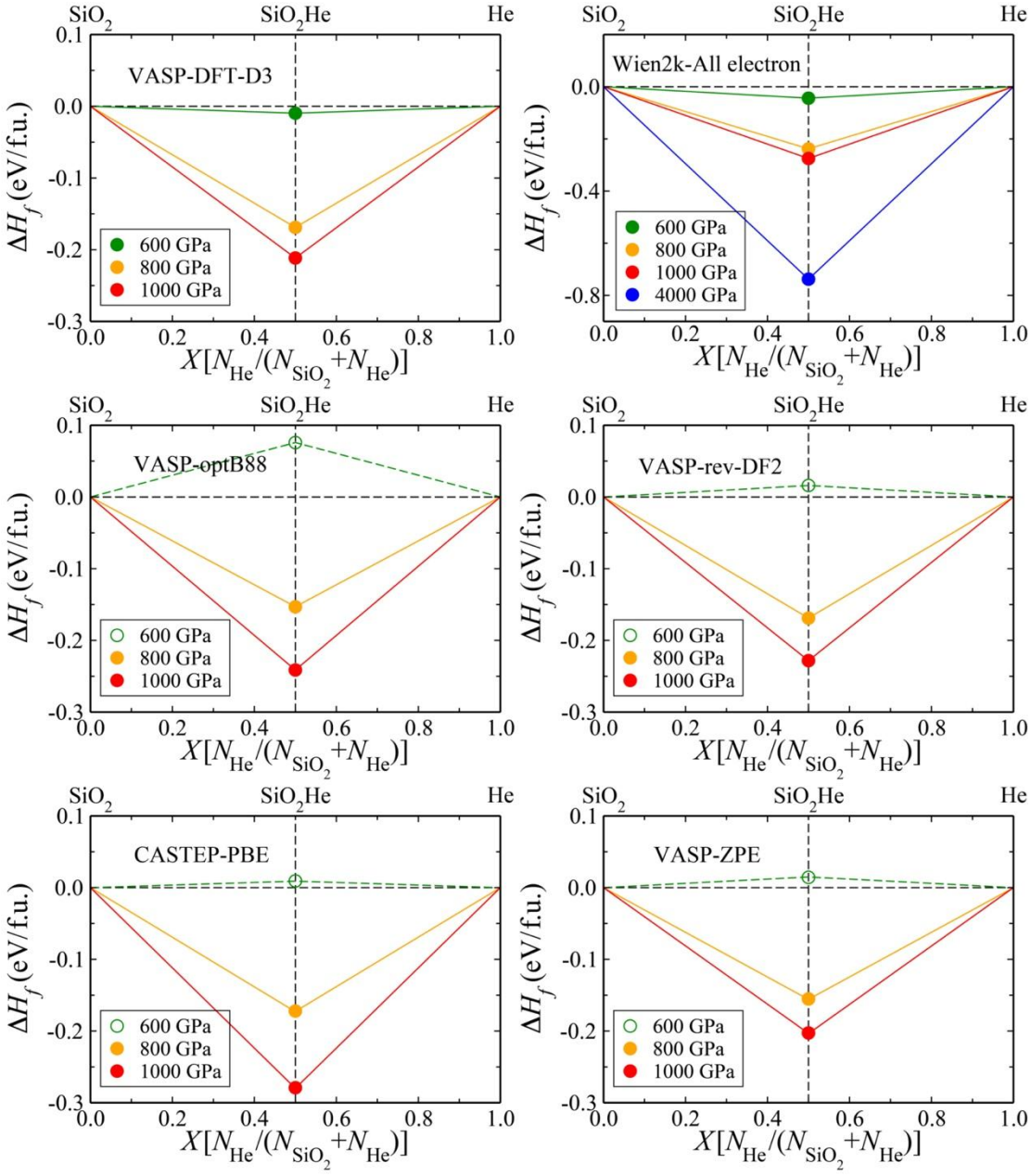

Fig. S1. Convexhull of formation enthalpies (ΔH_f) calculated from DFT-D3[1], all electron potentials (Wien2k[2]), vdw-optB88[3] and rev-vdw-DF2[4], CASTEP[5], and with zero point energy (ZPE). The results are robust and consistent with different functionals and methods.

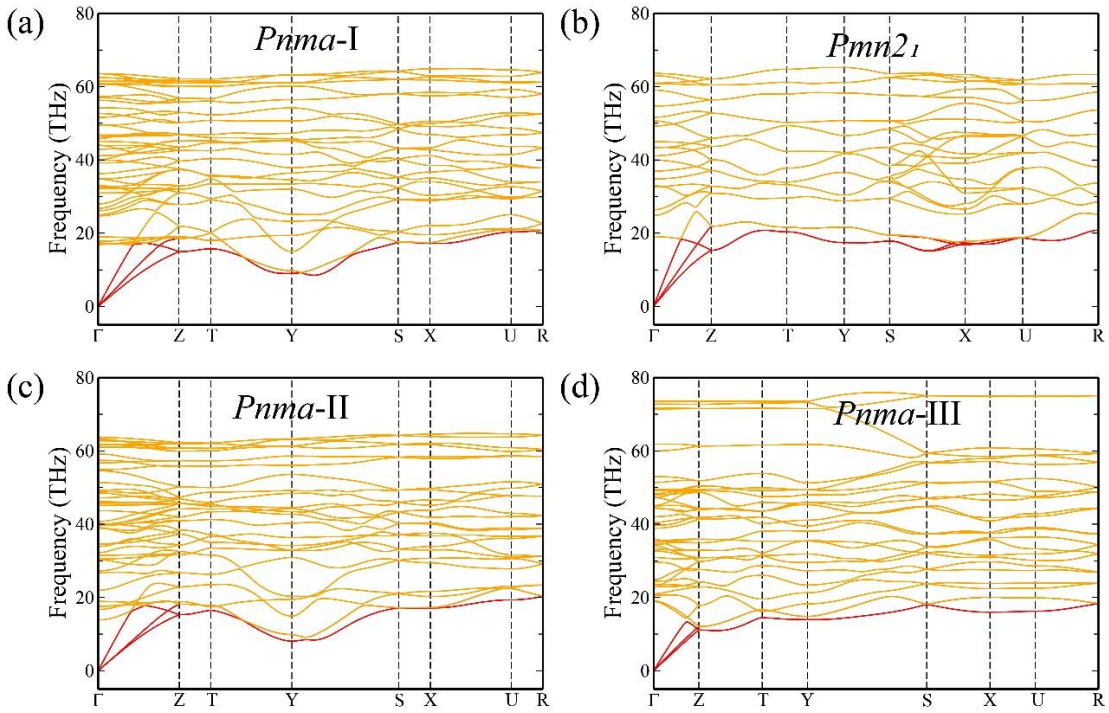

Fig. S2. Calculated Phonon spectra of the thermodynamically stable/metastable phases: (a) *Pnma*-I, (b) *Pmn2*$_1$, (c) *Pnma*-II, and (d) *Pnma*-III. The orange curves correspond to optical branches and the red curves correspond to acoustic branches. No imaginary vibrational frequencies were found in the phonon spectra.

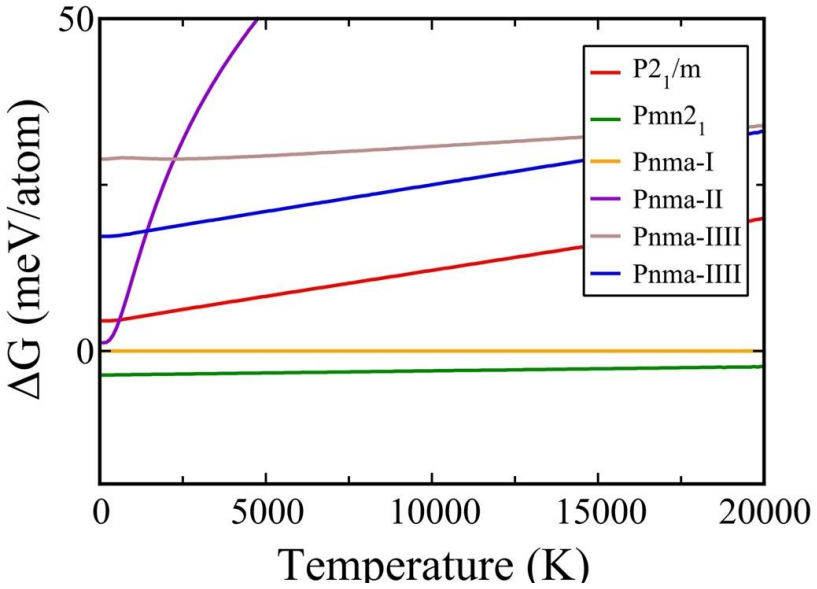

Fig. S3. Gibbs free energy at 2000 GPa based on QHA calculations.

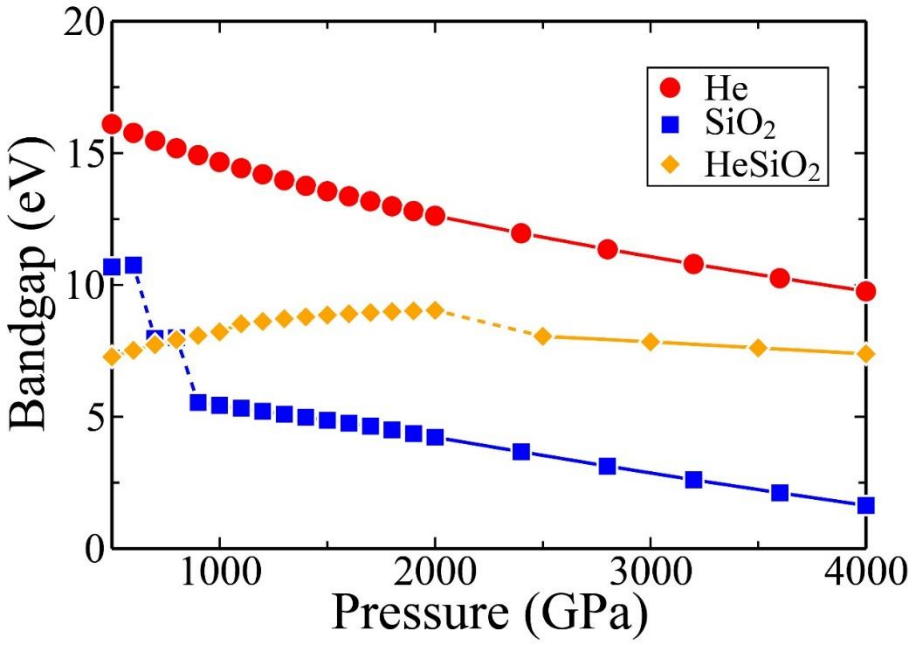

Fig. S4. Calculated Band gaps of He, SiO_2, and $HeSiO_2$ over the pressure range 500-4000 GPa based on simply pure PBE functional.

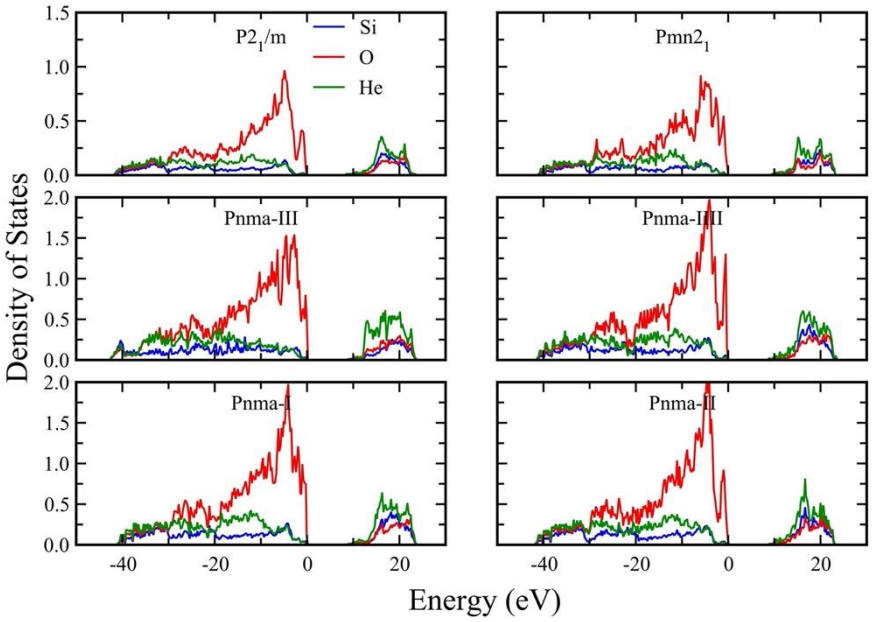

Fig. S5. Density of states for all $HeSiO_2$ canidates at 2000 GPa based on simply pure PBE functional.

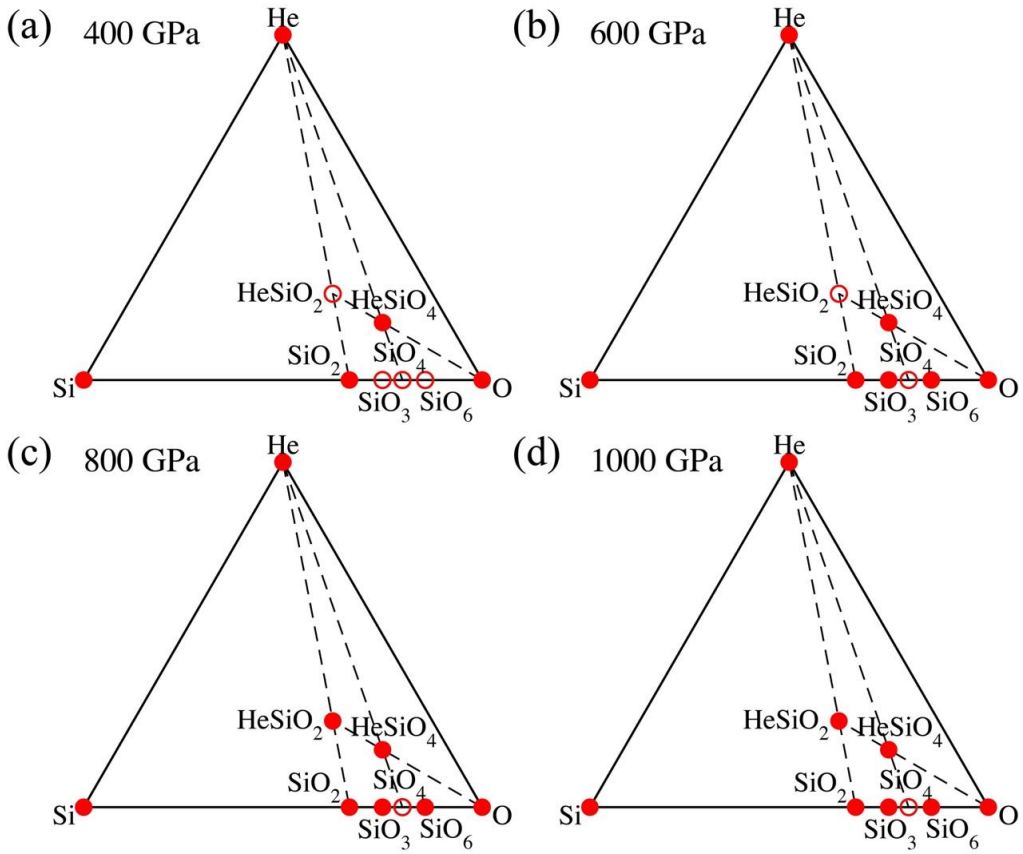

Fig. S6. Ternary phase diagram of the He-Si-O system at 400, 600, 800, and 1000 GPa. The stable/unstable phases are marked in solid/open red points.

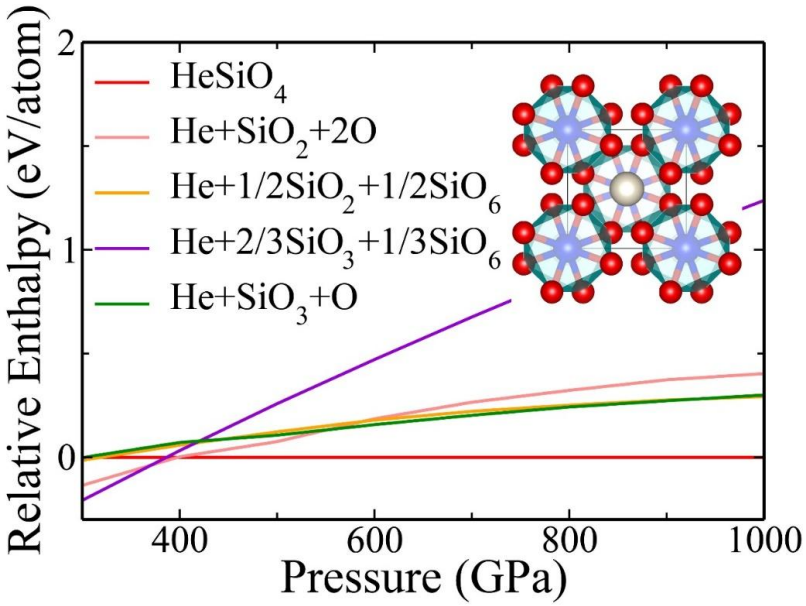

Fig. S7. Enthalpies of the $HeSiO_4$ compounds, as well as its possible decompositions in the pressure range between 300 and 1000 GPa. Insert figure show the crystal structure of *I422* phase $HeSiO_4$.

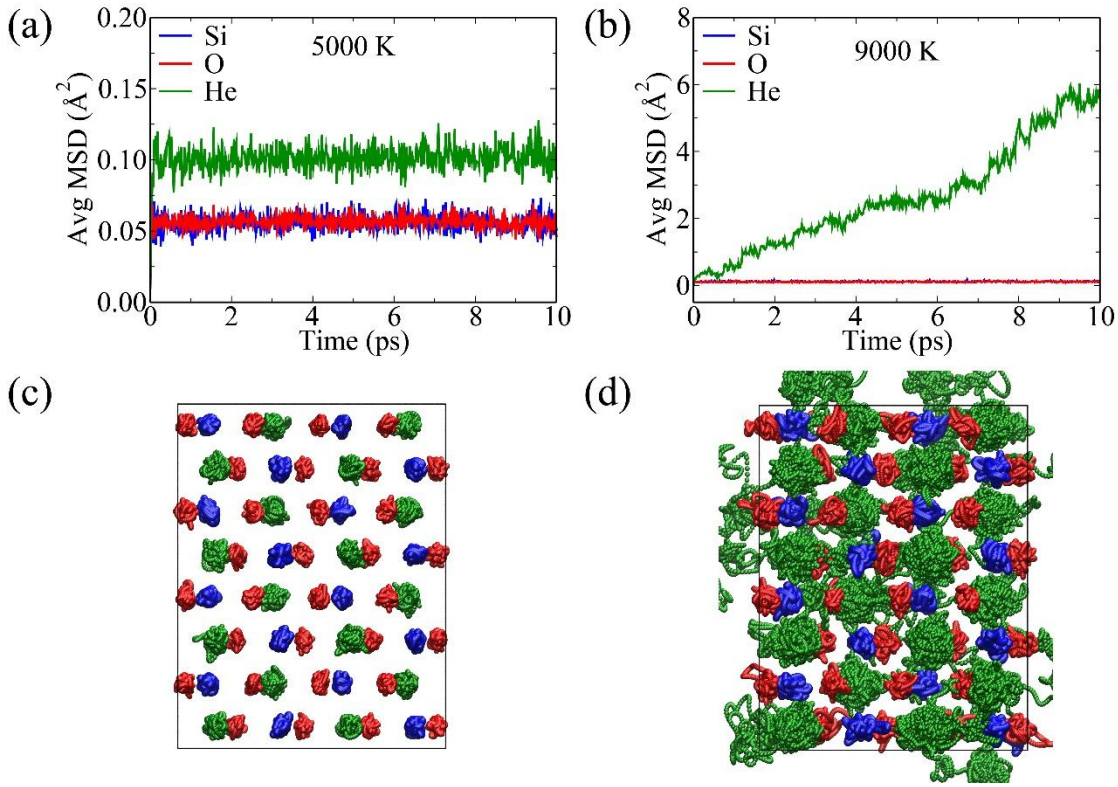

Fig S8. Dynamical behavior of Si (blue), O (red), and He atoms (dark green) in the $HeSiO_2$ compound under high pressures and high temperatures. AIMD simulations were performed at initial pressure of 600 GPa for the *Pnma* $HeSiO_2$ compound. (a-b) The averaged mean-squared displacements (MSD). (c-d) Atomic trajectories from the simulations representing the plastic phase. The Si, O and He atoms are respectively plotted with blue, red, and dark green.

Table I. Bader charge on helium atoms in different phases.

Pressure	$P2_1/m$	$Pmn2_1$	Pnma-III	Pnma-IIII	Pnma-I	Pnma-II
500 GPa	2.075	2.078	2.072	2.079	2.078	2.075
1000 GPa	2.088	2.085	2.069	2.090	2.083	2.087
2000 GPa	2.095	2.083	2.056	2.089	2.088	2.093
3000 GPa	2.105	2.079	2.064	2.106	2.082	2.083
4000 GPa	2.112	2.090	2.074	2.116	2.092	2.079

Table II. Thermodynamic data from our simulations affect by different box size (number of atoms in supercells: *N*) and *k-mesh* on motion behaviors of each species of atom in *Pnma*-I phase.

V (Å^3)	T (K)	P (GPa)	N	*k-mesh*	D_{Si} D_O D_{He} ($10^{-8}\,m^2/s$)	State
659.04	5000	663.84	192	$1 \times 1 \times 1$	0.00 0.00 0.00	Solid
659.04	5000	663.97	192	$2 \times 2 \times 2$	0.00 0.00 0.00	Solid
1318.09	5000	663.93	384	$1 \times 1 \times 1$	0.00 0.00 0.00	Solid
659.04	9000	721.66	192	$1 \times 1 \times 1$	0.00 0.00 0.12	*SI*
659.04	9000	719.64	192	$2 \times 2 \times 2$	0.00 0.00 0.10	*SI*
1318.09	9000	721.45	384	$1 \times 1 \times 1$	0.00 0.00 0.08	*SI*
659.04	9000	820.87	192	$1 \times 1 \times 1$	1.08 1.48 3.37	Fluid
659.04	12000	822.06	192	$2 \times 2 \times 2$	1.07 1.51 4.02	Fluid
1318.09	12000	820.75	384	$1 \times 1 \times 1$	1.06 1.40 3.98	Fluid

Table III. Structural information for $HeSiO_2$ compounds at 1000 GPa.

Space group	Lattice parameters (Å)	Atomic coordinates (fractional)	
Pnma-I	a = 7.3530 b = 2.2022 c = 2.8982	Si	0.6125 0.7500 0.2546
		O	0.9667 0.2500 0.2499
		O	0.2153 0.2500 0.0276
		He	0.3531 0.7500 0.0657
Pnma-II	a = 7.4130 b = 2.1865 c = 2.8849	Si	0.8618 0.7500 0.5341
		O	0.0339 0.7500 0.2387
		O	0.2835 0.7500 0.4700
		He	0.1023 0.7500 0.7868
Pnma-III	a = 3.9635 b = 2.1028 c = 5.5564	Si	0.8139 0.7500 0.1580
		O	0.6865 0.7500 0.4528
		O	0.9774 0.7500 0.7208
		He	0.4570 0.2500 0.9751
Pnma-IV	a = 5.4683 b = 2.1832 c = 3.9197	Si	0.3271 0.2500 0.1362
		O	0.3930 0.7500 0.8795
		O	0.6083 0.2500 0.6175
		He	0.6496 0.7500 0.3703
$Pmn2_1$	a = 2.2011 b = 3.6785 c = 2.8973	Si	0.0000 0.7249 0.7610
		O	0.0000 0.0697 0.4804
		O	0.5000 0.4334 0.7582
		He	0.5000 0.7940 0.4424
$P2_1/m$	a = 2.8890 b = 2.1869 c = 4.0453	Si	0.3805 0.7500 0.7236
		O	0.2124 0.2500 0.4332
		O	0.7235 0.2500 0.9325
		He	0.0984 0.2500 0.7953

Table V. Structural information for $HeSiO_4$ compounds at 1000 GPa.

Space group	Lattice parameters (Å)	Atomic coordinates (fractional)	
I422	a = 3.2944	Si	0.5000 0.5000 0.5000
		O	0.6312 0.8688 0.7500
		He	0.5000 0.5000 0.0000

Reference

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