Supporting information

for

Volume dependence of the dielectric properties of amorphous SiO_2

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Table S1. Monkhorst-Pack grids used in the first principles calculations. For non am-SiO_2 polymorphs, Materials Project id of each SiO_2 is given[1]

System	Type of calculations	Size
All systems	BOMD	single Γ-point
	Density functional perturbation theory	2×2×2
am-SiO_2	Frequency dependent dielectric function	4×4×4
α-SiO_2		4×4×4
SiO_2 (mp-604717)		5×5×5
SiO_2 (mp-560527)		5×4×5
SiO_2 (mp-559273)		2×3×3
SiO_2 (mp-555960)		4×4×4
SiO_2 (mp-11684)		6×4×7
SiO_2 (mp-10948)		5×5×4

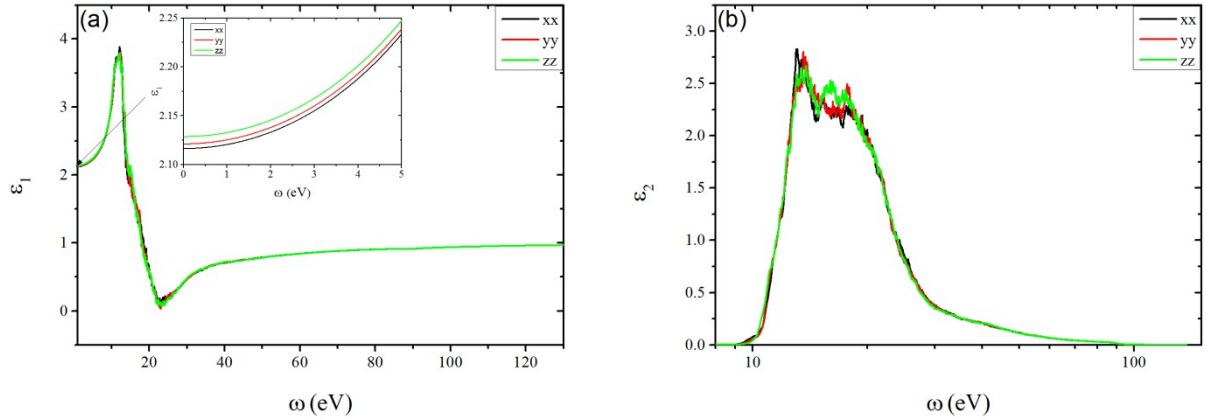

Figure S1 (a) Real and (b) imaginary parts of frequency dependent dielectric tensor computed for most anisotropic am-SiO_2 sample (Δ = 3.6 eV). The ionic contribution to the dielectric function is not shown.

Visualization

The visualization of computed structures was made by VESTA software.[2]

Structures used in calculations of dielectric functions

Amorphous SiO_2

am-SiO_2(generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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am-SiO_2 (generated by BOMD: 10ps at 5000 K, 10ps from 5000 to 2500 K, 20ps at 2500K, 30ps from 2500 to 1 K)

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am-SiO_2 (generated by BOMD: 10ps at 5000 K, 5ps from 5000 to 2500 K, 10ps at 2500K, 30ps from 2500 to 1 K)

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  O  O25  1  0.851224  0.971737  0.157465  1
  O  O26  1  0.390548  0.941543  0.695250  1
  O  O27  1  0.733354  0.799296  0.680404  1
  O  O28  1  0.197928  0.310841  0.130378  1
  O  O29  1  0.947107  0.528908  0.977322  1
  O  O30  1  0.521090  0.089266  0.898434  1
  O  O31  1  0.828981  0.294457  0.453571  1
  O  O32  1  0.194613  0.561900  0.199214  1
  O  O33  1  0.325240  0.530530  0.973487  1
  O  O34  1  0.227522  0.986483  0.862879  1
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O O35 1 0.675397 0.019658 0.032788 1
O O36 1 0.841740 0.236581 0.884402 1
O O37 1 0.147997 0.012124 0.338958 1
O O38 1 0.364787 0.413149 0.627557 1
O O39 1 0.405932 0.758065 0.366764 1
O O40 1 0.309289 0.781318 0.893586 1
O O41 1 0.034459 0.019529 0.737480 1
O O42 1 0.683802 0.381863 0.095377 1
O O43 1 0.530050 0.439946 0.249030 1
O O44 1 0.046919 0.309626 0.326785 1
O O45 1 0.860053 0.444241 0.756935 1
O O46 1 0.123659 0.484859 0.824771 1
O O47 1 0.400330 0.139096 0.185915 1
O O48 1 0.329541 0.425344 0.407364 1
Si Si49 1 0.359604 0.949096 0.836728 1
Si Si50 1 0.507039 0.320845 0.141325 1
Si Si51 1 0.018031 0.401322 0.436012 1
Si Si52 1 0.505302 0.383937 0.608036 1
Si Si53 1 0.911724 0.854623 0.667910 1
Si Si54 1 0.233586 0.348651 0.529021 1
Si Si55 1 0.936275 0.890974 0.088246 1
Si Si56 1 0.786295 0.088279 0.145462 1
Si Si57 1 0.238803 0.690739 0.307582 1
Si Si58 1 0.511433 0.490722 0.378797 1
Si Si59 1 0.124282 0.997000 0.477226 1
Si Si60 1 0.580836 0.802247 0.707588 1
Si Si61 1 0.230004 0.984625 0.225136 1
Si Si62 1 0.408623 0.042155 0.582691 1
Si Si63 1 0.107670 0.043109 0.864303 1
Si Si64 1 0.693862 0.118277 0.403596 1
Si Si65 1 0.946087 0.423896 0.862234 1
Si Si66 1 0.290739 0.359150 0.005010 1
Si Si67 1 0.788752 0.552037 0.770579 1
Si Si68 1 0.801010 0.542581 0.022689 1
Si Si69 1 0.093983 0.368601 0.194162 1
Si Si70 1 0.299126 0.614917 0.868361 1
Si Si71 1 0.553886 0.796282 0.443167 1
Si Si72 1 0.672168 0.076081 0.903444 1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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_cell_length_c   12.14878968
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_cell_angle_beta   91.56996482
_cell_angle_gamma   121.46101606
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si24 O48'
_cell_volume   1036.16672418
_cell_formula_units_Z   24
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  O  O1  1  0.483003  0.650035  0.176743  1
  O  O2  1  0.892410  0.969880  0.683315  1
  O  O3  1  0.825616  0.155272  0.544636  1
  O  O4  1  0.448883  0.273904  0.763945  1
  O  O5  1  0.015886  0.439962  0.926165  1
  O  O6  1  0.781413  0.796036  0.203119  1
  O  O7  1  0.153715  0.508916  0.668636  1
  O  O8  1  0.680264  0.504493  0.617970  1
  O  O9  1  0.147502  0.250428  0.673448  1
  O  O10  1  0.450229  0.209033  0.354693  1
  O  O11  1  0.250316  0.428691  0.853233  1
  O  O12  1  0.427202  0.508731  0.676395  1
  O  O13  1  0.492062  0.976155  0.448829  1
  O  O14  1  0.378369  0.926370  0.051000  1
  O  O15  1  0.049120  0.046873  0.506338  1
  O  O16  1  0.036803  0.964136  0.303078  1
  O  O17  1  0.214162  0.939878  0.449950  1
  O  O18  1  0.837385  0.426077  0.496660  1
  O  O19  1  0.225315  0.465239  0.069033  1
  O  O20  1  0.138492  0.648398  0.466810  1
  O  O21  1  0.390681  0.657484  0.463349  1
  O  O22  1  0.033740  0.993265  0.082833  1
  O  O23  1  0.816730  0.253486  0.335825  1
  O  O24  1  0.916494  0.801574  0.912823  1
  O  O25  1  0.221700  0.548177  0.277425  1
  O  O26  1  0.732132  0.088067  0.749143  1
  O  O27  1  0.650709  0.633624  0.024481  1
  O  O28  1  0.329897  0.804887  0.622926  1
  O  O29  1  0.895731  0.731989  0.467773  1
  O  O30  1  0.995355  0.648951  0.642671  1
  O  O31  1  0.615726  0.481444  0.224579  1
  O  O32  1  0.734265  0.205411  0.939424  1
  O  O33  1  0.187950  0.014229  0.690854  1
  O  O34  1  0.283504  0.697724  0.914030  1
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O O35 1 0.079275 0.373599 0.450201 1
O O36 1 0.179081 0.086306 0.891632 1
O O37 1 0.873367 0.346874 0.124565 1
O O38 1 0.893877 0.057156 0.919284 1
O O39 1 0.614507 0.861568 0.596178 1
O O40 1 0.577407 0.905049 0.921000 1
O O41 1 0.449660 0.199600 0.138350 1
O O42 1 0.312328 0.341118 0.233259 1
O O43 1 0.903342 0.108512 0.203364 1
O O44 1 0.339281 0.934042 0.262145 1
O O45 1 0.657597 0.572986 0.817550 1
O O46 1 0.374997 0.990022 0.839011 1
O O47 1 0.799160 0.496742 0.972465 1
O O48 1 0.624503 0.069826 0.182235 1
Si Si49 1 0.555253 0.462131 0.718258 1
Si Si50 1 0.804578 0.194180 0.212882 1
Si Si51 1 0.300330 0.094870 0.798064 1
Si Si52 1 0.405522 0.882384 0.930431 1
Si Si53 1 0.890864 0.305645 0.457507 1
Si Si54 1 0.847509 0.576460 0.554471 1
Si Si55 1 0.198697 0.509460 0.942540 1
Si Si56 1 0.373932 0.016609 0.380705 1
Si Si57 1 0.153227 0.657417 0.604265 1
Si Si58 1 0.212978 0.555905 0.410622 1
Si Si59 1 0.765823 0.018837 0.642514 1
Si Si60 1 0.306434 0.498844 0.189255 1
Si Si61 1 0.450165 0.033425 0.155520 1
Si Si62 1 0.455798 0.307100 0.238625 1
Si Si63 1 0.939235 0.967965 0.196452 1
Si Si64 1 0.072269 0.070402 0.638113 1
Si Si65 1 0.855698 0.373295 0.992419 1
Si Si66 1 0.457523 0.823392 0.531163 1
Si Si67 1 0.636286 0.640230 0.156558 1
Si Si68 1 0.041574 0.912161 0.431444 1
Si Si69 1 0.740664 0.064345 0.882359 1
Si Si70 1 0.006191 0.985192 0.949273 1
Si Si71 1 0.757744 0.627509 0.929676 1
Si Si72 1 0.246697 0.426253 0.718326 1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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_cell_angle_beta   89.96162115
_cell_angle_gamma   121.30465328
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si24 O48'
_cell_volume   1039.52507081
_cell_formula_units_Z   24
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 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  O  O1  1  0.380782  0.754167  0.558927  1
  O  O2  1  0.539217  0.480724  0.435512  1
  O  O3  1  0.236095  0.006976  0.260721  1
  O  O4  1  0.852671  0.749373  0.167139  1
  O  O5  1  0.387876  0.328619  0.853203  1
  O  O6  1  0.666022  0.858166  0.447081  1
  O  O7  1  0.344921  0.707353  0.109998  1
  O  O8  1  0.616918  0.798475  0.183542  1
  O  O9  1  0.827532  0.349090  0.208530  1
  O  O10  1  0.329541  0.192298  0.063085  1
  O  O11  1  0.617803  0.043513  0.574724  1
  O  O12  1  0.701720  0.250658  0.982293  1
  O  O13  1  0.945254  0.807013  0.952637  1
  O  O14  1  0.877687  0.983408  0.280314  1
  O  O15  1  0.506941  0.158369  0.219106  1
  O  O16  1  0.932531  0.564827  0.368908  1
  O  O17  1  0.829391  0.526299  0.043836  1
  O  O18  1  0.112569  0.574284  0.686401  1
  O  O19  1  0.001061  0.344963  0.379181  1
  O  O20  1  0.817889  0.938260  0.837697  1
  O  O21  1  0.366300  0.322441  0.261332  1
  O  O22  1  0.791596  0.555151  0.558843  1
  O  O23  1  0.246849  0.389029  0.009113  1
  O  O24  1  0.519209  0.855427  0.838074  1
  O  O25  1  0.102268  0.364270  0.824103  1
  O  O26  1  0.983649  0.366176  0.034684  1
  O  O27  1  0.535384  0.124758  0.804214  1
  O  O28  1  0.414795  0.858768  0.291201  1
  O  O29  1  0.107263  0.742846  0.097673  1
  O  O30  1  0.238437  0.340246  0.455242  1
  O  O31  1  0.190804  0.616659  0.929694  1
  O  O32  1  0.715347  0.267115  0.413844  1
  O  O33  1  0.647331  0.816114  0.660744  1
  O  O34  1  0.108502  0.108620  0.912562  1
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O O35 1 0.418205 0.045803 0.435826 1
O O36 1 0.837504 0.316999 0.764171 1
O O37 1 0.383146 0.581507 0.306506 1
O O38 1 0.548253 0.269221 0.578794 1
O O39 1 0.109336 0.753426 0.532409 1
O O40 1 0.679139 0.433389 0.823353 1
O O41 1 0.868170 0.987733 0.056393 1
O O42 1 0.961153 0.082885 0.482600 1
O O43 1 0.298243 0.872511 0.719210 1
O O44 1 0.524954 0.487355 0.661564 1
O O45 1 0.906069 0.805990 0.432765 1
O O46 1 0.021335 0.307618 0.605514 1
O O47 1 0.332877 0.909566 0.947970 1
O O48 1 0.590977 0.638572 0.847837 1
Si Si49 1 0.937857 0.670893 0.473151 1
Si Si50 1 0.420222 0.940502 0.824328 1
Si Si51 1 0.689273 0.279833 0.845233 1
Si Si52 1 0.870276 0.384921 0.340339 1
Si Si53 1 0.015543 0.390780 0.717370 1
Si Si54 1 0.936287 0.962230 0.938669 1
Si Si55 1 0.852082 0.929692 0.413977 1
Si Si56 1 0.545472 0.473096 0.797464 1
Si Si57 1 0.131095 0.435379 0.949047 1
Si Si58 1 0.572632 0.865267 0.558468 1
Si Si59 1 0.267226 0.253077 0.959070 1
Si Si60 1 0.644116 0.811324 0.797624 1
Si Si61 1 0.226666 0.740547 0.623172 1
Si Si62 1 0.440489 0.734809 0.225242 1
Si Si63 1 0.803041 0.879070 0.171679 1
Si Si64 1 0.576823 0.157028 0.502674 1
Si Si65 1 0.934070 0.707290 0.067114 1
Si Si66 1 0.392874 0.003563 0.303636 1
Si Si67 1 0.601403 0.449932 0.555967 1
Si Si68 1 0.830470 0.369021 0.071323 1
Si Si69 1 0.381649 0.432322 0.363911 1
Si Si70 1 0.355983 0.180243 0.196020 1
Si Si71 1 0.054260 0.269692 0.480203 1
Si Si72 1 0.246091 0.748086 0.023167 1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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_cell_length_c   11.59950077
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_cell_angle_beta   89.67427424
_cell_angle_gamma   118.75564696
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si24 O48'
_cell_volume   1046.29853076
_cell_formula_units_Z   24
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  O  O1  1  0.253560  0.011711  0.140606  1
  O  O2  1  0.500098  0.371445  0.099657  1
  O  O3  1  0.126911  0.172756  0.661575  1
  O  O4  1  0.459778  0.475493  0.298011  1
  O  O5  1  0.925054  0.056309  0.831021  1
  O  O6  1  0.836677  0.873198  0.313423  1
  O  O7  1  0.736927  0.776216  0.922958  1
  O  O8  1  0.092168  0.363957  0.800959  1
  O  O9  1  0.654741  0.462536  0.912297  1
  O  O10  1  0.280739  0.885363  0.336843  1
  O  O11  1  0.661018  0.004799  0.879349  1
  O  O12  1  0.936759  0.439240  0.243867  1
  O  O13  1  0.463146  0.641296  0.581868  1
  O  O14  1  0.105989  0.128844  0.031154  1
  O  O15  1  0.902898  0.674620  0.825906  1
  O  O16  1  0.604387  0.374564  0.438732  1
  O  O17  1  0.715615  0.614351  0.190739  1
  O  O18  1  0.953847  0.110890  0.451946  1
  O  O19  1  0.871446  0.453812  0.479596  1
  O  O20  1  0.142805  0.650919  0.831924  1
  O  O21  1  0.519698  0.154126  0.973121  1
  O  O22  1  0.449560  0.915928  0.579146  1
  O  O23  1  0.968658  0.844155  0.129334  1
  O  O24  1  0.618037  0.225030  0.625630  1
  O  O25  1  0.437700  0.999589  0.788857  1
  O  O26  1  0.407493  0.183846  0.311342  1
  O  O27  1  0.879851  0.180050  0.643355  1
  O  O28  1  0.985265  0.590004  0.027895  1
  O  O29  1  0.328055  0.090006  0.621664  1
  O  O30  1  0.248438  0.540163  0.991891  1
  O  O31  1  0.640975  0.628546  0.736374  1
  O  O32  1  0.322491  0.304813  0.482741  1
  O  O33  1  0.823731  0.017352  0.051052  1
  O  O34  1  0.945596  0.684377  0.325990  1
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O	O35	1	0.443247	0.764007	0.391717	1
O	O36	1	0.142006	0.591971	0.392761	1
O	O37	1	0.739401	0.339917	0.087852	1
O	O38	1	0.726617	0.167485	0.447892	1
O	O39	1	0.126606	0.881265	0.943473	1
O	O40	1	0.417808	0.846662	0.998610	1
O	O41	1	0.402187	0.372807	0.696946	1
O	O42	1	0.291212	0.683586	0.193871	1
O	O43	1	0.124048	0.028327	0.339677	1
O	O44	1	0.370339	0.595658	0.792871	1
O	O45	1	0.690147	0.906596	0.533396	1
O	O46	1	0.993590	0.163977	0.228608	1
O	O47	1	0.497633	0.645272	0.101337	1
O	O48	1	0.980807	0.321343	0.051512	1
Si	Si49	1	0.508259	0.000595	0.913138	1
Si	Si50	1	0.263831	0.026374	0.280404	1
Si	Si51	1	0.703977	0.308356	0.500302	1
Si	Si52	1	0.913349	0.425935	0.104812	1
Si	Si53	1	0.291973	0.727914	0.328508	1
Si	Si54	1	0.811944	0.091048	0.522304	1
Si	Si55	1	0.977420	0.043633	0.333907	1
Si	Si56	1	0.972307	0.538352	0.362042	1
Si	Si57	1	0.038632	0.697741	0.907320	1
Si	Si58	1	0.978746	0.159659	0.089858	1
Si	Si59	1	0.115489	0.967608	0.058228	1
Si	Si60	1	0.785089	0.960948	0.919015	1
Si	Si61	1	0.734617	0.635168	0.849773	1
Si	Si62	1	0.470521	0.560196	0.703376	1
Si	Si63	1	0.209914	0.531768	0.853644	1
Si	Si64	1	0.364574	0.680705	0.070350	1
Si	Si65	1	0.292328	0.233849	0.615939	1
Si	Si66	1	0.864260	0.750099	0.240151	1
Si	Si67	1	0.446952	0.335485	0.385474	1
Si	Si68	1	0.463348	0.059755	0.654563	1
Si	Si69	1	0.541360	0.528109	0.171161	1
Si	Si70	1	0.512776	0.810955	0.520024	1
Si	Si71	1	0.007473	0.198113	0.734538	1
Si	Si72	1	0.603051	0.330731	0.017170	1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 10ps from 5000 to 2500 K, 10ps at 2500K, 30ps from 2500 to 1 K)

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_cell_length_c   11.86869266
_cell_angle_alpha   87.91591373
_cell_angle_beta   94.00161934
_cell_angle_gamma   124.51111958
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si24 O48'
_cell_volume   1058.12172326
_cell_formula_units_Z   24
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 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  O  O1  1  0.620361  0.461817  0.413578  1
  O  O2  1  0.164719  0.151437  0.168118  1
  O  O3  1  0.974750  0.385906  0.396162  1
  O  O4  1  0.079597  0.195944  0.371156  1
  O  O5  1  0.703255  0.925388  0.147526  1
  O  O6  1  0.079721  0.628046  0.547818  1
  O  O7  1  0.795570  0.393940  0.534850  1
  O  O8  1  0.183450  0.486802  0.168982  1
  O  O9  1  0.915482  0.208616  0.085846  1
  O  O10  1  0.753047  0.756296  0.036148  1
  O  O11  1  0.059763  0.481327  0.972728  1
  O  O12  1  0.119131  0.371730  0.804722  1
  O  O13  1  0.249413  0.875341  0.687256  1
  O  O14  1  0.041821  0.086921  0.779245  1
  O  O15  1  0.446802  0.729268  0.283041  1
  O  O16  1  0.376052  0.911127  0.359886  1
  O  O17  1  0.058161  0.588448  0.771034  1
  O  O18  1  0.193213  0.930761  0.480617  1
  O  O19  1  0.061384  0.937611  0.010724  1
  O  O20  1  0.509505  0.162635  0.485855  1
  O  O21  1  0.306572  0.625421  0.456866  1
  O  O22  1  0.691810  0.472976  0.193911  1
  O  O23  1  0.601160  0.093144  0.079165  1
  O  O24  1  0.346818  0.417703  0.294001  1
  O  O25  1  0.350233  0.335618  0.786354  1
  O  O26  1  0.765437  0.885806  0.663975  1
  O  O27  1  0.902042  0.433224  0.151456  1
  O  O28  1  0.002919  0.876285  0.638950  1
  O  O29  1  0.572640  0.374536  0.638660  1
  O  O30  1  0.529952  0.110611  0.862094  1
  O  O31  1  0.361246  0.119556  0.032966  1
  O  O32  1  0.129396  0.359085  0.564333  1
  O  O33  1  0.906745  0.604739  0.364722  1
  O  O34  1  0.864804  0.784436  0.836333  1
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O O35 1 0.716320 0.021999 0.920242 1
O O36 1 0.652268 0.354821 0.996676 1
O O37 1 0.486024 0.609216 0.122091 1
O O38 1 0.654577 0.049141 0.690310 1
O O39 1 0.574778 0.883665 0.494880 1
O O40 1 0.315031 0.148736 0.335693 1
O O41 1 0.276424 0.154921 0.618949 1
O O42 1 0.900552 0.632679 0.017445 1
O O43 1 0.202894 0.244217 0.966730 1
O O44 1 0.830677 0.297800 0.818940 1
O O45 1 0.305001 0.647388 0.673314 1
O O46 1 0.416198 0.486525 0.593723 1
O O47 1 0.855556 0.118352 0.516378 1
O O48 1 0.737441 0.721493 0.270955 1
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Si Si50 1 0.734641 0.061458 0.057820 1
Si Si51 1 0.008478 0.260551 0.457204 1
Si Si52 1 0.526966 0.164814 0.991810 1
Si Si53 1 0.669892 0.750696 0.147705 1
Si Si54 1 0.916654 0.908571 0.731841 1
Si Si55 1 0.786269 0.474634 0.089721 1
Si Si56 1 0.349659 0.038239 0.412729 1
Si Si57 1 0.943247 0.505738 0.457862 1
Si Si58 1 0.018890 0.401202 0.096384 1
Si Si59 1 0.182406 0.963713 0.610583 1
Si Si60 1 0.292427 0.533057 0.573928 1
Si Si61 1 0.177454 0.258383 0.832185 1
Si Si62 1 0.430511 0.794804 0.400286 1
Si Si63 1 0.221461 0.226582 0.294863 1
Si Si64 1 0.621954 0.350070 0.517112 1
Si Si65 1 0.173472 0.686818 0.671173 1
Si Si66 1 0.712750 0.987651 0.591397 1
Si Si67 1 0.738992 0.567644 0.313782 1
Si Si68 1 0.403591 0.337540 0.660492 1
Si Si69 1 0.202845 0.113519 0.047633 1
Si Si70 1 0.013976 0.431324 0.841278 1
Si Si71 1 0.895879 0.780259 0.972714 1
Si Si72 1 0.680022 0.115556 0.819354 1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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_cell_angle_gamma   119.97620760
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
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_cell_volume   1063.08639043
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 _atom_site_fract_x
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 _atom_site_occupancy
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  O  O2  1  0.400634  0.273731  0.275388  1
  O  O3  1  0.492512  0.363554  0.972470  1
  O  O4  1  0.796435  0.627565  0.601478  1
  O  O5  1  0.695931  0.494875  0.300842  1
  O  O6  1  0.246700  0.955642  0.279857  1
  O  O7  1  0.423706  0.594857  0.932977  1
  O  O8  1  0.818646  0.936259  0.738369  1
  O  O9  1  0.034098  0.641325  0.492335  1
  O  O10  1  0.161930  0.012590  0.026811  1
  O  O11  1  0.994842  0.135059  0.110737  1
  O  O12  1  0.957159  0.024704  0.913934  1
  O  O13  1  0.059472  0.902805  0.565798  1
  O  O14  1  0.580548  0.915788  0.256749  1
  O  O15  1  0.855942  0.153724  0.297221  1
  O  O16  1  0.724797  0.301942  0.960234  1
  O  O17  1  0.154846  0.470679  0.564253  1
  O  O18  1  0.611576  0.828839  0.062328  1
  O  O19  1  0.741051  0.766994  0.223363  1
  O  O20  1  0.810678  0.203810  0.795341  1
  O  O21  1  0.328192  0.523401  0.393819  1
  O  O22  1  0.402947  0.392426  0.783372  1
  O  O23  1  0.721834  0.732012  0.900326  1
  O  O24  1  0.975558  0.708363  0.224343  1
  O  O25  1  0.437750  0.735610  0.550201  1
  O  O26  1  0.091270  0.107002  0.298659  1
  O  O27  1  0.276814  0.131248  0.451220  1
  O  O28  1  0.866077  0.758382  0.406815  1
  O  O29  1  0.606459  0.296548  0.136499  1
  O  O30  1  0.219928  0.818894  0.890708  1
  O  O31  1  0.563768  0.328459  0.624214  1
  O  O32  1  0.990433  0.517177  0.872425  1
  O  O33  1  0.440941  0.064048  0.995507  1
  O  O34  1  0.206042  0.294545  0.955161  1
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O O37 1 0.739789 0.443789 0.780850 1
O O38 1 0.117354 0.665058 0.696572 1
O O39 1 0.136487 0.384366 0.233039 1
O O40 1 0.271453 0.146868 0.658097 1
O O41 1 0.602760 0.996693 0.664876 1
O O42 1 0.976770 0.787953 0.805258 1
O O43 1 0.399569 0.450234 0.578827 1
O O44 1 0.430746 0.611096 0.201216 1
O O45 1 0.612472 0.194502 0.325684 1
O O46 1 0.362438 0.958323 0.556420 1
O O47 1 0.591231 0.905858 0.864558 1
O O48 1 0.224547 0.800747 0.098343 1
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Si Si56 1 0.592366 0.779411 0.185950 1
Si Si57 1 0.252099 0.116255 0.325561 1
Si Si58 1 0.740654 0.450625 0.652459 1
Si Si59 1 0.261201 0.923488 0.000800 1
Si Si60 1 0.082050 0.119796 0.003433 1
Si Si61 1 0.583730 0.765872 0.940557 1
Si Si62 1 0.015980 0.194028 0.234443 1
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Si Si66 1 0.579253 0.315722 0.260059 1
Si Si67 1 0.674118 0.068908 0.334704 1
Si Si68 1 0.560318 0.254171 0.015075 1
Si Si69 1 0.509375 0.928251 0.555958 1
Si Si70 1 0.706181 0.012995 0.765274 1
Si Si71 1 0.935004 0.733698 0.514570 1
Si Si72 1 0.820425 0.683089 0.287340 1

am-SiO_2 (generated by BOMD: 10ps at 5000 K, 25ps from 5000 to 2500 K, 20ps at 2500K, 25ps from 2500 to 1 K)

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  O  O3  1  0.944125  0.177828  0.679066  1
  O  O4  1  0.490524  0.414455  0.855183  1
  O  O5  1  0.679119  0.228555  0.189980  1
  O  O6  1  0.848946  0.517512  0.190600  1
  O  O7  1  0.481374  0.212208  0.738736  1
  O  O8  1  0.768247  0.485939  0.769751  1
  O  O9  1  0.343440  0.977710  0.122936  1
  O  O10  1  0.508436  0.658025  0.240166  1
  O  O11  1  0.340884  0.926885  0.697735  1
  O  O12  1  0.409569  0.795795  0.010558  1
  O  O13  1  0.913178  0.184878  0.087847  1
  O  O14  1  0.811949  0.711918  0.302844  1
  O  O15  1  0.542378  0.403873  0.248515  1
  O  O16  1  0.965655  0.273751  0.395053  1
  O  O17  1  0.648428  0.734765  0.982901  1
  O  O18  1  0.668560  0.957757  0.188746  1
  O  O19  1  0.183491  0.950366  0.537264  1
  O  O20  1  0.257462  0.016939  0.325404  1
  O  O21  1  0.655600  0.848665  0.383842  1
  O  O22  1  0.340642  0.536149  0.945977  1
  O  O23  1  0.391177  0.841516  0.298664  1
  O  O24  1  0.562404  0.439227  0.623616  1
  O  O25  1  0.722783  0.340469  0.376789  1
  O  O26  1  0.101230  0.759527  0.234638  1
  O  O27  1  0.380848  0.005919  0.900224  1
  O  O28  1  0.924300  0.987684  0.953649  1
  O  O29  1  0.190564  0.244459  0.974584  1
  O  O30  1  0.194374  0.196537  0.455094  1
  O  O31  1  0.737464  0.724501  0.738173  1
  O  O32  1  0.966520  0.951207  0.408532  1
  O  O33  1  0.194513  0.444209  0.513902  1
  O  O34  1  0.953143  0.253939  0.879500  1
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O O38 1 0.506818 0.771709 0.809565 1
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Si Si69 1 0.798564 0.805764 0.402304 1
Si Si70 1 0.189975 0.834854 0.626819 1
Si Si71 1 0.756144 0.095834 0.653469 1
Si Si72 1 0.153424 0.027691 0.431258 1

SiO_2 polymorphs

SiO_2 (mp-10948)

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_cell_length_b   9.05432510
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  Si  Si2  1  0.250000  0.375000  0.673845  1
  Si  Si3  1  0.250000  0.875000  0.173845  1
  Si  Si4  1  0.250000  0.875000  0.673845  1
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  Si  Si12  1  0.000000  0.625000  0.576155  1
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  Si  Si14  1  0.500000  0.125000  0.576155  1
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  Si  Si19  1  0.250000  0.625000  0.326156  1
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O O93 1 0.865449 0.210016 0.191211 1
O O94 1 0.865449 0.210016 0.691211 1

O O95 1 0.865449 0.710016 0.191211 1
O O96 1 0.865449 0.710016 0.691211 1

SiO_2 (mp-11684)

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_cell_angle_alpha   90.00000000
_cell_angle_beta   119.96224213
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
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_chemical_formula_sum   'Si16 O32'
_cell_volume   570.879451833
_cell_formula_units_Z   16
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  1  'x, y, z'
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Si  Si2  1  0.217022  0.091310  0.461002  1
  Si  Si3  1  0.217022  0.908690  0.961002  1
  Si  Si4  1  0.282978  0.408690  0.538998  1
  Si  Si5  1  0.181128  0.642363  0.573122  1
  Si  Si6  1  0.318872  0.142363  0.926878  1
  Si  Si7  1  0.318872  0.857637  0.426878  1
  Si  Si8  1  0.181128  0.357637  0.073122  1
  Si  Si9  1  0.782978  0.091310  0.038998  1
  Si  Si10  1  0.717022  0.591310  0.461002  1
  Si  Si11  1  0.717022  0.408690  0.961002  1
  Si  Si12  1  0.782978  0.908690  0.538998  1
  Si  Si13  1  0.681128  0.142363  0.573122  1
  Si  Si14  1  0.818872  0.642363  0.926878  1
  Si  Si15  1  0.818872  0.357637  0.426878  1
  Si  Si16  1  0.681128  0.857637  0.073122  1
  O  O17  1  0.217860  0.038639  0.982206  1
  O  O18  1  0.282140  0.538639  0.517794  1
  O  O19  1  0.282140  0.461361  0.017794  1
  O  O20  1  0.217860  0.961361  0.482206  1
  O  O21  1  0.270974  0.645085  0.829069  1
  O  O22  1  0.229026  0.145085  0.670931  1
  O  O23  1  0.229026  0.854915  0.170931  1
  O  O24  1  0.270974  0.354915  0.329069  1
  O  O25  1  0.250000  0.250000  0.000000  1
  O  O26  1  0.250000  0.750000  0.500000  1
  O  O27  1  0.500000  0.369420  0.750000  1
  O  O28  1  0.000000  0.130580  0.250000  1
  O  O29  1  0.923016  0.370257  0.944517  1
  O  O30  1  0.076984  0.370257  0.555483  1
  O  O31  1  0.576984  0.129743  0.055483  1
  O  O32  1  0.423016  0.129743  0.444517  1
  O  O33  1  0.717860  0.538639  0.982206  1
  O  O34  1  0.782140  0.038639  0.517794  1
  O  O35  1  0.782140  0.961361  0.017794  1
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O O36 1 0.717860 0.461361 0.482206 1
O O37 1 0.770974 0.145085 0.829069 1
O O38 1 0.729026 0.645085 0.670931 1
O O39 1 0.729026 0.354915 0.170931 1
O O40 1 0.770974 0.854915 0.329069 1
O O41 1 0.750000 0.750000 0.000000 1
O O42 1 0.750000 0.250000 0.500000 1
O O43 1 0.000000 0.869420 0.750000 1
O O44 1 0.500000 0.630580 0.250000 1
O O45 1 0.423016 0.870257 0.944517 1
O O46 1 0.576984 0.870257 0.555483 1
O O47 1 0.076984 0.629743 0.055483 1
O O48 1 0.923016 0.629743 0.444517 1

SiO_2 (mp-560527)

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_cell_length_c   9.05719280
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_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si16 O32'
_cell_volume   911.308801252
_cell_formula_units_Z   16
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loop_
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 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Si  Si3  1  0.164463  0.134499  0.925059  1
  Si  Si4  1  0.835537  0.865501  0.074941  1
  Si  Si5  1  0.164463  0.134499  0.574941  1
  Si  Si6  1  0.164463  0.865501  0.425059  1
  Si  Si7  1  0.835537  0.134499  0.574941  1
  Si  Si8  1  0.164463  0.865501  0.074941  1
  Si  Si9  1  0.335537  0.365501  0.425059  1
  Si  Si10  1  0.335537  0.634499  0.925059  1
  Si  Si11  1  0.664463  0.634499  0.925059  1
  Si  Si12  1  0.335537  0.365501  0.074941  1
  Si  Si13  1  0.664463  0.634499  0.574941  1
  Si  Si14  1  0.664463  0.365501  0.425059  1
  Si  Si15  1  0.335537  0.634499  0.574941  1
  Si  Si16  1  0.664463  0.365501  0.074941  1
  O  O17  1  0.212038  0.000000  0.000000  1
  O  O18  1  0.000000  0.158808  0.547537  1
  O  O19  1  0.000000  0.841192  0.047537  1
  O  O20  1  0.787962  0.000000  0.500000  1
  O  O21  1  0.198917  0.129191  0.750000  1
  O  O22  1  0.801083  0.129191  0.750000  1
  O  O23  1  0.750000  0.250000  0.500000  1
  O  O24  1  0.212038  0.000000  0.500000  1
  O  O25  1  0.000000  0.158808  0.952463  1
  O  O26  1  0.787962  0.000000  0.000000  1
  O  O27  1  0.000000  0.841192  0.452463  1
  O  O28  1  0.198917  0.870809  0.250000  1
  O  O29  1  0.801083  0.870809  0.250000  1
  O  O30  1  0.750000  0.750000  0.000000  1
  O  O31  1  0.750000  0.750000  0.500000  1
  O  O32  1  0.750000  0.250000  0.000000  1
  O  O33  1  0.712038  0.500000  0.000000  1
  O  O34  1  0.500000  0.658808  0.547537  1
  O  O35  1  0.500000  0.341192  0.047537  1
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O O36 1 0.287962 0.500000 0.500000 1
O O37 1 0.698917 0.629191 0.750000 1
O O38 1 0.301083 0.629191 0.750000 1
O O39 1 0.250000 0.750000 0.500000 1
O O40 1 0.712038 0.500000 0.500000 1
O O41 1 0.500000 0.658808 0.952463 1
O O42 1 0.287962 0.500000 0.000000 1
O O43 1 0.500000 0.341192 0.452463 1
O O44 1 0.698917 0.370809 0.250000 1
O O45 1 0.301083 0.370809 0.250000 1
O O46 1 0.250000 0.250000 0.000000 1
O O47 1 0.250000 0.250000 0.500000 1
O O48 1 0.250000 0.750000 0.000000 1

SiO_2 (mp-604717)

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_cell_angle_gamma   90.00000000
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_chemical_formula_sum   'Si12 O24'
_cell_volume   825.871259522
_cell_formula_units_Z   12
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Si  Si2  1  0.024799  0.369934  0.891693  1
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  Si  Si4  1  0.176638  0.823362  0.250000  1
  Si  Si5  1  0.975201  0.630066  0.391693  1
  Si  Si6  1  0.869934  0.475201  0.641693  1
  Si  Si7  1  0.676638  0.676638  0.500000  1
  Si  Si8  1  0.630066  0.975201  0.608307  1
  Si  Si9  1  0.369934  0.024799  0.108307  1
  Si  Si10  1  0.524799  0.130066  0.858307  1
  Si  Si11  1  0.475201  0.869934  0.358307  1
  Si  Si12  1  0.130066  0.524799  0.141693  1
  O  O13  1  0.944916  0.491518  0.793930  1
  O  O14  1  0.301709  0.835765  0.369442  1
  O  O15  1  0.461579  0.292344  0.897780  1
  O  O16  1  0.698291  0.164235  0.869442  1
  O  O17  1  0.198291  0.335765  0.880558  1
  O  O18  1  0.707656  0.538421  0.602220  1
  O  O19  1  0.207656  0.961579  0.147780  1
  O  O20  1  0.164235  0.698291  0.130558  1
  O  O21  1  0.444916  0.008482  0.956070  1
  O  O22  1  0.801709  0.664235  0.380558  1
  O  O23  1  0.055084  0.508482  0.293930  1
  O  O24  1  0.008482  0.444916  0.043930  1
  O  O25  1  0.038421  0.792344  0.352220  1
  O  O26  1  0.555084  0.991518  0.456070  1
  O  O27  1  0.538421  0.707656  0.397780  1
  O  O28  1  0.292344  0.461579  0.102220  1
  O  O29  1  0.792344  0.038421  0.647780  1
  O  O30  1  0.491518  0.944916  0.206070  1
  O  O31  1  0.335765  0.198291  0.119442  1
  O  O32  1  0.508482  0.055084  0.706070  1
  O  O33  1  0.835765  0.301709  0.630558  1
  O  O34  1  0.961579  0.207656  0.852220  1
  O  O35  1  0.664235  0.801709  0.619442  1
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O O36 1 0.991518 0.555084 0.543930 1

SiO_2 (mp-555960)

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_cell_angle_beta   95.66514587
_cell_angle_gamma   91.60611725
_symmetry_Int_Tables_number   1
_chemical_formula_structural   SiO2
_chemical_formula_sum   'Si16 O32'
_cell_volume   1702.29137627
_cell_formula_units_Z   16
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Si  Si2  1  0.436052  0.602298  0.698901  1
  Si  Si3  1  0.395725  0.739013  0.359927  1
  Si  Si4  1  0.563948  0.397702  0.301099  1
  Si  Si5  1  0.328245  0.250920  0.566817  1
  Si  Si6  1  0.672100  0.249728  0.433228  1
  Si  Si7  1  0.563804  0.579035  0.301089  1
  Si  Si8  1  0.671755  0.749080  0.433183  1
  Si  Si9  1  0.603957  0.761976  0.639999  1
  Si  Si10  1  0.604275  0.260987  0.640073  1
  Si  Si11  1  0.436196  0.420965  0.698911  1
  Si  Si12  1  0.234496  0.080255  0.430477  1
  Si  Si13  1  0.396043  0.238025  0.360001  1
  Si  Si14  1  0.765675  0.101023  0.569646  1
  Si  Si15  1  0.765504  0.919745  0.569523  1
  Si  Si16  1  0.327900  0.750272  0.566772  1
  O  O17  1  0.276221  0.820294  0.334717  1
  O  O18  1  0.535412  0.493280  0.386240  1
  O  O19  1  0.211037  0.830123  0.529978  1
  O  O20  1  0.788963  0.169877  0.470021  1
  O  O21  1  0.535914  0.806785  0.390787  1
  O  O22  1  0.723779  0.179706  0.665283  1
  O  O23  1  0.464086  0.193215  0.609213  1
  O  O24  1  0.536297  0.180480  0.390873  1
  O  O25  1  0.692511  0.658074  0.342947  1
  O  O26  1  0.692743  0.329826  0.342935  1
  O  O27  1  0.723440  0.851771  0.665168  1
  O  O28  1  0.463703  0.819520  0.609127  1
  O  O29  1  0.276560  0.148229  0.334832  1
  O  O30  1  0.211419  0.161188  0.530040  1
  O  O31  1  0.407668  0.516701  0.786192  1
  O  O32  1  0.354621  0.307219  0.461155  1
  O  O33  1  0.431853  0.318345  0.273308  1
  O  O34  1  0.464588  0.506720  0.613760  1
  O  O35  1  0.645379  0.692781  0.538845  1
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O	O37	1	0.881769	0.014927	0.601178	1
O	O38	1	0.307489	0.341926	0.657053	1
O	O39	1	0.118231	0.985073	0.398822	1
O	O40	1	0.568147	0.681655	0.726692	1
O	O41	1	0.652079	0.005944	0.538207	1
O	O42	1	0.788581	0.838812	0.469960	1
O	O43	1	0.307257	0.670174	0.657065	1
O	O44	1	0.568362	0.351087	0.726689	1
O	O45	1	0.645762	0.318706	0.538873	1
O	O46	1	0.431638	0.648913	0.273311	1
O	O47	1	0.347921	0.994056	0.461793	1
O	O48	1	0.354238	0.681294	0.461127	1

SiO_2 (mp-559273)

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_cell_angle_gamma   120.00000000
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_cell_formula_units_Z   24
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  Si  Si2  1  0.836477  0.276170  0.283869  1
  Si  Si3  1  0.125828  0.562915  0.166667  1
  Si  Si4  1  0.836477  0.560307  0.049465  1
  Si  Si5  1  0.620205  0.000000  0.500000  1
  Si  Si6  1  0.276170  0.439693  0.950535  1
  Si  Si7  1  0.562915  0.125828  0.500000  1
  Si  Si8  1  0.439693  0.163523  0.617202  1
  Si  Si9  1  0.276170  0.836477  0.382798  1
  Si  Si10  1  0.379795  0.379795  0.833333  1
  Si  Si11  1  0.163523  0.439693  0.049465  1
  Si  Si12  1  0.379795  -0.000000  0.500000  1
  Si  Si13  1  0.620205  0.620205  0.833333  1
  Si  Si14  1  0.000000  0.620205  0.166667  1
  Si  Si15  1  0.437085  0.562915  0.833333  1
  Si  Si16  1  0.560307  0.836477  0.617202  1
  Si  Si17  1  0.437085  0.874172  0.500000  1
  Si  Si18  1  0.723830  0.560307  0.950535  1
  Si  Si19  1  -0.000000  0.379795  0.166667  1
  Si  Si20  1  0.439693  0.276170  0.716131  1
  Si  Si21  1  0.163523  0.723830  0.283869  1
  Si  Si22  1  0.560307  0.723830  0.716131  1
  Si  Si23  1  0.723830  0.163523  0.382798  1
  Si  Si24  1  0.562915  0.437085  0.833333  1
  O  O25  1  0.253721  0.431699  0.076233  1
  O  O26  1  0.934457  0.529672  0.232697  1
  O  O27  1  0.295892  0.362206  0.907099  1
  O  O28  1  0.538252  0.181427  0.581723  1
  O  O29  1  0.362206  0.295892  0.759568  1
  O  O30  1  0.461748  0.818573  0.581723  1
  O  O31  1  0.704108  0.637794  0.907099  1
  O  O32  1  0.568301  0.746279  0.590433  1
  O  O33  1  0.404784  0.934457  0.566030  1
  O  O34  1  0.568301  0.822022  0.742900  1
  O  O35  1  0.404784  0.470328  0.767303  1
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O O36 1 0.595216 0.065543 0.566030 1
O O37 1 0.746279 0.568301 0.076233 1
O O38 1 0.643175 0.461748 0.915056 1
O O39 1 0.595216 0.529672 0.767303 1
O O40 1 0.470328 0.065543 0.433970 1
O O41 1 0.529672 0.595216 0.899363 1
O O42 1 0.065543 0.470328 0.232697 1
O O43 1 0.822022 0.568301 0.923767 1
O O44 1 0.356825 0.538252 0.915056 1
O O45 1 0.362206 0.066313 0.573766 1
O O46 1 0.066313 0.704108 0.240432 1
O O47 1 0.643175 0.181427 0.418277 1
O O48 1 0.746279 0.177978 0.257100 1
O O49 1 0.822022 0.253721 0.409567 1
O O50 1 0.637794 0.704108 0.759568 1
O O51 1 0.253721 0.822022 0.257100 1
O O52 1 0.818573 0.356825 0.248390 1
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O O54 1 0.431699 0.177978 0.742900 1
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O O57 1 0.181427 0.643175 0.248390 1
O O58 1 0.637794 0.933687 0.573766 1
O O59 1 0.529672 0.934457 0.433970 1
O O60 1 0.356825 0.818573 0.418277 1
O O61 1 0.934457 0.404784 0.100637 1
O O62 1 0.066313 0.362206 0.092901 1
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O O64 1 0.295892 0.933687 0.426234 1
O O65 1 0.538252 0.356825 0.751610 1
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O O67 1 0.470328 0.404784 0.899363 1
O O68 1 0.181427 0.538252 0.084944 1
O O69 1 0.461748 0.643175 0.751610 1
O O70 1 0.177978 0.431699 0.923767 1
O O71 1 0.818573 0.461748 0.084944 1
O O72 1 0.933687 0.637794 0.092901 1

References

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