Supplementary Materials: Multiscale Computational Simulation of Amorphous Silicates' Structural, Dielectric, and Vibrational Spectroscopic Properties

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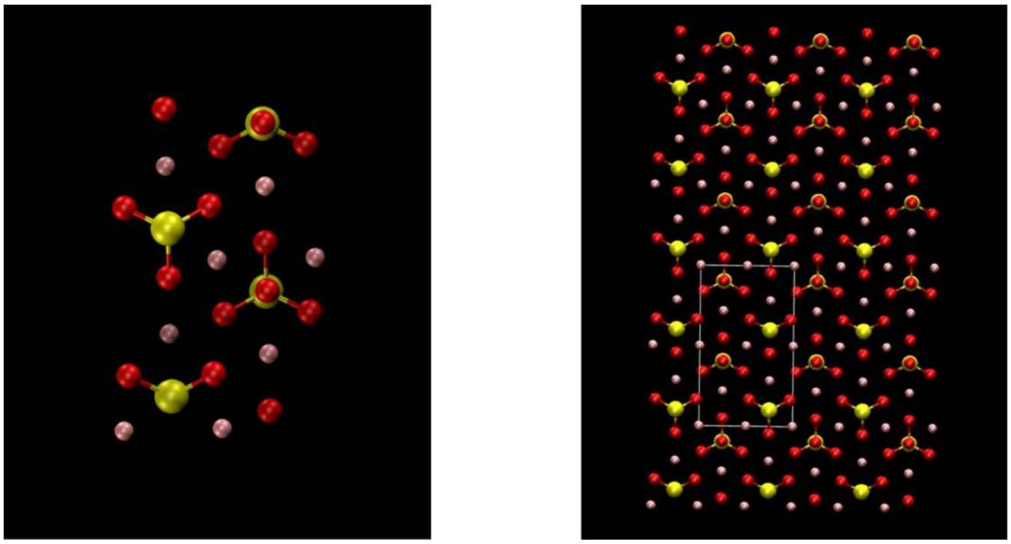


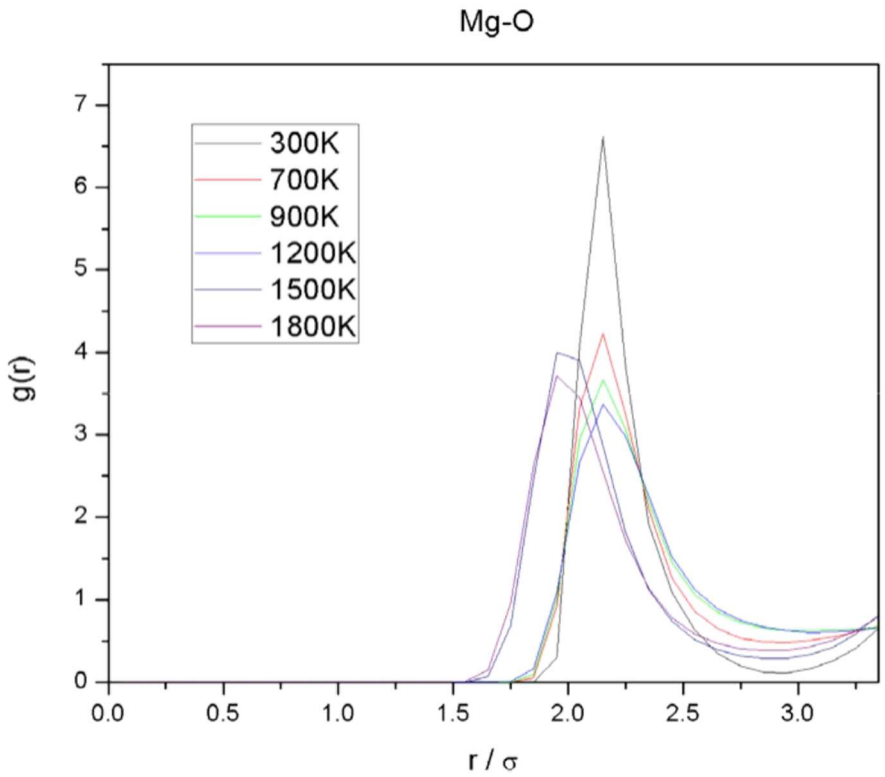
Figure S1. GULP-optimized structure for the bulk of the crystal Mg_2SiO_4. View of the unit cell (left), view of the extended periodic system (right).

Table S1. Bond distance ranges (in Å) of the crystalline 1 × 1 × 1 Mg_2SiO_4 bulk structures: experimental, GULP-optimized, and B3LYP and B3LYP-D2 optimized values.

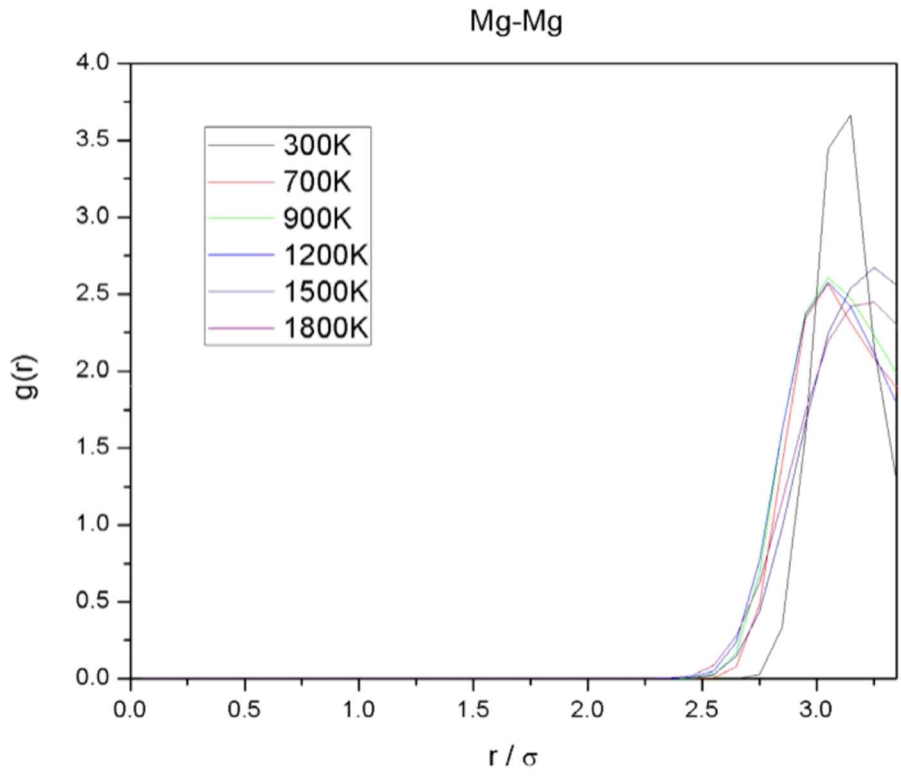
Parameters	Experimental	GULP	B3LYP	B3LYP-D2
Si–O	1.616–1.649	1.61–1.67	1.628–1.673	1.618–1.666
Mg1–O	2.069–2.126	2.05–2.15	2.073–2.131	2.023–2.036
Mg2–O	2.040–2.166	2.01–2.26	2.062–2.223	2.000–2.154

Table S2. Bond distance ranges (in Å) and lattice parameters (distances in Å, angles in degrees) of the amorphous 1 × 1 × 2 Mg_2SiO_4 bulk structure optimized at B3LYP and B3LYP-D2 theory level.

Parameters	B3LYP	B3LYP-D2
Si–O	1.618–1.693	1.610–1.702
Mg–O	1.929–2.226	1.918–2.239
a	4.93	4.95
b	9.37	9.22
c	11.94	11.88
α	87.4	86.8
β	90.6	89.9
γ	88.6	88.5



(**a**)



(**b**)

Figure S2. Mg–Mg (**a**) and Mg–O (**b**) pair correlation functions derived from the MD simulations at the different temperatures accounting for periodic boundary conditions.

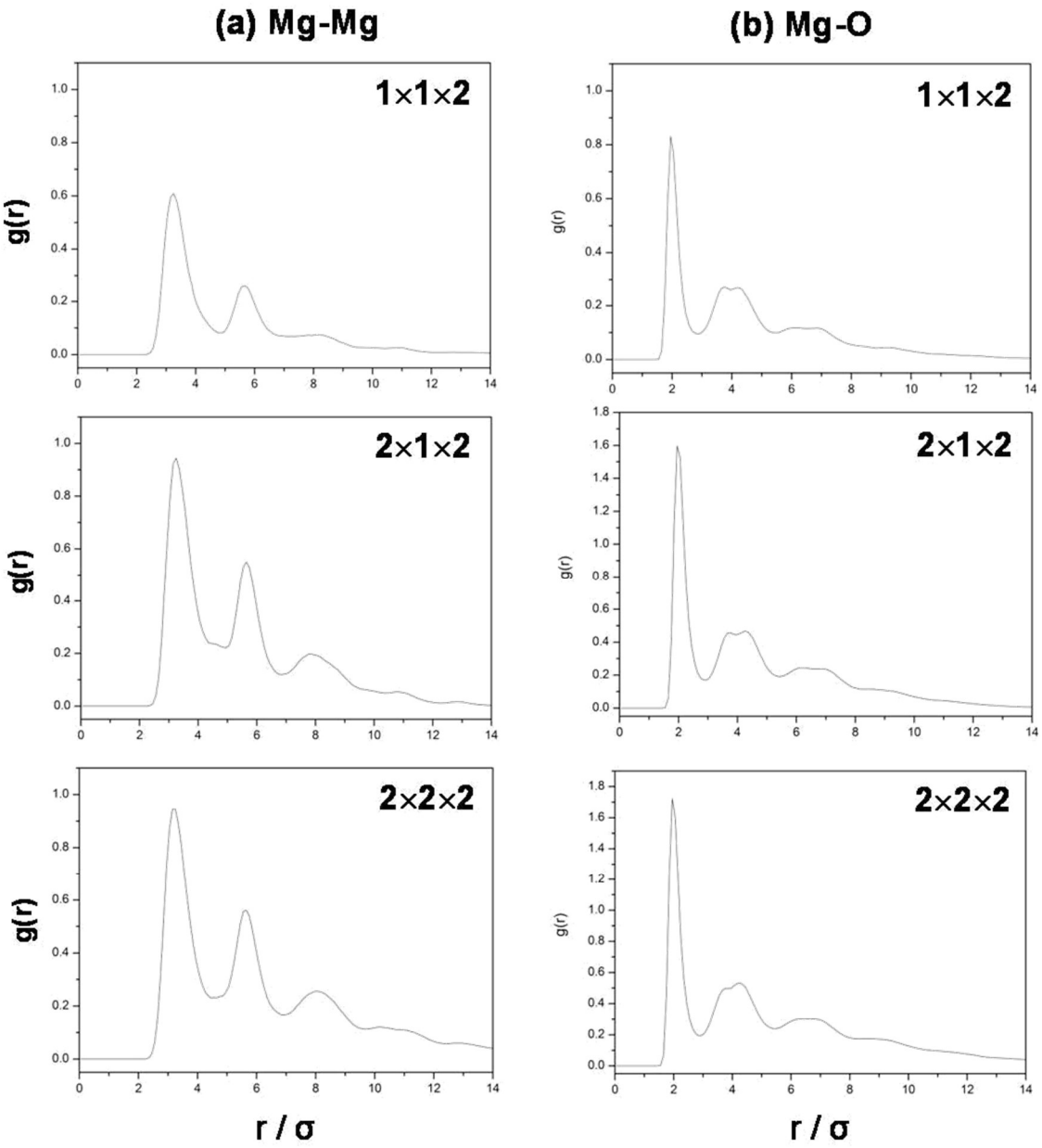


Figure S3. Mg–Mg (**a**) and Mg–O (**b**) pair correlation functions derived from the classical MD simulations for the 1 × 1 × 2, 2 × 1 × 2 and 2 × 2 × 2 systems.

Scheme S1. Cell parameters and fractionary coordinates of the optimized systems.

Amorphous 1 × 1 × 2 Mg_2SiO_4 structure.

a = 4.93304476000	α = 87.441554
b = 9.37079363000	β = 90.613072
c = 11.93606723000	γ = 88.598256

12	0.088033963245	0.071404847491	−0.025783798004
12	−0.023814722733	0.301748472438	−0.333035975045
12	0.473861984392	0.495792988074	0.280404977664
12	0.384569679244	−0.437358025828	−0.191627039204
12	0.437838847985	0.455077110139	−0.437571512971
12	−0.002081268047	−0.044678425945	−0.263148562494
12	0.091303279227	−0.114512819647	0.209388284349
12	0.033010380761	−0.004458243938	0.452832521894
12	0.004546685846	0.243279398245	0.196227733413
12	0.386709360423	0.369960484776	0.044446552325
12	0.495302036361	0.148045197659	0.348584327379
12	0.474109828445	0.201356888186	−0.177051653109
12	0.431241533794	−0.282190068864	0.083483126707
12	0.405005901730	−0.216901158402	−0.392879646620
12	0.070641801819	−0.333455448660	0.406633240999
12	−0.048630992965	−0.287918985156	−0.073566220372
14	−0.456992531532	0.075445737893	0.103434226889
14	−0.498697091246	0.107502367173	−0.399197800553
14	−0.033136132237	0.342781091159	0.413643382933
14	−0.063645498613	0.367384153800	−0.088196958255
14	−0.079776129076	−0.432055956585	0.163472860318
14	−0.062431662068	−0.359032876833	−0.332296590138
14	−0.461515731510	−0.193447505037	0.348933389726
14	−0.445182514108	−0.119392912848	−0.151458036929
8	0.133839397184	0.496546080134	−0.322649386510
8	0.114380911747	−0.488198834049	−0.070375068121
8	0.164631015667	0.447250178740	0.174950570940
8	−0.357813591684	−0.144579031624	−0.280231314476
8	−0.168000082991	−0.401573505571	0.290921016603
8	−0.163680576118	−0.067540243039	−0.092058472000
8	0.336211660607	0.257834950709	−0.384017257585
8	−0.145449269708	−0.142011245524	0.343487832427
8	0.005635826397	−0.283621629084	0.090728881016
8	0.246300226491	−0.011489825222	−0.399534030733
8	0.096783307291	−0.270242311284	−0.231485482184
8	−0.267661085174	0.129552586805	−0.296111457330
8	0.491606370706	0.171062113504	−0.012665473377
8	−0.203254840595	0.373288935816	−0.474371910933
8	0.221881387721	0.461112860791	0.414649852784
8	0.010712668052	−0.263297242874	−0.443875389219
8	0.393139685251	0.183073529774	0.188752117185
8	−0.366354936987	−0.478166125302	0.103657065664
8	−0.267581206392	0.323875026960	0.311116820889
8	−0.014430683760	0.273700779709	0.029090259956
8	0.472917955969	−0.291138000797	0.460402675040
8	−0.478026688476	−0.278117367337	−0.082221853187
8	−0.143491864884	0.046978611362	0.147319919495
8	−0.379833400304	−0.408324081084	−0.326798331950
8	0.363270904931	−0.068070637805	0.086418181465
8	−0.376298304045	0.397604224513	−0.132524289194
8	−0.325681403323	0.076396353108	0.489573712254
8	0.126255256760	0.191725828878	0.390497464230

8	0.087536182341	0.261603274225	−0.174199441117
8	0.341357544219	−0.049030183237	0.340229627315
8	0.307690329745	−0.002106125139	−0.158411620105

Amorphous 2 × 1 × 2 Mg_2SiO_4 structure.

a = 10.16843999000	α = 89.634659
b = 10.17756989000	β = 83.909210
c = 11.32973798000	γ = 97.083695

12	0.073460850068	−0.493977325015	−0.246394144523
12	−0.135925146351	−0.398740076291	0.111827092155
12	−0.034187419415	0.297895009031	−0.045494235902
12	0.412711638588	−0.303783645109	0.320407541182
12	−0.182372037422	0.056105938736	−0.167613052425
12	0.140723243551	−0.053976326826	−0.301646552408
12	−0.355101059202	−0.229620684904	0.028886945242
12	0.211817118888	−0.400095498556	−0.005022211422
12	0.484758101519	−0.069709678301	0.463237802126
12	−0.336328446534	0.065614169462	−0.397021139924
12	0.211801094404	−0.155040812056	0.419696197893
12	−0.496824930667	−0.414183706234	−0.180363616838
12	−0.485522029003	−0.485966314524	0.074995896003
12	0.208714618074	0.486124706260	0.468839510002
12	0.181727116951	0.076545330968	−0.061863081008
12	0.248795072453	0.324298976875	0.156925151764
12	0.472840562436	0.088650628260	0.021461249437
12	0.312532000891	0.186888661124	0.442429421675
12	−0.033311959130	−0.263693447213	0.391303036198
12	−0.379481921387	0.051168939897	0.262189357342
12	0.455781472610	0.405856309854	−0.357390581600
12	0.335174401835	−0.144844857974	−0.151166862277
12	−0.086703131806	−0.023809170988	0.276335152573
12	−0.101554683130	0.457700562588	0.420754682306
12	−0.016129642691	0.014925971566	−0.475071693554
12	−0.249919031363	0.499453420111	−0.365090021861
12	−0.307127958117	0.394177831434	−0.136195528195
12	−0.298366608270	−0.280729588524	−0.481232495486
12	−0.349394148137	0.270124843836	0.458154998645
12	0.298892106843	0.032380421263	0.253966641327
12	−0.022531506445	−0.311807142651	−0.374652163848
12	−0.194575424933	−0.325747249442	−0.162674711358
14	0.405493415694	−0.193714870492	0.106263692371
14	0.125079602292	−0.122914556018	0.148997286553
14	−0.468640211687	0.284573243264	0.211049119949
14	−0.133592446413	−0.017332915749	0.047049914770
14	0.101287263800	−0.405141179625	0.234769249704
14	−0.467265491869	0.474749213281	0.371856556743
14	0.166378966189	0.222810896569	−0.348638804044
14	−0.169005989323	0.315789283115	0.195215112159
14	0.304144440980	−0.304386954409	−0.381597190985
14	0.473091344676	0.186192969651	−0.198816628647
14	−0.384284894960	−0.162877424234	−0.278451086096
14	−0.314051989880	−0.231502260870	0.292275082255
14	0.270453818453	0.361812782935	−0.093880661057
14	0.048331872387	−0.238146901597	−0.127242564387
14	0.044303080806	0.234659899379	0.330497128647
14	−0.113958354253	0.262850558828	−0.326887027253
8	−0.212973259924	−0.102318287754	−0.050497855654

8	−0.061450282068	−0.424276754129	0.268709459368
8	0.153424531370	−0.345064735946	−0.154528411012
8	0.393290131075	−0.411308969032	−0.330792337296
8	−0.207752068599	0.340563492564	0.334450078895
8	0.154262310592	−0.397587126908	−0.395458669469
8	−0.400237210754	0.455490185122	−0.257119480461
8	0.102488311660	−0.286121241999	0.129956333143
8	0.378310141565	−0.491923826091	0.371014391581
8	0.040863682969	−0.156744721149	−0.476850823652
8	0.485796621210	0.288269381969	0.361105956426
8	−0.470539086858	0.184445387017	−0.338608303541
8	−0.429975197559	0.229386177763	−0.094637455898
8	−0.472335413383	−0.083350315330	0.056106412021
8	0.179602266515	0.493415609938	0.154200514248
8	0.141964517231	−0.099909132498	−0.110831773448
8	−0.191789920576	−0.172564245439	0.372759948609
8	−0.125489524020	0.101735212077	−0.351069263604
8	−0.349356754477	−0.414505731282	−0.052635825116
8	0.124770671172	0.403163261733	−0.119625213971
8	−0.391572438013	−0.355685650743	0.379976397441
8	−0.216281176072	0.012239608829	0.172799871196
8	0.336158626351	0.008111241339	0.413370029953
8	0.287973544200	0.322146974072	−0.427364494009
8	−0.409174821638	0.443398769226	−0.498323681727
8	−0.281368799379	−0.276599087046	−0.303665129419
8	0.469104675343	0.121607127345	0.194406215203
8	0.233625463803	0.000561068117	0.096574658798
8	−0.111446323463	−0.461932322149	−0.255765866159
8	−0.050949129070	0.108212714607	0.391273274570
8	0.220017591509	0.248246455174	0.006921499018
8	−0.369731690197	0.085736380180	0.438678918538
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8	0.381831601425	0.054907811636	−0.131302154374
8	−0.397048904471	0.456219093971	0.230318359067
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8	0.435998954392	0.339798964445	0.118787308745
8	−0.021409420046	0.250922541897	0.200137759470
8	0.361844311383	0.496733120111	−0.055757004427
8	0.288729450989	−0.160470011483	−0.318290308968
8	−0.432427533597	−0.137050877673	0.307565191080
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8	0.147043302218	−0.356220066640	0.362446418963
8	−0.161965727136	0.272205085052	−0.182778647603
8	0.201106520808	0.203825617674	0.295496224527
8	−0.021540606956	−0.190649801820	−0.243209389433
8	0.363500635482	0.303302830393	−0.204591152834
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8	0.084385779956	−0.101455910260	0.293387092015
8	0.146130417063	0.132939795110	−0.227923862024
8	0.150065494670	0.100856586949	−0.440833477832
8	0.046785551725	0.325906578020	−0.342845125079
8	−0.142434925855	−0.388499258301	−0.490775399311
8	−0.405744616378	−0.135165183041	−0.419437221964
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8	−0.072137404128	−0.317011029120	−0.039061934258

8	−0.335937385300	−0.014451244617	−0.238140750988
8	−0.314607463479	0.234398625389	0.166129965578
8	−0.061792298288	0.109852639277	−0.034837907705
8	0.319137615755	−0.167416288441	0.232970457398
8	0.060941608204	0.372196786092	0.403908797668
8	0.474378959863	−0.324817887587	0.142449156725
8	−0.195918553017	0.328349786087	−0.423406501955

Amorphous 2 × 2 × 2 Mg_2SiO_4 structure.

a = 9.58976422000	α = 85.714872
b = 20.57419425000	β = 93.367506
c = 11.93781887000	γ = 91.743204

12	−0.366764219280	−0.377918300554	0.025564748863
12	0.238206216175	0.221995226492	−0.401543809988
12	−0.013433567011	−0.318347340150	−0.327954181383
12	0.106944543489	0.104852079097	−0.019908418561
12	−0.005139231183	−0.164052806005	0.168114627911
12	−0.239923147384	−0.384194519302	−0.487513299107
12	−0.380846211971	0.315133726243	0.409574531082
12	−0.280421998652	−0.035352411866	0.423347739102
12	0.346979496471	−0.492684099996	0.102628055207
12	0.343163035900	−0.353595324136	−0.315082329188
12	0.086566255360	−0.401305993028	−0.163244723639
12	−0.391655791235	−0.404943126082	0.249229638090
12	−0.139225353645	−0.247573391449	0.388224214179
12	−0.012718639680	0.418891666554	−0.229705397225
12	0.062286303112	0.175834641213	0.345344244712
12	0.426983054391	0.324500102006	0.243313568109
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12	0.255367667208	−0.216177097495	0.370744652007
12	0.093993139980	−0.303406419558	0.220097812121
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12	0.049992871997	−0.161454525102	−0.200174781859
12	0.366243029205	0.187332906784	0.090119970058
12	0.032832494311	0.150109800813	−0.281738867706
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12	−0.214205230931	0.354524515741	−0.408358714077
12	−0.478911863176	0.285631122694	−0.062310027940
12	−0.188607927055	−0.158318857349	−0.420971227376
12	−0.080217508913	−0.265527379336	−0.061097993865
12	0.432546568761	−0.068431269198	0.229314605457
12	0.420034252572	−0.189158354610	−0.345596754617
12	−0.496104966363	−0.241818862279	0.190273411376
12	−0.291409244453	−0.129858986138	0.185259183516
12	−0.145316414421	−0.031886694552	0.012205494865
12	0.272873426054	0.071940521842	−0.466587820800
12	0.086668666059	0.482483895485	0.274166124779
12	−0.365104281101	−0.279643847973	−0.380632557098
12	−0.228900766514	0.132232125537	0.129968483255
12	−0.019942618135	0.058770610847	0.217981234441
12	0.444688202943	0.375994152200	−0.455215633096
12	−0.496973764856	−0.099316316465	0.023431355635
12	−0.390411157326	−0.084130186698	−0.362079758623
12	0.083558251362	0.008644657723	−0.186847313165
12	0.459973204880	−0.435015243957	−0.484347942575
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12	0.270571371215	0.219645293121	−0.138490906161
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12	0.016196135452	−0.457565866254	−0.362247472172
12	0.433381872002	0.450286148993	0.314605402646
12	−0.421241692369	0.005491025692	−0.193801910476
12	−0.447290861968	0.397489809867	−0.222865773232
12	0.387485903802	0.029458874071	−0.004378463748
12	−0.254069681262	0.474250513356	0.402965122533
12	0.105764544109	0.350713097792	0.486724259290
12	0.184342580553	−0.028283215787	0.337462545654
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