

P1 7.5 GPa job P1Cm 0069
Cell volume 134.422 Angstrom**3
Enthalpy -107.805 eV/f.u.

SPGNAM= P1
CELEDG= 4.989231192 4.851069078 6.583991660 Angstroms
CELANG= 83.476317778 104.243860922 119.502303678 degrees.
ATOM= 1 Si 1a 1 0.364869439 0.641991350 0.115152933
ATOM= 2 Si 1a 1 0.706711835 0.304963801 0.112334841
ATOM= 3 Al 1a 1 0.523887536 -0.002309260 0.533595915
ATOM= 4 Al 1a 1 0.179809305 0.319726950 0.534854060
ATOM= 5 O 1a 1 0.426092686 0.654397681 0.367486396
ATOM= 6 O 1a 1 0.801397098 0.285910258 0.366578792
ATOM= 7 O 1a 1 0.392190318 -0.020751446 0.028127209
ATOM= 8 O 1a 1 0.008334410 0.362277766 0.023191791
ATOM= 9 O 1a 1 0.646268142 0.607243775 0.057974584
ATOM= 10 O 1a 1 0.899915730 -0.003544698 0.688642153
ATOM= 11 O 1a 1 0.269284692 0.665401659 0.689131513
ATOM= 12 O 1a 1 0.547692544 0.315490913 0.686614285
ATOM= 13 O 1a 1 0.178797777 0.033804107 0.371941161
ATOM= 14 H 1a 1 0.947420205 0.054060280 0.836062187
ATOM= 15 H 1a 1 0.109758744 0.717912847 0.703361933
ATOM= 16 H 1a 1 0.710433772 0.538040902 0.690383345
ATOM= 17 H 1a 1 -0.012062903 -0.141273653 0.296943896

Cm 7.5 GPa job P1Cm 0070
Cell volume 268.475 Angstrom**3
Enthalpy -107.730 eV/f.u.

SPGNAM= Cm
CELEDG= 4.824223129 8.634056145 6.692884157 Angstroms
CELANG= 90.000000000 105.623861424 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.050967280 0.332164737 -0.049279328
ATOM= 2 Al 4b 1 0.079962233 0.162462339 0.531513788
ATOM= 3 O 4b 1 -0.036447710 0.321957493 0.698694891
ATOM= 4 O 4b 1 0.770076405 0.309875129 0.034346786
ATOM= 5 O 2a .m. -0.300418342 0.000000000 0.024142762
ATOM= 6 O 4b 1 0.696889080 0.181352692 0.382352018
ATOM= 7 O 2a .m. 0.193052361 0.000000000 0.375931331
ATOM= 8 O 2a .m. 0.008282610 0.000000000 -0.308714020
ATOM= 9 H 4b 1 0.549912091 0.100815822 0.365778461
ATOM= 10 H 2a .m. 0.087815855 0.000000000 0.228766843
ATOM= 11 H 2a .m. -0.183092353 0.000000000 -0.286827534

P1 10 GPa job P1Cm 0009
Cell volume 131.601 Angstrom**3
Enthalpy -105.648 eV/f.u.

SPGNAM= P1
CELEDG= 4.963327790 4.820626825 6.521411258 Angstroms
CELANG= 83.368359617 104.358017313 119.467404347 degrees.
ATOM= 1 Si 1a 1 0.364687041 0.643074720 0.112660718

ATOM=	2	Si	1a	1	0.706322809	0.306543942	0.110043061
ATOM=	3	Al	1a	1	0.524459450	-0.002969118	0.534533028
ATOM=	4	Al	1a	1	0.179752344	0.318949367	0.535737596
ATOM=	5	O	1a	1	0.427581160	0.653738239	0.367646073
ATOM=	6	O	1a	1	0.801426343	0.287852397	0.366927955
ATOM=	7	O	1a	1	0.386421636	-0.018777548	0.027778796
ATOM=	8	O	1a	1	0.008413412	0.357723147	0.022541675
ATOM=	9	O	1a	1	0.652329457	0.615056305	0.056728912
ATOM=	10	O	1a	1	0.900246116	-0.007941783	0.690475216
ATOM=	11	O	1a	1	0.268323320	0.664373464	0.692499003
ATOM=	12	O	1a	1	0.550152357	0.316360145	0.689752739
ATOM=	13	O	1a	1	0.177552406	0.031702558	0.372596963
ATOM=	14	H	1a	1	0.948603723	0.048465344	0.839676324
ATOM=	15	H	1a	1	0.106227313	0.719137347	0.700136313
ATOM=	16	H	1a	1	0.711493789	0.540913849	0.689609733
ATOM=	17	H	1a	1	-0.013197058	-0.140861931	0.293035107

Cm 10 GPa job P1Cm 0010
 Cell volume 262.896 Angstrom**3
 Enthalpy -105.577 eV/f.u.

SPGNAM= Cm

CELEDG=	4.789286926	8.589318298	6.633550910	Angstroms			
CELANG=	90.000000000	105.548872001	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.051890916	0.332387386	-0.046863818
ATOM=	2	Al	4b	1	0.080546442	0.162326090	0.531058256
ATOM=	3	O	4b	1	-0.034602592	0.322951208	0.698959778
ATOM=	4	O	4b	1	0.766594571	0.312883950	0.035140045
ATOM=	5	O	2a	.m.	-0.294569723	0.000000000	0.026446335
ATOM=	6	O	4b	1	0.696228616	0.180596445	0.380018949
ATOM=	7	O	2a	.m.	0.196458026	0.000000000	0.374549063
ATOM=	8	O	2a	.m.	0.005993504	0.000000000	-0.308721959
ATOM=	9	H	4b	1	0.548009833	0.099931140	0.366724092
ATOM=	10	H	2a	.m.	0.090861554	0.000000000	0.226019580
ATOM=	11	H	2a	.m.	-0.187722223	0.000000000	-0.288251812

P1 12.5 GPa job P1Cm 0071
 Cell volume 128.786 Angstrom**3
 Enthalpy -103.512 eV/f.u.

SPGNAM= P1

CELEDG=	4.942391057	4.792251982	6.449371988	Angstroms			
CELANG=	83.244688944	104.518744134	119.434460271	degrees.			
ATOM=	1	Si	1a	1	0.364203126	0.644198881	0.109688333
ATOM=	2	Si	1a	1	0.705648328	0.308292420	0.107267626
ATOM=	3	Al	1a	1	0.525102550	-0.003728363	0.535491731
ATOM=	4	Al	1a	1	0.179488839	0.317987605	0.536633357
ATOM=	5	O	1a	1	0.428680327	0.652827549	0.367860989
ATOM=	6	O	1a	1	0.801376580	0.289640999	0.367333039
ATOM=	7	O	1a	1	0.380436189	-0.016670191	0.027733497
ATOM=	8	O	1a	1	0.008300089	0.353178586	0.022122752
ATOM=	9	O	1a	1	0.658240995	0.622998779	0.055753683
ATOM=	10	O	1a	1	0.900509066	-0.012088210	0.692384151

ATOM=	11	O	1a	1	0.267759845	0.663278376	0.696477391
ATOM=	12	O	1a	1	0.552564652	0.317002696	0.693376134
ATOM=	13	O	1a	1	0.176265818	0.029208609	0.373651387
ATOM=	14	H	1a	1	0.949892461	0.042541849	0.843734306
ATOM=	15	H	1a	1	0.103268237	0.719998752	0.697004626
ATOM=	16	H	1a	1	0.712345265	0.543288200	0.688664729
ATOM=	17	H	1a	1	-0.013290159	-0.138619563	0.287198943

Cm 12.5 GPa job P1Cm 0072
Cell volume 257.634 Angstrom**3
Enthalpy -103.456 eV/f.u.

SPGNAM= Cm

CELEDG=	4.757604266	8.550188893	6.571471563	Angstroms			
CELANG=	90.000000000	105.468632748	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.052787036	0.332584684	-0.044359220
ATOM=	2	Al	4b	1	0.081018547	0.162224580	0.530621154
ATOM=	3	O	4b	1	-0.032947601	0.323822234	0.699135089
ATOM=	4	O	4b	1	0.763146736	0.315680713	0.035699953
ATOM=	5	O	2a	.m.	-0.289359146	0.000000000	0.028538756
ATOM=	6	O	4b	1	0.695569540	0.179939955	0.377429303
ATOM=	7	O	2a	.m.	0.199470156	0.000000000	0.373352170
ATOM=	8	O	2a	.m.	0.003660312	0.000000000	-0.308821832
ATOM=	9	H	4b	1	0.546556954	0.099118354	0.367762364
ATOM=	10	H	2a	.m.	0.094052832	0.000000000	0.223312489
ATOM=	11	H	2a	.m.	-0.191732327	0.000000000	-0.288845535

P1 15 GPa job P1Cm 0005
Cell volume 126.299 Angstrom**3
Enthalpy -101.437 eV/f.u.

SPGNAM= P1

CELEDG=	4.923841771	4.767395440	6.384514498	Angstroms			
CELANG=	83.151566200	104.661618334	119.412231253	degrees.			
ATOM=	1	Si	1a	1	0.363604415	0.645054822	0.106643496
ATOM=	2	Si	1a	1	0.704777594	0.309688586	0.104372129
ATOM=	3	Al	1a	1	0.525818394	-0.004223682	0.536114369
ATOM=	4	Al	1a	1	0.179210467	0.317267052	0.537219967
ATOM=	5	O	1a	1	0.429553678	0.651864192	0.367892826
ATOM=	6	O	1a	1	0.801237944	0.291424065	0.367505673
ATOM=	7	O	1a	1	0.374822561	-0.015059730	0.027949215
ATOM=	8	O	1a	1	0.008188212	0.348554536	0.022032837
ATOM=	9	O	1a	1	0.663518005	0.629956987	0.055002463
ATOM=	10	O	1a	1	0.900716988	-0.015276049	0.693881235
ATOM=	11	O	1a	1	0.267605808	0.662464306	0.700220865
ATOM=	12	O	1a	1	0.554859436	0.317781107	0.696872028
ATOM=	13	O	1a	1	0.174797451	0.026357856	0.375035945
ATOM=	14	H	1a	1	0.950926466	0.037827604	0.847174923
ATOM=	15	H	1a	1	0.101312914	0.720975621	0.694341937
ATOM=	16	H	1a	1	0.713116556	0.545449215	0.687888253
ATOM=	17	H	1a	1	-0.013275094	-0.136760284	0.282229896

Cm 15 GPa job P1Cm 0006

Cell volume 252.899 Angstrom**3
Enthalpy -101.380 eV/f.u.

SPGNAM= Cm
CELEDG= 4.729431416 8.513944932 6.515107613 Angstroms
CELANG= 90.000000000 105.416061781 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.053773495 0.332745875 -0.041952559
ATOM= 2 Al 4b 1 0.081417010 0.162154979 0.530345604
ATOM= 3 O 4b 1 -0.031424680 0.324588598 0.699329489
ATOM= 4 O 4b 1 0.760102833 0.318231784 0.036010746
ATOM= 5 O 2a .m. -0.284514369 0.000000000 0.030314259
ATOM= 6 O 4b 1 0.694909903 0.179404401 0.374943301
ATOM= 7 O 2a .m. 0.202005815 0.000000000 0.372504576
ATOM= 8 O 2a .m. 0.001375040 0.000000266 -0.308955394
ATOM= 9 H 4b 1 0.545296658 0.098447854 0.368582041
ATOM= 10 H 2a .m. 0.096789766 0.000000000 0.221042900
ATOM= 11 H 2a .m. -0.195438028 0.000000000 -0.289303379

P1 17.5 GPa job P1Cm 0073
Cell volume 123.374 Angstrom**3
Enthalpy -99.334 eV/f.u.

SPGNAM= P1
CELEDG= 4.913999561 4.745240767 6.284064872 Angstroms
CELANG= 82.992560556 104.922493620 119.383627422 degrees.
ATOM= 1 Si 1a 1 0.362484378 0.646314215 0.101227616
ATOM= 2 Si 1a 1 0.703272103 0.311827442 0.099010627
ATOM= 3 Al 1a 1 0.526952801 -0.004831581 0.536583709
ATOM= 4 Al 1a 1 0.178479260 0.316249615 0.537724203
ATOM= 5 O 1a 1 0.429511259 0.650074167 0.367795785
ATOM= 6 O 1a 1 0.800861793 0.293380732 0.367513976
ATOM= 7 O 1a 1 0.368162971 -0.012726189 0.028704575
ATOM= 8 O 1a 1 0.008194001 0.342977445 0.022411262
ATOM= 9 O 1a 1 0.670057651 0.638759955 0.054660161
ATOM= 10 O 1a 1 0.900639878 -0.018895765 0.695760632
ATOM= 11 O 1a 1 0.268013779 0.661297154 0.706283464
ATOM= 12 O 1a 1 0.557891058 0.318848882 0.702450576
ATOM= 13 O 1a 1 0.172878773 0.021943916 0.377839838
ATOM= 14 H 1a 1 0.952034895 0.031650355 0.852125257
ATOM= 15 H 1a 1 0.099706531 0.721642091 0.690841595
ATOM= 16 H 1a 1 0.713373764 0.547445089 0.686437819
ATOM= 17 H 1a 1 -0.011724012 -0.132610750 0.275006830

Cm 17.5 GPa job P1Cm 0074
Cell volume 247.874 Angstrom**3
Enthalpy -99.292 eV/f.u.

SPGNAM= Cm
CELEDG= 4.702078552 8.482351489 6.444845734 Angstroms
CELANG= 90.000000000 105.355803305 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.054652222 0.332869547 -0.038978552
ATOM= 2 Al 4b 1 0.081781606 0.162105817 0.529986083
ATOM= 3 O 4b 1 -0.030051884 0.325184312 0.699414730

ATOM=	4	O	4b	1	0.756385138	0.320961765	0.036128631
ATOM=	5	O	2a	.m.	-0.279984746	0.000000000	0.031761848
ATOM=	6	O	4b	1	0.694087920	0.178819388	0.371775070
ATOM=	7	O	2a	.m.	0.204664856	0.000000000	0.371608534
ATOM=	8	O	2a	.m.	-0.001049333	0.000000000	-0.309298201
ATOM=	9	H	4b	1	0.544450458	0.097696821	0.369798679
ATOM=	10	H	2a	.m.	0.100537021	0.000000000	0.218237156
ATOM=	11	H	2a	.m.	-0.198414155	0.000000000	-0.288438451

P1 20 GPa job P1Cm 0007
Cell volume 121.191 Angstrom**3
Enthalpy -97.363 eV/f.u.

SPGNAM= P1
CELEDG= 4.903258319 4.727410818 6.213080621 Angstroms
CELANG= 82.891782156 105.085049111 119.361443118 degrees.
ATOM= 1 Si 1a 1 0.361566408 0.647135521 0.096608822
ATOM= 2 Si 1a 1 0.701781905 0.313255255 0.094057599
ATOM= 3 Al 1a 1 0.528063967 -0.005015561 0.536352906
ATOM= 4 Al 1a 1 0.177759114 0.315774244 0.537594004
ATOM= 5 O 1a 1 0.429679223 0.648658129 0.367415887
ATOM= 6 O 1a 1 0.800488491 0.295233855 0.366975722
ATOM= 7 O 1a 1 0.362904211 -0.011273396 0.029589243
ATOM= 8 O 1a 1 0.008437605 0.338157880 0.022947498
ATOM= 9 O 1a 1 0.675344217 0.645470917 0.054586972
ATOM= 10 O 1a 1 0.900546845 -0.021152087 0.696812758
ATOM= 11 O 1a 1 0.268467432 0.660629945 0.710875478
ATOM= 12 O 1a 1 0.560437095 0.319905723 0.706953718
ATOM= 13 O 1a 1 0.171244229 0.018097857 0.380325275
ATOM= 14 H 1a 1 0.952526019 0.027887498 0.855342232
ATOM= 15 H 1a 1 0.099179035 0.722697707 0.688466271
ATOM= 16 H 1a 1 0.713772257 0.549224203 0.685895943
ATOM= 17 H 1a 1 -0.011400167 -0.131347022 0.271584271

Cm 20 GPa job P1Cm 0008
Cell volume 244.033 Angstrom**3
Enthalpy -97.317 eV/f.u.

SPGNAM= Cm
CELEDG= 4.680220664 8.453487712 6.395958602 Angstroms
CELANG= 90.000000000 105.341973970 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.055667647 0.332929791 -0.036591550
ATOM= 2 Al 4b 1 0.082118595 0.162086436 0.529910780
ATOM= 3 O 4b 1 -0.028853502 0.325684070 0.699630987
ATOM= 4 O 4b 1 0.753816298 0.323146175 0.036059317
ATOM= 5 O 2a .m. -0.276067591 0.000000000 0.032859098
ATOM= 6 O 4b 1 0.693406424 0.178440409 0.369363946
ATOM= 7 O 2a .m. 0.206688682 0.000000000 0.371187505
ATOM= 8 O 2a .m. -0.003221631 0.000000000 -0.309652652
ATOM= 9 H 4b 1 0.543585016 0.097212350 0.370408740
ATOM= 10 H 2a .m. 0.102791041 0.000000000 0.216507867
ATOM= 11 H 2a .m. -0.201307513 0.000000000 -0.288350990

P1 22.5 GPa job P1Cm 0075
Cell volume 118.133 Angstrom**3
Enthalpy -95.346 eV/f.u.

SPGNAM= P1
CELEDG= 4.923219728 4.717679955 6.060516153 Angstroms
CELANG= 82.548864792 105.638829678 119.365971571 degrees.
ATOM= 1 Si 1a 1 0.359062620 0.648513504 0.086005031
ATOM= 2 Si 1a 1 0.697786671 0.316423332 0.080383564
ATOM= 3 Al 1a 1 0.531029765 -0.004650921 0.534373059
ATOM= 4 Al 1a 1 0.174724496 0.314144483 0.536158392
ATOM= 5 O 1a 1 0.428356256 0.645140749 0.367334776
ATOM= 6 O 1a 1 0.799707571 0.297697482 0.365079042
ATOM= 7 O 1a 1 0.355869967 -0.008681850 0.031824218
ATOM= 8 O 1a 1 0.009063668 0.331706196 0.024938146
ATOM= 9 O 1a 1 0.682726920 0.656042379 0.056515339
ATOM= 10 O 1a 1 0.899790279 -0.024061531 0.698828406
ATOM= 11 O 1a 1 0.270200514 0.659232666 0.720264979
ATOM= 12 O 1a 1 0.565936957 0.323076564 0.717084287
ATOM= 13 O 1a 1 0.169526947 0.010960173 0.386016317
ATOM= 14 H 1a 1 0.953637199 0.022183699 0.862258561
ATOM= 15 H 1a 1 0.100493002 0.723506998 0.683301905
ATOM= 16 H 1a 1 0.713112484 0.552378608 0.684671062
ATOM= 17 H 1a 1 -0.010222208 -0.130261078 0.267352006

Cm 22.5 GPa job P1Cm 0076
Cell volume 239.451 Angstrom**3
Enthalpy -95.295 eV/f.u.

SPGNAM= Cm
CELEDG= 4.659019509 8.438112704 6.315489919 Angstroms
CELANG= 90.000000000 105.328396043 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.056591249 0.332931105 -0.032790232
ATOM= 2 Al 4b 1 0.082357696 0.162077783 0.529611417
ATOM= 3 O 4b 1 -0.027899857 0.325801078 0.699567227
ATOM= 4 O 4b 1 0.749669396 0.325843788 0.035452976
ATOM= 5 O 2a .m. -0.272449111 0.000000000 0.033044317
ATOM= 6 O 4b 1 0.692055929 0.177928951 0.365155981
ATOM= 7 O 2a .m. 0.209100483 0.000000000 0.370515738
ATOM= 8 O 2a .m. -0.005952909 0.000000000 -0.310779998
ATOM= 9 H 4b 1 0.543519622 0.096569875 0.372209613
ATOM= 10 H 2a .m. 0.107206700 0.000000000 0.213448219
ATOM= 11 H 2a .m. -0.202127805 0.000000000 -0.284528256

P1 25 GPa job P1Cm 0011
Cell volume 116.640 Angstrom**3
Enthalpy -93.465 eV/f.u.

SPGNAM= P1
CELEDG= 4.908032555 4.698663434 6.027618100 Angstroms
CELANG= 82.520675090 105.682428204 119.359256440 degrees.

ATOM=	1	Si	1a	1	0.358631587	0.648562327	0.083750558
ATOM=	2	Si	1a	1	0.697033673	0.316853119	0.077794815
ATOM=	3	Al	1a	1	0.531614737	-0.004555871	0.533784506
ATOM=	4	Al	1a	1	0.174297847	0.313944582	0.535755093
ATOM=	5	O	1a	1	0.429474002	0.644343953	0.367184998
ATOM=	6	O	1a	1	0.799708211	0.299499911	0.364742541
ATOM=	7	O	1a	1	0.353125602	-0.008250672	0.032560320
ATOM=	8	O	1a	1	0.009315233	0.328297736	0.025750743
ATOM=	9	O	1a	1	0.685579109	0.659479175	0.056189270
ATOM=	10	O	1a	1	0.899733801	-0.025342662	0.699154804
ATOM=	11	O	1a	1	0.270060721	0.658909227	0.722174904
ATOM=	12	O	1a	1	0.567485829	0.323783066	0.718987587
ATOM=	13	O	1a	1	0.168136684	0.008248147	0.387182927
ATOM=	14	H	1a	1	0.953723473	0.021696681	0.863437163
ATOM=	15	H	1a	1	0.100383938	0.724769260	0.682529608
ATOM=	16	H	1a	1	0.713907621	0.554395947	0.685110780
ATOM=	17	H	1a	1	-0.011424185	-0.131293928	0.266281569

Cm 25 GPa job P1Cm 0085
Cell volume 231.687 Angstrom**3
Enthalpy -93.314 eV/f.u.

SPGNAM= Cm

CELEDG=	4.696121713	8.544045467	5.986914086	Angstroms			
CELANG=	90.000000000	105.315286917	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.054932862	0.331647114	-0.018019859
ATOM=	2	Al	4b	1	0.078598006	0.162126150	0.527247350
ATOM=	3	O	4b	1	-0.038624209	0.319840901	0.694443490
ATOM=	4	O	4b	1	0.731167329	0.333544418	0.025091578
ATOM=	5	O	2a	.m.	-0.273899524	0.000000000	0.016691659
ATOM=	6	O	4b	1	0.679589407	0.175830301	0.338951351
ATOM=	7	O	2a	.m.	0.204941920	0.000000000	0.366491710
ATOM=	8	O	2a	.m.	-0.033212144	0.000000000	-0.329883589
ATOM=	9	H	4b	1	0.553412287	0.095190601	0.383475742
ATOM=	10	H	2a	.m.	0.122835311	0.000000000	0.199028086
ATOM=	11	H	2a	.m.	-0.110467493	0.000000000	-0.194603862

P1 27.5 GPa job P1Cm 0077
Cell volume 114.874 Angstrom**3
Enthalpy -91.532 eV/f.u.

SPGNAM= P1

CELEDG=	4.910454615	4.680355091	5.962965395	Angstroms			
CELANG=	82.389928674	105.894519465	119.361564009	degrees.			
ATOM=	1	Si	1a	1	0.357360552	0.648863978	0.079560100
ATOM=	2	Si	1a	1	0.696121755	0.318327034	0.073660164
ATOM=	3	Al	1a	1	0.532866139	-0.004166528	0.532925434
ATOM=	4	Al	1a	1	0.173361176	0.312864453	0.535212570
ATOM=	5	O	1a	1	0.429847644	0.642920521	0.367245881
ATOM=	6	O	1a	1	0.800336391	0.301910289	0.364996039
ATOM=	7	O	1a	1	0.351009462	-0.006540667	0.033659209
ATOM=	8	O	1a	1	0.009093452	0.325447999	0.026936770
ATOM=	9	O	1a	1	0.688112887	0.663754866	0.056649907

ATOM=	10	O	1a	1	0.899410541	-0.027344848	0.699954205
ATOM=	11	O	1a	1	0.270383201	0.658169909	0.725464081
ATOM=	12	O	1a	1	0.569648492	0.325264611	0.721562210
ATOM=	13	O	1a	1	0.166893741	0.004397732	0.389026464
ATOM=	14	H	1a	1	0.954083387	0.019783478	0.866220357
ATOM=	15	H	1a	1	0.100736910	0.725162002	0.680061085
ATOM=	16	H	1a	1	0.714213815	0.557108622	0.684537220
ATOM=	17	H	1a	1	-0.012689411	-0.132581423	0.264702554

Cm 27.5 GPa job P1Cm 0081
 Cell volume 228.851 Angstrom**3
 Enthalpy -91.454 eV/f.u.

SPGNAM= Cm

CELEDG=	4.676096882	8.525888450	5.951732130	Angstroms
CELANG=	90.000000000	105.319960845	90.000000000	degrees.

ATOM=	1	Si	4b	1	0.055985184	0.331669677	-0.015770763
ATOM=	2	Al	4b	1	0.079372357	0.161950681	0.527847384
ATOM=	3	O	4b	1	-0.037160779	0.320350849	0.694614078
ATOM=	4	O	4b	1	0.729347073	0.334917420	0.024293096
ATOM=	5	O	2a	.m.	-0.271519823	0.000000000	0.017252623
ATOM=	6	O	4b	1	0.679120025	0.175748514	0.337360653
ATOM=	7	O	2a	.m.	0.206774714	0.000000000	0.366483030
ATOM=	8	O	2a	.m.	-0.036524233	0.000000000	-0.331076249
ATOM=	9	H	4b	1	0.552762995	0.095128273	0.383537490
ATOM=	10	H	2a	.m.	0.123790344	0.000000000	0.198046097
ATOM=	11	H	2a	.m.	-0.113012794	0.000000000	-0.194362055

P1 30 GPa job P1Cm 0015
 Cell volume 113.667 Angstrom**3
 Enthalpy -89.707 eV/f.u.

SPGNAM= P1

CELEDG=	4.893635176	4.661414197	5.943697904	Angstroms
CELANG=	82.394289636	105.892710648	119.346236942	degrees.

ATOM=	1	Si	1a	1	0.357128964	0.648775376	0.078484623
ATOM=	2	Si	1a	1	0.695828102	0.318433039	0.072615462
ATOM=	3	Al	1a	1	0.533137219	-0.004079777	0.532661329
ATOM=	4	Al	1a	1	0.173314105	0.312782601	0.535051981
ATOM=	5	O	1a	1	0.431090768	0.642452743	0.367166512
ATOM=	6	O	1a	1	0.800460905	0.303410246	0.364940347
ATOM=	7	O	1a	1	0.349076541	-0.006282396	0.034169971
ATOM=	8	O	1a	1	0.009228453	0.322858920	0.027533412
ATOM=	9	O	1a	1	0.690014836	0.666052041	0.056143527
ATOM=	10	O	1a	1	0.899448740	-0.028382147	0.700109624
ATOM=	11	O	1a	1	0.270077690	0.657962389	0.726379383
ATOM=	12	O	1a	1	0.570566023	0.325545744	0.722387768
ATOM=	13	O	1a	1	0.165681701	0.002387607	0.389550890
ATOM=	14	H	1a	1	0.954174568	0.019890097	0.866776811
ATOM=	15	H	1a	1	0.100374069	0.726181308	0.679633883
ATOM=	16	H	1a	1	0.715072318	0.558772200	0.685000416
ATOM=	17	H	1a	1	-0.013884058	-0.133420013	0.263773478

Cm 30 GPa job P1Cm 0087
Cell volume 226.149 Angstrom**3
Enthalpy -89.600 eV/f.u.

SPGNAM= Cm
CELEDG= 4.657493065 8.513578188 5.913163187 Angstroms
CELANG= 90.000000000 105.308148620 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.056898762 0.331706591 -0.013687973
ATOM= 2 Al 4b 1 0.080092590 0.161734581 0.528361046
ATOM= 3 O 4b 1 -0.035762509 0.320825150 0.694595989
ATOM= 4 O 4b 1 0.727572877 0.336060812 0.023483187
ATOM= 5 O 2a .m. -0.269648257 0.000000000 0.017745943
ATOM= 6 O 4b 1 0.678693079 0.175664094 0.335966581
ATOM= 7 O 2a .m. 0.208483832 0.000000000 0.366357254
ATOM= 8 O 2a .m. -0.039539542 0.000000000 -0.332147957
ATOM= 9 H 4b 1 0.552334917 0.095091627 0.383932094
ATOM= 10 H 2a .m. 0.124861873 0.000000000 0.196849538
ATOM= 11 H 2a .m. -0.115469909 0.000000000 -0.193994343

P1 32.5 GPa job P1Cm 0079
Cell volume 112.351 Angstrom**3
Enthalpy -87.855 eV/f.u.

SPGNAM= P1
CELEDG= 4.885108082 4.641080890 5.912577109 Angstroms
CELANG= 82.349609096 105.970371415 119.335515805 degrees.
ATOM= 1 Si 1a 1 0.356571421 0.648739664 0.076855688
ATOM= 2 Si 1a 1 0.695541952 0.318984672 0.071041429
ATOM= 3 Al 1a 1 0.533694341 -0.003789912 0.532329071
ATOM= 4 Al 1a 1 0.173074445 0.312267293 0.534910638
ATOM= 5 O 1a 1 0.432062489 0.641681713 0.367239661
ATOM= 6 O 1a 1 0.800915602 0.305097097 0.365102041
ATOM= 7 O 1a 1 0.347450997 -0.005436585 0.034818255
ATOM= 8 O 1a 1 0.009110669 0.320654857 0.028202670
ATOM= 9 O 1a 1 0.691646029 0.668724824 0.055971392
ATOM= 10 O 1a 1 0.899338174 -0.029783917 0.700457777
ATOM= 11 O 1a 1 0.269944496 0.657547211 0.727684808
ATOM= 12 O 1a 1 0.571706378 0.326103091 0.723378439
ATOM= 13 O 1a 1 0.164562260 -0.000081161 0.390287104
ATOM= 14 H 1a 1 0.954377185 0.019395258 0.867972187
ATOM= 15 H 1a 1 0.100161493 0.726715820 0.678379727
ATOM= 16 H 1a 1 0.715784786 0.560883640 0.685128818
ATOM= 17 H 1a 1 -0.015153886 -0.134364919 0.262625179

Cm 32.5 GPa job P1Cm 0080
Cell volume 223.811 Angstrom**3
Enthalpy -87.790 eV/f.u.

SPGNAM= Cm
CELEDG= 4.638368680 8.495921176 5.888235895 Angstroms
CELANG= 90.000000000 105.303798794 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.057524416 0.331750959 -0.012400942
ATOM= 2 Al 4b 1 0.080580347 0.161604607 0.528703321

ATOM= 3 O 4b 1 -0.034479504 0.321324780 0.694675072
ATOM= 4 O 4b 1 0.726095652 0.337052327 0.022864497
ATOM= 5 O 2a .m. -0.267775624 0.000000000 0.018383088
ATOM= 6 O 4b 1 0.678428398 0.175644285 0.335110596
ATOM= 7 O 2a .m. 0.210041276 0.000000000 0.366354138
ATOM= 8 O 2a .m. -0.041731219 0.000000000 -0.332906551
ATOM= 9 H 4b 1 0.551587997 0.095003235 0.383948618
ATOM= 10 H 2a .m. 0.125448298 0.000000000 0.196180333
ATOM= 11 H 2a .m. -0.117106282 0.000000000 -0.193698390

P1 35 GPa job P1Cm 0021
Cell volume 111.278 Angstrom**3
Enthalpy -86.070 eV/f.u.

SPGNAM= P1
CELEDG= 4.869973112 4.624455041 5.894963606 Angstroms
CELLANG= 82.355099992 105.967354377 119.328996022 degrees.
ATOM= 1 Si 1a 1 0.356379709 0.648635833 0.076035534
ATOM= 2 Si 1a 1 0.695320213 0.319037793 0.070286617
ATOM= 3 Al 1a 1 0.533897963 -0.003689319 0.532153494
ATOM= 4 Al 1a 1 0.173118315 0.312187141 0.534812731
ATOM= 5 O 1a 1 0.433245836 0.641321731 0.367211694
ATOM= 6 O 1a 1 0.801095381 0.306424422 0.365125790
ATOM= 7 O 1a 1 0.345864793 -0.005263096 0.035264864
ATOM= 8 O 1a 1 0.009199541 0.318484535 0.028724546
ATOM= 9 O 1a 1 0.693158885 0.670566084 0.055514355
ATOM= 10 O 1a 1 0.899371530 -0.030690361 0.700595321
ATOM= 11 O 1a 1 0.269639112 0.657363252 0.728340870
ATOM= 12 O 1a 1 0.572466398 0.326333276 0.723971718
ATOM= 13 O 1a 1 0.163514172 -0.001769191 0.390636403
ATOM= 14 H 1a 1 0.954493889 0.019561635 0.868482830
ATOM= 15 H 1a 1 0.099731540 0.727482319 0.677907267
ATOM= 16 H 1a 1 0.716594641 0.562455866 0.685535914
ATOM= 17 H 1a 1 -0.016297409 -0.135100925 0.261778503

Cm 35 GPa job P1Cm 0022
Cell volume 221.724 Angstrom**3
Enthalpy -86.017 eV/f.u.

SPGNAM= Cm
CELEDG= 4.619087046 8.467235997 5.877902225 Angstroms
CELLANG= 90.000000000 105.317511233 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.058010449 0.331772130 -0.011734837
ATOM= 2 Al 4b 1 0.080868573 0.161604473 0.528955008
ATOM= 3 O 4b 1 -0.033310494 0.321892742 0.694961963
ATOM= 4 O 4b 1 0.725009674 0.338045246 0.022432127
ATOM= 5 O 2a .m. -0.265489191 0.000000000 0.019226850
ATOM= 6 O 4b 1 0.678269667 0.175689953 0.334607047
ATOM= 7 O 2a .m. 0.211432239 0.000000000 0.366529211
ATOM= 8 O 2a .m. -0.043440933 0.000000000 -0.333474270
ATOM= 9 H 4b 1 0.550400041 0.094838118 0.383387309
ATOM= 10 H 2a .m. 0.125359475 0.000000000 0.196133041
ATOM= 11 H 2a .m. -0.117993609 0.000000000 -0.193522191

P1 40 GPa job P1Cm 0025
Cell volume 109.193 Angstrom**3
Enthalpy -82.520 eV/f.u.

SPGNAM= P1
CELEDG= 4.843879671 4.590377606 5.857945624 Angstroms
CELANG= 82.343550200 105.992782133 119.300162602 degrees.
ATOM= 1 Si 1a 1 0.355862748 0.648377705 0.074452554
ATOM= 2 Si 1a 1 0.694958741 0.319222143 0.068847151
ATOM= 3 Al 1a 1 0.534376971 -0.003415800 0.531852591
ATOM= 4 Al 1a 1 0.173189067 0.311906455 0.534714375
ATOM= 5 O 1a 1 0.435436551 0.640508028 0.367239575
ATOM= 6 O 1a 1 0.801600770 0.308994138 0.365280450
ATOM= 7 O 1a 1 0.343094687 -0.004657686 0.036146897
ATOM= 8 O 1a 1 0.009235011 0.314654891 0.029680614
ATOM= 9 O 1a 1 0.695703483 0.674069811 0.054693055
ATOM= 10 O 1a 1 0.899438909 -0.032571635 0.700929521
ATOM= 11 O 1a 1 0.269093121 0.656962706 0.729572815
ATOM= 12 O 1a 1 0.573886564 0.326753068 0.725019061
ATOM= 13 O 1a 1 0.161578680 -0.005056689 0.391276335
ATOM= 14 H 1a 1 0.954806828 0.019689395 0.869652615
ATOM= 15 H 1a 1 0.098961050 0.728883067 0.676626292
ATOM= 16 H 1a 1 0.718150058 0.565625654 0.686226221
ATOM= 17 H 1a 1 -0.018582101 -0.136608924 0.260175147

Cm 40 GPa job P1Cm 0026
Cell volume 217.522 Angstrom**3
Enthalpy -82.477 eV/f.u.

SPGNAM= Cm
CELEDG= 4.581473176 8.434649534 5.836317757 Angstroms
CELANG= 90.000000000 105.317370608 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.058968174 0.331890494 -0.009905449
ATOM= 2 Al 4b 1 0.081589290 0.161391412 0.529422766
ATOM= 3 O 4b 1 -0.030857172 0.322872929 0.695061751
ATOM= 4 O 4b 1 0.722389343 0.339634740 0.021380185
ATOM= 5 O 2a .m. -0.262251805 0.000000000 0.020511226
ATOM= 6 O 4b 1 0.677917636 0.175678906 0.333463236
ATOM= 7 O 2a .m. 0.214173061 0.000000000 0.366506691
ATOM= 8 O 2a .m. -0.046606562 0.000000000 -0.334528976
ATOM= 9 H 4b 1 0.548768413 0.094632266 0.383345310
ATOM= 10 H 2a .m. 0.125973563 0.000000000 0.195027253
ATOM= 11 H 2a .m. -0.120477911 0.000000000 -0.192939146

P1 45 GPa job P1Cm 0029
Cell volume 107.308 Angstrom**3
Enthalpy -79.044 eV/f.u.

SPGNAM= P1
CELEDG= 4.818661788 4.558099173 5.826866950 Angstroms
CELANG= 82.348282183 106.001664511 119.276512913 degrees.
ATOM= 1 Si 1a 1 0.355473045 0.648100740 0.073260725

ATOM=	2	Si	1a	1	0.694672422	0.319267297	0.067769170
ATOM=	3	Al	1a	1	0.534765943	-0.003151721	0.531607540
ATOM=	4	Al	1a	1	0.173345217	0.311676308	0.534635131
ATOM=	5	O	1a	1	0.437525068	0.639778903	0.367244723
ATOM=	6	O	1a	1	0.802071563	0.311243546	0.365380524
ATOM=	7	O	1a	1	0.340564785	-0.004211392	0.036923810
ATOM=	8	O	1a	1	0.009280959	0.311208151	0.030534344
ATOM=	9	O	1a	1	0.697925884	0.677114910	0.053900085
ATOM=	10	O	1a	1	0.899470733	-0.034213416	0.701158887
ATOM=	11	O	1a	1	0.268569741	0.656539408	0.730523327
ATOM=	12	O	1a	1	0.575091765	0.327021865	0.725849504
ATOM=	13	O	1a	1	0.159786692	-0.008105173	0.391791779
ATOM=	14	H	1a	1	0.955089660	0.020348843	0.870507000
ATOM=	15	H	1a	1	0.098157093	0.730025220	0.675512224
ATOM=	16	H	1a	1	0.719677764	0.568678161	0.687064626
ATOM=	17	H	1a	1	-0.020667461	-0.137987002	0.258711023

Cm 45 GPa job P1Cm 0030
Cell volume 213.754 Angstrom**3
Enthalpy -79.016 eV/f.u.

SPGNAM= Cm

CELEDG=	4.544424272	8.405129961	5.802110046	Angstroms			
CELANG=	90.000000000	105.310941588	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.059729506	0.332001112	-0.008506927
ATOM=	2	Al	4b	1	0.082244518	0.161213778	0.529816069
ATOM=	3	O	4b	1	-0.028444080	0.323766731	0.695245158
ATOM=	4	O	4b	1	0.719894186	0.341023696	0.020435913
ATOM=	5	O	2a	.m.	-0.259510436	0.000000000	0.021812231
ATOM=	6	O	4b	1	0.677709347	0.175755520	0.332666451
ATOM=	7	O	2a	.m.	0.216925449	0.000000000	0.366604923
ATOM=	8	O	2a	.m.	-0.049313956	0.000000000	-0.335501409
ATOM=	9	H	4b	1	0.547124873	0.094435952	0.383141479
ATOM=	10	H	2a	.m.	0.126522740	0.000000000	0.194226588
ATOM=	11	H	2a	.m.	-0.122780568	0.000000000	-0.192623018

P1 50 GPa job P1Cm 0033
Cell volume 105.590 Angstrom**3
Enthalpy -75.636 eV/f.u.

SPGNAM= P1

CELEDG=	4.794286196	4.528414450	5.799945942	Angstroms			
CELANG=	82.347847837	106.002619798	119.266344286	degrees.			
ATOM=	1	Si	1a	1	0.355133075	0.647800270	0.072350175
ATOM=	2	Si	1a	1	0.694375851	0.319193976	0.066925150
ATOM=	3	Al	1a	1	0.535084154	-0.002901042	0.531409065
ATOM=	4	Al	1a	1	0.173621404	0.311517430	0.534609048
ATOM=	5	O	1a	1	0.439556582	0.639192040	0.367262425
ATOM=	6	O	1a	1	0.802567771	0.313253840	0.365445269
ATOM=	7	O	1a	1	0.338193820	-0.003962009	0.037650291
ATOM=	8	O	1a	1	0.009273542	0.308063789	0.031276535
ATOM=	9	O	1a	1	0.699812690	0.679697870	0.053134682
ATOM=	10	O	1a	1	0.899496699	-0.035620588	0.701322710

ATOM=	11	O	1a	1	0.268088996	0.656147372	0.731278725
ATOM=	12	O	1a	1	0.576157453	0.327198931	0.726570145
ATOM=	13	O	1a	1	0.158137287	-0.010831557	0.392204292
ATOM=	14	H	1a	1	0.955351636	0.021260116	0.871172215
ATOM=	15	H	1a	1	0.097306200	0.730910658	0.674408119
ATOM=	16	H	1a	1	0.721212730	0.571603858	0.687968033
ATOM=	17	H	1a	1	-0.022578099	-0.139191048	0.257386977

Cm 50 GPa job P1Cm 0034
Cell volume 210.338 Angstrom**3
Enthalpy -75.618 eV/f.u.

SPGNAM= Cm

CELEDG=	4.512943902	8.369111937	5.774340070	Angstroms			
CELANG=	90.000000000	105.324599974	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.060400988	0.332058875	-0.007431322
ATOM=	2	Al	4b	1	0.082715256	0.161125610	0.530135043
ATOM=	3	O	4b	1	-0.026435388	0.324615855	0.695449729
ATOM=	4	O	4b	1	0.717969809	0.342298219	0.019605437
ATOM=	5	O	2a	.m.	-0.256782704	0.000000000	0.023055228
ATOM=	6	O	4b	1	0.677480739	0.175849175	0.332035341
ATOM=	7	O	2a	.m.	0.219198476	0.000000000	0.366707521
ATOM=	8	O	2a	.m.	-0.051676330	0.000000000	-0.336285926
ATOM=	9	H	4b	1	0.545493396	0.094190305	0.382840976
ATOM=	10	H	2a	.m.	0.126839390	0.000000000	0.193604718
ATOM=	11	H	2a	.m.	-0.124462547	0.000000000	-0.192235526

P1 55 GPa job P1Cm 0037
Cell volume 104.008 Angstrom**3
Enthalpy -72.282 eV/f.u.

SPGNAM= P1

CELEDG=	4.770835556	4.501208127	5.774825100	Angstroms			
CELANG=	82.350324552	105.998362921	119.250516285	degrees.			
ATOM=	1	Si	1a	1	0.354853979	0.647522941	0.071580794
ATOM=	2	Si	1a	1	0.694098347	0.319037931	0.066213498
ATOM=	3	Al	1a	1	0.535341398	-0.002707640	0.531252290
ATOM=	4	Al	1a	1	0.173901759	0.311411176	0.534585234
ATOM=	5	O	1a	1	0.441486170	0.638702641	0.367296214
ATOM=	6	O	1a	1	0.802985265	0.315065328	0.365505761
ATOM=	7	O	1a	1	0.336074367	-0.003787920	0.038295835
ATOM=	8	O	1a	1	0.009345855	0.305236934	0.032032492
ATOM=	9	O	1a	1	0.701449120	0.681889632	0.052374665
ATOM=	10	O	1a	1	0.899567357	-0.036828900	0.701507321
ATOM=	11	O	1a	1	0.267579030	0.655763070	0.731887862
ATOM=	12	O	1a	1	0.577116785	0.327308767	0.727137392
ATOM=	13	O	1a	1	0.156613197	-0.013264234	0.392517313
ATOM=	14	H	1a	1	0.955644520	0.022266342	0.871798781
ATOM=	15	H	1a	1	0.096489651	0.731787668	0.673362000
ATOM=	16	H	1a	1	0.722685608	0.574315653	0.688777499
ATOM=	17	H	1a	1	-0.024437472	-0.140387438	0.256250055

Cm 55 GPa job P1Cm 0038

Cell volume 207.168 Angstrom**3
Enthalpy -72.274 eV/f.u.

SPGNAM= Cm
CELEDG= 4.482342047 8.337145480 5.748294935 Angstroms
CELANG= 90.000000000 105.332467270 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.060966681 0.332120745 -0.006504283
ATOM= 2 Al 4b 1 0.083179574 0.161036804 0.530411220
ATOM= 3 O 4b 1 -0.024451759 0.325413452 0.695635161
ATOM= 4 O 4b 1 0.716076229 0.343428108 0.018818448
ATOM= 5 O 2a .m. -0.254421413 0.000000000 0.024288690
ATOM= 6 O 4b 1 0.677314292 0.175972193 0.331510096
ATOM= 7 O 2a .m. 0.221376710 0.000000000 0.366793718
ATOM= 8 O 2a .m. -0.053753560 0.000000000 -0.336993807
ATOM= 9 H 4b 1 0.543976881 0.093966669 0.382584933
ATOM= 10 H 2a .m. 0.127082120 0.000000000 0.193021629
ATOM= 11 H 2a .m. -0.126036599 0.000000000 -0.191913722

P1 60 GPa job P1Cm 0043
Cell volume 102.536 Angstrom**3
Enthalpy -68.978 eV/f.u.

SPGNAM= P1
CELEDG= 4.747980382 4.475492617 5.751235348 Angstroms
CELANG= 82.359427572 105.988773190 119.218143183 degrees.
ATOM= 1 Si 1a 1 0.354607151 0.647276394 0.070906037
ATOM= 2 Si 1a 1 0.693839734 0.318818707 0.065617758
ATOM= 3 Al 1a 1 0.535551332 -0.002605826 0.531106641
ATOM= 4 Al 1a 1 0.174186413 0.311357583 0.534576788
ATOM= 5 O 1a 1 0.443298369 0.638207879 0.367331794
ATOM= 6 O 1a 1 0.803325931 0.316669017 0.365570559
ATOM= 7 O 1a 1 0.334178444 -0.003607347 0.038906495
ATOM= 8 O 1a 1 0.009486462 0.302715467 0.032735949
ATOM= 9 O 1a 1 0.702925336 0.683834269 0.051630874
ATOM= 10 O 1a 1 0.899685032 -0.037892383 0.701679648
ATOM= 11 O 1a 1 0.267056509 0.655407075 0.732411943
ATOM= 12 O 1a 1 0.577937264 0.327298008 0.727635332
ATOM= 13 O 1a 1 0.155188925 -0.015491868 0.392762998
ATOM= 14 H 1a 1 0.955966110 0.023413555 0.872365905
ATOM= 15 H 1a 1 0.095697254 0.732723738 0.672405539
ATOM= 16 H 1a 1 0.724046928 0.576713020 0.689531135
ATOM= 17 H 1a 1 -0.026177844 -0.141505576 0.255200042

Cm 60 GPa job P1Cm 0044
Cell volume 204.221 Angstrom**3
Enthalpy -68.983 eV/f.u.

SPGNAM= Cm
CELEDG= 4.452955261 8.308451771 5.723984510 Angstroms
CELANG= 90.000000000 105.345858733 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.061466067 0.332179058 -0.005688174
ATOM= 2 Al 4b 1 0.083622219 0.160949714 0.530666873
ATOM= 3 O 4b 1 -0.022505698 0.326153011 0.695815556

ATOM=	4	O	4b	1	0.714251695	0.344441498	0.018067448
ATOM=	5	O	2a	.m.	-0.252372345	0.000000000	0.025494506
ATOM=	6	O	4b	1	0.677185385	0.176122685	0.331072575
ATOM=	7	O	2a	.m.	0.223452836	0.000000000	0.366888660
ATOM=	8	O	2a	.m.	-0.055591432	0.000000000	-0.337634948
ATOM=	9	H	4b	1	0.542533941	0.093760121	0.382328385
ATOM=	10	H	2a	.m.	0.127238133	0.000000000	0.192486858
ATOM=	11	H	2a	.m.	-0.127463188	0.000000000	-0.191642471

P1 65 GPa job P1Cm 0045
 Cell volume 101.165 Angstrom**3
 Enthalpy -65.725 eV/f.u.

SPGNAM= P1

CELEDG=	4.727364723	4.452279127	5.728668841	Angstroms
CELANG=	82.357112739	105.984292143	119.217736066	degrees.

ATOM=	1	Si	1a	1	0.354355491	0.647000578	0.070322253
ATOM=	2	Si	1a	1	0.693535353	0.318579700	0.065054080
ATOM=	3	Al	1a	1	0.535774445	-0.002428768	0.530999561
ATOM=	4	Al	1a	1	0.174534532	0.311270743	0.534577466
ATOM=	5	O	1a	1	0.445080788	0.637855814	0.367397940
ATOM=	6	O	1a	1	0.803758597	0.318191061	0.365626004
ATOM=	7	O	1a	1	0.332337854	-0.003603821	0.039462480
ATOM=	8	O	1a	1	0.009517639	0.300298038	0.033455174
ATOM=	9	O	1a	1	0.704124425	0.685465943	0.050945571
ATOM=	10	O	1a	1	0.899760942	-0.038782154	0.701868616
ATOM=	11	O	1a	1	0.266573958	0.655007010	0.732861556
ATOM=	12	O	1a	1	0.578786495	0.327381677	0.728082296
ATOM=	13	O	1a	1	0.153871244	-0.017588449	0.393012339
ATOM=	14	H	1a	1	0.956300325	0.024746678	0.872914689
ATOM=	15	H	1a	1	0.094874117	0.733241174	0.671203331
ATOM=	16	H	1a	1	0.725468992	0.579314552	0.690346732
ATOM=	17	H	1a	1	-0.027847470	-0.142610912	0.254240883

Cm 65 GPa job P1Cm 0046
 Cell volume 201.474 Angstrom**3
 Enthalpy -65.741 eV/f.u.

SPGNAM= Cm

CELEDG=	4.425321637	8.281850363	5.700930424	Angstroms
CELANG=	90.000000000	105.361534688	90.000000000	degrees.

ATOM=	1	Si	4b	1	0.061899248	0.332226279	-0.004959450
ATOM=	2	Al	4b	1	0.084050109	0.160868478	0.530896361
ATOM=	3	O	4b	1	-0.020642938	0.326834373	0.695980388
ATOM=	4	O	4b	1	0.712521829	0.345357310	0.017351135
ATOM=	5	O	2a	.m.	-0.250590728	0.000000000	0.026654414
ATOM=	6	O	4b	1	0.677087048	0.176289149	0.330705817
ATOM=	7	O	2a	.m.	0.225388612	0.000000000	0.366968708
ATOM=	8	O	2a	.m.	-0.057213676	0.000000000	-0.338212115
ATOM=	9	H	4b	1	0.541208983	0.093564765	0.382112260
ATOM=	10	H	2a	.m.	0.127371734	0.000000000	0.191955403
ATOM=	11	H	2a	.m.	-0.128835075	0.000000000	-0.191426169

P1 70 GPa job P1Cm 0052
Cell volume 99.877 Angstrom**3
Enthalpy -62.517 eV/f.u.

SPGNAM= P1
CELEDG= 4.707193042 4.430635314 5.707535726 Angstroms
CELANG= 82.348804068 105.983091966 119.214765270 degrees.
ATOM= 1 Si 1a 1 0.354125224 0.646749505 0.069807741
ATOM= 2 Si 1a 1 0.693237734 0.318307249 0.064558031
ATOM= 3 Al 1a 1 0.535963624 -0.002289468 0.530903774
ATOM= 4 Al 1a 1 0.174903488 0.311216370 0.534596527
ATOM= 5 O 1a 1 0.446786607 0.637571034 0.367465996
ATOM= 6 O 1a 1 0.804142492 0.319602426 0.365679356
ATOM= 7 O 1a 1 0.330628557 -0.003644008 0.039974001
ATOM= 8 O 1a 1 0.009588543 0.298062628 0.034164744
ATOM= 9 O 1a 1 0.705209085 0.686901703 0.050285589
ATOM= 10 O 1a 1 0.899854124 -0.039555280 0.702060200
ATOM= 11 O 1a 1 0.266085953 0.654598957 0.733244532
ATOM= 12 O 1a 1 0.579588263 0.327420225 0.728478981
ATOM= 13 O 1a 1 0.152615834 -0.019499724 0.393227154
ATOM= 14 H 1a 1 0.956642173 0.026111042 0.873433779
ATOM= 15 H 1a 1 0.094051701 0.733689691 0.669943382
ATOM= 16 H 1a 1 0.726870377 0.581794920 0.691137220
ATOM= 17 H 1a 1 -0.029487221 -0.143695214 0.253399809

Cm 70 GPa job P1Cm 0053
Cell volume 198.903 Angstrom**3
Enthalpy -62.547 eV/f.u.

SPGNAM= Cm
CELEDG= 4.399633551 8.256301888 5.678980985 Angstroms
CELANG= 90.000000000 105.376115244 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.062288616 0.332261522 -0.004310034
ATOM= 2 Al 4b 1 0.084447325 0.160797814 0.531112297
ATOM= 3 O 4b 1 -0.018902661 0.327470039 0.696132539
ATOM= 4 O 4b 1 0.710924632 0.346197326 0.016657029
ATOM= 5 O 2a .m. -0.248986636 0.000000000 0.027768181
ATOM= 6 O 4b 1 0.676998632 0.176471064 0.330391178
ATOM= 7 O 2a .m. 0.227163734 0.000000000 0.367043636
ATOM= 8 O 2a .m. -0.058726247 0.000000149 -0.338748975
ATOM= 9 H 4b 1 0.540000415 0.093374970 0.381941240
ATOM= 10 H 2a .m. 0.127521028 0.000000000 0.191440885
ATOM= 11 H 2a .m. -0.130120296 0.000000000 -0.191227443

P1 75 GPa job P1Cm 0054
Cell volume 98.669 Angstrom**3
Enthalpy -59.352 eV/f.u.

SPGNAM= P1
CELEDG= 4.687961479 4.410664711 5.687448316 Angstroms
CELANG= 82.344615637 105.977143621 119.221287529 degrees.
ATOM= 1 Si 1a 1 0.353898082 0.646505828 0.069341231
ATOM= 2 Si 1a 1 0.692919926 0.318004914 0.064118471
ATOM= 3 Al 1a 1 0.536151093 -0.002149727 0.530837746

ATOM=	4	Al	1a	1	0.175316042	0.311188793	0.534622975
ATOM=	5	O	1a	1	0.448412789	0.637349529	0.367525779
ATOM=	6	O	1a	1	0.804542204	0.320912914	0.365732538
ATOM=	7	O	1a	1	0.328987166	-0.003771692	0.040467313
ATOM=	8	O	1a	1	0.009627458	0.295955600	0.034852927
ATOM=	9	O	1a	1	0.706155990	0.688127275	0.049667996
ATOM=	10	O	1a	1	0.899949865	-0.040211589	0.702245696
ATOM=	11	O	1a	1	0.265620361	0.654206319	0.733576190
ATOM=	12	O	1a	1	0.580346696	0.327468412	0.728838950
ATOM=	13	O	1a	1	0.151435714	-0.021303763	0.393441010
ATOM=	14	H	1a	1	0.956976355	0.027519728	0.873924262
ATOM=	15	H	1a	1	0.093251984	0.734046861	0.668570269
ATOM=	16	H	1a	1	0.728289744	0.584254863	0.691942956
ATOM=	17	H	1a	1	-0.031074496	-0.144768102	0.252660489

Cm 75 GPa job P1Cm 0055
Cell volume 196.480 Angstrom**3
Enthalpy -59.390 eV/f.u.

SPGNAM= Cm

CELEDG=	4.375072362	8.232212704	5.658307064	Angstroms			
CELANG=	90.000000000	105.395151686	90.000000000	degrees.			
ATOM=	1	Si	4b	1	0.062638067	0.332287867	-0.003725990
ATOM=	2	Al	4b	1	0.084827455	0.160732115	0.531310817
ATOM=	3	O	4b	1	-0.017218677	0.328062083	0.696281679
ATOM=	4	O	4b	1	0.709392346	0.346973478	0.015988849
ATOM=	5	O	2a	.m.	-0.247559061	0.000000000	0.028859352
ATOM=	6	O	4b	1	0.676940693	0.176665080	0.330123285
ATOM=	7	O	2a	.m.	0.228839538	0.000000000	0.367119768
ATOM=	8	O	2a	.m.	-0.060083765	0.000000000	-0.339239900
ATOM=	9	H	4b	1	0.538859487	0.093193174	0.381774902
ATOM=	10	H	2a	.m.	0.127626298	0.000000000	0.190952880
ATOM=	11	H	2a	.m.	-0.131341168	0.000000000	-0.191074683