

Supplementary Table ST1 (Mercier et al., 2010)

Table 1 a: Repeated application of (R,T)

Translation	Rotation R					
T	0	$\pi/3$	$2\pi/3$	$\pi$	$4\pi/3$	$5\pi/3$
-a/3	[KP01]a	[KP11]a	[KP21]a	[KP31]a	[KP22]a*	[KP12]a*
Space grp	P1	P61	P31	P21		
INITIAL	job0001	job0002	job0003	job0004		
FINAL	job0151	job0169	job0159	job0160		
H (eV/f.u.)	-105.645	-105.550	-105.609	-105.659		
Vol./f.u ( $\text{\AA}^3$ )	131.84	132.15	132.21	132.27		
-b/3	[KP01]a*	[KP12]a	[KP22]a	[KP31]a*	[KP21]a*	[KP11]a*
Space grp		P61	P31			
INITIAL		job0005	job0006			
FINAL		job0170	job0161			
H (eV/f.u.)		-105.642	-105.539			
Vol./f.u ( $\text{\AA}^3$ )		132.59	132.21			
(a+b)/3	[KP03]a	[KP13]a	[KP23]a	[KP33]a	[KP23]a*	[KP13]a*
Space grp	Cm	P61	P31	Cmc21		
INITIAL	job0008	job0009	job0010	job0011		
FINAL	job0140	job0172	job0162	job0143		
H (eV/f.u.)	-105.576	-105.632	-105.620	-105.579		
Vol./f.u ( $\text{\AA}^3$ )	131.51	132.25	132.14	131.61		

Supplementary Table ST1 (Mercier et al., 2010)

Table 1 b: Repeated application of the sequence [(R,T):(R\*,T\*)]

Translation T	Rotation R					
	0	$\pi/3$	$2\pi/3$	$\pi$	$4\pi/3$	$5\pi/3$
-a/3	[KP01]b	[KP11]b	[KP21]b	[KP31]b	=[KP22]b	=[KP12]b
	Cc	Cc	Cc	Cc		
INITIAL	job0012	job0013	job0014	job0015		
FINAL	job0134	job0135	job0136	job0137		
H (eV/f.u.)	-105.608	-105.557	-105.622	-105.636		
Vol./f.u (Å <sup>3</sup> )	131.88	132.10	131.62	132.38		
-b/3	=[KP01]b	[KP12]b	[KP22]b	=[KP31]b	=[KP21]b	=[KP11]b
Space grp		Cc	Cc			
INITIAL		job0016	job0017			
FINAL		job0138	job0139			
H (eV/f.u.)		-105.633	-105.535			
Vol./f.u (Å <sup>3</sup> )		131.93	131.84			
(a+b)/3	=[KP03]a	[KP13]b	[KP23]b	=[KP33]a	=[KP23]b	=[KP13]b
Space grp	Cm	Cc	Cc	Cmc21		
INITIAL	job0008	job0018	job0019	job0011		
FINAL	job0140	job0141	job0142	job0143		
H (eV/f.u.)	-105.576	-105.648	-105.624	-105.579		
Vol./f.u (Å <sup>3</sup> )	131.51	132.24	131.76	131.62		

# Supplementary Table ST1 (Mercier et al., 2010)

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 Kaolinite can transform to models in the following family:  
 [KP01]a, [KP03]a, [KP01]b  
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Model [KP01]a

Initial job0001

SPGNAM= P1  
 CELEDG= 5.326700000 5.326700000 7.468045407 Angstroms  
 CELANG= 83.172669732 103.754088527 120.000000000 degrees.  
 ATOM= 1 Si 1a 1 0.379310345 0.666666667 0.137931035  
 ATOM= 2 Si 1a 1 0.712643679 0.333333333 0.137931035  
 ATOM= 3 Al 1a 1 0.505044611 0.000000000 0.515133834  
 ATOM= 4 Al 1a 1 0.171711278 0.333333333 0.515133834  
 ATOM= 5 O 1a 1 0.453350151 0.666666667 0.360050455  
 ATOM= 6 O 1a 1 0.786683485 0.333333333 0.360050455  
 ATOM= 7 O 1a 1 0.517961949 0.000000000 0.053885848  
 ATOM= 8 O 1a 1 0.017961949 0.500000000 0.053885848  
 ATOM= 9 O 1a 1 0.517961949 0.500000000 0.053885848  
 ATOM= 10 O 1a 1 0.885069715 0.000000000 0.655209145  
 ATOM= 11 O 1a 1 0.218403048 0.666666667 0.655209145  
 ATOM= 12 O 1a 1 0.551736381 0.333333333 0.655209145  
 ATOM= 13 O 1a 1 0.119683306 0.000000000 0.359049917  
 ATOM= 14 H 1a 1 0.927759334 0.000000000 0.783278000  
 ATOM= 15 H 1a 1 0.261092667 0.666666667 0.783278000  
 ATOM= 16 H 1a 1 0.594426000 0.333333333 0.783278000  
 ATOM= 17 H 1a 1 0.079995301 0.000000000 0.239985904

Final job0151

SPGNAM= P1  
 CELEDG= 4.962150295 4.821909718 6.531644089 Angstroms  
 CELANG= 83.391403147 104.310867685 119.466334795 degrees.  
 ATOM= 1 Si 1a 1 0.364834373 0.642959564 0.112897391  
 ATOM= 2 Si 1a 1 0.706415027 0.306261636 0.110322219  
 ATOM= 3 Al 1a 1 0.524436773 -0.002793857 0.534352940  
 ATOM= 4 Al 1a 1 0.179955956 0.319327412 0.535586384  
 ATOM= 5 O 1a 1 0.427704628 0.653913003 0.367457825  
 ATOM= 6 O 1a 1 0.801422708 0.287848444 0.366766267  
 ATOM= 7 O 1a 1 0.386858108 -0.019048312 0.027758847  
 ATOM= 8 O 1a 1 0.008510390 0.358033548 0.022514642  
 ATOM= 9 O 1a 1 0.651831781 0.614239407 0.056603332  
 ATOM= 10 O 1a 1 0.900230307 -0.007396127 0.690137001  
 ATOM= 11 O 1a 1 0.268342563 0.664617137 0.691932267  
 ATOM= 12 O 1a 1 0.549983956 0.316436296 0.689240973  
 ATOM= 13 O 1a 1 0.177476909 0.031809994 0.372519124  
 ATOM= 14 H 1a 1 0.948329028 0.049194687 0.839033196  
 ATOM= 15 H 1a 1 0.106636603 0.719417812 0.700472052  
 ATOM= 16 H 1a 1 0.711628409 0.540845153 0.689765193  
 ATOM= 17 H 1a 1 -0.013801968 -0.142322341 0.295020318

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 Model [KP03]a

Initial job0008

SPGNAM= Cm  
 CELEDG= 5.326700000 9.226115037 7.468045407 Angstroms  
 CELANG= 90.000000000 103.754088528 90.000000000 degrees.  
 ATOM= 1 Si 4b 1 0.016522976 0.333333333 -0.075431047  
 ATOM= 2 Al 4b 1 0.057455377 0.166666667 0.547366154  
 ATOM= 3 O 4b 1 -0.057516830 0.333333333 0.702449533  
 ATOM= 4 O 4b 1 0.794538039 0.250000000 0.008614140  
 ATOM= 5 O 2a .m. 0.544538039 0.000000000 0.008614140  
 ATOM= 6 O 4b 1 0.677430274 0.166666667 0.407290843  
 ATOM= 7 O 2a .m. 0.177430273 0.000000000 0.407290843  
 ATOM= 8 O 2a .m. -0.057183318 0.000000000 0.703450071  
 ATOM= 9 H 4b 1 0.634740655 0.166666667 0.279221988  
 ATOM= 10 H 2a .m. 0.134740654 0.000000000 0.279221988  
 ATOM= 11 H 2a .m. -0.017495313 0.000000000 0.822514084

# Supplementary Table ST1 (Mercier et al., 2010)

Final job0140

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SPGNAM= Cm
CELEDG= 4.790498413 8.588613932 6.635928591 Angstroms
CELANG= 90.000000000 105.564879345 90.000000000 degrees.
ATOM= 1 Si 4b 1 0.051903986 0.332369307 -0.046929396
ATOM= 2 Al 4b 1 0.080513511 0.162351191 0.531065993
ATOM= 3 O 4b 1 -0.034655863 0.322931214 0.698966947
ATOM= 4 O 4b 1 0.766752727 0.312843403 0.035114394
ATOM= 5 O 2a .m. -0.294585852 0.000000000 0.026407968
ATOM= 6 O 4b 1 0.696210836 0.180607850 0.380073549
ATOM= 7 O 2a .m. 0.196328043 0.000000000 0.374605620
ATOM= 8 O 2a .m. 0.006030331 0.000000000 -0.308743547
ATOM= 9 H 4b 1 0.548034882 0.099925421 0.366684925
ATOM= 10 H 2a .m. 0.090669718 0.000000000 0.226122276
ATOM= 11 H 2a .m. -0.187600070 0.000000000 -0.288228597
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Model [KP01]b

Initial job0012

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SPGNAM= Cc
CELEDG= 5.326700000 9.226115037 14.616049324 Angstroms
CELANG= 90.000000000 96.977560803 90.000000000 degrees.
ATOM= 1 Si 4a 1 0.326312407 0.083333335 0.131465505
ATOM= 2 Si 4a 1 0.826312407 0.249999999 0.131465506
ATOM= 3 Al 4a 1 0.055846207 0.750000001 0.320066905
ATOM= 4 Al 4a 1 0.055846207 0.083333332 0.320066905
ATOM= 5 O 4a 1 0.363332310 0.083333335 0.242525215
ATOM= 6 O 4a 1 0.863332311 0.249999999 0.242525216
ATOM= 7 O 4a 1 0.062304876 0.666666668 0.089442912
ATOM= 8 O 4a 1 0.062304876 0.166666666 0.089442912
ATOM= 9 O 4a 1 0.312304876 -0.083333332 0.089442912
ATOM= 10 O 4a 1 0.745858759 0.083333334 0.390104560
ATOM= 11 O 4a 1 0.245858759 0.249999999 0.390104560
ATOM= 12 O 4a 1 0.245858758 -0.083333332 0.390104560
ATOM= 13 O 4a 1 0.863165554 -0.083333332 0.242024946
ATOM= 14 H 4a 1 0.767203568 -0.083333334 -0.045861012
ATOM= 15 H 4a 1 0.767203568 0.250000001 -0.045861012
ATOM= 16 H 4a 1 0.267203567 0.083333332 -0.045861012
ATOM= 17 H 4a 1 0.843321552 -0.083333332 0.182492940
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Final job0134

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SPGNAM= Cc
CELEDG= 4.949468843 8.424144693 12.766272261 Angstroms
CELANG= 90.000000000 97.690147798 90.000000000 degrees.
ATOM= 1 Si 4a 1 0.307010839 0.090534939 0.118419382
ATOM= 2 Si 4a 1 0.808856392 0.250564259 0.118098297
ATOM= 3 Al 4a 1 0.061466943 0.755631686 0.330039247
ATOM= 4 Al 4a 1 0.055262042 0.090882633 0.329747897
ATOM= 5 O 4a 1 0.347278788 0.106570904 0.245914709
ATOM= 6 O 4a 1 0.843836957 0.237512404 0.246187483
ATOM= 7 O 4a 1 -0.012031583 0.730819840 0.073559782
ATOM= 8 O 4a 1 -0.013718476 0.107948034 0.076685319
ATOM= 9 O 4a 1 0.435091368 -0.079262953 0.090183532
ATOM= 10 O 4a 1 0.753354401 0.091048760 0.407775611
ATOM= 11 O 4a 1 0.268035436 0.244766426 0.407742109
ATOM= 12 O 4a 1 0.233787266 -0.072988350 0.407394723
ATOM= 13 O 4a 1 0.908711845 -0.077579785 0.248516223
ATOM= 14 H 4a 1 0.806002961 -0.118674064 -0.017791825
ATOM= 15 H 4a 1 0.717615031 0.143571261 -0.087773393
ATOM= 16 H 4a 1 0.426588427 0.047370389 -0.090839051
ATOM= 17 H 4a 1 0.726424842 -0.078778700 0.209833975
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# Supplementary Table ST1 (Mercier et al., 2010)

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No low-pressure representative currently known for this family:  
[KP11]a, [KP12]a, [KP13]a

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Model [KP11]a

Initial job0002

SPGNAM= P61  
CELEDG= 5.326700000 5.326700000 43.523400000 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 6a 1 0.666666666 -0.000000002 -0.085488494  
ATOM= 2 Si 6a 1 0.333333334 0.333333332 -0.085488494  
ATOM= 3 Al 6a 1 0.333333333 0.666666665 0.851644373  
ATOM= 4 Al 6a 1 0.666666667 0.333333332 0.851644373  
ATOM= 5 O 6a 1 0.333333334 0.000000002 0.377491603  
ATOM= 6 O 6a 1 0.333333332 -0.000000002 0.710824936  
ATOM= 7 O 6a 1 0.500000000 0.666666665 -0.071480963  
ATOM= 8 O 6a 1 0.500000000 0.166666665 -0.071480963  
ATOM= 9 O 6a 1 0.000000000 0.166666665 -0.071480963  
ATOM= 10 O 6a 1 0.333333335 0.000000002 0.161631821  
ATOM= 11 O 6a 1 0.333333333 -0.000000002 0.828298488  
ATOM= 12 O 6a 1 0.000000000 0.333333332 0.828298488  
ATOM= 13 O 6a 1 0.000000000 0.333333335 0.377658359  
ATOM= 14 H 6a 1 0.333333335 0.000000002 0.140287012  
ATOM= 15 H 6a 1 0.333333333 -0.000000002 0.806953679  
ATOM= 16 H 6a 1 0.000000000 0.333333332 0.806953679  
ATOM= 17 H 6a 1 0.000000000 0.333333335 0.397502361

Final job0169

SPGNAM= P61  
CELEDG= 4.895367750 4.895367750 38.205713606 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 6a 1 0.662742383 0.019033255 -0.080866533  
ATOM= 2 Si 6a 1 0.341585510 0.359211353 -0.080783300  
ATOM= 3 Al 6a 1 0.330122857 0.666079203 0.848859423  
ATOM= 4 Al 6a 1 0.665958553 0.340395706 0.848585642  
ATOM= 5 O 6a 1 0.360297793 -0.004529104 0.376725328  
ATOM= 6 O 6a 1 0.368807619 0.004538483 0.710032020  
ATOM= 7 O 6a 1 0.376450330 0.685763100 -0.067009182  
ATOM= 8 O 6a 1 0.626816812 0.310455916 -0.066927257  
ATOM= 9 O 6a 1 0.002545212 0.062634567 -0.069298630  
ATOM= 10 O 6a 1 0.333250384 -0.007310101 0.156330806  
ATOM= 11 O 6a 1 0.355526083 0.000351672 0.823455369  
ATOM= 12 O 6a 1 -0.006023896 0.348540711 0.823493845  
ATOM= 13 O 6a 1 0.001554211 0.364768388 0.375652714  
ATOM= 14 H 6a 1 0.370912035 -0.014803865 0.131319887  
ATOM= 15 H 6a 1 0.139118650 -0.047656843 0.820052475  
ATOM= 16 H 6a 1 -0.064828322 0.126727417 0.822233824  
ATOM= 17 H 6a 1 -0.001550968 0.171282110 0.381912249

Model [KP12]a

Initial job0005

SPGNAM= P61  
CELEDG= 5.326700000 5.326700000 43.523400000 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 6a 1 -0.000000002 0.333333331 0.081178172  
ATOM= 2 Si 6a 1 -0.000000001 0.666666667 -0.085488494  
ATOM= 3 Al 6a 1 0.000000002 0.000000000 0.351644373  
ATOM= 4 Al 6a 1 0.333333332 0.666666667 0.851644373  
ATOM= 5 O 6a 1 -0.000000002 0.333333331 0.044158269  
ATOM= 6 O 6a 1 0.000000001 0.333333333 0.377491603  
ATOM= 7 O 6a 1 0.166666665 0.000000000 -0.071480963  
ATOM= 8 O 6a 1 0.166666665 0.500000000 -0.071480963  
ATOM= 9 O 6a 1 0.666666665 0.500000000 -0.071480963  
ATOM= 10 O 6a 1 0.333333332 0.000000000 0.828298488

# Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	11	O	6a	1	-0.000000002	0.333333333	0.828298488
ATOM=	12	O	6a	1	0.333333333	-0.000000002	0.161631821
ATOM=	13	O	6a	1	0.333333335	0.000000000	0.377658359
ATOM=	14	H	6a	1	0.333333332	0.000000000	0.806953679
ATOM=	15	H	6a	1	-0.000000002	0.333333333	0.806953679
ATOM=	16	H	6a	1	0.333333333	-0.000000002	0.140287012
ATOM=	17	H	6a	1	0.333333335	0.000000000	0.397502361

Final job0170

SPGNAM= P61  
CELEDG= 4.914870931 4.914870931 38.030310463 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.

ATOM=	1	Si	6a	1	-0.013431151	0.309214417	0.085815497
ATOM=	2	Si	6a	1	-0.014161213	0.661492792	-0.081629638
ATOM=	3	Al	6a	1	0.011427706	0.013260018	0.348460211
ATOM=	4	Al	6a	1	0.320734177	0.647551093	0.848249715
ATOM=	5	O	6a	1	-0.035390435	0.280429561	0.043254972
ATOM=	6	O	6a	1	-0.021506978	0.318276047	0.376190723
ATOM=	7	O	6a	1	0.025155686	-0.011866004	-0.067085449
ATOM=	8	O	6a	1	0.263538032	0.605950243	-0.065834079
ATOM=	9	O	6a	1	0.648454866	0.358161625	-0.071774867
ATOM=	10	O	6a	1	0.305418318	-0.035258823	0.822982763
ATOM=	11	O	6a	1	-0.001868331	0.320482144	0.822659074
ATOM=	12	O	6a	1	0.319556627	-0.020549224	0.156290073
ATOM=	13	O	6a	1	0.347265216	0.063502111	0.375834166
ATOM=	14	H	6a	1	0.523153439	0.134233232	0.825130261
ATOM=	15	H	6a	1	0.027493035	0.307440099	0.797491517
ATOM=	16	H	6a	1	0.487306599	0.184752352	0.149055580
ATOM=	17	H	6a	1	0.350175816	-0.105202775	0.388679446

Model [KP13]a

Initial job0009

SPGNAM= P61  
CELEDG= 5.326700000 5.326700000 43.523400000 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.

ATOM=	1	Si	6a	1	0.000000001	0.666666668	-0.085488494
ATOM=	2	Si	6a	1	0.666666669	0.000000002	-0.085488494
ATOM=	3	Al	6a	1	0.666666665	0.333333333	0.184977706
ATOM=	4	Al	6a	1	-0.000000002	0.000000000	0.184977706
ATOM=	5	O	6a	1	-0.000000001	0.333333332	0.377491603
ATOM=	6	O	6a	1	0.333333331	-0.000000002	0.377491603
ATOM=	7	O	6a	1	0.833333335	0.333333335	-0.071480963
ATOM=	8	O	6a	1	0.833333335	0.833333335	-0.071480963
ATOM=	9	O	6a	1	0.333333335	0.833333335	-0.071480963
ATOM=	10	O	6a	1	0.000000002	0.333333335	0.828298488
ATOM=	11	O	6a	1	0.333333332	0.000000000	0.161631821
ATOM=	12	O	6a	1	0.333333335	0.000000002	0.828298488
ATOM=	13	O	6a	1	0.333333335	0.000000000	0.710991692
ATOM=	14	H	6a	1	0.000000002	0.333333335	0.806953679
ATOM=	15	H	6a	1	0.333333332	0.000000000	0.140287012
ATOM=	16	H	6a	1	0.333333335	0.000000002	0.806953679
ATOM=	17	H	6a	1	0.333333335	0.000000000	0.730835694

Final job0172

SPGNAM= P61  
CELEDG= 4.902539746 4.902539746 38.120305743 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.

ATOM=	1	Si	6a	1	0.009295912	0.697627714	-0.081057475
ATOM=	2	Si	6a	1	0.684883573	0.034514719	-0.080740059
ATOM=	3	Al	6a	1	0.650094994	0.321432182	0.181837996
ATOM=	4	Al	6a	1	-0.024377176	-0.008832918	0.182078812
ATOM=	5	O	6a	1	0.020966894	0.314978739	0.376656213
ATOM=	6	O	6a	1	0.291455448	-0.051436705	0.376808363
ATOM=	7	O	6a	1	0.730498169	0.363806937	-0.065569404
ATOM=	8	O	6a	1	0.970472702	0.986614040	-0.066808114
ATOM=	9	O	6a	1	0.346305829	0.732479124	-0.070865532

Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	10	O	6a	1	-0.012938218	0.337170492	0.823384005
ATOM=	11	O	6a	1	0.306755360	0.016458383	0.156746644
ATOM=	12	O	6a	1	0.344413569	0.019699980	0.822928342
ATOM=	13	O	6a	1	0.308758683	-0.036241848	0.709463355
ATOM=	14	H	6a	1	0.155108659	0.557517594	0.823128498
ATOM=	15	H	6a	1	0.264985509	-0.193864874	0.150811487
ATOM=	16	H	6a	1	0.332310857	0.051496126	0.797820201
ATOM=	17	H	6a	1	0.498334574	0.151523589	0.717144825

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# Supplementary Table ST1 (Mercier et al., 2010)

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No low-pressure representative currently known for this family:  
[KP21]a, [KP22]a, [KP23]a

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Model [KP21]a

Initial job0003

SPGNAM= P31  
CELEDG= 5.326700000 5.326700000 21.761700000 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 3a 1 0.22222221 0.11111114 0.108477000  
ATOM= 2 Si 3a 1 0.55555555 0.77777778 0.108477000  
ATOM= 3 Al 3a 1 0.22222221 0.44444447 0.234211266  
ATOM= 4 Al 3a 1 0.88888888 0.77777778 0.234211266  
ATOM= 5 O 3a 1 0.22222221 0.11111114 0.182516806  
ATOM= 6 O 3a 1 0.55555555 0.77777778 0.182516806  
ATOM= 7 O 3a 1 0.38888888 0.44444447 0.080461937  
ATOM= 8 O 3a 1 0.88888888 -0.05555553 0.080461937  
ATOM= 9 O 3a 1 0.38888888 -0.05555553 0.080461937  
ATOM= 10 O 3a 1 0.55555555 0.44444447 0.280903036  
ATOM= 11 O 3a 1 0.22222225 0.11111112 -0.052430297  
ATOM= 12 O 3a 1 0.22222221 0.77777778 0.280903036  
ATOM= 13 O 3a 1 0.88888888 0.44444447 0.182183294  
ATOM= 14 H 3a 1 0.55555555 0.44444447 0.323592655  
ATOM= 15 H 3a 1 0.22222225 0.11111112 -0.009740678  
ATOM= 16 H 3a 1 0.22222221 0.77777778 0.323592655  
ATOM= 17 H 3a 1 0.88888888 0.44444447 0.142495289

Final job0159

SPGNAM= P31  
CELEDG= 4.908312000 4.908312000 19.011072143 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 3a 1 0.204400217 0.109286136 0.100083782  
ATOM= 2 Si 3a 1 0.544842649 0.773151454 0.100042227  
ATOM= 3 Al 3a 1 0.220114678 0.458232064 0.240625040  
ATOM= 4 Al 3a 1 0.880405494 0.786095209 0.240813352  
ATOM= 5 O 3a 1 0.185783586 0.124417488 0.184934336  
ATOM= 6 O 3a 1 0.552002376 0.752472868 0.185162098  
ATOM= 7 O 3a 1 0.259023129 0.444721608 0.070090208  
ATOM= 8 O 3a 1 0.877199650 -0.180049777 0.072223702  
ATOM= 9 O 3a 1 0.509672077 0.076537009 0.081048033  
ATOM= 10 O 3a 1 0.548668006 0.458538115 0.292585287  
ATOM= 11 O 3a 1 0.218897580 0.091087104 -0.040817905  
ATOM= 12 O 3a 1 0.191693493 0.768683791 0.292408548  
ATOM= 13 O 3a 1 0.929584351 0.500326065 0.186298278  
ATOM= 14 H 3a 1 0.547469851 0.513318734 0.342048042  
ATOM= 15 H 3a 1 0.438455504 0.259211956 -0.040858408  
ATOM= 16 H 3a 1 0.355708408 0.988138089 0.297526618  
ATOM= 17 H 3a 1 0.763731598 0.332535306 0.159080981

Model [KP22]a

Initial job0006

SPGNAM= P31  
CELEDG= 5.326700000 5.326700000 21.761700000 Angstroms  
CELANG= 90.000000000 90.000000000 120.000000000 degrees.  
ATOM= 1 Si 3a 1 0.88888889 0.11111114 0.108477000  
ATOM= 2 Si 3a 1 0.22222225 0.77777778 0.108477000  
ATOM= 3 Al 3a 1 0.55555555 0.111111109 -0.099122067  
ATOM= 4 Al 3a 1 0.22222221 0.444444442 -0.099122067  
ATOM= 5 O 3a 1 0.88888889 0.11111114 0.182516806  
ATOM= 6 O 3a 1 0.22222225 0.77777778 0.182516806  
ATOM= 7 O 3a 1 0.05555558 0.44444447 0.080461937  
ATOM= 8 O 3a 1 0.55555558 -0.05555553 0.080461937  
ATOM= 9 O 3a 1 0.05555558 -0.05555553 0.080461937  
ATOM= 10 O 3a 1 0.22222225 0.44444447 0.280903036



# Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	11	O	3a	1	0.555555558	0.111111114	0.280903036
ATOM=	12	O	3a	1	0.888888888	0.111111109	-0.052430297
ATOM=	13	O	3a	1	0.555555558	0.444444447	0.182183294
ATOM=	14	H	3a	1	0.222222225	0.444444447	0.323592655
ATOM=	15	H	3a	1	0.555555558	0.111111114	0.323592655
ATOM=	16	H	3a	1	0.888888888	0.111111109	-0.009740678
ATOM=	17	H	3a	1	0.555555558	0.444444447	0.142495289

Final job0161

```
SPGNAM= P31
CELEDG= 4.891602195 4.891602195 19.140011077 Angstroms
CELANG= 90.000000000 90.000000000 120.000000000 degrees.
ATOM= 1 Si 3a 1 0.890743692 0.108741160 0.098671834
ATOM= 2 Si 3a 1 0.231082927 0.769205891 0.099607048
ATOM= 3 Al 3a 1 0.540689941 0.090493584 -0.093374088
ATOM= 4 Al 3a 1 0.205628714 0.416110991 -0.093645770
ATOM= 5 O 3a 1 0.881148906 0.120187661 0.183744930
ATOM= 6 O 3a 1 0.245057972 0.761548141 0.184259559
ATOM= 7 O 3a 1 -0.059871955 0.442830954 0.071297764
ATOM= 8 O 3a 1 0.563586404 -0.183782739 0.071570491
ATOM= 9 O 3a 1 0.189290575 0.067036182 0.076336424
ATOM= 10 O 3a 1 0.248648097 0.479445680 0.290489383
ATOM= 11 O 3a 1 0.585141546 0.117760800 0.291739643
ATOM= 12 O 3a 1 0.868977552 0.100481438 -0.042519363
ATOM= 13 O 3a 1 0.613289956 0.487316105 0.186368231
ATOM= 14 H 3a 1 0.301640617 0.313496143 0.295772556
ATOM= 15 H 3a 1 0.634175570 0.115657542 0.341237002
ATOM= 16 H 3a 1 0.807711993 -0.121958710 -0.039067432
ATOM= 17 H 3a 1 0.419232854 0.296625066 0.174136263
```

Model [KP23]a

Initial job0010

```
SPGNAM= P31
CELEDG= 5.326700000 5.326700000 21.761700000 Angstroms
CELANG= 90.000000000 90.000000000 120.000000000 degrees.
ATOM= 1 Si 3a 1 0.888888886 0.777777779 0.108477000
ATOM= 2 Si 3a 1 0.222222220 0.444444445 0.108477000
ATOM= 3 Al 3a 1 0.888888886 0.111111112 0.234211266
ATOM= 4 Al 3a 1 0.555555553 0.444444445 0.234211266
ATOM= 5 O 3a 1 0.888888886 0.777777779 0.182516806
ATOM= 6 O 3a 1 0.222222220 0.444444445 0.182516806
ATOM= 7 O 3a 1 0.055555553 0.111111112 0.080461937
ATOM= 8 O 3a 1 0.555555553 0.611111112 0.080461937
ATOM= 9 O 3a 1 0.055555553 0.611111112 0.080461937
ATOM= 10 O 3a 1 0.222222220 0.111111112 0.280903036
ATOM= 11 O 3a 1 0.222222225 0.444444447 -0.052430297
ATOM= 12 O 3a 1 0.555555558 0.111111114 -0.052430297
ATOM= 13 O 3a 1 0.555555553 0.111111112 0.182183294
ATOM= 14 H 3a 1 0.222222220 0.111111112 0.323592655
ATOM= 15 H 3a 1 0.222222225 0.444444447 -0.009740678
ATOM= 16 H 3a 1 0.555555558 0.111111114 -0.009740678
ATOM= 17 H 3a 1 0.555555553 0.111111112 0.142495289
```

Final job0162

```
SPGNAM= P31
CELEDG= 4.897503424 4.897503424 19.084496512 Angstroms
CELANG= 90.000000000 90.000000000 120.000000000 degrees.
ATOM= 1 Si 3a 1 0.868648083 0.753807133 0.099652616
ATOM= 2 Si 3a 1 0.204565087 0.413749132 0.099195700
ATOM= 3 Al 3a 1 0.878661591 0.096123358 0.240204398
ATOM= 4 Al 3a 1 0.551301231 0.424422811 0.240196538
ATOM= 5 O 3a 1 0.851680672 0.760868574 0.184434522
ATOM= 6 O 3a 1 0.217415770 0.397751832 0.183984943
ATOM= 7 O 3a 1 -0.085208941 0.085911977 0.071482630
ATOM= 8 O 3a 1 0.539997732 0.468163707 0.069208009
ATOM= 9 O 3a 1 0.170228746 0.717240522 0.079441970
```

Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	10	O	3a	1	0.209157103	0.117852027	0.291243209
ATOM=	11	O	3a	1	0.185544677	0.433415081	-0.041967914
ATOM=	12	O	3a	1	0.544873121	0.113129620	-0.041540866
ATOM=	13	O	3a	1	0.592571990	0.138095814	0.185739770
ATOM=	14	H	3a	1	0.155483079	-0.101290858	0.297181537
ATOM=	15	H	3a	1	0.352016189	0.654338306	-0.039174547
ATOM=	16	H	3a	1	0.544674683	0.166707038	0.007902750
ATOM=	17	H	3a	1	0.405131173	-0.049776350	0.169442772

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# Supplementary Table ST1 (Mercier et al., 2010)

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No low-pressure representative currently known for this family:  
[KP31]a, [KP33]a, [KP31]b

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Model [KP31]a

Initial job0004

SPGNAM= P21  
CELEDG= 5.326700000 14.507800000 5.326700000 Angstroms  
CELANG= 90.000000000 120.000000000 90.000000000 degrees.  
ATOM= 1 Si 2a 1 0.166666667 0.131465505 -0.000000002  
ATOM= 2 Si 2a 1 0.833333333 0.131465505 0.333333332  
ATOM= 3 Al 2a 1 0.500000000 0.320066905 -0.000000002  
ATOM= 4 Al 2a 1 0.833333333 0.320066905 0.666666665  
ATOM= 5 O 2a 1 0.166666667 0.242525215 -0.000000002  
ATOM= 6 O 2a 1 0.833333333 0.242525215 0.333333332  
ATOM= 7 O 2a 1 0.500000000 0.089442912 0.166666665  
ATOM= 8 O 2a 1 0.000000000 0.089442912 0.666666665  
ATOM= 9 O 2a 1 0.000000000 0.089442912 0.166666665  
ATOM= 10 O 2a 1 0.500000000 0.390104560 0.333333332  
ATOM= 11 O 2a 1 0.166666667 0.390104560 0.666666665  
ATOM= 12 O 2a 1 0.833333333 0.390104560 -0.000000002  
ATOM= 13 O 2a 1 0.500000000 0.242024946 0.666666665  
ATOM= 14 H 2a 1 0.500000000 0.454138988 0.333333332  
ATOM= 15 H 2a 1 0.166666667 0.454138988 0.666666665  
ATOM= 16 H 2a 1 0.166666667 -0.045861012 0.000000002  
ATOM= 17 H 2a 1 0.500000000 0.182492940 0.666666665

Final job0160

SPGNAM= P21  
CELEDG= 4.845743523 12.658460466 4.964051551 Angstroms  
CELANG= 90.000000000 119.687365408 90.000000000 degrees.  
ATOM= 1 Si 2a 1 0.160458699 0.118485183 -0.023663488  
ATOM= 2 Si 2a 1 0.825164656 0.118011981 0.319297501  
ATOM= 3 Al 2a 1 0.509998890 0.329270689 -0.004217181  
ATOM= 4 Al 2a 1 0.831869622 0.330607344 0.653102668  
ATOM= 5 O 2a 1 0.169198945 0.245741574 -0.044707844  
ATOM= 6 O 2a 1 0.802242688 0.245851382 0.329804981  
ATOM= 7 O 2a 1 0.499259304 0.076126161 0.027751387  
ATOM= 8 O 2a 1 -0.120795172 0.072801112 0.649535584  
ATOM= 9 O 2a 1 0.131076127 0.090662684 0.281162497  
ATOM= 10 O 2a 1 0.507496751 0.406873333 0.322161539  
ATOM= 11 O 2a 1 0.175537420 0.407616709 0.691635615  
ATOM= 12 O 2a 1 0.828094198 0.406163926 -0.026386690  
ATOM= 13 O 2a 1 0.547472701 0.248109951 0.703490285  
ATOM= 14 H 2a 1 0.535153080 0.482550782 0.305933387  
ATOM= 15 H 2a 1 0.218269759 0.419050169 0.522041538  
ATOM= 16 H 2a 1 -0.051216367 -0.095950884 -0.136710838  
ATOM= 17 H 2a 1 0.371363374 0.211717689 0.533711977

Model [KP33a]

Initial job0011

SPGNAM= Cmc21  
CELEDG= 9.226115037 5.326700000 14.507800000 Angstroms  
CELANG= 90.000000000 90.000000000 90.000000000 degrees.  
ATOM= 1 Si 8b 1 0.333333333 0.166666665 0.131465505  
ATOM= 2 Al 8b 1 0.166666667 -0.000000002 0.320066905  
ATOM= 3 O 8b 1 0.333333333 0.166666665 0.242525215  
ATOM= 4 O 8b 1 0.250000000 -0.083333335 0.089442912  
ATOM= 5 O 4a m.. 0.000000000 0.666666665 0.089442912  
ATOM= 6 O 8b 1 0.166666667 0.333333331 0.390104560  
ATOM= 7 O 4a m.. 0.000000000 0.833333332 0.390104560  
ATOM= 8 O 4a m.. 0.000000000 0.166666665 0.242024946  
ATOM= 9 H 8b 1 0.166666667 0.333333331 0.454138988  
ATOM= 10 H 4a m.. 0.000000000 0.166666668 -0.045861012

# Supplementary Table ST1 (Mercier et al., 2010)

ATOM= 11 H 4a m.. 0.000000000 0.166666665 0.182492940

Final job0143

SPGNAM= Cmc21

CELEDG= 8.583435259 4.805264844 12.764243879 Angstroms

CELANG= 90.000000000 90.000000000 90.000000000 degrees.

ATOM=	1	Si	8b	1	0.332281879	0.186416364	0.117293278
ATOM=	2	Al	8b	1	0.162599234	0.001080065	0.328641480
ATOM=	3	O	8b	1	0.322163553	0.179088984	0.244432810
ATOM=	4	O	8b	1	0.187179137	0.001142497	0.076018604
ATOM=	5	O	4a	m..	0.000000000	0.561380592	0.080910394
ATOM=	6	O	8b	1	0.179955309	0.329707113	0.403642397
ATOM=	7	O	4a	m..	0.000000000	-0.173183466	0.406328808
ATOM=	8	O	4a	m..	0.000000000	0.132671147	0.248013124
ATOM=	9	H	8b	1	0.098194338	0.470354928	0.410335312
ATOM=	10	H	4a	m..	0.000000000	0.132454718	-0.018623420
ATOM=	11	H	4a	m..	0.000000000	0.332666367	0.236339107

Model [KP31]b

Initial job0015

SPGNAM= Cc

CELEDG= 9.226115037 5.326700000 14.830177740 Angstroms

CELANG= 90.000000000 101.968420863 90.000000000 degrees.

ATOM=	1	Si	4a	1	-0.020622082	0.583333332	0.006465529
ATOM=	2	Si	4a	1	0.812711252	0.083333335	0.006465530
ATOM=	3	Al	4a	1	0.375578385	0.249999999	0.195066929
ATOM=	4	Al	4a	1	0.042245052	0.250000001	0.195066929
ATOM=	5	O	4a	1	0.016397821	0.583333332	0.117525239
ATOM=	6	O	4a	1	0.849731155	0.083333335	0.117525240
ATOM=	7	O	4a	1	0.382037054	0.333333332	-0.035557064
ATOM=	8	O	4a	1	0.882037054	0.333333334	-0.035557064
ATOM=	9	O	4a	1	0.132037054	0.583333332	-0.035557064
ATOM=	10	O	4a	1	0.065590937	-0.083333334	0.265104584
ATOM=	11	O	4a	1	0.398924270	-0.083333332	0.265104584
ATOM=	12	O	4a	1	0.732257603	-0.083333335	0.265104584
ATOM=	13	O	4a	1	0.182897732	0.083333332	0.117024970
ATOM=	14	H	4a	1	0.086935746	-0.083333334	0.329139012
ATOM=	15	H	4a	1	-0.079730921	0.416666668	0.329139012
ATOM=	16	H	4a	1	0.753602412	-0.083333335	0.329139012
ATOM=	17	H	4a	1	0.163053730	0.083333332	0.057492964

Final job0137

SPGNAM= Cc

CELEDG= 8.476414692 4.933084155 12.950307907 Angstroms

CELANG= 90.000000000 102.089438954 90.000000000 degrees.

ATOM=	1	Si	4a	1	-0.015312262	0.570278480	-0.005829433
ATOM=	2	Si	4a	1	0.823094947	0.070867440	-0.007921608
ATOM=	3	Al	4a	1	0.383694556	0.252177481	0.204397368
ATOM=	4	Al	4a	1	0.051185731	0.244900247	0.205093429
ATOM=	5	O	4a	1	0.007770971	0.566995019	0.121012829
ATOM=	6	O	4a	1	0.877648210	0.063035212	0.120045419
ATOM=	7	O	4a	1	0.330943969	0.265492261	-0.052878125
ATOM=	8	O	4a	1	0.951831371	0.263907073	-0.049227943
ATOM=	9	O	4a	1	0.144432550	0.705099135	-0.035186476
ATOM=	10	O	4a	1	0.071988917	-0.080256855	0.281941995
ATOM=	11	O	4a	1	0.423141351	-0.066167163	0.281018388
ATOM=	12	O	4a	1	0.739194524	-0.098263697	0.280939536
ATOM=	13	O	4a	1	0.191927140	0.127927478	0.122280184
ATOM=	14	H	4a	1	0.074131341	-0.074768918	0.357521506
ATOM=	15	H	4a	1	-0.175473339	0.368966520	0.299495744
ATOM=	16	H	4a	1	0.712294055	0.094488632	0.277322876
ATOM=	17	H	4a	1	0.183186113	-0.048454112	0.088662165

# Supplementary Table ST1 (Mercier et al., 2010)

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Nacrite can transform to the models in the following family:  
[KP11]b, [KP12]b, [KP13]b

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Model [KP11]b

Initial job0013

SPGNAM= Cc  
CELEDG= 9.226115037 5.326700000 14.507800000 Angstroms  
CELANG= 90.000000000 90.000000000 90.000000000 degrees.  
ATOM= 1 Si 4a 1 0.158320528 0.166666667 0.868534495  
ATOM= 2 Si 4a 1 -0.008346139 0.333333334 0.368534494  
ATOM= 3 Al 4a 1 0.324987195 -0.000000001 0.179933095  
ATOM= 4 Al 4a 1 -0.008346139 0.000000001 0.179933095  
ATOM= 5 O 4a 1 0.158320528 0.166666667 0.757474785  
ATOM= 6 O 4a 1 -0.008346139 0.333333334 0.257474784  
ATOM= 7 O 4a 1 0.324987195 0.166666668 -0.089442912  
ATOM= 8 O 4a 1 0.074987195 -0.083333335 -0.089442912  
ATOM= 9 O 4a 1 0.574987195 -0.083333332 -0.089442912  
ATOM= 10 O 4a 1 0.324987195 0.333333335 0.609895440  
ATOM= 11 O 4a 1 0.158320528 0.166666668 0.109895440  
ATOM= 12 O 4a 1 0.491653861 0.166666666 0.109895440  
ATOM= 13 O 4a 1 0.324987195 0.333333332 0.257975054  
ATOM= 14 H 4a 1 0.324987195 0.333333335 0.545861012  
ATOM= 15 H 4a 1 0.158320528 0.166666668 0.045861012  
ATOM= 16 H 4a 1 0.491653861 0.166666666 0.045861012  
ATOM= 17 H 4a 1 0.324987195 0.333333332 0.317507060

Final job0135

SPGNAM= Cc  
CELEDG= 8.382680249 4.942851686 12.753045365 Angstroms  
CELANG= 90.000000000 90.388338712 90.000000000 degrees.  
ATOM= 1 Si 4a 1 0.148837215 0.147570442 0.881485510  
ATOM= 2 Si 4a 1 -0.018288337 0.342811879 0.384060685  
ATOM= 3 Al 4a 1 0.327467407 0.010495072 0.172174678  
ATOM= 4 Al 4a 1 -0.013228110 0.009893211 0.170818335  
ATOM= 5 O 4a 1 0.156791994 0.131533422 0.754906656  
ATOM= 6 O 4a 1 -0.023615957 0.326121413 0.256308140  
ATOM= 7 O 4a 1 0.316886791 0.028590187 -0.075004666  
ATOM= 8 O 4a 1 0.004025551 -0.034943426 -0.075986444  
ATOM= 9 O 4a 1 0.629250861 -0.038466616 -0.081811147  
ATOM= 10 O 4a 1 0.324495611 0.317321027 0.594699538  
ATOM= 11 O 4a 1 0.157456953 0.146645655 0.096079538  
ATOM= 12 O 4a 1 0.486512050 0.184491731 0.096268665  
ATOM= 13 O 4a 1 0.339815319 0.325750130 0.252224820  
ATOM= 14 H 4a 1 0.341538313 0.289373745 0.519727872  
ATOM= 15 H 4a 1 0.174045195 0.334276740 0.077008399  
ATOM= 16 H 4a 1 0.600259913 0.138746709 0.097239639  
ATOM= 17 H 4a 1 0.239198154 0.415569358 0.266111343

=====

Model [KP12]b

Initial job0016

SPGNAM= Cc  
CELEDG= 9.226115037 5.326700000 14.830177740 Angstroms  
CELANG= 90.000000000 101.968420863 90.000000000 degrees.  
ATOM= 1 Si 4a 1 -0.073043657 0.583333333 0.131465505  
ATOM= 2 Si 4a 1 0.260289676 0.416666666 0.631465506  
ATOM= 3 Al 4a 1 0.156490143 0.749999999 0.320066905  
ATOM= 4 Al 4a 1 0.323156809 0.250000001 0.320066905  
ATOM= 5 O 4a 1 -0.036023754 0.583333333 0.242525215  
ATOM= 6 O 4a 1 0.297309579 0.416666666 0.742525216  
ATOM= 7 O 4a 1 0.079615478 0.583333332 0.089442912  
ATOM= 8 O 4a 1 0.329615478 0.333333334 0.089442912  
ATOM= 9 O 4a 1 0.329615478 0.833333332 0.089442912  
ATOM= 10 O 4a 1 0.179836028 0.416666665 0.390104560

# Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	11	O	4a	1	0.013169361	-0.083333332	0.390104560
ATOM=	12	O	4a	1	0.346502694	-0.083333334	0.390104560
ATOM=	13	O	4a	1	0.130476157	0.083333332	0.242024946
ATOM=	14	H	4a	1	0.201180837	0.416666666	0.454138988
ATOM=	15	H	4a	1	0.034514171	0.083333332	-0.045861012
ATOM=	16	H	4a	1	0.367847504	0.083333334	-0.045861012
ATOM=	17	H	4a	1	0.110632154	0.083333332	0.182492940

Final job0138

SPGNAM= Cc  
CELEDG= 8.635004399 4.835323896 12.965116397 Angstroms  
CELANG= 90.000000000 102.884178391 90.000000000 degrees.

ATOM=	1	Si	4a	1	-0.076614274	0.584678799	0.117950195
ATOM=	2	Si	4a	1	0.251969356	0.423892068	0.618491373
ATOM=	3	Al	4a	1	0.161755638	0.741733042	0.330753178
ATOM=	4	Al	4a	1	0.333003394	0.239426992	0.329410481
ATOM=	5	O	4a	1	-0.028735463	0.611768758	0.246115661
ATOM=	6	O	4a	1	0.284915104	0.441050941	0.746151785
ATOM=	7	O	4a	1	0.074119354	0.695159651	0.073126842
ATOM=	8	O	4a	1	0.263471281	0.262416672	0.076778776
ATOM=	9	O	4a	1	0.395629807	0.758526723	0.090300118
ATOM=	10	O	4a	1	0.203606676	0.412886009	0.407665162
ATOM=	11	O	4a	1	0.021894126	-0.095539705	0.407280789
ATOM=	12	O	4a	1	0.344408738	-0.086063503	0.407014828
ATOM=	13	O	4a	1	0.159657872	0.052513058	0.247940329
ATOM=	14	H	4a	1	0.120610115	0.275933419	0.407830534
ATOM=	15	H	4a	1	0.049178141	0.130279028	-0.016703826
ATOM=	16	H	4a	1	0.429113876	0.222723667	-0.086518279
ATOM=	17	H	4a	1	0.063196683	0.141657407	0.210101801

Model [KP13]b

Initial job0018

SPGNAM= Cc  
CELEDG= 9.226115037 5.326700000 14.830177740 Angstroms  
CELANG= 90.000000000 101.968420863 90.000000000 degrees.

ATOM=	1	Si	4a	1	0.083284646	-0.083333333	0.131465505
ATOM=	2	Si	4a	1	0.249951313	0.416666666	0.131465506
ATOM=	3	Al	4a	1	0.479485112	0.250000001	0.320066905
ATOM=	4	Al	4a	1	0.312818446	0.250000001	0.820066905
ATOM=	5	O	4a	1	0.120304549	-0.083333333	0.242525215
ATOM=	6	O	4a	1	0.286971216	0.416666666	0.242525216
ATOM=	7	O	4a	1	-0.097389552	-0.083333333	0.089442912
ATOM=	8	O	4a	1	0.652610448	0.166666666	0.089442912
ATOM=	9	O	4a	1	0.152610448	0.166666667	0.089442912
ATOM=	10	O	4a	1	0.002830997	0.083333335	0.390104560
ATOM=	11	O	4a	1	0.669497664	0.083333333	0.390104560
ATOM=	12	O	4a	1	0.336164331	0.083333334	0.390104560
ATOM=	13	O	4a	1	0.453471126	-0.083333332	0.242024946
ATOM=	14	H	4a	1	0.024175807	-0.083333335	-0.045861012
ATOM=	15	H	4a	1	0.690842473	-0.083333332	-0.045861012
ATOM=	16	H	4a	1	0.357509140	-0.083333335	-0.045861012
ATOM=	17	H	4a	1	0.433627124	-0.083333333	0.182492940

Final job0141

SPGNAM= Cc  
CELEDG= 8.382139559 4.957144718 13.052774100 Angstroms  
CELANG= 90.000000000 102.756583617 90.000000000 degrees.

ATOM=	1	Si	4a	1	0.069222871	-0.104446406	0.117335727
ATOM=	2	Si	4a	1	0.236166754	0.401516202	0.117840889
ATOM=	3	Al	4a	1	0.466678888	0.237109328	0.328754752
ATOM=	4	Al	4a	1	0.306820225	0.256914721	0.829064002
ATOM=	5	O	4a	1	0.108417768	-0.125555243	0.244244058
ATOM=	6	O	4a	1	0.287105100	0.423512851	0.244692907
ATOM=	7	O	4a	1	-0.113304636	-0.223943029	0.075035617
ATOM=	8	O	4a	1	0.694766693	0.205250781	0.071473027
ATOM=	9	O	4a	1	0.075192508	0.212281902	0.087102643

Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	10	O	4a	1	-0.010318850	0.058106261	0.403561812
ATOM=	11	O	4a	1	0.664991354	0.106000030	0.404829916
ATOM=	12	O	4a	1	0.328396530	0.073395819	0.405900076
ATOM=	13	O	4a	1	0.420363704	-0.069796630	0.246567924
ATOM=	14	H	4a	1	0.102986738	-0.109312034	-0.095885669
ATOM=	15	H	4a	1	0.688213724	0.081021994	-0.075284360
ATOM=	16	H	4a	1	0.370840491	-0.049038825	-0.018783166
ATOM=	17	H	4a	1	0.512226321	-0.160021747	0.227236726

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# Supplementary Table ST1 (Mercier et al., 2010)

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Dickite can transform to models in this family:  
[KP21]b, [KP22]b, [KP23]b

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Model [KP21]b

Initial job0014

SPGNAM= Cc  
CELEDG= 5.326700000 9.226115037 14.616049324 Angstroms  
CELANG= 90.000000000 96.977560803 90.000000000 degrees.  
ATOM= 1 Si 4a 1 0.481642204 0.249999999 0.868534495  
ATOM= 2 Si 4a 1 0.481642204 0.083333332 0.368534494  
ATOM= 3 Al 4a 1 0.752108404 0.249999999 0.679933095  
ATOM= 4 Al 4a 1 0.252108403 -0.083333334 0.179933095  
ATOM= 5 O 4a 1 0.444622301 0.249999999 0.757474785  
ATOM= 6 O 4a 1 0.444622300 0.083333332 0.257474784  
ATOM= 7 O 4a 1 0.245649735 0.833333332 -0.089442912  
ATOM= 8 O 4a 1 0.495649735 0.083333334 -0.089442912  
ATOM= 9 O 4a 1 0.245649735 0.333333332 -0.089442912  
ATOM= 10 O 4a 1 0.062095852 0.083333334 0.109895440  
ATOM= 11 O 4a 1 0.562095852 -0.083333334 0.109895440  
ATOM= 12 O 4a 1 0.062095852 0.249999999 0.609895440  
ATOM= 13 O 4a 1 -0.055210943 -0.083333332 0.257975054  
ATOM= 14 H 4a 1 0.040751043 0.083333334 0.045861012  
ATOM= 15 H 4a 1 0.540751043 -0.083333334 0.045861012  
ATOM= 16 H 4a 1 0.040751043 0.249999999 0.545861012  
ATOM= 17 H 4a 1 -0.035366941 -0.083333332 0.317507060

Final job0136

SPGNAM= Cc  
CELEDG= 4.819929192 8.643644962 12.722259212 Angstroms  
CELANG= 90.000000000 96.659912373 90.000000000 degrees.  
ATOM= 1 Si 4a 1 0.464818364 0.242596589 0.880590521  
ATOM= 2 Si 4a 1 0.456738930 0.086081602 0.382430258  
ATOM= 3 Al 4a 1 0.738060814 0.252363220 0.670569755  
ATOM= 4 Al 4a 1 0.235064239 -0.079724978 0.169178407  
ATOM= 5 O 4a 1 0.443092839 0.231770145 0.753071473  
ATOM= 6 O 4a 1 0.391238975 0.081551126 0.253980490  
ATOM= 7 O 4a 1 0.291644010 0.767626441 -0.077144184  
ATOM= 8 O 4a 1 0.357691539 0.080189442 -0.073950170  
ATOM= 9 O 4a 1 0.292495995 0.395707672 -0.090636583  
ATOM= 10 O 4a 1 0.046505036 0.084786831 0.092190829  
ATOM= 11 O 4a 1 0.541227881 -0.095861781 0.091469919  
ATOM= 12 O 4a 1 0.039923228 0.237065184 0.592263292  
ATOM= 13 O 4a 1 -0.051108107 -0.106067944 0.251635548  
ATOM= 14 H 4a 1 0.078934381 0.086272306 0.017618131  
ATOM= 15 H 4a 1 0.681351451 -0.013844341 0.092515178  
ATOM= 16 H 4a 1 0.179586438 0.317915293 0.587560623  
ATOM= 17 H 4a 1 -0.125601902 -0.025155600 0.292965323

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Model [KP22]b

Initial job0017

SPGNAM= Cc  
CELEDG= 5.326700000 9.226115037 14.616049324 Angstroms  
CELANG= 90.000000000 96.977560803 90.000000000 degrees.  
ATOM= 1 Si 4a 1 0.335488493 -0.083333333 0.006465529  
ATOM= 2 Si 4a 1 0.335488495 0.416666667 0.506465530  
ATOM= 3 Al 4a 1 0.065022294 -0.083333333 0.195066929  
ATOM= 4 Al 4a 1 0.065022294 0.250000000 0.195066929  
ATOM= 5 O 4a 1 0.372508397 -0.083333333 0.117525239  
ATOM= 6 O 4a 1 0.372508399 0.416666667 0.617525240  
ATOM= 7 O 4a 1 0.071480963 0.000000000 -0.035557064  
ATOM= 8 O 4a 1 0.321480963 0.250000000 0.464442936  
ATOM= 9 O 4a 1 0.071480963 0.500000000 -0.035557064  
ATOM= 10 O 4a 1 0.255034846 0.083333333 0.265104584



# Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	11	O	4a	1	0.255034845	0.250000000	0.765104584
ATOM=	12	O	4a	1	0.255034846	0.416666667	0.265104584
ATOM=	13	O	4a	1	0.372341640	0.250000000	0.117024970
ATOM=	14	H	4a	1	0.276379655	0.083333333	0.329139012
ATOM=	15	H	4a	1	0.276379654	0.250000000	0.829139012
ATOM=	16	H	4a	1	0.276379655	0.416666667	0.329139012
ATOM=	17	H	4a	1	0.352497639	0.250000000	0.057492964

Final job0139

SPGNAM= Cc  
CELEDG= 4.945721876 8.363951786 12.877022631 Angstroms  
CELANG= 90.000000000 98.112245905 90.000000000 degrees.

ATOM=	1	Si	4a	1	0.311675957	-0.084260286	-0.008067694
ATOM=	2	Si	4a	1	0.321634601	0.416437488	0.492581246
ATOM=	3	Al	4a	1	0.055226007	-0.077615778	0.203621716
ATOM=	4	Al	4a	1	0.054685697	0.262397623	0.203412133
ATOM=	5	O	4a	1	0.341314044	-0.088471977	0.119657101
ATOM=	6	O	4a	1	0.383466314	0.408337358	0.619718356
ATOM=	7	O	4a	1	-0.010482857	-0.062869700	-0.048411259
ATOM=	8	O	4a	1	0.426468112	0.248680668	0.450292917
ATOM=	9	O	4a	1	-0.007338235	0.564747719	-0.041886363
ATOM=	10	O	4a	1	0.222313197	0.092657392	0.280390401
ATOM=	11	O	4a	1	0.256916096	0.239657718	0.781198430
ATOM=	12	O	4a	1	0.261097372	0.420881377	0.279619394
ATOM=	13	O	4a	1	0.341217978	0.273850307	0.123713413
ATOM=	14	H	4a	1	0.416767929	0.115012850	0.286816725
ATOM=	15	H	4a	1	0.309970457	0.214761654	0.855563071
ATOM=	16	H	4a	1	0.219880553	0.534919115	0.284465247
ATOM=	17	H	4a	1	0.424748775	0.174435559	0.106009941

Model [KP23]b

Initial job0019

SPGNAM= Cc  
CELEDG= 5.326700000 9.226115037 14.616049324 Angstroms  
CELANG= 90.000000000 96.977560803 90.000000000 degrees.

ATOM=	1	Si	4a	1	0.364975539	-0.083333334	0.368534495
ATOM=	2	Si	4a	1	0.364975539	0.250000001	0.368534494
ATOM=	3	Al	4a	1	0.135441739	0.416666666	0.179933095
ATOM=	4	Al	4a	1	0.135441739	0.083333334	0.179933095
ATOM=	5	O	4a	1	0.327955636	-0.083333334	0.257474785
ATOM=	6	O	4a	1	0.327955636	0.250000001	0.257474784
ATOM=	7	O	4a	1	0.628983070	0.166666668	-0.089442912
ATOM=	8	O	4a	1	0.378983070	-0.083333334	-0.089442912
ATOM=	9	O	4a	1	0.128983070	0.166666668	-0.089442912
ATOM=	10	O	4a	1	-0.054570813	0.249999999	0.109895440
ATOM=	11	O	4a	1	-0.054570812	0.583333334	0.109895440
ATOM=	12	O	4a	1	-0.054570813	-0.083333334	0.109895440
ATOM=	13	O	4a	1	0.328122392	0.416666668	0.757975054
ATOM=	14	H	4a	1	-0.075915622	0.249999999	0.045861012
ATOM=	15	H	4a	1	-0.075915622	0.583333334	0.045861012
ATOM=	16	H	4a	1	-0.075915622	-0.083333334	0.045861012
ATOM=	17	H	4a	1	0.347966394	0.416666668	0.817507060

Final job0142

SPGNAM= Cc  
CELEDG= 4.960956514 8.359770285 12.835613614 Angstroms  
CELANG= 90.000000000 98.089790441 90.000000000 degrees.

ATOM=	1	Si	4a	1	0.384502286	-0.072520757	0.382918357
ATOM=	2	Si	4a	1	0.378045720	0.260466264	0.381937308
ATOM=	3	Al	4a	1	0.147562544	0.425167118	0.170411852
ATOM=	4	Al	4a	1	0.141698319	0.085009412	0.171441407
ATOM=	5	O	4a	1	0.359822961	-0.065759728	0.255278603
ATOM=	6	O	4a	1	0.310317490	0.255876501	0.254848737
ATOM=	7	O	4a	1	0.706094448	0.096880103	-0.072267440
ATOM=	8	O	4a	1	0.271559278	-0.092776437	-0.075879362
ATOM=	9	O	4a	1	0.205641173	0.224002044	-0.087856883

Supplementary Table ST1 (Mercier et al., 2010)

ATOM=	10	O	4a	1	-0.020386100	0.257304892	0.093586053
ATOM=	11	O	4a	1	-0.067898161	0.581540474	0.094848451
ATOM=	12	O	4a	1	-0.049279181	-0.082255310	0.093461945
ATOM=	13	O	4a	1	0.363753701	0.432394238	0.752316800
ATOM=	14	H	4a	1	-0.214728328	0.280056712	0.084758420
ATOM=	15	H	4a	1	-0.020327574	0.695373749	0.091890324
ATOM=	16	H	4a	1	-0.101391296	-0.054970990	0.019128355
ATOM=	17	H	4a	1	0.283332496	0.335161884	0.775486067

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