Supplementary Table ST1 (Mercier et al., 2010)

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

Translation T	Rotation R					
	0	π/3	2π/3	π	4π/3	5π/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 ($Å^3$)	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 ($Å^3$)		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 ($Å^3$)	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	π/3	2π/3	π	4π/3	5π/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 ($Å^3$)	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 ($Å^3$)		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 ($Å^3$)	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
==================================================
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
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Supplementary Table ST1 (Mercier et al., 2010)

Final job0140

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

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

Final job0134

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

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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
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Supplementary Table ST1 (Mercier et al., 2010)

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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

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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

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         0.222222221    0.111111114    0.108477000
ATOM=    2  Si   3a    1         0.555555555    0.777777780    0.108477000
ATOM=    3  Al   3a    1         0.222222221    0.444444447    0.234211266
ATOM=    4  Al   3a    1         0.888888888    0.777777780    0.234211266
ATOM=    5  O    3a    1         0.222222221    0.111111114    0.182516806
ATOM=    6  O    3a    1         0.555555555    0.777777780    0.182516806
ATOM=    7  O    3a    1         0.388888888    0.444444447    0.080461937
ATOM=    8  O    3a    1         0.888888888   -0.055555553    0.080461937
ATOM=    9  O    3a    1         0.388888888   -0.055555553    0.080461937
ATOM=   10  O    3a    1         0.555555555    0.444444447    0.280903036
ATOM=   11  O    3a    1         0.222222225    0.111111112   -0.052430297
ATOM=   12  O    3a    1         0.222222221    0.777777780    0.280903036
ATOM=   13  O    3a    1         0.888888888    0.444444447    0.182183294
ATOM=   14  H    3a    1         0.555555555    0.444444447    0.323592655
ATOM=   15  H    3a    1         0.222222225    0.111111112   -0.009740678
ATOM=   16  H    3a    1         0.222222221    0.777777780    0.323592655
ATOM=   17  H    3a    1         0.888888888    0.444444447    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

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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         0.888888891    0.111111114    0.108477000
ATOM=    2  Si   3a    1         0.222222225    0.777777780    0.108477000
ATOM=    3  Al   3a    1         0.555555555    0.111111109   -0.099122067
ATOM=    4  Al   3a    1         0.222222221    0.444444442   -0.099122067
ATOM=    5  O    3a    1         0.888888891    0.111111114    0.182516806
ATOM=    6  O    3a    1         0.222222225    0.777777780    0.182516806
ATOM=    7  O    3a    1         0.055555558    0.444444447    0.080461937
ATOM=    8  O    3a    1         0.555555558   -0.055555553    0.080461937
ATOM=    9  O    3a    1         0.055555558   -0.055555553    0.080461937
ATOM=   10  O    3a    1         0.222222225    0.444444447    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

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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

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

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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

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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
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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

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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
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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

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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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