

Table 5. Rietveld results for runs at 400 MPa

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
2-98A 500 °C	mica 1M	5.205 (3)	8.989 (5)	10.340 (5)	101.60 (4)	0.10 (1)	0.197 (26)	0.082	1.81	1.091
	mica 2M1	5.195 (2)	8.996 (8)	20.327 (13)	95.58 (7)	0.06 (1)				
	mica 2M2	8.998 (6)	5.229 (9)	20.529 (13)	100.00 (6)	<0.01				
	mica 3T	5.214 (7)		30.065 (94)		<0.01				
	fsp	8.658 (2)	13.048 (2)	7.185 (1)	116.02 (1)	0.57 (1)	0.243 (8)			
	qtz	4.912 (1)		5.403 (1)		0.27 (1)				
4-98 500 °C	mica 1M	5.211 (2)	8.999 (4)	10.400 (4)	101.52 (2)	0.18 (1)	0.456 (21)	0.086	1.76	1.128
	mica 2M1	5.197 (3)	9.010 (8)	20.489 (9)	95.90 (6)	0.10 (1)				
	mica 2M2	9.017 (4)	5.206 (7)	20.694 (9)	100.12 (6)	0.07 (1)				
	mica 3T	5.224 (6)		30.603 (41)		<0.01				
	fsp	8.739 (2)	13.053 (3)	7.192 (2)	116.11 (2)	0.25 (1)	0.597 (12)			
	qtz	4.915 (1)		5.407 (1)		0.40 (1)				
5-98A 500 °C	fsp	8.621 (1)	13.034 (1)	7.177 (1)	116.03 (1)	0.94 (1)	0.077 (3)	0.054	1.60	1.236
	qtz	4.914 (1)		5.405 (1)		0.06 (1)				
6-98 600 °C	mica 1M	5.206 (1)	8.995 (2)	10.395 (2)	101.51 (2)	0.28 (1)	0.422 (13)	0.097	1.60	1.227
	mica 2M1	5.196 (2)	9.007 (3)	20.453 (6)	95.81 (4)	0.17 (1)				
	mica 2M2	9.010 (3)	5.201 (5)	20.686 (6)	100.17 (4)	0.10 (1)				
	mica 3T	5.225 (5)		30.374 (38)		<0.01				
	qtz	4.913 (1)		5.404 (1)		0.44 (1)				
7-98 600 °C	mica 1M	5.210 (2)	8.991 (4)	10.332 (4)	101.63 (3)	0.13 (1)	0.181 (19)	0.086	1.84	1.106
	mica 2M1	5.196 (2)	9.009 (3)	20.333 (8)	95.81 (4)	0.14 (1)				
	mica 2M2	9.001 (5)	5.189 (4)	20.567 (8)	100.19 (4)	0.08 (1)				
	mica 3T	5.223 (6)		29.897 (78)		<0.01				
	fsp	8.658 (2)	13.050 (2)	7.189 (1)	116.02 (2)	0.31 (1)	0.247 (11)			
	qtz	4.916 (1)		5.407 (1)		0.35 (1)				
8-98 600 °C	fsp	8.614 (1)	13.029 (1)	7.178 (1)	116.01 (1)	0.92 (1)	0.042 (4)	0.052	1.58	1.280
	qtz	4.911 (1)		5.401 (1)		0.08 (1)				
9-98 500 °C	mica 1M	5.211 (4)	9.010 (7)	10.437 (6)	101.43 (5)	0.14 (2)	0.622 (31)	0.075	1.77	1.149
	mica 2M1	5.203 (4)	9.018 (8)	20.572 (13)	95.74 (8)	0.11 (2)				
	mica 2M2	9.021 (7)	5.221 (7)	20.780 (18)	100.04 (9)	0.05 (1)				
	mica 3T	5.220 (4)		30.586 (66)		<0.01				
	fsp	8.744 (3)	13.068 (4)	7.189 (2)	116.05 (2)	0.25 (1)	0.624 (16)			
	qtz	4.915 (1)		5.407 (1)		0.45 (1)				
10-98 500 °C	mica 1M	5.204 (4)	8.996 (9)	10.326 (7)	101.68 (6)	0.06 (1)	0.141 (37)	0.076	1.84	1.060
	mica 2M1	5.184 (3)	9.001 (6)	20.313 (16)	95.83 (8)	0.05 (1)				
	mica 2M2	8.996 (8)	5.189 (6)	20.530 (21)	100.09 (9)	0.03 (1)				
	mica 3T	5.234 (4)		29.911 (63)		0.01 (1)				
	fsp	8.663 (2)	13.035 (2)	7.177 (1)	116.05 (1)	0.54 (1)	0.256 (8)			
	qtz	4.911 (1)		5.402 (1)		0.31 (1)				
11-98 500 °C	fsp	8.629 (1)	13.036 (1)	7.183 (1)	116.04 (1)	0.87 (1)	0.114 (6)	0.058	1.64	1.239
	qtz	4.915 (1)		5.407 (1)		0.13 (1)				
1-99 500 °C	mica 1M	5.206 (4)	9.005 (5)	10.465 (6)	101.27 (5)	0.16 (2)	0.691 (27)	0.107	1.70	1.231
	mica 2M1	5.201 (3)	9.016 (8)	20.580 (11)	95.65 (6)	0.16 (2)				
	mica 2M2	9.016 (6)	5.198 (7)	20.851 (16)	100.27 (12)	0.02 (1)				
	mica 3T	5.218 (5)		30.778 (33)		<0.01				
	fsp	8.779 (4)	13.057 (4)	7.184 (3)	116.05 (3)	0.07 (1)	0.769 (19)			
	qtz	4.912 (1)		5.404 (1)		0.58 (1)				

Table 5. Rietveld results for runs at 400 MPa (continued)

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
2-99 500 °C	mica 1M	5.204(3)	8.986(4)	10.377(4)	101.53(4)	0.10(1)	0.319(23)	0.088	1.84	1.084
	mica 2M1	5.196(3)	9.002(4)	20.381(10)	95.81(7)	0.10(1)				
	mica 2M2	9.011(6)	5.210(10)	20.665(11)	100.34(7)	0.04(1)				
	mica 3T	5.209(4)		30.411(67)		<0.01				
	fsp	8.715(2)	13.045(2)	7.184(1)	116.10(2)	0.38(1)	0.489(10)			
	qtz	4.912(1)		5.404(1)		0.38(1)				
3-99 500 °C	mica 1M	5.210(4)	8.985(6)	10.349(7)	101.50(6)	0.09(1)	0.238(34)	0.091	1.84	1.114
	mica 2M1	5.195(5)	8.999(17)	20.350(15)	95.73(8)	0.05(1)				
	mica 2M2	9.014(7)	5.214(8)	20.574(14)	100.15(7)	<0.01				
	mica 3T	5.211(6)		30.259(67)		<0.01				
	fsp	8.689(2)	13.044(2)	7.184(1)	116.08(1)	0.59(1)	0.376(7)			
	qtz	4.913(1)		5.405(1)		0.27(1)				
4-99 500 °C	mica 1M	5.211(6)	8.979(15)	10.341(8)	101.40(9)	0.04(1)	0.239(46)	0.081	1.79	1.126
	mica 2M1	5.203(4)	8.983(15)	20.378(24)	95.78(9)	<0.01				
	mica 2M2	9.010(11)	5.186(6)	20.605(34)	100.36(14)	<0.01				
	mica 3T	5.209(4)		29.986(47)		<0.01				
	fsp	8.648(1)	13.046(1)	7.188(1)	116.00(1)	0.79(1)	0.199(6)			
	qtz	4.913(1)		5.405(1)		0.17(1)				
5-99 500 °C	mica 1M	5.210(6)	8.983(10)	10.312(8)	101.51(6)	0.01(1)	0.075(43)	0.058	1.62	1.189
	mica 2M1	5.193(5)	8.988(5)	20.241(14)	95.96(8)	<0.01				
	mica 2M2	9.005(11)	5.189(6)	20.451(26)	100.10(11)	<0.01				
	mica 3T	5.224(3)		29.906(62)		<0.01				
	fsp	8.635(1)	13.038(1)	7.183(1)	116.04(1)	0.90(1)	0.137(4)			
	qtz	4.915(1)		5.406(1)		0.09(1)				
6-99 500 °C	fsp	8.606(1)	13.027(1)	7.180(1)	116.03(1)	0.94(1)	0.008(4)	0.053	1.55	1.240
	qtz	4.913(1)		5.403(1)		0.06(1)				
7-99 600 °C	mica 1M	5.208(2)	9.004(4)	10.471(5)	101.47(3)	0.28(3)	0.719(23)	0.111	1.72	1.237
	mica 2M1	5.204(3)	9.016(10)	20.604(9)	95.74(6)	0.15(1)				
	mica 2M2	9.024(5)	5.202(9)	20.827(13)	99.92(8)	0.05(2)				
	mica 3T	5.221(6)		30.784(24)		<0.01				
	qtz	4.913(1)		5.404(1)		0.52(2)				
8-99 600 °C	mica 1M	5.205(2)	8.991(3)	10.377(3)	101.55(3)	0.26(1)	0.351(14)	0.102	1.71	1.184
	mica 2M1	5.192(2)	8.999(3)	20.417(6)	95.80(4)	0.16(1)				
	mica 2M2	9.007(3)	5.197(4)	20.652(5)	100.19(4)	0.10(1)				
	mica 3T	5.226(4)		30.084(52)		<0.01				
	qtz	4.912(1)		5.404(1)		0.48(1)				
9-99 600 °C	mica 1M	5.206(2)	8.988(2)	10.339(3)	101.61(2)	0.19(1)	0.194(14)	0.110	1.84	1.148
	mica 2M1	5.192(2)	9.004(3)	20.337(6)	95.89(3)	0.14(1)				
	mica 2M2	9.008(4)	5.172(4)	20.575(7)	100.23(4)	0.06(1)				
	mica 3T	5.215(6)		29.857(35)		<0.01				
	fsp	8.677(5)	13.039(4)	7.180(3)	116.08(3)	0.13(1)	0.322(24)			
	qtz	4.914(1)		5.405(1)		0.48(1)				
10-99 600 °C	mica 1M	5.204(5)	8.990(10)	10.322(8)	101.64(9)	0.05(1)	0.068(32)	0.079	1.89	1.099
	mica 2M1	5.190(2)	8.998(6)	20.258(11)	95.71(8)	0.08(1)				
	mica 2M2	8.989(9)	5.189(6)	20.514(15)	100.13(10)	0.03(1)				
	mica 3T	5.215(6)		29.854(91)		<0.01				
	fsp	8.645(1)	13.045(1)	7.185(1)	116.02(1)	0.62(1)	0.186(5)			
	qtz	4.914(1)		5.405(1)		0.23(1)				
12-99 600 °C	fsp	8.607(1)	13.041(1)	7.188(1)	115.98(1)	0.92(1)	0.021(3)	0.056	1.57	1.251
	qtz	4.914(1)		5.406(1)		0.08(1)				

Table 5. Rietveld results for runs at 400 MPa (continued)

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
13-99 500 °C	mica 1M	5.210(3)	9.005(5)	10.542(8)	101.28(4)	0.40(3)	1.034(32)	0.089	0.81	2.528
	mica 2M1	5.205(3)	9.018(6)	20.767(11)	95.50(7)	0.40(1)				
	mica 2M2	9.021(5)	5.202(7)	21.010(16)	99.94(10)	0.11(3)				
	mica 3T	5.222(5)		31.003(33)		0.06(3)				
	qtz	4.910(3)		5.402(5)		0.03(1)				
14-99 500 °C	mica 1M	5.207(4)	9.005(5)	10.471(8)	101.38(5)	0.41(4)	0.721(36)	0.078	0.69	2.920
	mica 2M1	5.202(4)	9.016(7)	20.601(13)	95.69(8)	0.38(1)				
	mica 2M2	9.020(5)	5.200(6)	20.836(20)	99.93(11)	0.12(4)				
	mica 3T	5.217(5)		30.784(37)		0.04(3)				
	qtz	4.912(2)		5.404(4)		0.03(1)				
15-99 500 °C	mica 1M	5.211(3)	9.001(3)	10.416(3)	101.34(4)	0.38(1)	0.534(14)	0.069	1.02	1.993
	mica 2M1	5.201(1)	9.015(3)	20.506(6)	95.58(4)	0.41(1)				
	mica 2M2	9.016(4)	5.202(4)	20.752(6)	100.19(5)	0.14(1)				
	mica 3T	5.223(3)		30.349(27)		0.04(1)				
	qtz	4.913(1)		5.404(2)		0.03(1)				
16-99 500 °C	mica 1M	5.206(2)	8.996(3)	10.385(3)	101.32(3)	0.41(1)	0.407(17)	0.061	1.05	1.860
	mica 2M1	5.197(2)	9.008(3)	20.434(7)	95.52(5)	0.39(1)				
	mica 2M2	9.009(4)	5.210(7)	20.688(7)	100.22(5)	0.17(1)				
	mica 3T	5.220(3)		30.229(33)		0.01(1)				
	qtz	4.912(1)		5.403(3)		0.02(1)				
16-99A 500 °C	mica 1M	5.204(2)	8.993(3)	10.375(3)	101.35(3)	0.41(1)	0.376(15)	0.063	0.87	2.291
	mica 2M1	5.195(1)	9.004(3)	20.423(7)	95.55(4)	0.40(1)				
	mica 2M2	9.005(3)	5.216(5)	20.671(5)	100.26(4)	0.17(1)				
	mica 3T	5.218(2)		30.232(32)		0.02(1)				
	qtz	4.911(4)		5.404(7)		0.01(1)				
17-99 500 °C	mica 1M	5.204(2)	8.990(3)	10.350(4)	101.48(2)	0.48(2)	0.254(18)	0.068	0.88	2.343
	mica 2M1	5.191(2)	9.001(3)	20.361(8)	95.75(5)	0.33(1)				
	mica 2M2	9.003(4)	5.198(6)	20.610(8)	100.23(5)	0.17(2)				
	mica 3T	5.221(4)		30.100(35)		0.01(1)				
	qtz	4.911(3)		5.405(5)		0.01(1)				
18-99 500 °C	mica 1M	5.203(2)	8.986(3)	10.327(4)	101.56(2)	0.49(3)	0.156(20)	0.065	0.73	2.794
	mica 2M1	5.190(2)	8.997(3)	20.312(8)	95.84(5)	0.30(1)				
	mica 2M2	9.002(4)	5.193(5)	20.551(9)	100.16(4)	0.20(3)				
	mica 3T	5.213(7)		30.043(69)		<0.01				
	qtz	4.912(4)		5.405(8)		0.01(1)				
19-99 500 °C	mica 1M	5.202(1)	8.983(2)	10.311(2)	101.63(1)	0.45(1)	0.085(10)	0.058	0.82	2.359
	mica 2M1	5.188(1)	8.995(2)	20.277(4)	95.85(3)	0.32(1)				
	mica 2M2	8.999(2)	5.190(2)	20.513(4)	100.12(3)	0.22(1)				
	mica 3T	5.212(6)		29.930(53)		<0.01				
	qtz	4.912(3)		5.408(5)		0.01(1)				
20-99 500 °C	mica 1M	5.201(2)	8.982(3)	10.303(3)	101.66(2)	0.45(2)	0.050(15)	0.070	0.79	2.740
	mica 2M1	5.188(2)	8.993(3)	20.261(6)	95.87(4)	0.32(1)				
	mica 2M2	8.998(3)	5.189(3)	20.494(7)	100.11(4)	0.22(2)				
	mica 3T	5.216(11)		29.891(91)		<0.01				
	qtz	4.910(4)		5.409(7)		0.02(1)				
21-99 500 °C	mica 1M	5.203(2)	8.983(3)	10.301(4)	101.65(2)	0.49(1)	0.046(19)	0.064	0.81	2.438
	mica 2M1	5.189(2)	8.996(3)	20.258(9)	95.85(4)	0.29(1)				
	mica 2M2	8.999(5)	5.192(4)	20.487(9)	100.07(4)	0.17(2)				
	mica 3T	5.214(14)		29.873(87)		<0.01				
	fsp	8.606(15)	13.022(14)	7.180(8)	116.10(11)	0.02(1)	0.009(73)			
	qtz	4.910(4)		5.411(8)		0.02(1)				

Table 5. Rietveld results for runs at 400 MPa (continued)

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
22-99 500 °C	mica 1M	5.204(2)	8.984(3)	10.296(3)	101.68(2)	0.48(1)	0.022(17)	0.061	0.86	2.306
	mica 2M1	5.189(2)	8.995(3)	20.248(7)	95.87(4)	0.29(1)				
	mica 2M2	8.997(5)	5.192(4)	20.477(8)	100.06(5)	0.17(1)				
	mica 3T	5.215(15)		29.846(85)		<0.01				
	fsp	8.609(9)	13.030(10)	7.178(5)	116.06(6)	0.04(1)	0.025(44)			
	qtz	4.907(15)		5.417(28)		0.01(1)				
23-99 500 °C	mica 1M	5.206(1)	8.987(2)	10.291(3)	101.72(2)	0.47(1)	0.000(14)	0.056	0.91	2.159
	mica 2M1	5.190(2)	9.000(2)	20.239(6)	95.88(4)	0.28(1)				
	mica 2M2	9.003(4)	5.191(3)	20.460(7)	100.04(4)	0.15(1)				
	fsp	8.602(4)	13.044(6)	7.183(3)	115.99(3)	0.09(1)	0.000(22)			
	qtz	4.895(11)		5.422(22)		0.01(1)				
38-99 400 °C	mica 1M	5.215(13)	9.004(11)	10.404(9)	101.42(14)	0.01(1)	0.488(63)	0.071	1.31	1.553
	mica 2M1	5.203(17)	9.004(46)	20.488(33)	95.53(19)	0.01(1)				
	mica 2M2	9.017(12)	5.217(6)	20.720(16)	99.88(14)	<0.01				
	mica 3T	5.221(8)		30.475(39)		0.01(1)				
	fsp	8.745(1)	13.043(1)	7.186(1)	116.10(1)	0.82(1)	0.615(5)			
	qtz	4.912(1)		5.404(1)		0.15(1)				
39-99 400 °C	mica 1M	5.201(9)	9.019(12)	10.415(11)	101.38(11)	0.02(1)	0.537(65)	0.075	1.52	1.332
	mica 2M1	5.203(10)	9.024(36)	20.523(44)	95.67(20)	0.01(1)				
	mica 2M2	9.011(7)	5.227(8)	20.735(21)	100.01(10)	0.02(1)				
	mica 3T	5.221(9)		30.490(29)		0.01(1)				
	fsp	8.740(1)	13.046(1)	7.190(1)	116.09(1)	0.78(1)	0.598(6)			
	qtz	4.914(1)		5.406(1)		0.17(1)				
40-99 400 °C	mica 1M	5.202(6)	8.998(8)	10.444(9)	101.32(6)	<0.01	0.541(38)	0.068	1.61	1.231
	mica 2M1	5.207(3)	8.997(12)	20.532(14)	95.64(7)	<0.01				
	mica 2M2	9.032(6)	5.200(6)	20.720(15)	100.00(8)	0.02(1)				
	mica 3T	5.216(4)		30.580(19)		0.01(1)				
	fsp	8.704(2)	13.047(2)	7.190(1)	116.07(1)	0.79(1)	0.441(7)			
	qtz	4.914(1)		5.406(1)		0.17(1)				
43-99 400 °C	fsp	8.647(1)	13.048(1)	7.184(1)	116.02(1)	0.87(1)	0.194(4)	0.068	1.70	1.168
	qtz	4.914(1)		5.406(1)		0.13(1)				
44-99 400 °C	fsp	8.625(1)	13.046(1)	7.183(1)	116.01(1)	0.89(1)	0.098(3)	0.061	1.74	1.177
	qtz	4.915(1)		5.406(1)		0.11(1)				
1-00 600 °C	mica 1M	5.208(2)	9.003(2)	10.432(3)	101.35(4)	0.23(1)	0.609(16)	0.082	1.19	1.726
	mica 2M1	5.200(1)	9.016(3)	20.547(7)	95.51(4)	0.23(1)				
	mica 2M2	9.019(3)	5.208(4)	20.795(7)	100.16(5)	0.11(1)				
	mica 3T	5.221(3)		30.352(28)		0.01(1)				
	qtz	4.914(1)		5.404(1)		0.16(1)				
	cor	4.757(1)		12.984(4)		0.27(1)				
2-00 600 °C	mica 1M	5.208(2)	8.993(2)	10.362(4)	101.48(2)	0.35(2)	0.310(23)	0.077	1.13	1.782
	mica 2M1	5.194(2)	9.007(3)	20.399(11)	95.74(5)	0.25(1)				
	mica 2M2	9.009(3)	5.200(6)	20.636(11)	100.26(5)	0.17(2)				
	mica 3T	5.226(4)		30.132(43)		0.01(1)				
	qtz	4.914(1)		5.405(1)		0.10(1)				
	cor	4.758(1)		12.988(5)		0.14(1)				

Table 5. Rietveld results for runs at 400 MPa (continued)

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{\text{NH}_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
3-00 600 °C	mica 1M	5.205(1)	8.985(1)	10.320(2)	101.65(1)	0.36(1)	0.116(8)	0.065	1.14	1.818
	mica 2M1	5.191(1)	9.001(1)	20.296(4)	95.86(2)	0.31(1)				
	mica 2M2	9.004(2)	5.190(1)	20.528(3)	100.13(2)	0.24(1)				
	mica 3T	5.220(18)		30.140(128)		<0.01				
	qtz	4.914(1)		5.404(1)		0.05(1)				
	cor	4.758(1)		12.990(7)		0.06(1)				
4-00 600 °C	mica 1M	5.202(1)	8.982(2)	10.298(3)	101.68(2)	0.50(1)	0.033(14)	0.074	0.76	2.620
	mica 2M1	5.188(2)	8.992(3)	20.254(6)	95.89(3)	0.30(1)				
	mica 2M2	8.997(3)	5.189(4)	20.485(6)	100.10(4)	0.19(1)				
	mica 3T	5.199(25)		29.919(237)		<0.01				
7-00 400 °C	mica 1M	5.214(3)	9.007(4)	10.445(3)	101.29(5)	0.36(1)	0.664(19)	0.082	0.81	2.497
	mica 2M1	5.205(2)	9.020(4)	20.577(8)	95.54(5)	0.42(1)				
	mica 2M2	9.025(4)	5.214(5)	20.804(8)	100.09(7)	0.16(1)				
	mica 3T	5.230(3)		30.413(31)		0.04(1)				
	qtz	4.913(2)		5.404(3)		0.03(1)				
8-00 400 °C	mica 1M	5.210(3)	8.995(4)	10.384(6)	101.39(3)	0.43(2)	0.407(27)	0.071	1.01	2.008
	mica 2M1	5.199(3)	9.012(4)	20.449(11)	95.69(6)	0.38(1)				
	mica 2M2	9.011(5)	5.215(7)	20.680(13)	100.27(6)	0.18(2)				
	mica 3T	5.229(4)		30.152(41)		0.01(1)				
	qtz	4.908(7)		5.410(12)		0.01(1)				
9-00 400 °C	mica 1M	5.206(2)	8.992(4)	10.345(5)	101.47(3)	0.44(2)	0.217(23)	0.059	0.98	1.997
	mica 2M1	5.196(2)	9.007(3)	20.332(9)	95.67(5)	0.41(1)				
	mica 2M2	9.003(5)	5.206(6)	20.598(11)	100.27(5)	0.14(2)				
	mica 3T	5.225(5)		29.908(46)		<0.01				
	qtz	4.911(3)		5.406(6)		0.01(1)				
10-00 400 °C	mica 1M	5.204(2)	8.986(4)	10.316(5)	101.53(3)	0.42(2)	0.100(23)	0.061	0.98	2.120
	mica 2M1	5.194(2)	9.002(3)	20.272(9)	95.72(5)	0.41(1)				
	mica 2M2	8.998(5)	5.201(5)	20.539(11)	100.18(5)	0.16(2)				
	mica 3T	5.223(5)		30.078(65)		<0.01				
	qtz	4.912(5)		5.408(9)		0.01(1)				

Table 6. Rietveld results for runs at 1500 MPa

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
28-99 500 °C	mica 1M	5.218(7)	8.989(6)	10.313(8)	101.41(7)	0.04(1)	0.079(25)	0.100	1.68	1.227
	mica 2M1	5.187(4)	8.997(4)	20.255(10)	95.36(6)	0.05(1)				
	mica 2M2	8.985(11)	5.178(7)	20.465(14)	99.98(11)	<0.01				
	mica 3T	5.194(5)		30.098(31)		0.03(1)				
	mica 2Or	5.197(5)	9.004(5)	20.085(18)		<0.01				
	fsp	8.660(1)	13.043(1)	7.183(1)	116.06(1)	0.63(1)	0.250(5)			
	qtz	4.914(1)		5.406(1)		0.25(1)				
41-99 500 °C	mica 1M	5.222(11)	8.987(10)	10.335(8)	101.38(11)	0.05(1)	0.281(31)	0.076	1.32	1.554
	mica 2M1	5.197(6)	9.003(4)	20.367(11)	94.96(10)	0.11(2)				
	mica 2M2	9.001(7)	5.188(6)	20.589(16)	100.17(6)	0.04(1)				
	mica 3T	5.204(5)		29.763(46)		<0.01				
	mica 2Or	5.217(6)	9.007(8)	19.843(33)		<0.01				
	fsp	8.730(1)	13.053(2)	7.190(1)	116.06(1)	0.59(1)	0.552(5)			
	qtz	4.914(1)		5.406(1)		0.21(1)				
42-99 500 °C	mica 1M	5.212(7)	8.975(9)	10.329(9)	101.71(11)	0.04(1)	0.141(32)	0.079	1.39	1.405
	mica 2M1	5.191(4)	8.992(4)	20.289(13)	95.20(7)	0.10(1)				
	mica 2M2	9.024(7)	5.204(5)	20.535(15)	100.03(6)	0.02(1)				
	mica 3T	5.191(4)		29.998(50)		0.03(1)				
	mica 2Or	5.211(10)	9.000(8)	20.240(41)		0.01(1)				
	fsp	8.683(1)	13.045(1)	7.184(1)	116.06(1)	0.73(1)	0.349(5)			
	qtz	4.912(1)		5.404(1)		0.07(1)				
45-99 500 °C	mica 1M	5.205(3)	9.012(7)	10.261(9)	101.69(8)	0.03(1)	-0.043(37)	0.082	1.64	1.284
	mica 2M1	5.200(3)	9.034(5)	20.231(14)	95.74(8)	0.03(1)				
	mica 2M2	9.004(6)	5.199(4)	20.448(14)	100.25(6)	<0.01				
	mica 3T	5.204(3)		29.936(51)		0.01(1)				
	mica 2Or	5.186(4)	9.019(6)	19.933(43)		<0.01				
	fsp	8.635(1)	13.036(1)	7.182(1)	116.05(1)	0.80(1)	0.139(4)			
	qtz	4.914(1)		5.405(1)		0.12(1)				
46-99 500 °C	mica 1M	5.193(10)	9.015(17)	10.266(21)	101.37(15)	<0.01	-0.083(40)	0.070	1.52	1.271
	mica 2M1	5.193(7)	9.023(8)	20.194(15)	95.89(9)	0.03(1)				
	mica 2M2	8.981(12)	5.208(10)	20.424(28)	100.16(17)	<0.01				
	mica 3T	5.215(5)		29.887(99)		<0.01				
	mica 2Or	5.207(12)	8.973(10)	19.857(53)		<0.01				
	fsp	8.616(1)	13.030(1)	7.180(1)	116.05(1)	0.87(1)	0.054(3)			
	qtz	4.912(1)		5.404(1)		0.08(1)				
5-00 500 °C	mica 1M	5.204(4)	9.010(8)	10.366(9)	101.61(10)	0.16(3)	0.414(17)	0.120	0.84	2.391
	mica 2M1	5.193(2)	8.999(3)	20.449(12)	95.51(5)	0.57(1)				
	mica 2M2	9.004(8)	5.202(4)	20.625(15)	100.11(10)	0.13(3)				
	mica 3T	5.214(3)		30.435(26)		0.06(2)				
	mica 2Or	5.196(4)	8.976(9)	20.101(30)		0.08(3)				
6-00 500 °C	mica 1M	5.204(3)	8.990(4)	10.334(5)	101.55(6)	0.18(1)	0.199(12)	0.073	1.11	1.748
	mica 2M1	5.191(1)	8.999(1)	20.334(5)	95.61(3)	0.58(1)				
	mica 2M2	9.002(3)	5.194(2)	20.561(6)	100.16(5)	0.13(1)				
	mica 3T	5.212(1)		30.338(9)		0.06(1)				
	mica 2Or	5.196(3)	8.994(14)	20.105(28)		0.05(1)				
11-00 500 °C	mica 1M	5.195(2)	8.975(3)	10.278(5)	101.46(6)	0.17(1)	-0.035(12)	0.082	0.90	1.816
	mica 2M1	5.185(1)	8.988(1)	20.203(5)	95.47(3)	0.59(1)				
	mica 2M2	8.989(3)	5.186(1)	20.469(6)	100.15(4)	0.16(1)				
	mica 3T	5.204(1)		30.226(9)		0.04(1)				
	mica 2Or	5.194(3)	8.955(4)	20.018(26)		0.04(1)				

Table 6. Rietveld results for runs at 1500 MPa (continued)

run	phase	$a(2\sigma)$ (Å)	$b(2\sigma)$ (Å)	$c(2\sigma)$ (Å)	$\beta(2\sigma)$ (°)	wt(2σ) fraction	$x_{NH_4}(2\sigma)$ ss	w_{Rp}	Durbin- Watson	χ^2
12-00 500 °C	mica 1M	5.195(2)	8.987(4)	10.262(5)	101.60(6)	0.16(1)				
	mica 2M1	5.187(1)	8.992(1)	20.178(4)	95.73(2)	0.60(1)				
	mica 2M2	8.990(4)	5.188(2)	20.428(6)	100.16(4)	0.13(1)	-0.103(7)	0.068	1.07	1.856
	mica 3T	5.205(1)		30.167(9)		0.09(1)				
	mica 2Or	5.189(4)	8.987(12)	20.051(24)		0.02(1)				
13-00 600 °C	mica 1M	5.206(4)	8.989(6)	10.369(9)	101.37(11)	0.08(1)				
	mica 2M1	5.196(3)	9.002(3)	20.344(8)	95.62(6)	0.21(2)	0.231(24)			
	mica 2M2	9.004(7)	5.190(5)	20.595(23)	100.25(8)	0.07(2)				
	mica 3T	5.213(4)		30.352(36)		0.05(1)		0.074	1.57	1.318
	mica 2Or	5.177(7)	9.002(9)	20.291(23)		0.01(1)				
	fsp	8.715(2)	13.048(2)	7.185(1)	116.06(2)	0.20(1)	0.486(8)			
	qtz	4.913(1)		5.404(1)		0.38(1)				
14-00 600 °C	mica 1M	5.182(4)	8.995(6)	10.309(5)	101.55(9)	0.07(1)				
	mica 2M1	5.191(2)	9.001(2)	20.260(5)	95.46(4)	0.24(1)	0.071(13)			
	mica 2M2	8.997(5)	5.193(2)	20.502(8)	100.01(6)	0.05(1)				
	mica 3T	5.209(4)		29.910(31)		0.01(1)		0.065	1.45	1.375
	mica 2Or	5.209(8)	8.996(5)	19.913(44)		0.01(1)				
	fsp	8.674(1)	13.045(1)	7.185(1)	116.06(1)	0.42(1)	0.308(4)			
	qtz	4.913(1)		5.405(1)		0.20(1)				
15-00 600 °C	mica 1M	5.198(3)	8.978(6)	10.266(5)	101.51(6)	0.05(1)				
	mica 2M1	5.187(2)	8.996(2)	20.202(5)	95.75(3)	0.16(1)	-0.061(13)			
	mica 2M2	8.983(3)	5.194(2)	20.428(7)	100.10(5)	0.03(1)				
	mica 3T	5.208(3)		29.616(25)		<0.01		0.073	1.37	1.539
	mica 2Or	5.199(3)	9.027(4)	19.692(24)		<0.01				
	fsp	8.633(1)	13.032(1)	7.184(1)	116.03(1)	0.680	0.127(4)			
	qtz	4.915(1)		5.406(1)		0.07(1)				
16-00 600 °C	mica 1M	5.204(3)	8.977(5)	10.288(6)	101.63(6)	0.04(1)				
	mica 2M1	5.196(2)	8.986(2)	20.206(11)	95.75(6)	0.06(1)	-0.040(26)			
	mica 2M2	8.993(5)	5.190(2)	20.463(10)	100.26(5)	<0.01				
	mica 3T	5.202(3)		29.801(47)		<0.01		0.061	1.38	1.403
	mica 2Or	5.199(4)	8.997(6)	19.699(42)		<0.01				
	fsp	8.621(1)	13.032(1)	7.182(1)	116.04(1)	0.85(1)	0.077(3)			
	qtz	4.914(1)	4.914(1)	5.405(1)		0.05(1)				
17-00 500 °C	mica 1M	5.194(4)	9.002(5)	10.442(6)	101.42(7)	0.14(1)				
	mica 2M1	5.203(3)	9.014(3)	20.525(11)	95.51(5)	0.26(2)	0.583(27)			
	mica 2M2	9.015(6)	5.200(4)	20.769(14)	99.93(8)	0.08(2)				
	mica 3T	5.218(3)		30.706(32)		<0.01		0.070	1.48	1.334
	mica 2Or	5.206(7)	8.977(10)	20.436(28)		0.02(1)				
	fsp	8.776(4)	13.058(6)	7.193(2)	116.06(3)	0.12(1)	0.755(19)			
	qtz	4.914(1)		5.405(1)		0.38(1)				
19-00 500 °C	mica 1M	5.209(5)	9.005(6)	10.432(8)	101.44(10)	0.17(2)				
	mica 2M1	5.201(3)	9.012(4)	20.522(15)	95.49(6)	0.33(2)	0.572(35)			
	mica 2M2	9.022(8)	5.205(6)	20.765(16)	99.99(11)	0.10(2)				
	mica 3T	5.218(4)		30.643(40)		0.01(1)		0.094	1.10	1.872
	mica 2Or	5.207(6)	8.986(11)	20.439(33)		0.02(1)				
	fsp	8.779(9)	13.062(15)	7.193(6)	115.98(8)	0.04(2)	0.771(45)			
	qtz	4.915(1)		5.407(1)		0.33(1)				
20-00 500 °C	mica 1M	5.207(4)	8.992(7)	10.411(8)	101.32(8)	0.21(1)				
	mica 2M1	5.196(2)	9.001(2)	20.494(10)	95.35(5)	0.54(1)	0.519(29)			
	mica 2M2	9.003(7)	5.203(3)	20.708(11)	100.14(10)	0.14(1)		0.103	0.80	2.558
	mica 3T	5.216(2)		30.704(23)		0.04(1)				
	mica 2Or	5.195(3)	8.974(5)	20.366(21)		0.05(1)				
	qtz	4.912(2)		5.402(4)		0.02(1)				