Appendix B

Parameterization of Holland and Powell (1992) plagioclase activity calculations for the revised plagioclase-liquid hygrometer

In order to calculate the activities of the anorthite and albite components in plagioclase for inputs into the plagioclase hygrometer without using a virtual basic for applications (VBA) script, the equations developed by Holland and Powell (1992) were parameterized and described in this appendix.

An initial dataset of plagioclase that ranged in composition from An_{18} to An_{89} were assembled from the data repositories of Crabtree and Lange (2010), Waters and Lange (2013), and Waters et al.,(in review)(Table B1). The plagioclase compositions listed in Table B1 were input into the Holland and Powel (1992) plagioclase activity model with constant pressure (1000 bars) and outputs of activities of anorthite and albite (a_{An} and a_{Ab}, respectively) were generated for temperatures ranging from 600 to 1350°C (Fig. B1). Individual temperature series were fitted with a fourth order polynomial equation to define how a_{An} and a_{Ab} changed as a function of the mole fraction of anorthite and albite (X_{An} and X_{Ab}, respectively) in plagioclase at a given temperature. Each temperature series is defined by a fourth order polynomial so that all R^2 values were >0.98 (shown in equation B1).

$$a_{An/Ab} = \mathbf{a}x^4 + \mathbf{b}x^3 + \mathbf{c}x^2 + \mathbf{d}x + \mathbf{e} \qquad \text{(equation B1)}$$

In equation B1, a, b, c, d, and e are fitted terms from the polynomial regressions (Fig. B1), and x is either X_{An} or X_{Ab}. The values of the fitted terms (a, b, c, d, and e) used in the calculations of a_{An} and a_{Ab} are plotted as a function of temperature in Fig. B2. The values of the fitted terms (a, b, c, d, and e) are defined as a function of temperature with polynomial equations. Temperature is a required input for the hygrometer, and therefore it is useful to have the fitted terms (a, b, c, d, and e) for the calculation of a_{An} and a_{Ab} defined as a function of temperature.

The results of this parameterization are compared to those of Holland and Powell (1992) in Fig. B3 with a plot of X_{An} v. a_{An} (Fig. B3a) and X_{Ab} v. a_{Ab} (Fig. B3b) for 750, 900, and 1200°C. The results of this parameterization are also compared to those of Holland and Powell (1992) in Fig. B3c-d with a 1:1 correspondence line. There is no major deviation of this parameterization from the activity calculations of Holland and Powell (1992). Lastly, the residuals of the calculations of a_{An} and a_{Ab} from this parameterization are shown in Fig. B3e-f. The average residual on both the a_{An} and a_{Ab} calculation is ~0.01

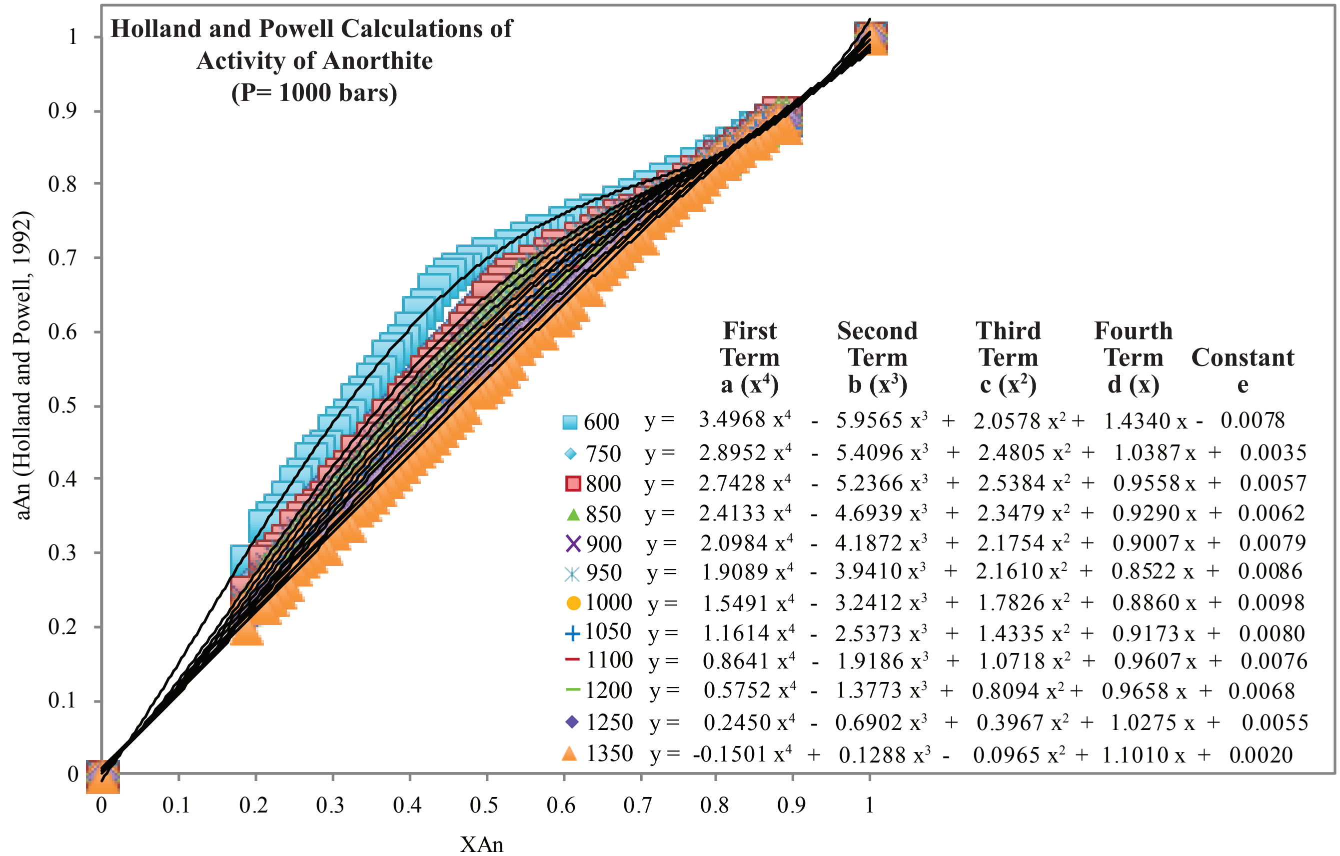
Table B1: Plagioclase compositions used in the parameterization of Holland and Powell (1992)

	An89	**An88**	**An87**	**An86**	**An85**	**An84**	**An83**	**An82**	**An81**	**An80**	**An79**	**An78**	**An77**	**An76**	**An75**	**An74**	**An73**	**An72**	**An71**	**An70**	**An69**	**An68**	**An67**	**An66**
SiO_2	46.6	45.9	46.6	46.6	46.5	43.8	47.1	47.6	47.5	48.4	47.9	48.7	47.7	48.3	48.5	48.9	49.1	50.3	49.6	50.7	50.8	51.3	50.6	51.4
TiO_2	0.05	0.03	0.05	0.00	0.01	0.03	0.00	0.00	0.06	0.00	0.02	0.01	0.06	0.04	0.03	0.03	0.01	0.05	0.07	0.00	0.01	0.02	0.07	0.02
Al_2O_3	34.6	33.5	34.6	34.3	34.5	37.1	33.5	34.5	33.7	33.2	33.1	32.7	32.8	32.8	33.3	32.1	31.9	31.5	32.1	31.2	31.9	31.3	31.2	30.7
CaO	17.8	17.85	17.8	18.07	17.81	16.32	17.07	16.62	16.94	16.5	16.12	16.28	15.86	15.86	14.9	15.0	15.29	14.84	14.32	14.28	13.82	14.01	14.01	13.35
Na_2O	1.45	1.28	1.45	1.6	1.68	1.68	1.91	1.97	2.14	2.2	2.31	2.51	2.57	2.79	2.73	2.81	3.08	3.18	3.24	3.42	3.37	3.58	3.74	3.71
K_2O	0.02	0.06	0.02	0.03	0.11	0.07	0.03	0.03	0.08	0.06	0.05	0.03	0.12	0.05	0.03	0.09	0.04	0.03	0.04	0.02	0.09	0.09	0.06	0.1
Total	100.5	98.6	100.5	100.7	100.5	99.0	99.6	100.8	100.3	100.4	99.4	100.3	99.1	99.8	99.4	98.9	99.5	99.9	99.4	99.6	100.0	100.3	99.7	99.3
X_{An}	0.89	0.88	0.87	0.86	0.85	0.84	0.83	0.82	0.81	0.8	0.79	0.78	0.77	0.76	0.75	0.74	0.73	0.72	0.71	0.7	0.69	0.68	0.67	0.66
X_{Ab}	0.11	0.12	0.13	0.14	0.15	0.16	0.17	0.18	0.19	0.2	0.21	0.22	0.23	0.24	0.25	0.26	0.27	0.28	0.29	0.3	0.31	0.32	0.33	0.34

	An65	**An64**	**An63**	**An62**	**An61**	**An59**	**An58**	**An57**	**An56**	**An55**	**An54**	**An53**	**An52**	**An51**	**An50**	**An49**	**An48**	**An47**	**An46**	**An45**	**An44**	**An43**	**An42**	**An41**
SiO_2	51.0	52.6	52.3	53.0	53.2	53.4	53.4	53.1	53.6	53.9	54.5	54.4	54.4	55.9	55.8	56.0	56.5	55.1	56.0	56.6	57.0	56.2	58.0	58.3
TiO_2	0.01	0.03	0.05	0.08	0.04	0.04	0.02	0.07	0.04	0.03	0.01	0.01	0.01	0.02	0.01	0.01	0.02	0.03	0.04	0.02	0.06	0.02	0.00	0.05
Al_2O_3	30.8	30.1	30.6	29.8	29.8	29.8	29.6	29.4	29.5	29.2	27.6	27.9	28.6	27.1	27.0	27.2	27.1	26.6	26.4	26.5	26.5	27.0	26.1	26.4
CaO	13.26	12.93	12.81	12.56	12.49	12.15	12.08	11.91	11.26	11.27	11.18	10.74	10.59	10.58	10.44	10.41	9.88	9.67	9.38	9.36	9.37	8.84	8.72	8.56
Na_2O	3.88	3.93	4.06	4.18	4.32	4.55	4.74	4.88	4.76	4.99	5.06	5.07	5.26	5.36	5.49	5.67	5.64	5.75	5.88	6.06	6.19	6.12	6.39	6.46
K_2O	0.07	0.09	0.2	0.13	0.2	0.23	0.11	0.14	0.15	0.14	0.25	0.31	0.22	0.39	0.38	0.42	0.34	0.38	0.44	0.41	0.5	0.46	0.42	0.49
Total	99.0	99.7	100.0	99.8	100.1	100.1	99.9	99.5	99.2	99.5	98.6	98.4	99.1	99.4	99.1	99.7	99.4	97.6	98.1	99.0	99.7	98.6	99.7	100.2
X_{An}	0.65	0.64	0.63	0.62	0.61	0.59	0.58	0.57	0.56	0.55	0.54	0.53	0.52	0.51	0.5	0.49	0.48	0.47	0.46	0.45	0.44	0.43	0.42	0.41
X_{Ab}	0.35	0.36	0.37	0.38	0.39	0.41	0.42	0.43	0.44	0.45	0.46	0.47	0.48	0.49	0.5	0.51	0.52	0.53	0.54	0.55	0.56	0.57	0.58	0.59

	An40	**An39**	**An38**	**An37**	**An36**	**An35**	**An34**	**An33**	**An32**	**An31**	**An30**	**An29**	**An28**	**An27**	**An26**	**An25**	**An24**	**An23**	**An22**	**An21**	**An20**	**An18.5**
SiO_2	59.3	58.3	58.8	58.9	59.9	60.0	60.1	59.8	60.3	62.3	61.6	62.1	62.0	62.2	62.7	62.8	62.8	63.9	64.9	64.6	64.3	64.8
TiO_2	0.02	0.03	0.00	0.04	0.02	0.05	0.04	0.00	0.01	0.02	0.04	0.02	0.05	0.03	0.03	0.04	0.01	0.02	0.06	0.02	0.01	0.06
Al_2O_3	26.4	26.2	25.0	25.6	24.9	25.4	24.5	23.9	24.3	24.0	24.5	24.1	24.6	24.5	24.1	23.3	23.7	23.6	23.4	22.8	22.7	22.7
CaO	8.22	7.91	7.72	7.86	7.54	7.12	7.04	6.44	6.49	6.27	6	5.83	5.7	5.52	5.25	5.12	4.7	4.52	4.46	4.31	3.95	3.65
Na_2O	6.47	6.5	6.6	6.94	7.04	6.96	7.1	6.72	7.19	7.43	7.23	7.61	7.7	7.71	7.73	8	7.73	7.91	8.28	8.32	8.14	8.35
K_2O	0.51	0.62	0.64	0.54	0.6	0.63	0.78	0.71	0.77	0.46	0.6	0.48	0.46	0.63	0.66	0.6	0.7	0.68	0.64	0.68	0.86	0.82
Total	100.9	99.5	98.7	99.9	100.0	100.2	99.6	97.6	99.0	100.4	100.0	100.2	100.5	100.6	100.5	99.9	99.7	100.7	101.7	100.7	100.0	100.4
X_{An}	0.4	0.39	0.38	0.37	0.36	0.35	0.34	0.33	0.32	0.31	0.3	0.29	0.28	0.27	0.26	0.25	0.24	0.23	0.22	0.21	0.2	0.19
X_{Ab}	0.6	0.61	0.62	0.63	0.64	0.65	0.66	0.67	0.68	0.69	0.7	0.71	0.72	0.73	0.74	0.75	0.76	0.77	0.78	0.79	0.8	0.81

Figure B1


Holland and Powell Calculations of
Activity of Anorthite
(P= 1000 bars)
aAn (Holland and Powell, 1992)
XAn
First Term a (x^4)
Second Term b (x^3)
Third Term c (x^2)
Fourth Term d (x)
Constant e
600 y = 3.4968 x^4 - 5.9565 x^3 + 2.0578 x^2 + 1.4340 x - 0.0078
750 y = 2.8952 x^4 - 5.4096 x^3 + 2.4805 x^2 + 1.0387 x + 0.0035
800 y = 2.7428 x^4 - 5.2366 x^3 + 2.5384 x^2 + 0.9558 x + 0.0057
850 y = 2.4133 x^4 - 4.6939 x^3 + 2.3479 x^2 + 0.9290 x + 0.0062
900 y = 2.0984 x^4 - 4.1872 x^3 + 2.1754 x^2 + 0.9007 x + 0.0079
950 y = 1.9089 x^4 - 3.9410 x^3 + 2.1610 x^2 + 0.8522 x + 0.0086
1000 y = 1.5491 x^4 - 3.2412 x^3 + 1.7826 x^2 + 0.8860 x + 0.0098
1050 y = 1.1614 x^4 - 2.5373 x^3 + 1.4335 x^2 + 0.9173 x + 0.0080
1100 y = 0.8641 x^4 - 1.9186 x^3 + 1.0718 x^2 + 0.9607 x + 0.0076
1200 y = 0.5752 x^4 - 1.3773 x^3 + 0.8094 x^2 + 0.9658 x + 0.0068
1250 y = 0.2450 x^4 - 0.6902 x^3 + 0.3967 x^2 + 1.0275 x + 0.0055
1350 y = -0.1501 x^4 + 0.1288 x^3 - 0.0965 x^2 + 1.1010 x + 0.0020

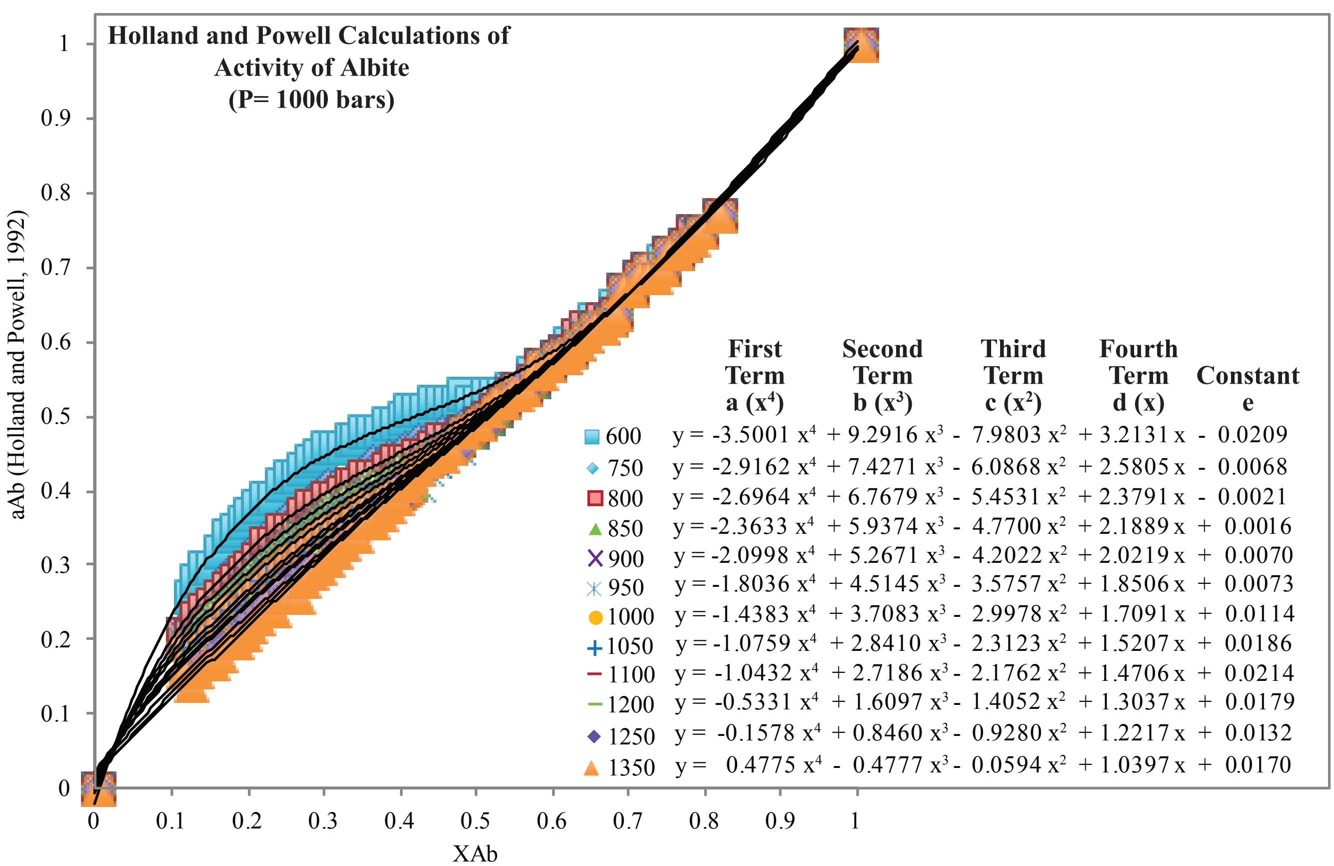
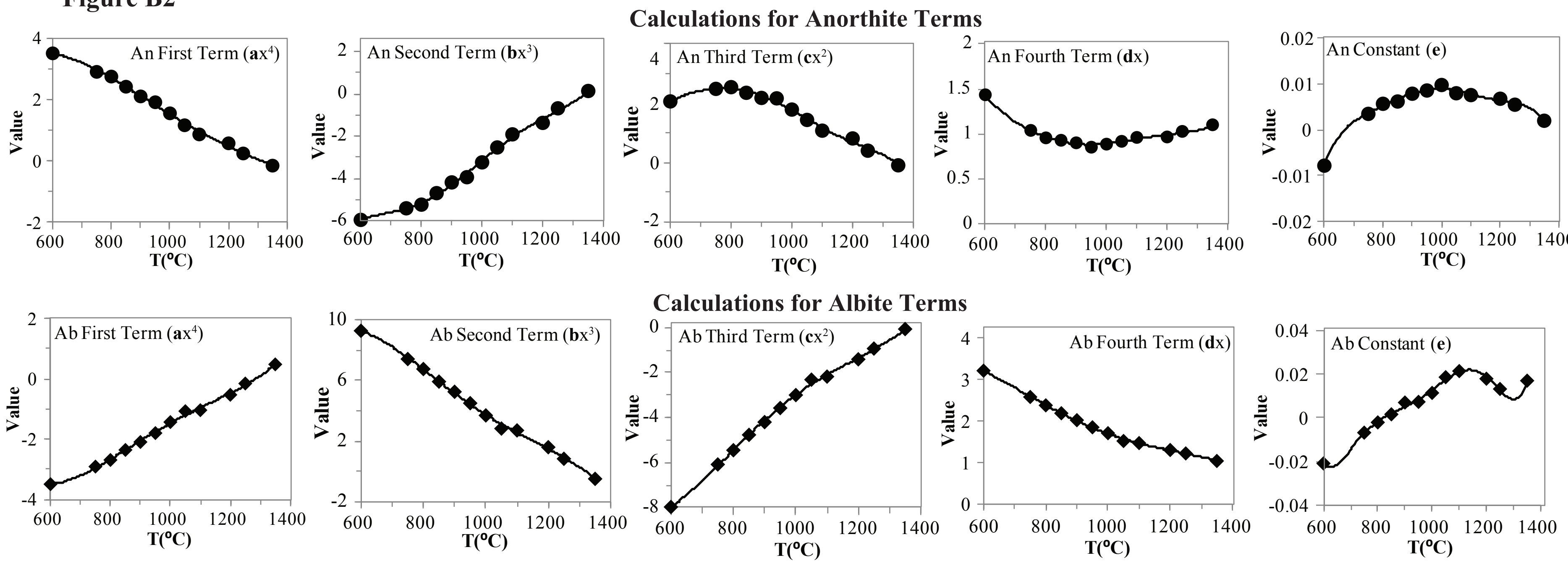

Holland and Powell Calculations of
Activity of Albite
(P= 1000 bars)
aAb (Holland and Powell, 1992)
XAb
First Term a (x^4)
Second Term b (x^3)
Third Term c (x^2)
Fourth Term d (x)
Constant e
600 y = -3.5001 x^4 + 9.2916 x^3 - 7.9803 x^2 + 3.2131 x - 0.0209
750 y = -2.9162 x^4 + 7.4271 x^3 - 6.0868 x^2 + 2.5805 x - 0.0068
800 y = -2.6964 x^4 + 6.7679 x^3 - 5.4531 x^2 + 2.3791 x - 0.0021
850 y = -2.3633 x^4 + 5.9374 x^3 - 4.7700 x^2 + 2.1889 x + 0.0016
900 y = -2.0998 x^4 + 5.2671 x^3 - 4.2022 x^2 + 2.0219 x + 0.0070
950 y = -1.8036 x^4 + 4.5145 x^3 - 3.5757 x^2 + 1.8506 x + 0.0073
1000 y = -1.4383 x^4 + 3.7083 x^3 - 2.9978 x^2 + 1.7091 x + 0.0114
1050 y = -1.0759 x^4 + 2.8410 x^3 - 2.3123 x^2 + 1.5207 x + 0.0186
1100 y = -1.0432 x^4 + 2.7186 x^3 - 2.1762 x^2 + 1.4706 x + 0.0214
1200 y = -0.5331 x^4 + 1.6097 x^3 - 1.4052 x^2 + 1.3037 x + 0.0179
1250 y = -0.1578 x^4 + 0.8460 x^3 - 0.9280 x^2 + 1.2217 x + 0.0132
1350 y = 0.4775 x^4 - 0.4777 x^3 - 0.0594 x^2 + 1.0397 x + 0.0170

Figure B2



Anorthite: Equations for fitted terms (a, b, c, d, and e)

$$a = -1.069600 \cdot 10^{-11} \cdot T^4 + 4.945054 \cdot 10^{-8} \cdot T^3 - 8.207491 \cdot 10^{-5} \cdot T^2 + 5.275448 \cdot 10^{-2} \cdot T - 7.914622$$

$$b = 2.194410 \cdot 10^{-13} \cdot T^5 - 1.062980 \cdot 10^{-9} \cdot T^4 + 2.003170 \cdot 10^{-6} \cdot T^3 - 1.827160 \cdot 10^{-3} \cdot T^2 + 0.811309 \cdot T^3 - 146.951$$

$$c = -2.443527 \cdot 10^{-16} \cdot T^6 + 1.318528 \cdot 10^{-12} \cdot T^5 - 2.899588 \cdot 10^{-9} \cdot T^4 + 3.337718 \cdot 10^{-6} \cdot T^3 - 2.140832 \cdot 10^{-3} \cdot T^2 + 0.734541 \cdot T - 104.25573$$

$$d = 9.642821 \cdot 10^{-17} \cdot T^6 - 5.482202 \cdot 10^{-13} \cdot T^5 + 1.280331 \cdot 10^{-9} \cdot T^4 - 1.576130 \cdot 10^{-6} \cdot T^3 + 1.084872 \cdot 10^{-3} \cdot T^2 - 0.399790 \cdot T + 63.39784$$

$$e = -6.798238 \cdot 10^{-18} \cdot T^6 + 4.008407 \cdot 10^{-14} \cdot T^5 - 9.724370 \cdot 10^{-11} \cdot T^4 + 1.242399 \cdot 10^{-7} \cdot T^3 - 8.824071 \cdot 10^{-5} \cdot T^2 + 3.310392 \cdot 10^{-2} \cdot T - 5.136283$$

Albite Equations for fitted terms (a, b, c, d, and e)

$$a = 3.118520 \cdot 10^{-11} \cdot T^4 - 1.241560 \cdot 10^{-7} \cdot T^3 + 1.816640 \cdot 10^{-4} \cdot T^2 - 0.110128 \cdot T + 19.960$$

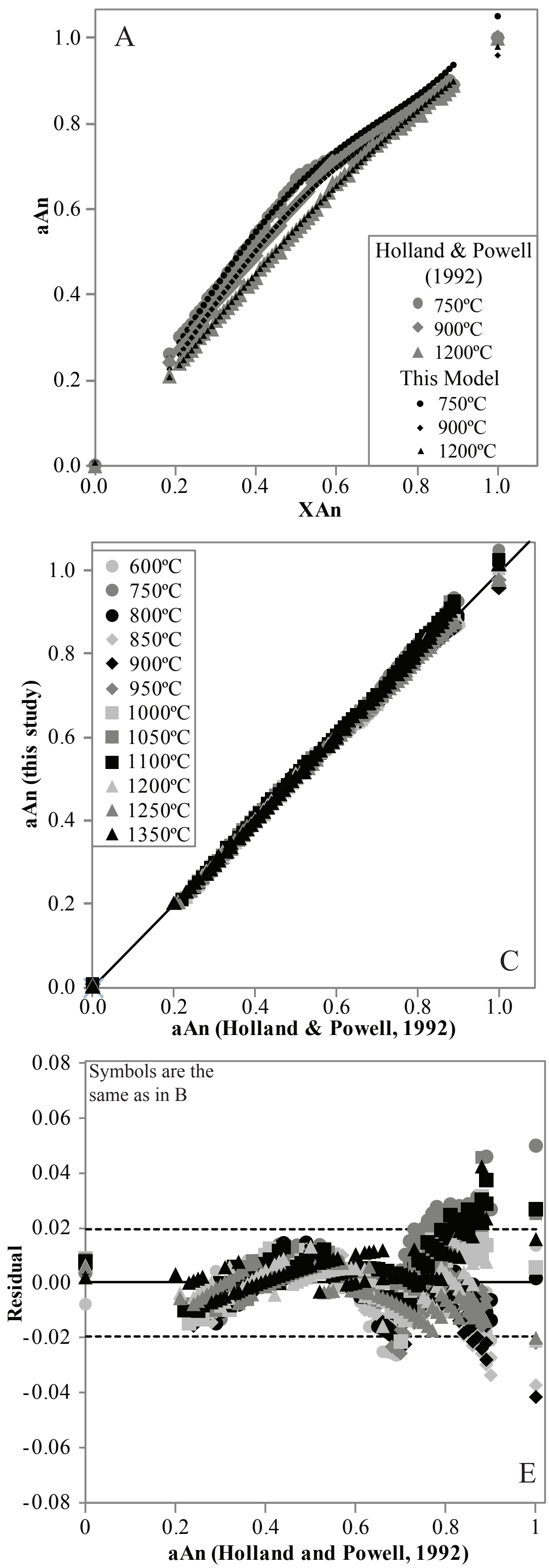
$$b = -6.683324 \cdot 10^{-11} \cdot T^4 + 2.646820 \cdot 10^{-7} \cdot T^3 - 3.813719 \cdot 10^{-4} \cdot T^2 + 2.230349 \cdot T - 35.75847$$

$$c = 4.556072 \cdot 10^{-11} \cdot T^4 - 1.790463 \cdot 10^{-7} \cdot T^3 + 2.520315 \cdot 10^{-4} \cdot T^2 - 1.390206 \cdot T + 17.47942$$

$$d = -1.038026 \cdot 10^{-11} \cdot T^4 + 4.046137 \cdot 10^{-8} \cdot T^3 - 5.510837 \cdot 10^{-5} \cdot T^2 + 2.766904 \cdot 10^{-2} \cdot T - 94.65208$$

$$e = 3.664241 \cdot 10^{-17} \cdot T^6 - 2.106807 \cdot 10^{-13} \cdot T^5 + 4.975989 \cdot 10^{-10} \cdot T^4 - 6.178773 \cdot 10^{-7} \cdot T^3 + 4.252932 \cdot 10^{-4} \cdot T^2 - 0.1537074 \cdot T + 22.74359$$

Figure B3


A
aAn
XAn
Holland & Powell (1992)
750ºC
900ºC
1200ºC
This Model
750ºC
900ºC
1200ºC
B
aAb
XAb
C
aAn (this study)
aAn (Holland & Powell, 1992)
600ºC
750ºC
800ºC
850ºC
900ºC
950ºC
1000ºC
1050ºC
1100ºC
1200ºC
1250ºC
1350ºC
D
1:1
aAb (this study)
aAb (Holland and Powell, 1992)
E
Symbols are the same as in B
Residual
aAn (Holland and Powell, 1992)
F
Symbols are the same as in B
Residual
aAn (Holland and Powell, 1992)