

Brownmillerite $\text{Ca}_2(\text{Fe}_{2-x}\text{Al}_x)\text{O}_5$ series; Redhammer et al.
Structural variations in the brownmillerite solid solution series: ...

sample BX000_1; x = 0.00

5.4268 14.7631 5.5969 90.000 90.000 90.000 Pnma

ANISOU

CA

0.480823 0.107976 0.022670 0.00940 0.00638 0.00618 -0.00021 0.00144 -0.00114

M (Fe=1.0)

0.000000 0.000000 0.000000 0.00268 0.00911 0.00293 0.00032 -0.00016 0.00066

T (Fe=1.0)

0.946054 0.250000 0.934030 0.00486 0.00432 0.00473 0.00000 -0.00001 0.00000

ANIONS

O1

0.262785 0.984263 0.237013 0.00526 0.00949 0.00636 0.00149 -0.00179 -0.00161

O2

0.023970 0.140632 0.073525 0.01363 0.00555 0.00703 0.00061 0.00023 0.00085

O3

0.599107 0.250000 0.874100 0.00548 0.01115 0.00547 0.00000 0.00034 0.00000

END

Sample BHT005_2; X = 0.115

5.4212 14.7432 5.5961 90.000 90.000 90.000 Pnma

ANISOU

CA

0.48141 0.10802 0.02331 0.00930 0.00368 0.00643 0.00002 0.00131 -0.00094

M (Fe=0.966,Al=0.034)

0.00000 0.00000 0.00000 0.00192 0.00551 0.00245 0.00020 -0.00010 0.00040

T (Fe=0.916,Al=0.084)

0.94628 0.25000 0.93351 0.00340 0.00074 0.00370 0.00000 0.00015 0.00000

ANIONS

O1

0.26221 0.98432 0.23753 0.00423 0.00806 0.00636 0.00048 -0.00222 -0.00051

O2

0.02358 0.14090 0.07234 0.01266 0.00355 0.00846 0.00052 0.00022 0.00129

O3

0.59917 0.25000 0.87360 0.00498 0.00603 0.00774 0.00000 -0.00156 0.00000

END

sample BHT015_1; x = 0.204

5.4140 14.7163 5.5947 90.000 90.000 90.000 Pnma

ANISOU

CA

0.48243 0.10813 0.02388 0.00892 0.00512 0.00625 0.00004 0.00117 -0.00101

M (Fe=0.952,Al=0.048)

0.00000 0.00000 0.00000 0.00121 0.00772 0.00194 0.00012 0.00002 0.00036

T (Fe=0.844,Al=0.156)

0.94682 0.25000 0.93280 0.00317 0.00260 0.00372 0.00000 0.00029 0.00000

ANIONS

O1
0.26100 0.98458 0.23858 0.00397 0.00942 0.00564 0.00041 -0.00254 -0.00085
O2
0.02317 0.14162 0.07196 0.01295 0.00548 0.00776 0.00030 0.00083 0.00108
O3
0.60067 0.25000 0.87201 0.00586 0.00802 0.00700 0.00000 -0.00094 0.00000
END

sample BF010_1; x = 0.212

5.4162 14.7155 5.5949 90.000 90.000 90.000 Pnma

ANISOU

CA

0.481848 0.108115 0.023637 0.01381 0.00657 0.00921 0.00017 0.00129 -0.00104

M (Fe=0.938,Al=0.062)

0.000000 0.000000 0.000000 0.00564 0.00820 0.00432 0.00022 0.00000 0.00034

T (Fe=0.850,Al=0.150)

0.946719 0.250000 0.933219 0.00767 0.00289 0.00619 0.00000 0.00041 0.00000

ANIONS

O1

0.261589 0.984361 0.238030 0.00863 0.01100 0.00788 0.00006 -0.00219 -0.00093

O2

0.023686 0.141256 0.072911 0.01703 0.00747 0.01113 0.00000 0.00077 0.00148

O3

0.599481 0.250000 0.872676 0.01205 0.00880 0.00831 0.00000 -0.00222 0.00000

END

sample BF060_1; x = 0.257

5.4068 14.6973 5.5930 90.000 90.000 90.000 Pnma

ANISOU

CA

0.482519 0.108198 0.024034 0.01058 0.00689 0.00771 0.00018 0.00115 -0.00102

M (Fe=0.966,Al=0.044)

0.000000 0.000000 0.000000 0.00275 0.00884 0.00359 0.00021 -0.00010 0.00033

T (Fe=0.787,Al=0.213)

0.946960 0.250000 0.932784 0.00458 0.00320 0.00490 0.00000 0.00019 0.00000

ANIONS

O1

0.261164 0.984523 0.238644 0.00630 0.01084 0.00681 0.00060 -0.00239 -0.00064

O2

0.023316 0.141453 0.071813 0.01386 0.00796 0.00945 0.00052 0.00082 0.00120

O3

0.600683 0.250000 0.871991 0.00890 0.00857 0.00796 0.00000 -0.00224 0.00000

END

sample BF070_1; x = 0.258

5.4051 14.6969 5.5942 90.000 90.000 90.000 Pnma

ANISOU

CA

0.482409 0.108116 0.023893 0.01020 0.00589 0.00693 0.00012 0.00119 -0.00098

M (Fe=0.939,Al=0.061)

0.000000 0.000000 0.000000 0.00235 0.00799 0.00275 0.00027 0.00005 0.00024

T (Fe=0.802,Al=0.197

0.946827	0.250000	0.932789	0.00422	0.00260	0.00418	0.00000	0.00019	0.00000
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ANIONS

O1

0.261012	0.984607	0.238574	0.00493	0.01032	0.00582	0.00063	-0.00267	-0.00106
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O2

0.023092	0.141560	0.072268	0.01333	0.00664	0.00843	0.00088	0.00019	0.00119
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O3

0.600347	0.250000	0.872051	0.00838	0.00830	0.00627	0.00000	-0.00140	0.00000
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END

sample BF020_2; x = 0.259

5.4073	14.6996	5.5948	90.000	90.000	90.000	Pnma		
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ANISOU

CA

0.482341	0.108130	0.023670	0.00864	0.00407	0.00652	0.00007	0.00102	-0.00116
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M (Fe=0.933,Al=0.067)

0.000000	0.000000	0.000000	0.00059	0.00588	0.00174	0.00027	-0.00013	0.00031
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T (Fe=0.808,Al=0.192

0.946820	0.250000	0.932906	0.00274	0.00036	0.00349	0.00000	0.00000	0.00000
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ANIONS

O1

0.261462	0.984593	0.238396	0.00481	0.00853	0.00590	0.00090	-0.00239	-0.00013
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O2

0.022902	0.141100	0.072590	0.01229	0.00490	0.00877	0.00090	0.00029	0.00131
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O3

0.600906	0.250000	0.871559	0.00712	0.00526	0.00766	0.00000	-0.00127	0.00000
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END

sample BF100_1; x = 0.271

5.4069	14.6974	5.5931	90.000	90.000	90.000	Pnma		
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ANISOU

CA

0.482357	0.108144	0.023898	0.01273	0.00770	0.00864	0.00000	0.00098	-0.00098
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M (Fe=0.936,Al=0.064)

0.000000	0.000000	0.000000	0.00462	0.00930	0.00404	0.00017	-0.00011	0.00027
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T (Fe=0.793,Al=0.207)

0.946937	0.250000	0.932898	0.00695	0.00416	0.00527	0.00000	0.00002	0.00000
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ANIONS

O1

0.261307	0.984440	0.238658	0.00869	0.01220	0.00682	0.00124	-0.00402	-0.00095
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O2

0.022945	0.141512	0.072301	0.01573	0.00798	0.01026	0.00026	0.00037	0.00040
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O3

0.600418	0.250000	0.872135	0.01097	0.01180	0.00753	0.00000	-0.00222	0.00000
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END

sample BHT025_2; x = 0.276

5.4071	14.6949	5.5941	90.000	90.000	90.000	Pnma		
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ANISOU

CA

0.48320	0.10819	0.02402	0.00930	0.00600	0.00682	0.00057	0.00099	-0.00087
M (Fe=0.963,Al=0.037)								
0.00000	0.00000	0.00000	0.00198	0.00959	0.00332	0.00037	0.00003	0.00030
T (Fe=0.760,Al=0.240)								
0.94715	0.25000	0.93249	0.00289	0.00274	0.00368	0.00000	-0.00006	0.00000
ANIONS								
O1								
0.26043	0.98471	0.23944	0.00500	0.00823	0.00546	0.00081	-0.00269	0.00037
O2								
0.02226	0.14146	0.07186	0.01221	0.00711	0.00837	0.00085	0.00067	0.00210
O3								
0.60255	0.25000	0.87106	0.00692	0.00560	0.00906	0.00000	-0.00117	0.00000
END								

sample BHT030_3; x = 0.365

5.4027	14.6779	5.5923	90.000	90.000	90.000	Pnma		
ANISOU								
CA								
0.48378	0.10821	0.02456	0.01119	0.00668	0.00873	0.00022	0.00094	-0.00090
M (Fe=0.932,Al=0.068)								
0.00000	0.00000	0.00000	0.00367	0.00954	0.00463	0.00046	0.00005	0.00043
T (Fe=0.703,Al=0.297)								
0.94757	0.25000	0.93200	0.00467	0.00373	0.00534	0.00000	0.00017	0.00000
ANIONS								
O1								
0.25961	0.98489	0.24038	0.00540	0.01165	0.00806	0.00057	-0.00285	-0.00091
O2								
0.02271	0.14189	0.07193	0.01513	0.00774	0.00983	0.00125	0.00012	0.00111
O3								
0.60342	0.25000	0.86977	0.01098	0.00759	0.01130	0.00000	-0.00220	0.00000
END								

sample BHT035_1, x = 0.408

5.3986	14.6631	5.5911	90.000	90.000	90.000	Pnma		
ANISOU								
CA								
0.48454	0.10834	0.02498	0.01088	0.00552	0.00738	0.00024	0.00092	-0.00109
M (Fe=0.906,Al=0.094)								
0.00000	0.00000	0.00000	0.00331	0.00832	0.00282	0.00031	0.00000	0.00025
T (Fe=0.686,Al=0.314)								
0.94803	0.25000	0.93142	0.00546	0.00237	0.00441	0.00000	0.00028	0.00000
ANIONS								
O1								
0.25888	0.98498	0.24121	0.00664	0.01015	0.00632	0.00037	-0.00190	-0.00061
O2								
0.02197	0.14226	0.07132	0.01445	0.00681	0.00914	0.00046	0.00073	0.00130
O3								
0.60453	0.25000	0.86871	0.01112	0.00623	0.00916	0.00000	-0.00251	0.00000
END								

sample BHT040_2, x = 0.441

5.3936 14.6476 5.5899 90.000 90.000 90.000 Pnma
 ANISOU
 CA
 0.48477 0.10835 0.02493 0.01053 0.00504 0.00756 0.00013 0.00108 -0.00101
 M (Fe=0.920,Al=0.080)
 0.00000 0.00000 0.00000 0.00281 0.00831 0.00339 0.00021 0.00003 0.00040
 T (Fe=0.639,Al=0.361)
 0.94805 0.25000 0.93132 0.00487 0.00226 0.00432 0.00000 0.00023 0.00000
 ANIONS
 O1
 0.25887 0.98509 0.24105 0.00591 0.01091 0.00657 0.00099 -0.00347 -0.00060
 O2
 0.02153 0.14222 0.07127 0.01385 0.00695 0.00964 0.00091 0.00061 0.00077
 O3
 0.60522 0.25000 0.86860 0.00965 0.00732 0.00914 0.00000 -0.00248 0.00000
 END

sample BF65I_1; x = 0.526

5.3859 14.6317 5.5871 90.000 90.000 90.000 Pnma
 ANISOU
 CA
 0.484957 0.108523 0.025257 0.01155 0.00681 0.00793 0.00025 0.00083 -0.00102
 M (Fe=0.881,Al=0.119)
 0.000000 0.000000 0.000000 0.00398 0.00925 0.00366 0.00023 0.00004 0.00042
 T (Fe=0.585,Al=0.415)
 0.948280 0.250000 0.931099 0.00577 0.00328 0.00506 0.00000 0.00014 0.00000
 ANIONS
 O1
 0.258470 0.985157 0.241669 0.00751 0.01222 0.00761 0.00088 -0.00208 -0.00038
 O2
 0.021303 0.142498 0.070976 0.01416 0.00901 0.00983 0.00143 0.00071 0.00110
 O3
 0.604834 0.250000 0.868523 0.01189 0.00886 0.00958 0.00000 -0.00199 0.00000
 END

sample BF120I_1, X = 0.527

5.3886 14.6314 5.5885 90.000 90.000 90.000 Pnma
 ANISOU
 CA
 0.485690 0.108570 0.025604 0.01245 0.00708 0.00905 0.00007 0.00094 -0.00089
 M (Fe=0.885,Al=0.115)
 0.000000 0.000000 0.000000 0.00483 0.01049 0.00495 0.00006 0.00002 0.00016
 T (Fe=0.411,Al=0.589)
 0.948868 0.250000 0.930985 0.00897 0.00389 0.00630 0.00000 0.00009 0.00000
 ANIONS
 O1
 0.257859 0.985081 0.241957 0.00855 0.01097 0.00843 0.00051 -0.00305 0.00023
 O2
 0.020713 0.142615 0.071488 0.01626 0.00916 0.01069 0.00076 0.00022 0.00087
 O3
 0.604457 0.250000 0.869120 0.01122 0.01086 0.01030 0.00000 -0.00201 0.00000
 END

sample BF90I_1; x = 0.541

5.3880 14.6306 5.5863 90.000 90.000 90.000 Pnma

ANISOU

CA

0.485062 0.108553 0.025327 0.01018 0.00366 0.00595 0.00011 0.00091 -0.00104

M (Fe=0.871,Al=0.129)

0.000000 0.000000 0.000000 0.00254 0.00669 0.00136 0.00022 0.00000 0.00033

T (Fe=0.587,Al=0.413)

0.948409 0.250000 0.930999 0.00439 0.00030 0.00218 0.00000 0.00042 0.00000

ANIONS

O1

0.258017 0.985173 0.241536 0.00597 0.00768 0.00564 0.00079 -0.00219 -0.00044

O2

0.021370 0.142591 0.070457 0.01386 0.00691 0.00664 0.00117 0.00125 0.00102

O3

0.605328 0.250000 0.868565 0.01049 0.00469 0.00811 0.00000 -0.00141 0.00000

END

sample BF80I_1; x = 0.560

5.3876 14.6302 5.5877 90.000 90.000 90.000 Pnma

ANISOU

CA

0.485588 0.108637 0.025692 0.00968 0.00682 0.00782 0.00033 0.00104 -0.00089

M (Fe=0.880,Al=0.120)

0.000000 0.000000 0.000000 0.00182 0.00958 0.00313 0.00014 -0.00003 0.00024

T (Fe=0.560,Al=0.440)

0.949031 0.250000 0.930841 0.00607 0.00376 0.00499 0.00000 0.00009 0.00000

ANIONS

O1

0.257942 0.985175 0.242317 0.00616 0.01090 0.00696 0.00053 -0.00166 -0.00042

O2

0.020644 0.142713 0.070736 0.01163 0.00945 0.00919 0.00057 0.00036 0.00041

O3

0.605550 0.250000 0.868333 0.00801 0.00942 0.01062 0.00000 -0.00112 0.00000

END

sample BHT055_1, x = 0.552

5.3808 14.6131 5.5911 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49099 0.10817 0.02643 0.00963 0.00324 0.00640 0.00046 0.00040 -0.00131

M (Fe=0.862,Al=0.138)

0.00101 0.00000 0.00000 0.00190 0.00563 0.00198 -0.00003 0.00000 0.00000

T (Fe=0.586,Al=0.414)

0.95256 0.25000 0.92986 0.00414 0.00001 0.00379 0.00000 -0.00009 0.00000

ANIONS

O1

0.24996	0.98578	0.25316	0.00437	0.00824	0.00563	0.00051	-0.00146	-0.00103
O2								
0.02465	0.14270	0.06992	0.01309	0.00570	0.00794	0.00079	0.00130	0.00012
O3								
0.60972	0.25000	0.86845	0.00982	0.00405	0.00820	0.00000	-0.00126	0.00000
END								

TITL BHT060_1, x = 0.583

5.3781 14.6016 5.5887 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49121	0.10829	0.02642	0.00914	0.00549	0.00778	0.00053	0.00056	-0.00091
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M (Fe=0.871,Al=0.129)

0.00080	0.00000	0.00000	0.00203	0.00816	0.00350	0.00011	0.00000	0.00000
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T (Fe=0.545,Al=0.454)

0.95243	0.25000	0.92969	0.00359	0.00221	0.00442	0.00000	-0.00007	0.00000
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ANIONS

O1

0.24998	0.98590	0.25269	0.00569	0.01014	0.00672	0.00080	-0.00168	-0.00098
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O2

0.02393	0.14257	0.06963	0.01170	0.00880	0.00917	0.00112	0.00145	-0.00005
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O3

0.61028	0.25000	0.86749	0.01089	0.00619	0.00990	0.00000	-0.00232	0.00000
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END

sample BHT050_2, x = 0.590

5.3832 14.6214 5.5916 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49118	0.10820	0.02655	0.00877	0.00441	0.00585	0.00049	0.00014	-0.00132
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M (Fe=0.849,Al=0.151)

0.00109	0.00000	0.00000	0.00084	0.00683	0.00117	0.00029	0.00000	0.00000
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T (Fe=0.561,Al=0.439)

0.95225	0.25000	0.92996	0.00301	0.00091	0.00295	0.00000	-0.00014	0.00000
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ANIONS

O1

0.24941	0.98593	0.25309	0.00386	0.00939	0.00484	0.00064	-0.00153	-0.00057
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O2

0.02380	0.14263	0.06973	0.00992	0.00599	0.00944	0.00042	0.00046	0.00064
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O3

0.61015	0.25000	0.86765	0.00993	0.00428	0.00723	0.00000	-0.00227	0.00000
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END

sample BHT065_3, x = 0.618

5.3725 14.5826 5.5870 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49106	0.10826	0.02652	0.01131	0.00579	0.00708	0.00029	0.00043	-0.00139
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M (Fe=0.867,Al=0.133)

0.00087	0.00000	0.00000	0.00430	0.00885	0.00299	0.00046	0.00000	0.00000
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T (Fe=0.515,Al=0.485)

0.95257	0.25000	0.92945	0.00718	0.00214	0.00298	0.00000	-0.00038	0.00000
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ANIONS

O1

0.24908	0.98589	0.25171	0.00652	0.00900	0.00582	0.00126	-0.00177	-0.00148
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O2

0.02400	0.14267	0.07029	0.00961	0.00895	0.01036	0.00128	0.00131	-0.00091
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O3

0.61145	0.25000	0.86542	0.01311	0.00499	0.00860	0.00000	-0.00261	0.00000
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END

sample BHT070_1; x = 0.663

5.3714	14.5804	5.5847	90.000	90.000	90.000	I2mb
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ANISOU

CA

0.49111	0.10826	0.02650	0.00997	0.00374	0.00607	0.00017	0.00068	-0.00139
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M (Fe=0.851,Al=0.149)

0.00060	0.00000	0.00000	0.00209	0.00627	0.00126	0.00028	0.00000	0.00000
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T (Fe=0.486,Al=0.514)

0.95281	0.25000	0.92959	0.00308	0.00008	0.00160	0.00000	-0.00003	0.00000
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ANIONS

O1

0.25007	0.98597	0.25304	0.00610	0.00859	0.00458	0.00192	-0.00289	-0.00054
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O2

0.02395	0.14294	0.06973	0.01379	0.00564	0.00963	0.00087	0.00147	0.00116
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O3

0.61062	0.25000	0.86616	0.01167	0.00595	0.00755	0.00000	-0.00260	0.00000
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END

sample BHT075_2; x = 0.749

5.3624	14.5526	5.5795	90.000	90.000	90.000	I2mb
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ANISOU

CA

0.49130	0.10849	0.02705	0.01076	0.00536	0.00637	0.00067	0.00043	-0.00127
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M (Fe=0.812,Al=0.188)

0.00064	0.00000	0.00000	0.00372	0.00825	0.00232	0.00032	0.00000	0.00000
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T (Fe=0.439,Al=0.561)

0.95255	0.25000	0.92867	0.00770	0.00174	0.00363	0.00000	-0.00010	0.00000
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ANIONS

O1

0.24882	0.98627	0.25224	0.00778	0.00901	0.00495	0.00049	-0.00120	-0.00099
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O2

0.02226	0.14344	0.06921	0.01229	0.00798	0.00934	0.00073	0.00147	0.00102
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O3

0.61417	0.25000	0.86356	0.01086	0.00712	0.00901	0.00000	-0.00310	0.00000
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END

sample bht120_6; x = 0.789

5.3569	14.5407	5.5735	90.000	90.000	90.000	I2mb
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ANISOU

CA

0.49115	0.10854	0.02705	0.00974	0.00615	0.00698	0.00047	0.00056	-0.00103
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M (Fe=0.791,Al=0.209)

0.00057	0.00000	0.00000	0.00238	0.00891	0.00270	0.00020	0.00000	0.00000
T (Fe=0.420,Al=0.580)								
0.95281	0.25000	0.92900	0.00505	0.00341	0.00431	0.00000	-0.00024	0.00000
ANIONS								
O1								
0.24938	0.98611	0.25295	0.00591	0.01045	0.00588	0.00079	-0.00280	-0.00129
O2								
0.02283	0.14334	0.06914	0.01256	0.00820	0.00958	0.00129	0.00149	0.00120
O3								
0.61351	0.25000	0.86396	0.01083	0.00577	0.00841	0.00000	-0.00233	0.00000
END								

sample bht095_2; x = 0.866

5.3510 14.5256 5.5685 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49127	0.10859	0.02718	0.00858	0.00561	0.00453	0.00034	0.00011	-0.00122
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M (Fe=0.783,Al=0.217)

0.00047	0.00000	0.00000	0.00132	0.00937	0.00053	0.00008	0.00000	0.00000
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T (Fe=0.351,Al=0.649)

0.95269	0.25000	0.92834	0.00303	0.00338	0.00158	0.00000	-0.00005	0.00000
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ANIONS

O1

0.24935	0.98635	0.25293	0.00498	0.01032	0.00328	-0.00026	-0.00140	-0.00041
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O2

0.02160	0.14333	0.06859	0.00992	0.00926	0.00720	0.00188	-0.00045	0.00086
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O3

0.61458	0.25000	0.86328	0.01075	0.00566	0.00447	0.00000	-0.00169	0.00000
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END

sample bht110_3, x = 0.880

5.3473 14.5156 5.5659 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49119	0.10852	0.02715	0.00989	0.00536	0.00665	0.00056	0.00030	-0.00122
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M (Fe=0.769,Al=0.231)

0.00057	0.00000	0.00000	0.00270	0.00874	0.00225	0.00004	0.00000	0.00000
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T (Fe=0.351,Al=0.649)

0.95279	0.25000	0.92862	0.00493	0.00238	0.00378	0.00000	-0.00032	0.00000
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ANIONS

O1

0.24926	0.98629	0.25312	0.00532	0.01003	0.00523	-0.00012	-0.00158	-0.00080
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O2

0.02197	0.14350	0.06864	0.01222	0.00838	0.00918	0.00153	0.00165	0.00062
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O3

0.61431	0.25000	0.86297	0.01080	0.00630	0.00726	0.00000	-0.00221	0.00000
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END

sample BHT100_2, X = 0.909

5.3469 14.5149 5.5640 90.000 90.000 90.000 I2mb

ANISOU

CA
0.49141 0.10855 0.02702 0.00968 0.00508 0.00593 0.00057 -0.00017 -0.00125
M (Fe=0.758,Al=0.242)
0.00055 0.00000 0.00000 0.00272 0.00842 0.00206 0.00056 0.00000 0.00000
T (Fe=0.333,Al=0.667)
0.95235 0.25000 0.92831 0.00577 0.00216 0.00294 0.00000 0.00004 0.00000
ANIONS
O1
0.24837 0.98646 0.25276 0.00615 0.00941 0.00480 0.00087 -0.00190 -0.00104
O2
0.02149 0.14347 0.06858 0.01169 0.00807 0.00823 0.00049 0.00127 0.00204
O3
0.61513 0.25000 0.86196 0.01022 0.00649 0.00630 0.00000 -0.00375 0.00000
END

sample BHT110n1, x = 0.986

5.3369 14.4945 5.5548 90.000 90.000 90.000 I2mb

ANISOU

CA
0.49139 0.10852 0.02709 0.00859 0.00425 0.00623 0.00022 0.00002 -0.00152
M (Fe=0.733,Al=0.267)
0.00040 0.00000 0.00000 0.00169 0.00759 0.00174 0.00036 0.00000 0.00000
T (Fe=0.281,Al=0.719)
0.95260 0.25000 0.92783 0.00370 0.00066 0.00319 0.00000 -0.00043 0.00000
ANIONS
O1
0.24863 0.98637 0.25194 0.00587 0.00687 0.00567 -0.00018 -0.00101 -0.00154
O2
0.02030 0.14399 0.06737 0.01115 0.00814 0.00912 0.00135 0.00125 0.00174
O3
0.61715 0.25000 0.86083 0.00814 0.00668 0.00409 0.00000 -0.00304 0.00000
END

sample BHT120N2; x = 1.078

5.3269 14.4687 5.5433 90.000 90.000 90.000 I2mb

ANISOU

CA
0.49144 0.10871 0.02713 0.00968 0.00689 0.00543 0.00039 -0.00036 -0.00134
M (Fe=0.684,Al=0.316)
0.00044 0.00000 0.00000 0.00143 0.01072 0.00099 0.00028 0.00000 0.00000
T (Fe=0.338,Al=0.762)
0.95260 0.25000 0.92749 0.00359 0.00365 0.00168 0.00000 -0.00002 0.00000
ANIONS
O1
0.24808 0.98675 0.25347 0.00491 0.01218 0.00455 -0.00033 -0.00161 -0.00021
O2
0.02002 0.14368 0.06660 0.00971 0.01149 0.00902 0.00345 0.00032 0.00233
O3
0.61683 0.25000 0.86104 0.00874 0.00938 0.00652 0.00000 -0.00030 0.00000
END

sample BHT130_2; x = 1.259

5.3093 14.4534 5.5230 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49171 0.10859 0.02695 0.00924 0.00554 0.00749 0.00073 0.00003 -0.00073

M (Fe=0.594,Al=0.406)

-0.00029 0.00000 0.00000 0.00247 0.00875 0.00338 0.00020 0.00000 0.00000

T (Fe=0.147,Al=0.853)

0.95269 0.25000 0.92700 0.00372 0.00254 0.00311 0.00000 -0.00036 0.00000

ANIONS

O1

0.24850 0.98713 0.25359 0.00603 0.00922 0.00655 -0.00069 -0.00109 0.00018

O2

0.01955 0.14381 0.06622 0.01208 0.00816 0.01269 0.00276 0.00260 0.00148

O3

0.61840 0.25000 0.85855 0.01007 0.00526 0.00568 0.00000 0.00108 0.00000

END

sample BHT140_2; x = 1.356

5.2991 14.4434 5.5099 90.000 90.000 90.000 I2mb

ANISOU

CA

0.49185 0.10859 0.02659 0.00927 0.00931 0.00868 0.00060 0.00004 -0.00077

M (Fe=0.541,Al=0.459)

-0.00040 0.00000 0.00000 0.00291 0.01306 0.00524 0.00057 0.00000 0.00000

T (Fe=0.897,Al=0.103)

0.95273 0.25000 0.92640 0.00555 0.00613 0.00448 0.00000 -0.00018 0.00000

ANIONS

O1

0.24814 0.98752 0.25221 0.00564 0.01221 0.00919 0.00121 -0.00041 -0.00004

O2

0.01851 0.14383 0.06476 0.01042 0.01232 0.01251 0.00231 0.00152 0.00123

O3

0.61827 0.25000 0.85930 0.00928 0.01143 0.00721 0.00000 -0.00087 0.00000

END