**Appendix 1**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Polyhedra | Na(AlFe2)(Al5Fe)(Si6O18)(BO3)3(OH)3O | | | | | | | | | Polyhedra | NaFe3Al6(Si6O18)(BO3)3(OH)4 | | |
| Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length |
| *Y* | Al 001 | O 031 | 18.0252 | Fe 002 | O 031 | 19.2951 | Fe 003 | O 031 | 19.2481 | *Y* | Fe 001 | O 031 | 19.7626 |
| O 001 | 18.4435 | O 027 | 19.8240 | O 027 | 19.6174 | O 025 | 20.0638 |
| O 025 | 18.8552 | O 004 | 19.8787 | O 007 | 19.8932 | O 029 | 20.0647 |
| O 029 | 19.0325 | O 010 | 20.1487 | O 029 | 20.2006 | O 001 | 20.0688 |
| O 013 | 19.9497 | O 025 | 20.2355 | O 016 | 20.2289 | O 013 | 20.0688 |
| O 019 | 20.6004 | O 021 | 21.4621 | O 023 | 21.4002 | O 019 | 20.7372 |
| Mean |  | 19.1511 | Mean |  | 20.1407 | Mean |  | 20.0981 | Mean |  | 20.1277 |
| *Z* | Fe 001 | O 005 | 19.6952 | Al 002 | O 008 | 18.0188 | Al 003 | O 007 | 18.1256 | *Z* | Al 001 | O 001 | 17.8230 |
| O 001 | 19.6964 | O 004 | 18.1696 | O 003 | 18.1886 | O 005 | 18.1881 |
| O 006 | 19.7626 | O 006 | 18.2712 | O 005 | 18.4979 | O 006 | 18.5892 |
| O 003 | 19.8887 | O 002 | 19.1264 | O 002 | 18.7145 | O 003 | 19.1170 |
| O 008 | 20.3691 | O 009 | 19.1749 | O 009 | 18.9744 | O 019 | 19.5782 |
| O 019 | 20.4667 | O 021 | 20.0299 | O 023 | 20.1227 | O 008 | 19.6735 |
| Mean |  | 19.9798 | Mean |  | 18.7985 | Mean |  | 18.7706 | Mean |  | 18.8282 |
| Al 004 | O 010 | 18.0492 | Al 005 | O 017 | 18.4094 | Al 006 | O 016 | 18.0174 |  |  |  |  |
| O 014 | 18.4465 | O 013 | 18.4996 | O 011 | 18.3957 |  |  |  |  |
| O 015 | 18.8766 | O 018 | 18.7120 | O 012 | 18.8997 |  |  |  |  |
| O 012 | 18.9530 | O 015 | 18.9011 | O 018 | 19.0678 |  |  |  |  |
| O 021 | 19.1758 | O 011 | 19.5386 | O 023 | 19.3910 |  |  |  |  |
| O 017 | 19.8055 | O 019 | 19.5996 | O 014 | 19.7072 |  |  |  |  |
| Mean |  | 18.8844 | Mean |  | 18.9434 | Mean |  | 18.9131 |  |  |  |  |

**Appendix 2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Polyhedra | Na(AlMg2)(Al5Mg)(Si6O18)(BO3)3(OH)3F | | | | | | | | | Polyhedra | NaMg3Al6(Si6O18)(BO3)3(OH)3F | | |
| Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length |
| *Y* | Al001 | O001 | 18.1124 | Mg002 | O004 | 20.3648 | Mg003 | O027 | 20.0374 | *Y* | Mg001 | O025 | 20.3510 |
| F001 | 18.2473 | O027 | 20.4301 | O007 | 20.2635 | O029 | 20.3510 |
| O029 | 18.5628 | O025 | 20.6768 | O029 | 20.9211 | F001 | 20.7602 |
| O019 | 18.8084 | O010 | 20.7691 | O016 | 20.9989 | O013 | 20.7776 |
| O025 | 18.9370 | O021 | 21.5497 | O023 | 21.1842 | O001 | 20.7776 |
| O013 | 19.3825 | F001 | 21.8536 | F001 | 21.5487 | O019 | 21.5005 |
| Mean |  | 18.6751 | Mean |  | 20.9407 | Mean |  | 20.8256 | Mean |  | 20.7530 |
| *Z* | Mg001 | O005 | 20.0199 | Al002 | O008 | 17.8133 | Al003 | O003 | 17.7160 | *Z* | Al001 | O001 | 17.8620 |
| O006 | 20.1111 | O004 | 17.9482 | O005 | 18.1373 | O005 | 18.2181 |
| O001 | 20.4133 | O006 | 18.2854 | O007 | 18.2296 | O006 | 18.3104 |
| O003 | 20.6625 | O002 | 19.0024 | O002 | 18.6788 | O003 | 19.2336 |
| O008 | 21.0376 | O009 | 19.2497 | O009 | 18.9204 | O008 | 19.4250 |
| O019 | 21.8167 | O021 | 20.0624 | O023 | 20.4302 | O019 | 19.7150 |
| Mean |  | 20.6769 | Mean |  | 18.7269 | Mean |  | 18.6854 | Mean |  | 18.7940 |
| Al004 | O010 | 17.9535 | Al005 | O017 | 18.2576 | Al006 | O016 | 17.8744 |  |  |  |  |
| O015 | 18.4257 | O018 | 18.4571 | O011 | 18.2891 |  |  |  |  |
| O014 | 18.4261 | O013 | 18.5878 | O012 | 18.8571 |  |  |  |  |
| O021 | 19.0678 | O015 | 18.8845 | O023 | 19.2718 |  |  |  |  |
| O012 | 19.1231 | O011 | 19.0891 | O018 | 19.3847 |  |  |  |  |
| O017 | 19.6191 | O019 | 19.2949 | O014 | 19.6386 |  |  |  |  |
| Mean |  | 18.7692 | Mean |  | 18.7618 | Mean |  | 18.8860 |  |  |  |  |

**Appendix 3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Polyhedra | Na(AlMg2)(Al5Mg)[Si6O18](BO3)3(OH)4 | | | | | | | | | Polyhedra | NaMg3Al6[Si6O18](BO3)3(OH)4 | | |
| Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length | Cation | Anion | Bond  length |
| *Y* | Al001 | O001 | 18.1518 | Mg002 | O004 | 20.4893 | Mg003 | O027 | 20.2000 | *Y* | Mg001 | O029 | 20.4790 |
| O029 | 18.4953 | O027 | 20.5065 | O007 | 20.2353 | O025 | 20.4797 |
| O031 | 18.6152 | O025 | 20.7735 | O016 | 20.7978 | O031 | 20.7195 |
| O019 | 18.9040 | O010 | 20.9974 | O029 | 21.1362 | O013 | 20.7850 |
| O025 | 18.9253 | O021 | 21.3958 | O031 | 21.2019 | O001 | 20.7859 |
| O013 | 19.7068 | O031 | 21.7519 | O023 | 21.4927 | O019 | 21.6276 |
| Mean |  | 18.7997 | Mean |  | 20.9857 |  |  | 20.8440 | Mean |  | 20.8128 |
| *Z* | Mg001 | O005 | 20.0136 | Al002 | O008 | 17.7383 | Al003 | O003 | 17.7356 | *Z* | Al001 | O001 | 17.8162 |
| O006 | 20.0813 | O004 | 17.8844 | O007 | 18.1227 | O005 | 18.1667 |
| O001 | 20.3314 | O006 | 18.2980 | O005 | 18.1819 | O006 | 18.3043 |
| O003 | 20.5683 | O002 | 18.8873 | O002 | 18.7081 | O003 | 19.2014 |
| O008 | 21.1252 | O009 | 19.4245 | O009 | 18.8350 | O008 | 19.4798 |
| O019 | 21.8195 | O021 | 20.1931 | O023 | 20.2056 | O019 | 19.6954 |
| Mean |  | 20.6566 | Mean |  | 18.7376 |  |  | 18.6315 | Mean |  | 18.7773 |
| Al004 | O010 | 17.8801 | Al005 | O017 | 18.2987 | Al006 | O016 | 17.8556 |  |  |  |  |
| O014 | 18.3713 | O018 | 18.3425 | O011 | 18.1940 |  |  |  |  |
| O015 | 18.4768 | O013 | 18.3890 | O012 | 18.7466 |  |  |  |  |
| O021 | 19.0165 | O015 | 18.7920 | O023 | 19.2634 |  |  |  |  |
| O012 | 19.2480 | O019 | 19.2816 | O018 | 19.5348 |  |  |  |  |
| O017 | 19.5071 | O011 | 19.3958 | O014 | 19.6143 |  |  |  |  |
| Mean |  | 18.7499 | Mean |  | 18.7499 | Mean |  | 18.8681 |  |  |  |  |