***Supplemental Material for Wander et al., The use of cation-cation and anion-anion bonds to augment the bond-valence model***

**Table S1.** Al-Si-H-O tempered calibration set.

|  |  |  |
| --- | --- | --- |
| **Name** | **Formula** | **Reference** |
| Quartz | SiO2 | ([Levien et al., 1980](#_ENREF_33)) |
| Coesite | SiO2 | ([Levien and Prewitt, 1981](#_ENREF_32)) |
| Cristobalite | SiO2 | ([Downs and Palmer, 1994](#_ENREF_20)) |
| Stishovite | SiO2 | ([Smyth et al., 1995](#_ENREF_40)) |
| Moganite | SiO2 | ([Heaney and Post, 2001](#_ENREF_25)) |
| Corundum | Al2O3 | ([Finger and Hazen, 1978](#_ENREF_21)) |
| Bayerite | Al(OH)3 | ([Balan et al., 2008](#_ENREF_2)) |
| Gibbsite | Al(OH)3 | ([Balan et al., 2006](#_ENREF_1)) |
| Boehmite | AlOOH | ([Hill, 1981](#_ENREF_27)) |
| Diaspore | AlOOH | ([Hill, 1979](#_ENREF_26)) |
| Kaolinite | Al2Si2O5(OH)4 | ([Bish, 1993](#_ENREF_4)) |
| Dickite | Al2Si2O5(OH)4 | ([Dera et al., 2003](#_ENREF_18)) |
| Ice-P1 | H2O | ([Pisani et al., 1996](#_ENREF_36)) |
| Hydrogen Peroxide | H2O2 | ([Busing and Levy, 1965](#_ENREF_9)) |
| Oxygen | O2 | ([Cox et al., 1973](#_ENREF_13)) |

**Table S2.** Al-Si-K-O tempered calibration set.

|  |  |  |
| --- | --- | --- |
| **Name** | **Formula** | **Reference** |
| Potassium Oxide | K2O | ([Wyckoff, 1963](#_ENREF_47)) |
| Potassium Superoxide | KO2 | ([Wyckoff, 1963](#_ENREF_47)) |
| Potassium Hydroxide | K2O2 | ([Bremm and Jansen, 1992](#_ENREF_7)) |
| Kalsilite | KAlSiO4 | ([Cellai et al., 1999](#_ENREF_10)) |
| Leucite | KAlSi2O6 | ([Dove et al., 1993](#_ENREF_19)) |
| Wadeite | K2Si(Si3O9) | ([Swanson and Prewitt, 1983](#_ENREF_41)) |
| Quartz | SiO2 | ([Levien et al., 1980](#_ENREF_33)) |
| Coesite | SiO2 | ([Levien and Prewitt, 1981](#_ENREF_32)) |
| Cristobalite | SiO2 | ([Downs and Palmer, 1994](#_ENREF_20)) |
| Stishovite | SiO2 | ([Smyth et al., 1995](#_ENREF_40)) |
| Moganite | SiO2 | ([Heaney and Post, 2001](#_ENREF_25)) |
| Corundum | Al2O3 | ([Finger and Hazen, 1978](#_ENREF_21)) |
| Oxygen | O2 | ([Cox et al., 1973](#_ENREF_13)) |

**Table S3.** Al-Si-H-O check set.

|  |  |  |
| --- | --- | --- |
| **Name** | **Formula** | **Reference** |
| Tridymite | SiO2 | ([Graetsch and Topalovic-Dierdorf, 1996](#_ENREF_22)) |
| Seifertite | SiO2 | ([Dera et al., 2002](#_ENREF_17)) |
| SiO2 | SiO2 | ([Boisen et al., 1994](#_ENREF_5)) |
| Mutinaite | SiO2 | ([van Konigsveld, 1990](#_ENREF_43)) |
| Post-quartz silica | SiO2 | ([Haines et al., 2001](#_ENREF_24)) |
| κ-Alumina | Al2O3 | ([Ollivier et al., 1997](#_ENREF_35)) |
| Doyleite | Al(OH)₃ | ([Clark et al., 1998](#_ENREF_11)) |
| Kyanite | Al2SiO5 | ([Comodi et al., 1997](#_ENREF_12)) |
| Andalusite | Al2SiO5 | ([Burt et al., 2006](#_ENREF_8)) |
| Sillimanite | Al2SiO5 | ([Burt et al., 2006](#_ENREF_8)) |
| Akdalaite | 5[Al](http://en.wikipedia.org/wiki/Aluminum)2[O](http://en.wikipedia.org/wiki/Oxygen)3·[H](http://en.wikipedia.org/wiki/Hydrogen)2O | ([Demichelis et al., 2008](#_ENREF_16)) |
| Dickite | Al2Si2O5(OH)4 | ([Joswig and Drits, 1986](#_ENREF_29)) |
| Phase egg | AlSiO3OH | ([Schmidt et al., 1998](#_ENREF_38)) |
| Pyrophyllite | Al2Si4O10(OH)2 | ([Wardle and Brindley, 1972](#_ENREF_45)) |
| Phase pi | Al3Si2O7(OH)3 | ([Daniels and Wunder, 1996](#_ENREF_14)) |
| Octahydridosilasesquioxane | H8Si8O12 | ([Törnroos, 1994](#_ENREF_42)) |

**Table S4.** Al-Si-K-O check set.

|  |  |  |
| --- | --- | --- |
| **Name** | **Formula** | **Reference** |
| Moganite | SiO2 | ([Miehe and Graetsch, 1992](#_ENREF_34)) |
| Tridymite | SiO2 | ([Graetsch and Topalovic-Dierdorf, 1996](#_ENREF_22)) |
| Seifertite | SiO2 | ([Dera et al., 2002](#_ENREF_17)) |
| Post-quartz silica | SiO2 | ([Haines et al., 2001](#_ENREF_24)) |
| Mutinaite | SiO2 | ([van Konigsveld, 1990](#_ENREF_43)) |
| κ-Alumina | Al2O3 | ([Ollivier et al., 1997](#_ENREF_35)) |
| Andalusite | Al2SiO5 | ([Burt et al., 2006](#_ENREF_8)) |
| Sillimanite | Al2SiO5 | ([Burt et al., 2006](#_ENREF_8)) |
| Megakalsilite | KAlSiO4 | ([Khomyakov et al., 2002](#_ENREF_30)) |
| K2Si2O5 | K2Si2O5 | ([de Jong et al., 1998](#_ENREF_15)) |
| Potassium cyclo-trisilicate | K2SiO3 | ([Werthmann and Hoppe, 1981](#_ENREF_46)) |
| Tripotassium aluminate | K3AlO3 | ([Bon et al., 1974](#_ENREF_6)) |
| Tetrapotassium phyllo-octasilicate | K4Si8O18 | ([Schweinsberg and Liebau, 1974](#_ENREF_39)) |
| Tetrapotassium silicate | K4SiO4 | ([Bernet and Hoppe, 1991](#_ENREF_3)) |
| Hexapotassium disilicate | K6Si2O7 | ([Jansen, 1982](#_ENREF_28)) |
| Hexapotassium dialuminate | K6Al2O6 | ([Schlaeger and Hoppe, 1994](#_ENREF_37)) |
| KAl9O14 | KAl9O14 | ([Lazic et al., 2013](#_ENREF_31)) |
| KAlO2 | KAlO2 | ([Voronin et al., 2012](#_ENREF_44)) |

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