Table 1.

Bond length, valence, distortion and strain parameters for selected compounds.

Symbols are: $<D_{obs}>$ = observed mean bond length; D' = mean bond length of regular polyhedron; ΔD = observed bond distortion; S_i = bond valence sum; V_i = atomic valence; $d1$ = discrepancy factor; $d2$ = bond discrepancy index; $<D_{th}>$ = theoretical mean bond length; D_{RU} = mean bond length of unstrained and regular polyhedron; ΔD_{top} = bond topological distortion; ΔD_{strain} = global strain; ΔD_{aniso} = anisotropic strain; ΔD_{iso} = isotropic strain. Bond valence parameters R_{Na+} = 1.803 Å, R_{Mg2+} = 1.693 Å, R_{Be2+} = 1.381 Å, R_{Zn2+} = 1.704 Å, R_{Mn2+} = 1.790 Å, R_{Al3+} = 1.651 Å, R_{Mn3+} = 1.760 Å, R_{Fe3+} = 1.759 Å and b_i = 0.37 Å from Brown & Altermatt (1985), R_{Si4+} = 1.622 Å from Brown (2009) and R_{V5+} = 1.788 Å and b_{V5+} = 0.32 Å from Hu & Zhou (2004).
The superscript a and b indicate that the observed site populations are: $^{IV}Zn^{VI}(Al_{1.95}Cr_{0.05})O_4$ and $^{IV}(Mn^{2+}{}_{0.99}Mg_{0.01})^{VI}Mn^{3+}{}_2O_4$, respectively.

	Cation site	$<D_{obs}>$ (Å)	D'(Å)	ΔD (Å)	S_i (vu)	V_i	$d1$ (vu)	$d2$ (vu)	$<D_{th}>$(Å)	D_{RU} (Å)	ΔD_{top} (Å)	ΔD_{strain} (Å)	ΔD_{aniso} (Å)	ΔD_{iso} (Å)
$ZnAl_2O_4$[a] (gahnite)	$^{IV}Zn^{2+}$	1.949	1.949	0	2.06	2	+0.06	0.01	1.960	1.960	0	-0.011	0	-0.011
	$^{VI}Al^{3+}$	1.917	1.915	0	2.93	3	-0.06	0.02	1.907	1.907	0	0.010	0	+0.010
$ZnFe_2O_4$ (franklinite)	$^{IV}Zn^{2+}$	1.980	1.980	0	1.90	2	-0.10	0.03	1.960	1.960	0	+0.020	0	+0.020
	$^{VI}Fe^{3+}$	2.026	2.026	0	2.91	3	-0.09	0.02	2.015	2.015	0	+0.011	0	+0.011
Mg_2SiO_4 (forsterite)	$^{VI}Mg^{2+}$(*M1*)	2.096	2.095	0.001	2.02	2	+0.02	0.02	2.099	2.099	0	-0.003	+0.001	-0.004
	$^{VI}Mg^{2+}$(*M2*)	2.130	2.123	0.007	1.88	2	-0.12	0.06	2.099	2.099	0	+0.030	+0.007	+0.023
	$^{IV}Si^{4+}$	1.636	1.636	0.0003	3.86	4	-0.14	0.05	1.622	1.622	0	+0.014	+0.0003	+0.014
$BeAl_2O_4$ (chrysoberyl)	$^{IV}Be^{2+}$	1.639	1.637	0.002	2.00	2	+0.00	0.05	1.637	1.637	0	-0.002	+0.002	0
	$^{VI}Al^{3+}$(*Al1*)	1.889	1.888	0.001	3.16	3	+0.16	0.04	1.907	1.907	0	-0.018	+0.001	-0.019
	$^{VI}Al^{3+}$(*Al2*)	1.939	1.934	0.005	2.80	3	-0.20	0.08	1.907	1.907	0	+0.031	+0.005	+0.026
$MnMn_2O_4$[b] (hausmannite)	$^{IV}Mn^{2+}$	2.040	2.040	0	2.04	2	+0.04	0.01	2.046	2.046	0	-0.006	0	-0.006
	$^{VI}Mn^{3+}$	2.049	2.015	0.034	3.01	3	+0.01	0.19	2.016	2.016	0	+0.033	+0.034	-0.001
$ZnMn_2O_4$ (heterolite)	$^{IV}Zn^{2+}$	1.983	1.983	0	1.88	2	-0.12	0.03	1.960	1.960	0	+0.023	0	+0.023
	$^{VI}Mn^{3+}$	2.038	2.008	0.030	3.07	3	+0.07	0.18	2.016	2.016	0	+0.022	+0.030	-0.009
ZnV_2O_6 (zinc vanadate)	$^{VI}Zn^{2+}$	2.159	2.136	0.023	1.87	2	-0.13	0.12	2.141	2.110	0.030	+0.018	-0.008	+0.026
	$^{VI}V^{5+}$	1.952	1.848	0.104	4.98	5	-0.02	0.44	1.854	1.846	0.008	+0.098	+0.097	+0.001
$NaMnSi_2O_6$ (namansilite)	$^{VIII}Na^{+}$	2.495	2.459	0.035	1.36	1	+0.36	0.10	2.642	2.572	0.069	-0.147	-0.034	-0.113
	$^{VI}Mn^{3+}$	2.025	2.005	0.020	3.09	3	+0.09	0.11	2.020	2.016	0.004	+0.005	+0.016	-0.011
	$^{IV}Si^{4+}$	1.631	1.631	0.000	3.91	4	-0.09	0.04	1.623	1.622	0.001	+0.008	-0.001	+0.009