Empirical electronic polarizabilities of ions for the prediction and interpretation of refractive indices: Oxides and oxysalts

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Table 3. Some reasons for not including data in the regression analysis.

	Example	Reference
A. Chemical composition		
poor or no analysis – composition uncertain	taikanite	Armbruster et al. (1993)
	cerchiaraite-Mn	Basso et al. (2000)
total amount of elements far below 100 %	haineaultite	McDonald and Chao(2004)
Rare earth ions not specified	thalenite	Fitzpatrick and Pabst (1986)
Fe^{2+}/Fe^{3+} ratio not known	morimotoite	Henmi et al. (1995)
H_2O content uncertain	hydroandradite	Peters (1965)
Crystal not homogeneous, e.g., zoned	morimotoite	Henmi et al.(1995)
	londonite	Simmons et al. (2001)
OH not found or OH:F variable in hydroxyfluorides		
Chemical analysis not determined on the samecrystal used for the refractive index measurement		
B. Crystal structure		
Structure unknown or incorrect	peprossiite-Ce	Callegari et al. (2000)
	fervanite	Hess and Henderson (1931)
Cation CN's or occupancies incorrect	khibinskite	Chernov et al. (1970)
C. Refractive index		
inaccurate nD	not common	
Not all indices measured	liebenbergite	DeWaal and Calk (1973)
wavelength is not λ(D) = 589 nm	Fe_3BO_6n(λ=630 nm)	Abe et al. (1980)
crystal reacts with immersion fluid	millosevichite	Miura et al. (1994)
nD calculated, not measured	$RbSr_4B_3O_9$	Xia and Li (2013)

Table 8. Comparison of polarizability analyses for 68 out of 205 examples where the compatibility index (CI) is listed as fair or poor by Mandarino (2006, 2007). Numbers in brackets refer to the number of minerals in the respective group.

Mineral	Composition	CI from Webmineral 2015	CI from Manda-rino 1981	α_{AE} (obs)	α_{AE} (calc)	$\Delta\alpha$
CARBONATES [5]						
tuliokite	$Na_6BaTh_{0.95}Fe^{3+}_{0.05}(CO_3)_6 \cdot 8H_2O$	CI calc= 0.09 (Poor)	fair	48.194	47.36	1.7%
comblainite	$Ni_{6.1}Co_{2.9}(CO_3)(OH)_{18} \cdot 4H_2O$	CI calc= 0.068 (Fair)	fair	55.679	55.76	-0.2%
mguinnessite	$Mg_{1.06}Cu_{0.94}(CO_3)(OH)_2$	CI calc= -0.146 (Poor)	poor	10.249	10.28	-0.3%
nullaginite	$Ni_{1.93}Mg_{0.05}Cr_{0.01}(CO_3)(OH)_2$	CI calc= 0.081 (Poor)	poor	10.584	10.84	-2.5%
azurite	$Cu_3[CO_3OH]_2$	CI calc= -0.08 (Poor)	poor	19.495	19.05	2.3%
BORATES [9]						
azoproite	$Mg_{1.82}Fe_{0.13}Fe^{3+}_{0.37}Ti_{0.36}Mg_{0.25}BO_5$	CI calc= 0.092 (Poor)	poor	11.665	12.77	-9.5%
hambergite	$Be_2BO_3(OH)_{0.96}F_{0.04}$	CI calc= -0.04 (Good)	poor	6.513	6.54	-0.5%
garrelsite	$Ba_3NaSi_2B_7O_{16}(OH)_4$	CI calc= 0.066 (Fair)	fair	40.007	41.95	-4.8%
peprossite-Ce	$Ce_{0.4}La_{0.32}r_{0.09}Nd_{0.05}Th_{0.02}Ca_{0.09}Al_2B_3O_9$	CI calc= 0.019 (Excellent)	poor	20.281	20.27	0.1%
wightmanite	$Mg_{4.7}Ca_{0.2}Fe_{0.1}BO_4(OH)_5 \cdot 2H_2O$	CI calc= 0.095 (Poor)	poor	18.892	21.21	-12.3%
				19.475	21.28	-9.2%
pinakiolite	$Mg_{1.75}Mn_{0.25}Mn^{3+}_{0.75}Sb^{3+}_{0.22}Al_{0.01}BO_5$	CI calc= -0.323 (Poor)	poor	14.676	13.64	7.0%
warwickite	$Mg_{1.33}Al_{0.21}Ti_{0.34}Fe^{3+}_{0.12}OBO_3$	CI calc= 0.241 (Poor)	poor	8.963	9.45	-5.4%
nordenskioldine	$CaSnB_2O_6$	CI calc= 0.029 (Excellent)	excellent	13.457	14.42	-7.1%
solongoite	$Ca_2B_3O_4Cl(OH)_4$	CI calc= 0.185 (Poor)	poor	15.762	18.69	-18.5%
SILICATES [4]						
zunyite	$Al_{13}Si_{4.69}Ti_{0.13}P_{0.12}O_{20}(OH)_{14.29}F_{3.59}Cl_{0.96}$	CI calc= 0.069 (Fair)		66.935	66.76	0.3%
baghdadite	$Ca_3Zr_{0.83}Ti_{0.15}Si_{1.99}Al_{0.01}Fe_{0.01}O_9$	CI calc= 0.118 (Poor)		24.206	24.29	-0.3%
huttonite	$Th_{0.96}U_{0.01}Y_{0.01}Ce_{0.02}SiO_4$	CI calc= 0.279 (Poor)		11.166	11.02	1.3%
lomonosovite	$Na_{9.5}Mn_{0.16}Ca_{0.11}Ti_{2.83}Nb_{0.51}Mn_{0.27}Zr_{0.11}Mg_{0.11}Fe_{0.1}Fe^{3+}_{0.06}Si_4O_{14}\ P_2O_8\ O_{3.5}F_{0.5}$	CI calc= 0.064 (Fair)		66.577	67.44	-1.3%
PHOSPHATES [19]						
attakolite	$Ca_{0.8}Sr_{0.2}MnAl_{3.6}Fe^{3+}_{0.4}Si_{0.7}P_{0.3}O_3(PO4)_3(OH)_5$	CI calc= 0.062 (Fair)	fair	36.604	37.50	-2.4%
kastningite	$Mn_{0.7}Fe_{0.3}Al_2(PO_4)_2\ (OH) \cdot 8H_2O$	CI calc= 0.005 (Superior)	poor	31.922	31.86	0.2%
kidwellite	$Na_{0.7}Fe_9(PO_4)_6(OH)_{10}5H_2O$	CI calc= 0.093 (Poor)	poor	92.144	95.13	-3.2%
kosnarite	$K_{0.9}Na_{0.2}Zr_{1.8}Mn_{0.1}(PO_4)_3$	CI calc= -0.047 (Good)	fair	28.820	28.83	0.0%
tiptopite	$K_2Li_{2.88}Na_{1.68}Ca_{0.66}(Be_6(PO_4)_6(OH)_2 \cdot 4H_2O$	CI calc= -0.064 (Fair)	fair	51.028	49.10	3.8%

Mineral	Composition	CI from Webmineral 2015	CI from Manda-rino 1981	α_{AE} (obs)	α_{AE} (calc)	$\Delta\alpha$
metaswitzerite	$Mn_{2.2}Fe_{0.6}Fe^{3+}_{0.2}(PO_4)_2 \cdot 4H_2O$	CI calc= 0.096 (Poor)	poor	24.776	25.92	-4.6%
barbosalite	$FeFe^{3+}_2(PO_4)_2(OH)_2$	CI calc= 0.119 (Poor)	poor	23.701	25.53	-7.7%
roscherite	$Ca_{1.2}Fe_{2.64}Mn_{0.04}Be_{2.5}(PO_4)_3 (OH)_3 \cdot 3H_2O$	CI calc= -0.055 (Good) -	poor	33.138	36.51	-10.2%
jahnsite	$Ca_{2.0}Mn_{2.3}Mg_{3.5}Fe_{3.3}Al_{0.8}(OH)_{4.1} (PO_4)_8 \cdot 15.8H_2O$	CI calc= 0.019 (Excellent)	superior	108.778	106.50	2.1%
switzerite	$Mn_{2.8}Fe_{0.2}(PO_4)_2 \cdot 7H_2O$	CI calc= 0.031 (Excellent)	excellent	29.970	30.51	-1.8%
strengite	$FePO_4 \cdot 2H_2O$	CI calc= 0.038 (Excellent)	fair	13.099	13.44	-2.6%
tavorite	$LiFePO_4OH$	CI calc= 0.073 (Fair)	fair	11.909	11.96	-0.5%
viitaniemiite	$Na_{0.9}Ca_{0.6}Mn_{0.4}AlPO_4F_{1.6}OH_{1.3}$	CI calc= 0.087 (Poor)	fair	11.816	12.18	-3.1%
zodacite	$Ca_4Mn_{0.8}Mg_{0.1}Fe^{3+}_{2.2}Al_{1.8}(PO_4)_6 (OH)_4 \cdot 12H_2O$	CI calc= 0.142 (Poor)	fair	77.444	77.58	-0.2%
wilhelmvierlin-gite	$Ca_{0.85}Zn_{0.13}MnFe^{3+}_{0.95}(PO_4)_2(OH) \cdot 4H_2O$	CI calc= -0.087 (Poor)	poor	27.710	28.39	-2.4%
cheralite-Ce	$Ca_{1.027}Th_{1.15}U_{0.148}Ce_{0.71}La_{0.306} Nd_{0.338}Sm_{0.100}Pr_{0.07}Gd_{0.02}P_{3.67} Si_{0.333}O_{16}$	CI calc= 0.14 (Poor)	poor	38.767	38.78	0.0%
benauite	$Sr_{0.67}Ba_{0.16}Pb_{0.07}Fe^{3+}_{2.90}Al_{0.03}P_{1.48}As_{0.04}S_{0.48}O_7(OH)_7$	CI calc= 0.053 (Good)	poor	36.975	35.35	4.4%
petersite-Y	$Y_{0.41}Ce_{0.28}Nd_{0.23}Sm_{0.13}La_{0.11}Fe_{0.20}Ca_{0.79}Cu_{12.07}(PO_4)_6(OH)_{12} \cdot 6H_2O$	CI calc= -0.079 (Fair)	fair	51.869	50.35	2.9%
monazite-Sm	$Sm_{0.18}Gd_{0.16}Th_{0.15}Ce_{0.15}Ca_{0.12} Nd_{0.09}La_{0.03}Y_{0.03}Pb_{0.02}Pr_{0.02}Tb_{0.02} Dy_{0.02}P_{0.94}Si_{0.06}O_4$	CI calc= -0.005 (Superior)	poor	9.569	9.91	-3.6%
ARSENATES[10]						
agardite-Ce	$Ce_{0.32}Ca_{0.22}La_{0.15}Nd_{0.15}Y_{0.08}Sm_{0.03}Gd_{0.03}Eu_{0.02}Dy_{0.01}Cu_{5.62}Fe_{0.05}As_{2.8}Si_{0.17}S_{0.05}O_{12.08}(OH)_6 \cdot 3H_2O$	CI calc= -0.108 (Poor)	fair	58.971	52.97	10.2%
arseno-crandallite	$Ca_{0.61}Sr_{0.29}Ba_{0.14}Bi_{0.05}Al_{2.79}Cu_{0.11}Fe^{3+}_{0.07}Zn_{0.02}A._{0.99}P_{0.75}Si_{0.26}O_4 (OH)_5 H_2O$	CI calc= 0.249 (Poor)	poor	26.062	27.51	-5.6%
arsenogoyazite	$Sr_{0.5}Ca_{0.25}Ba_{0.25}Al_3As_{1.2}P_{0.6}O_8 (OH)_4F \cdot H_2O$	CI calc= 0.025 (Excellent)	poor	26.661	26.21	1.7%
bradaczekite	$Na_{1.16}K_{0.05}Cu_{3.74}Zn_{0.07}Fe^{3+}_{0.03}As_3O_{12}$	CI calc= -0.01 (Superior)	poor	34.899	33.29	4.6%
clinoclase	$Cu_3AsO_4(OH)_3$	CI calc= -0.068 (Fair)	fair	19.884	19.48	2.0%
dussertite	$BaFe^{3+}_{2.52}Sb^{5+}_{0.483}As_2O_8(OH)_6$	CI calc= 0.023 (Excellent)	fair	39.233	39.34	-0.3%
olivenite	Cu_2AsO_4OH	CI calc= -0.047 (Good)	fair	14.100	14.09	-0.1%
symplesite	$Fe_3As_2O_8 \cdot 8H_2O$	CI calc= 0.18 (Poor)	fair	36.243	35.17	3.0%
weilite	$CaHAsO_4$	CI calc= -0.035 (Excellent)	poor	9.391	9.65	-2.28%
zalesiite	$Ca_{0.81}Y_{0.13}Al_{0.05}La_{0.01}Cu_{5.75}Ca_{0.15} As_{1.95}P_{0.05}O_4AsO_3OH(OH)_6 \cdot 3H_2O$	CI calc= -0.079 (Poor)	fair	55.707	53.55	3.9%

Mineral	Composition	CI from Webmineral 2015	CI from Manda-rino 1981	α_{AE} (obs)	α_{AE} (calc)	Δα
SULFATES [15]						
alunite	$KAl_3(SO_4)_2(OH)_6$	CI calc= 0.268 (Poor)	poor	23.673	23.84	-0.7%
argentojarosite	$AgFe_3(SO_4)_2(OH)_6$	CI calc= 0.084 (Poor)	fair	36.401	36.06	1.0%
bassanite	$2CaSO_4 \cdot H_2O$	CI calc= -0.026 (Excellent)	fair	8.257	8.71	-5.6%
bentorite	$Ca_{5.88}Cr_{1.61}Al_{0.32}Fe^{3+}_{0.02}(SO_4)_3(OH)_{12} \cdot 26H_2O$	CI calc= 0.033 (Excellent)	poor	92.726	95.69	-3.2%
caminite	$Mg_3(SO_4)_2(OH)_2$	CI calc= 0.214 (Poor)	fair	15.943	17.72	-11.0%
caminite	$Mg_7(SO_4)_5(OH)_4 \cdot H_2O$	CI calc= 0.214 (Poor)	fair	15.896	17.52	-10.0%
cesanite	$Ca_{2.92}Sr_{0.06}Na_{6.98}K_{0.04}(SO_4)_6(OH)_{0.88}Cl_{0.12} \cdot 0.88H_2O$	CI calc= -0.081 (Poor)	fair	50.433	49.81	1.2%
chalcocyanite	$CuSO_4$	CI calc= -0.076 (Fair)	poor	8.300	8.37	-0.7%
dolerophanite	Cu_2OSO_4	CI calc= -0.117 (Poor)	poor	12.748	12.31	3.4%
chalcoalumite	$CuAl_4SO_4(OH)_{12} \cdot 3H_2O$	CI calc= 0.047 (Good)	fair	34.151	33.57	1.7%
fedotovite	$K_2Cu_3O(SO_4)_3$	CI calc= -0.054 (Good)	poor	29.699	29.79	-0.3%
kamchatkite	$KCu_3(SO_4)OCl$	CI calc= -0.068 (Fair)	poor	26.414	25.85	2.1%
millosevichite	$Al_{1.5}Fe_{0.5}(SO_4)_3$	CI calc= 0.144 (Poor)	fair	21.924	21.35	2.6%
felsobanyite	$Al_4(SO_4)(OH)_{10} \cdot 4H_2O$	CI calc= 0.064 (Fair)	poor	30.627	30.54	-0.1%
walthierite	$Ba_{0.5}Al_3(SO_4)_2(OH)_6$	CI calc= 0.01 (Superior)	fair	24.073	24.11	0.2%
CHROMATES [1]						
chromatite	$CaCrO_4$	CI calc= 0.072 (Fair)	poor	11.204	12.46	-11.2%
MOLYBDATES [5]						
bamfordite	$Fe^{3+}Mo_2O_6(OH)_3 \cdot H_2O$	CI calc= -0.067 (Fair)	fair	31.438	27.15	13.6%
betpakdalite	$Ca_{1.89}Na_{0.42}K_{0.09}Cu^{2+}_{0.03}Mg_{1.01}Fe^{3+}_{3.01}Mo_8As_{1.8}P_{0.06}Si_{0.04}O_{36}(OH)1 \cdot 23H_2O$	CI calc= -0.071 (Fair)	poor	169.427	144.02	14.9%
lindgrenite	$Cu_3Mo_2O_8(OH)_2$	CI calc= -0.087 (Poor)	poor	33.784	31.90	5.7%
mendozavilite	$Na_{1.2}K_{1.1}CaFe^{3+}_{0.5}Ca_{0.4}Fe^{3+}_{2.9}Al_{0.1}Mo_{7.77}P_{1.95}O_{31.62}(OH)_2Cl_{0.09} \cdot 19.6H_2O$	CI calc= 0.193 (Poor)	poor	151.403	139.48	7.9%
obradovicite	$K_{1.72}Cu^{2+}_{0.58}Na_{0.38}Cu^{2+}Mo_8As_{1.53}Fe^{3+}_{2.64}O_{31.11}(OH)_{5.89} \cdot 18.25H_2O$	CI calc= -0.011 (Superior)	poor	163.741	144.50	11.7%
TUNGSTATES [4]						
scheelite	$CaWO_4$	CI calc= 0.152 (Poor)	poor	11.887	11.91	-0.2%
yttrotungstite-Y	$YW_2O_6(OH)_3$	CI calc= 0.067 (Fair)	poor	26.439	23.99	9.3%
yttrotungstite	$Y_{1.1}Nd_{0.17}Ce_{0.15}Dy_{0.09}RE_{0.3}Al_{0.2}W_{3.7}O_{11.4}(OH)_{6.6}$	CI calc= 0.067 (Fair)	poor	53.074	47.54	10.4%
paraniite-Y	$Ca_{1.64}Y_{1.13}Gd_{0.03}Dy_{0.08}Er_{0.07}Yb_{0.03}As_{1.07}W_{0.93}O_{12}$	CI calc= 0.143 (Poor)	poor	32.661	30.76	5.8%
tungstibite	Sb_2WO_6	CI calc= -0.091 (Poor)	poor	27.796	23.34	16.0%

Mineral	Composition	CI from Webmineral 2015	CI from Manda-rino 1981	α_{AE} (obs)	α_{AE} (calc)	$\Delta\alpha$
COMPLEX STRUCTURES [10]						
apjohnite	$Mn_{0.64}Mg_{0.28}Zn_{0.06}Fe_{0.02}Al_2(SO_4)_4 \cdot 22H_2O$	**CI calc= -0.009 (Superior)**		63.315	63.48	-0.3%
bannisterite	$Ca_{0.40}K_{0.44}Na_{0.05}Mn_{6.22}Fe_{1.45}Mg_{1.43}Zn_{1.01}Fe^{3+}_{0.18}Si_{14.42}Al_{1.43}O_{38}(OH)_8 \cdot 6H_2O$	**CI calc= 0.02 (Excellent)**		107.148	107.83	-0.6%
farnesite	$Na_{36.43}K_{9.18}Ca_{8.75}Si_{42.50}Al_{41.50}O_{213.72}F_{0.16}Cl_{0.48} \cdot 3H_2O$	**CI calc= 0.038 (Excellent)**		443.929	430.65	3.0%
giuseppetite	$Na_5K_{1.8}CaAl_{6.05}Si_{5.95}O_{24}(SO_4)_{1.8}Cl_{0.25}$	**CI calc= -0.029 (Excellent)**		62.518	61.24	2.0%
megacyclite	$Na_8KSi_9O_{18}(OH)_9 \cdot 19H_2O$	**CI calc= -0.016 (Superior)**		86.600	84.23	2.7%
nechelelyrusto-vite	$Na_4Ba_2Mn_{1.5}Ti_5NbSi_80_{28}(OH)_3F \cdot 6H_2O$	CI calc= 0.113 (Poor)		108.952	108.73	0.2%
polyphite	$Na_{8.72}Ca_{1.4}Sr_{0.03}Mg_{0.3}Mn_{0.68}Fe_{0.07}Ti_{1.41}Nb_{0.19}Zr_{0.19}P_{2.96}Si_{2.04}O_{20.94}F_{2.06}$	**CI calc= 0.004 (Superior)**		53.626	54.47	-1.6%
quadruphite	$Na_{13.59}Ca_{1.44}Sr_{0.06}Mg_{0.5}Mn_{0.85}Fe_{0.10}Ti_{2.55}Nb_{0.44}Zr_{0.47}Si_4P_4O_{33}F_{2.6}$	**CI calc= 0.059 (Good)**		86.742	86.54	0.2%
roger-mitchellite	$Na_{12}Sr_{21.16}Na_{1.17}Ca_{0.21}Ba_4Zr_{25.33}Ti_{0.93}Si_{77.02}B_{0.98}B_{12}O_{246}(OH)_{24} \cdot 18H_2O$			655.788	661.85	-0.9%
sobolevite	$Na_{13.62}Ca_{1.63}Sr_{0.03}Mg_{0.39}Mn_{1.02}Fe_{0.1}Ti_{2.42}Nb_{0.51}Zr_{0.09}Si_{4.1}P_4O_{33.08}F_{2.92}$	**CI calc= 0.013 (Superior)**		86.419	86.02	0.5%