Supplementary Material for Bickmore et al., Electronic structure effects in the vectorial bond valence model

Table S1. Data compilation for all atoms analyzed. The columns, from left to right, compile 1) the chemical formula of the compound, 2) the mineral name, if applicable, 3) the element represented by the atom, 4) its oxidation state, 5) the valence of the strongest bond to the atom, 6) the "minimum coordination number," 7) the valence sum of bonds to the atom, 8) the vectorial valence sum of bonds to the atom, and 8) the reference where the crystal structure was found. See the references after the table.

Compound	Mineral Name	Element	z_i	s_{max}	N_{min}	S_i	$\vec{S}_i$	Ref.
AgO	N/A	Ag	2	0.402	4.977	1.413	0.000	(Wyckoff, 1963)
AgO		Ag	2	0.560	3.574	2.500	0.000	
AgO		O	-2	0.560	3.574	1.956	0.000	
Al_2O_3	Corundum	Al	3	0.548	5.472	3.069	0.098	(Kirfel and Eichhorn, 1990)
Al_2O_3		O	-2	0.548	3.648	2.046	0.070	
κ-Al_2O_3	N/A	Al	3	0.665	4.514	3.075	0.108	(Ollivier et al., 1997)
κ-Al_2O_3		Al	3	0.742	4.043	2.990	0.306	
κ-Al_2O_3		Al	3	0.728	4.124	2.928	0.165	
κ-Al_2O_3		Al	3	0.618	4.858	2.870	0.159	
κ-Al_2O_3		O	-2	0.683	2.927	2.077	0.069	
κ-Al_2O_3		O	-2	0.651	3.073	2.006	0.125	
κ-Al_2O_3		O	-2	0.728	2.749	2.075	0.218	
κ-Al_2O_3		O	-2	0.441	4.535	1.749	0.324	
κ-Al_2O_3		O	-2	0.742	2.695	1.971	0.314	
κ-Al_2O_3		O	-2	0.665	3.010	1.986	0.261	
θ-Al_2O_3	N/A	Al	3	0.794	3.777	2.910	0.237	(Husson and Repelin, 1996)
θ-Al_2O_3		Al	3	0.595	5.039	2.975	0.108	
θ-Al_2O_3		O	-2	0.601	3.327	1.888	0.365	
θ-Al_2O_3		O	-2	0.638	3.134	2.013	0.175	
θ-Al_2O_3		O	-2	0.794	2.518	1.985	0.259	
Al_2SiO_5	Andalusite	Al	3	0.584	5.138	2.932	0.102	(Winter and Ghose, 1979)
Al_2SiO_5		Al	3	0.602	4.980	2.990	0.038	

Al_2SiO_5		O	-2	0.917	2.181	2.018	0.472	
Al_2SiO_5		O	-2	0.978	2.045	2.107	0.357	
Al_2SiO_5		O	-2	0.599	3.337	1.933	0.269	
Al_2SiO_5		O	-2	0.952	2.101	1.950	0.520	
Al_2SiO_5		Si	4	0.978	4.090	4.035	0.114	
Al_2SiO_5	Kyanite	Al	3	0.560	5.352	3.113	0.158	(Comodi et al., 1997)
Al_2SiO_5		Al	3	0.514	5.839	3.005	0.023	
Al_2SiO_5		Al	3	0.539	5.563	3.004	0.100	
Al_2SiO_5		Al	3	0.595	5.038	3.161	0.088	
Al_2SiO_5		O	-2	0.925	2.163	2.052	0.427	
Al_2SiO_5		O	-2	0.558	3.587	2.029	0.574	
Al_2SiO_5		O	-2	0.950	2.105	2.041	0.428	
Al_2SiO_5		O	-2	0.945	2.116	2.049	0.429	
Al_2SiO_5		O	-2	0.921	2.171	2.048	0.423	
Al_2SiO_5		O	-2	0.511	3.911	2.008	0.518	
Al_2SiO_5		O	-2	0.958	2.087	1.997	0.479	
Al_2SiO_5		O	-2	0.970	2.062	2.020	0.504	
Al_2SiO_5		O	-2	0.914	2.188	2.044	0.404	
Al_2SiO_5		O	-2	0.918	2.180	2.048	0.436	
Al_2SiO_5		Si	4	0.970	4.123	4.037	0.045	
Al_2SiO_5		Si	4	0.958	4.174	4.015	0.024	
$AlAsO_4$	Alarsite	Al	3	0.714	4.199	2.914	0.031	(Sowa, 1991)
$AlAsO_4$		As	5	1.269	3.939	5.148	0.026	
$AlAsO_4$		O	-2	1.269	1.576	2.034	0.908	
$AlAsO_4$		O	-2	1.249	1.601	1.996	0.915	
$AlPO_4$	Berlinite	Al	3	0.734	4.089	3.009	0.017	(Muraoka and Kihara, 1997)
$AlPO_4$		O	-2	1.243	1.609	2.030	0.796	
$AlPO_4$		O	-2	1.257	1.591	2.027	0.817	
$AlPO_4$		P	5	1.257	3.978	5.102	0.031	
$AlTaO_4$	Alumotantite	Al	3	0.533	5.629	3.139	0.073	(Ercit et al., 1992)

$AlTaO_4$		O	-2	0.699	2.861	2.032	0.203	
$AlTaO_4$		O	-2	0.901	2.221	2.060	0.324	
$AlTaO_4$		Ta	5	0.901	5.552	5.044	0.048	
As_2O_5	Paulmooreite	As	5	0.981	5.096	5.431	0.084	(Jansen, 1978)
As_2O_5		As	5	1.318	3.792	5.293	0.092	
As_2O_5		O	-2	0.981	2.038	2.072	0.717	
As_2O_5		O	-2	1.295	1.544	2.178	0.918	
As_2O_5		O	-2	1.318	1.517	2.218	0.963	
As_2O_5		O	-2	1.188	1.684	2.111	1.026	
As_2O_5		O	-2	1.201	1.665	2.145	1.017	
$AsSbO_3$	Stibioclaudetite	As	3	0.921	3.257	2.860	1.373	(Bodenstein et al., 1983)
$AsSbO_3$		O	-2	0.986	2.028	2.036	0.773	
$AsSbO_3$		O	-2	0.916	2.184	1.947	0.900	
$AsSbO_3$		O	-2	0.938	2.133	2.019	0.834	
$AsSbO_3$		Sb	3	0.986	3.043	3.141	1.618	
$BaCO_3$	Witherite	Ba	2	0.262	7.625	2.126	0.016	(Antoa and Hassan, 2009)
$BaCO_3$		C	4	1.275	3.136	3.875	0.119	
$BaCO_3$		O	-2	1.253	1.597	1.962	1.253	
$BaCO_3$		O	-2	1.275	1.568	2.020	1.275	
$Ba(NO_3)_2$	Nitrobarite	Ba	2	0.193	10.352	2.209	0.000	(Nowotny and Heger, 1983)
$Ba(NO_3)_2$		N	5	1.615	3.096	4.938	0.025	
$Ba(NO_3)_2$		O	-2	1.615	1.238	2.014	1.615	
BaO	N/A	Ba	2	0.252	7.922	1.535	0.000	(Wyckoff, 1963)
BaO		O	-2	0.252	7.922	1.535	0.000	
$BaSO_4$	Barite	Ba	2	0.242	8.258	2.203	0.084	(Jacobsen et al., 1998)
$BaSO_4$		O	-2	1.526	1.311	1.987	1.526	
$BaSO_4$		O	-2	1.489	1.343	2.010	1.489	
$BaSO_4$		O	-2	1.412	1.416	2.073	1.412	
$BaSO_4$		S	6	1.526	3.933	5.940	0.011	
Be_2SiO_4	Phenakite	Be	2	0.451	4.434	2.091	0.043	(Hazen and Au, 1986)

Be_2SiO_4		Be	2	0.456	4.388	2.087	0.042	
Be_2SiO_4		O	-2	0.949	2.107	2.067	0.453	
Be_2SiO_4		O	-2	0.953	2.099	2.089	0.499	
Be_2SiO_4		O	-2	0.952	2.101	2.046	0.532	
Be_2SiO_4		O	-2	0.953	2.098	2.051	0.528	
Be_2SiO_4		Si	4	0.953	4.197	4.075	0.072	
$BeAl_2O_4$	Chrysoberyl	Al	3	0.537	5.585	3.201	0.000	(Hazen, 1987)
$BeAl_2O_4$		Al	3	0.535	5.607	2.883	0.031	
$BeAl_2O_4$		Be	2	0.502	3.981	2.184	0.112	
$BeAl_2O_4$		O	-2	0.537	3.724	2.207	0.258	
$BeAl_2O_4$		O	-2	0.535	3.738	2.121	0.284	
$BeAl_2O_4$		O	-2	0.499	4.009	1.970	0.284	
BeO	Brommelite	Be	2	0.445	4.492	2.176	0.005	(Xu and Ching, 1993)
BeO		O	-2	0.445	4.492	2.176	0.005	
Bi_2CuO_4	Kusachiite	Bi	3	0.794	3.778	2.967	1.319	(Garcia-Munoz et al., 1990)
Bi_2CuO_4		Cu	2	0.448	4.463	1.919	0.078	
Bi_2CuO_4		O	-2	0.794	2.519	1.963	0.665	
Bi_2MoO_6	Koechlinite	Bi	3	0.710	4.223	3.052	1.105	(Teller et al., 1984)
Bi_2MoO_6		Bi	3	0.690	4.351	3.045	1.083	
Bi_2MoO_6		Mo	6	1.495	4.013	6.110	0.645	
Bi_2MoO_6		O	-2	1.159	1.726	1.931	0.948	
Bi_2MoO_6		O	-2	0.690	2.900	2.105	0.263	
Bi_2MoO_6		O	-2	0.710	2.816	2.180	0.263	
Bi_2MoO_6		O	-2	1.495	1.338	2.128	1.079	
Bi_2MoO_6		O	-2	1.424	1.405	2.019	1.129	
Bi_2MoO_6		O	-2	1.127	1.775	1.844	0.830	
β-Bi_2O_3	N/A	Bi	3	0.866	3.465	2.965	1.322	(Blower and Greaves, 1988)
β-Bi_2O_3		O	-2	0.803	2.492	1.891	0.312	
β-Bi_2O_3		O	-2	0.866	2.310	2.147	0.723	
Bi_2WO_6	Russellite	Bi	3	0.723	4.149	3.051	1.114	(Knight, 1992)

Bi_2WO_6		Bi	3	0.707	4.244	3.081	1.107	
Bi_2WO_6		O	-2	1.110	1.802	1.870	0.934	
Bi_2WO_6		O	-2	0.707	2.829	2.176	0.254	
Bi_2WO_6		O	-2	0.723	2.766	2.158	0.272	
Bi_2WO_6		O	-2	1.275	1.568	1.983	0.784	
Bi_2WO_6		O	-2	1.319	1.516	2.071	0.881	
Bi_2WO_6		O	-2	1.066	1.876	1.814	0.772	
Bi_2WO_6		W	6	1.319	4.549	5.940	0.410	
$BiAsO_4$	Rooseveltite	As	5	1.275	3.921	5.063	0.166	(Bedlivy and Mereiter, 1982)
$BiAsO_4$		Bi	3	0.491	6.114	2.945	0.584	
$BiAsO_4$		O	-2	1.275	1.569	1.862	1.275	
$BiAsO_4$		O	-2	1.231	1.625	2.040	1.009	
$BiAsO_4$		O	-2	1.171	1.708	2.134	0.815	
$BiAsO_4$		O	-2	1.238	1.615	1.972	0.963	
$BiPO_4$	Ximengite	Bi	3	0.516	5.819	3.016	0.362	(Mooney-Slater, 1962)
$BiPO_4$		O	-2	1.149	1.741	1.881	0.807	
$BiPO_4$		O	-2	1.149	1.740	1.972	0.830	
$BiPO_4$		P	5	1.150	4.348	4.691	0.004	
$BiVO_4$	Clinobisvanite	Bi	3	0.465	6.455	3.059	0.425	(Sleight et al., 1979)
$BiVO_4$		O	-2	1.055	1.895	2.143	0.529	
$BiVO_4$		O	-2	1.223	1.635	1.936	1.106	
$BiVO_4$		V	5	1.223	4.088	5.098	0.249	
$BiVO_4$	Dreyerite	Bi	3	0.402	7.466	2.816	0.000	(Dreyer and Tillmanns, 1981)
$BiVO_4$		O	-2	1.197	1.670	1.971	0.860	
$BiVO_4$		V	5	1.197	4.176	5.067	0.000	
$BiVO_4$	Pucherite	Bi	3	0.497	6.042	3.002	0.578	(Mereiter and Preisinger, 1986)
$BiVO_4$		O	-2	1.037	1.929	2.225	0.505	
$BiVO_4$		O	-2	1.285	1.557	1.855	1.285	
$BiVO_4$		V	5	1.285	3.892	5.159	0.617	

Ca_2SiO_4	Larnite	Ca	2	0.381	5.254	1.776	0.236	(Tsurumi et al., 1994)
Ca_2SiO_4		Ca	2	0.280	7.141	1.878	0.033	
Ca_2SiO_4		O	-2	1.024	1.954	1.926	0.670	
Ca_2SiO_4		O	-2	1.191	1.680	2.135	1.191	
Ca_2SiO_4		O	-2	1.378	1.452	2.269	1.378	
Ca_2SiO_4		O	-2	0.863	2.317	1.861	0.583	
Ca_2SiO_4		Si	4	1.378	2.903	4.536	0.279	
$Ca_3(BO_3)_2$	Takedaite	B	3	0.936	3.206	2.860	0.062	(Vegas et al., 1975)
$Ca_3(BO_3)_2$		Ca	2	0.315	6.357	2.039	0.006	
$Ca_3(BO_3)_2$		O	-2	0.936	2.137	1.974	0.723	
$Ca_3(PO_4)_2$	Tuite	Ca	2	0.258	7.750	2.056	0.000	(Sugiyama and Tokonami, 1987)
$Ca_3(PO_4)_2$		Ca	2	0.394	5.081	2.078	0.069	
$Ca_3(PO_4)_2$		O	-2	1.242	1.610	1.970	0.848	
$Ca_3(PO_4)_2$		O	-2	1.216	1.644	2.066	1.216	
$Ca_3(PO_4)_2$		P	5	1.242	4.025	5.060	0.021	
$CaAl_2O_4$	Dmitryivanovite	Al	3	0.718	4.180	2.928	0.139	(Lazic et al., 2007)
$CaAl_2O_4$		Al	3	0.722	4.154	2.872	0.112	
$CaAl_2O_4$		Al	3	0.704	4.259	2.850	0.094	
$CaAl_2O_4$		Al	3	0.727	4.128	2.918	0.103	
$CaAl_2O_4$		Ca	2	0.356	5.618	1.769	0.186	
$CaAl_2O_4$		Ca	2	0.316	6.327	1.655	0.226	
$CaAl_2O_4$		O	-2	0.718	2.786	1.895	0.409	
$CaAl_2O_4$		O	-2	0.727	2.752	1.835	0.462	
$CaAl_2O_4$		O	-2	0.696	2.874	1.803	0.385	
$CaAl_2O_4$		O	-2	0.713	2.804	1.881	0.337	
$CaAl_2O_4$		O	-2	0.722	2.769	1.954	0.497	
$CaAl_2O_4$		O	-2	0.688	2.909	1.806	0.530	
$CaAl_2O_4$		O	-2	0.699	2.860	1.949	0.378	
$CaAl_2O_4$		O	-2	0.712	2.810	1.869	0.392	

$CaAl_4O_7$	Grossite	Al	3	0.735	4.080	2.867	0.115	(Goodwin and Lindop, 1970)
$CaAl_4O_7$		Al	3	0.761	3.944	2.947	0.115	
$CaAl_4O_7$		Ca	2	0.325	6.153	1.811	0.100	
$CaAl_4O_7$		O	-2	0.758	2.639	1.931	0.434	
$CaAl_4O_7$		O	-2	0.710	2.818	1.866	0.359	
$CaAl_4O_7$		O	-2	0.761	2.630	1.889	0.265	
$CaAl_4O_7$		O	-2	0.655	3.053	1.999	0.283	
$CaCO_3$	Aragonite	C	4	1.301	3.076	4.047	0.193	(Antao and Hassan, 2009)
$CaCO_3$		Ca	2	0.279	7.173	2.078	0.020	
$CaCO_3$		O	-2	1.301	1.538	2.006	1.301	
$CaCO_3$		O	-2	1.293	1.547	2.060	1.293	
$CaCO_3$	Calcite	C	4	1.302	3.073	4.007	0.000	(Markgraf and Reeder, 1985)
$CaCO_3$		Ca	2	0.306	6.538	2.081	0.000	
$CaCO_3$		O	-2	1.302	1.537	2.029	1.302	
$CaMn_2O_4$	Marokite	Ca	2	0.376	5.313	2.307	0.146	(Zouari et al., 2003)
$CaMn_2O_4$		Mn	3	0.614	4.890	2.834	0.117	
$CaMn_2O_4$		O	-2	0.551	3.631	1.878	0.379	
$CaMn_2O_4$		O	-2	0.600	3.331	2.061	0.086	
$CaMn_2O_4$		O	-2	0.614	3.260	2.018	0.433	
$CaMoO_4$	Powellite	Ca	2	0.252	7.928	2.116	0.000	(Hazen et al., 1985)
$CaMoO_4$		Mo	6	1.425	4.210	6.045	0.000	
$CaMoO_4$		O	-2	1.425	1.403	2.040	1.425	
CaO	Lime	Ca	2	0.276	7.239	1.725	0.000	(Fiquet et al., 1999)
CaO		O	-2	0.276	7.239	1.725	0.000	
$CaSiO_3$	Wollastonite	Ca	2	0.384	5.203	1.905	0.152	(Ohashi, 1984)
$CaSiO_3$		Ca	2	0.374	5.343	1.897	0.113	
$CaSiO_3$		Ca	2	0.317	6.306	2.023	0.041	
$CaSiO_3$		O	-2	0.991	2.019	1.952	0.575	
$CaSiO_3$		O	-2	1.026	1.950	1.974	0.614	
$CaSiO_3$		O	-2	1.023	1.955	1.779	0.959	

$CaSiO_3$		O	-2	1.057	1.893	1.788	0.653	
$CaSiO_3$		O	-2	1.083	1.847	1.855	0.665	
$CaSiO_3$		O	-2	0.998	2.004	1.883	0.679	
$CaSiO_3$		O	-2	0.927	2.157	2.125	0.468	
$CaSiO_3$		O	-2	0.914	2.187	2.153	0.347	
$CaSiO_3$		O	-2	0.917	2.180	2.158	0.362	
$CaSiO_3$		Si	4	1.057	3.786	3.948	0.064	
$CaSiO_3$		Si	4	1.083	3.694	4.020	0.138	
$CaSiO_3$		Si	4	1.023	3.910	3.874	0.154	
$CaSO_4$	Anhydrite	Ca	2	0.308	6.499	2.101	0.003	(Bezou et al., 1995)
$CaSO_4$		Ca	2	0.273	7.332	2.052	0.000	
$CaSO_4$		O	-2	1.400	1.428	1.976	1.400	
$CaSO_4$		O	-2	1.450	1.380	2.007	1.450	
$CaSO_4$		O	-2	1.434	1.395	1.944	1.434	
$CaSO_4$		S	6	1.400	4.285	5.707	0.000	
$CaSO_4$		S	6	1.450	4.139	5.873	0.079	
$CaTiO_3$	Perovskite	Ca	2	0.336	5.950	2.090	0.091	(Yamanaka et al., 2002)
$CaTiO_3$		O	-2	0.643	3.111	2.011	0.089	
$CaTiO_3$		O	-2	0.636	3.143	2.028	0.079	
$CaTiO_3$		Ti	4	0.643	6.223	3.976	0.000	
$CaWO_4$	Scheelite	Ca	2	0.257	7.768	2.108	0.000	(Hazen et al., 1985)
$CaWO_4$		O	-2	1.365	1.465	1.988	1.365	
$CaWO_4$		W	6	1.365	4.395	5.845	0.000	
$CdCO_3$	Otavite	C	4	1.305	3.066	4.045	0.000	(Bromiley et al., 2007)
$CdCO_3$		Cd	2	0.329	6.087	2.138	0.000	
$CdCO_3$		O	-2	1.305	1.533	2.061	0.966	
CdO	Monteponite	Cd	2	0.287	6.974	1.760	0.000	(Wyckoff, 1963)
CdO		O	-2	0.287	6.974	1.760	0.000	
$CeAsO_4$	Ce-Gasparite	As	5	1.229	4.068	4.968	0.174	(Brahim et al., 2002)
$CeAsO_4$		Ce	3	0.385	7.791	2.872	0.241	

$CeAsO_4$		O	-2	1.229	1.627	1.965	1.075	
$CeAsO_4$		O	-2	1.179	1.696	1.958	0.967	
$CeAsO_4$		O	-2	1.200	1.667	1.945	0.833	
$CeAsO_4$		O	-2	1.219	1.641	1.973	0.893	
CoO	N/A	Co	2	0.305	6.559	1.927	0.000	(Wyckoff, 1963)
CoO		O	-2	0.305	6.559	1.927	0.000	
CrO_2	(Rutile structure)	Cr	4	0.744	5.377	4.419	0.000	(Baur and Khan, 1971)
CrO_2		O	-2	0.744	2.688	2.210	0.142	
CrO_3	N/A	Cr	6	1.645	3.648	5.808	0.512	(Stephens and Cruickshank, 1970)
CrO_3		O	-2	1.177	1.699	2.378	0.740	
CrO_3		O	-2	1.633	1.225	1.656	1.645	
CrO_3		O	-2	1.645	1.216	1.773	1.595	
Cs_2O	N/A	Cs	1	0.237	4.223	0.716	0.364	(Wyckoff, 1963)
Cs_2O		O	-2	0.237	8.446	1.432	0.000	
$Cs(NO_3)$	N/A	Cs	1	0.117	8.562	1.025	0.018	(Pohl and Gross, 1993)
$Cs(NO_3)$		Cs	1	0.120	8.362	1.088	0.022	
$Cs(NO_3)$		Cs	1	0.118	8.460	1.065	0.041	
$Cs(NO_3)$		N	5	1.743	2.869	5.102	0.043	
$Cs(NO_3)$		N	5	1.760	2.841	5.069	0.145	
$Cs(NO_3)$		N	5	1.935	2.584	5.117	0.299	
$Cs(NO_3)$		O	-2	1.658	1.207	2.068	1.658	
$Cs(NO_3)$		O	-2	1.743	1.147	2.066	1.743	
$Cs(NO_3)$		O	-2	1.621	1.234	2.021	1.621	
$Cs(NO_3)$		O	-2	1.645	1.216	2.079	1.645	
$Cs(NO_3)$		O	-2	1.760	1.137	2.122	1.760	
$Cs(NO_3)$		O	-2	1.583	1.263	1.919	1.583	
$Cs(NO_3)$		O	-2	1.935	1.034	2.269	1.935	
$Cs(NO_3)$		O	-2	1.519	1.316	1.899	1.519	
$Cs(NO_3)$		O	-2	1.579	1.266	2.020	1.579	

$CuAs_2O_4$	Trippkeite	As	3	1.006	2.984	2.915	1.394	(Pertlik, 1975)
$CuAs_2O_4$		Cu	2	0.438	4.568	2.092	0.000	
$CuAs_2O_4$		O	-2	0.889	2.250	1.977	0.790	
$CuAs_2O_4$		O	-2	1.006	1.989	1.985	0.684	
CuB_2O_4	Santarosaite	B	3	0.798	3.759	3.195	0.048	(Martinez-Ripoll et al., 1971)
CuB_2O_4		B	3	0.745	4.027	3.039	0.110	
CuB_2O_4		Cu	2	0.388	5.149	1.891	0.000	
CuB_2O_4		Cu	2	0.500	4.002	2.146	0.052	
CuB_2O_4		O	-2	0.752	2.658	2.011	0.394	
CuB_2O_4		O	-2	0.745	2.683	2.118	0.322	
CuB_2O_4		O	-2	0.772	2.590	2.178	0.300	
CuB_2O_4		O	-2	0.798	2.506	2.102	0.544	
$CuSO_4$	Chalcocyanite	Cu	2	0.467	4.283	2.119	0.000	(Wildner and Giester, 1988)
$CuSO_4$		O	-2	1.534	1.303	1.934	1.534	
$CuSO_4$		O	-2	1.310	1.526	2.060	0.935	
$CuSO_4$		O	-2	1.489	1.343	2.069	1.192	
$CuSO_4$		S	6	1.534	3.910	6.013	0.045	
$CuTe_2O_5$	Rajite	Cu	2	0.435	4.596	2.021	0.135	(Hanke et al., 1973)
$CuTe_2O_5$		O	-2	1.263	1.583	1.964	1.150	
$CuTe_2O_5$		O	-2	1.056	1.895	2.042	0.958	
$CuTe_2O_5$		O	-2	1.206	1.659	2.023	0.891	
$CuTe_2O_5$		O	-2	1.199	1.668	1.882	0.984	
$CuTe_2O_5$		O	-2	1.238	1.616	1.956	1.077	
$CuTe_2O_5$		Te	4	1.206	3.318	3.917	1.903	
$CuTe_2O_5$		Te	4	1.263	3.166	3.929	1.790	
$CuTeO_3$	Balyakinite	Cu	2	0.450	4.440	1.927	0.153	(Lindqvist, 1972)
$CuTeO_3$		O	-2	1.163	1.720	2.119	0.678	
$CuTeO_3$		O	-2	1.198	1.670	1.804	0.953	
$CuTeO_3$		O	-2	0.990	2.020	1.994	0.514	
$CuTeO_3$		O	-2	1.262	1.585	2.042	1.018	

$CuTeO_3$		Te	4	1.262	3.170	4.068	1.899	
$CuTeO_3$		Te	4	1.198	3.339	3.960	1.649	
$DyPO_4$	Dy-Xenotime	Dy	3	0.432	6.938	3.304	0.000	(Ni et al., 1995)
$DyPO_4$		O	-2	1.210	1.653	2.077	0.785	
$DyPO_4$		P	5	1.210	4.134	5.004	0.000	
$ErPO_4$	Er-Xenotime	Er	3	0.447	6.710	3.330	0.000	(Ni et al., 1995)
$ErPO_4$		O	-2	1.214	1.647	2.091	0.777	
$ErPO_4$		P	5	1.214	4.118	5.035	0.000	
EuO	N/A	Eu	2	0.252	7.928	1.568	0.000	(Wyckoff, 1963)
EuO		O	-2	0.252	7.928	1.568	0.000	
$Fe_2MO_3O_8$	Kamiokite	Fe	2	0.421	4.745	1.961	0.126	(Kanazawa and Sasaki, 1986)
$Fe_2MO_3O_8$		Fe	2	0.352	5.676	2.147	0.019	
$Fe_2MO_3O_8$		Mo	4	0.666	6.010	3.862	0.159	
$Fe_2MO_3O_8$		O	-2	0.564	3.548	1.907	1.182	
$Fe_2MO_3O_8$		O	-2	0.481	4.156	2.004	0.268	
$Fe_2MO_3O_8$		O	-2	0.530	3.770	1.993	0.242	
$Fe_2MO_3O_8$		O	-2	0.666	3.005	1.935	0.678	
Fe_2O_3	Hematite	Fe	3	0.568	5.278	2.977	0.038	(Blake et al., 1966)
Fe_2O_3		O	-2	0.568	3.519	1.984	0.020	
Fe_2SiO_4	Fayalite	Fe	2	0.323	6.192	1.947	0.000	(Smyth, 1975)
Fe_2SiO_4		Fe	2	0.352	5.678	1.884	0.022	
Fe_2SiO_4		O	-2	0.937	2.135	1.960	0.475	
Fe_2SiO_4		O	-2	0.905	2.210	1.977	0.697	
Fe_2SiO_4		O	-2	0.990	2.021	1.929	0.817	
Fe_2SiO_4		Si	4	0.990	4.042	3.964	0.258	
$Fe_2(SO_4)_3$	Mikasaite	Fe	3	0.523	5.732	3.234	0.074	(Christidis and Rentzeperis, 1976)
$Fe_2(SO_4)_3$		Fe	3	0.519	5.786	3.177	0.015	
$Fe_2(SO_4)_3$		O	-2	1.493	1.339	2.087	1.051	
$Fe_2(SO_4)_3$		O	-2	1.484	1.348	2.065	1.145	

$Fe_2(SO_4)_3$		O	-2	1.500	1.333	2.055	1.161	
$Fe_2(SO_4)_3$		O	-2	1.496	1.337	2.057	1.113	
$Fe_2(SO_4)_3$		S	6	1.500	4.000	6.129	0.042	
$FeAl_2O_4$	Hercynite	Al	3	0.451	6.651	2.813	0.000	(Hill, 1984)
$FeAl_2O_4$		Fe	2	0.458	4.364	2.459	0.000	
$FeAl_2O_4$		O	-2	0.458	4.364	2.021	0.134	
$FeCO_3$	Siderite	C	4	1.285	3.112	4.063	0.000	(Graf, 1961a)
$FeCO_3$		Fe	2	0.309	6.470	2.119	0.000	
$FeCO_3$		O	-2	1.285	1.556	2.061	1.285	
$FeCr_2O_4$	Chromite	Cr	3	0.463	6.483	2.881	0.000	(Lenaz et al., 2004)
$FeCr_2O_4$		Fe	2	0.419	4.775	1.925	0.000	
$FeCr_2O_4$		O	-2	0.463	4.323	1.921	0.296	
FeO	Wustite	Fe	2	0.301	6.644	1.924	0.000	(Wyckoff, 1963)
FeO		O	-2	0.301	6.644	1.924	0.000	
$FePO_4$	Rodolicoite	Fe	3	0.759	3.953	3.013	0.020	(Long et al., 1983)
$FePO_4$		O	-2	1.275	1.569	2.085	0.836	
$FePO_4$		O	-2	1.190	1.681	1.929	0.834	
$FePO_4$		P	5	1.275	3.922	5.018	0.015	
$FeSB_2O_4$	Schafarzikite	Fe	2	0.336	5.953	1.999	0.000	(Fischer and Pertlik, 1975)
$FeSB_2O_4$		O	-2	0.852	2.346	2.082	0.504	
$FeSB_2O_4$		O	-2	1.008	1.984	1.860	0.773	
$FeSB_2O_4$		Sb	3	1.008	2.977	2.943	1.451	
$FeTiO_3$	Ilmenite	Fe	2	0.354	5.652	2.066	0.103	(Wechsler and Prewitt, 1984)
$FeTiO_3$		O	-2	0.741	2.701	2.001	0.376	
$FeTiO_3$		Ti	4	0.742	5.392	3.939	0.006	
FeV_2O_4	Coulsonite	Fe	2	0.424	4.719	1.931	0.000	(Reuter et al., 1969)
FeV_2O_4		O	-2	0.454	4.404	1.900	0.289	
FeV_2O_4		V	3	0.454	6.606	2.835	0.000	
Ga_2O_3	N/A	Ga	3	0.732	4.099	2.996	0.119	(Åhman et al., 1996)
Ga_2O_3		Ga	3	0.555	5.404	2.955	0.076	

Ga_2O_3		O	-2	0.727	2.751	1.911	0.390	
Ga_2O_3		O	-2	0.674	2.967	1.946	0.113	
Ga_2O_3		O	-2	0.732	2.733	2.094	0.276	
GeO_2	(Quartz structure)	Ge	4	1.007	3.973	4.108	0.050	(Smith and Isaacs, 1964)
GeO_2		O	-2	1.007	1.986	2.054	0.823	
GeO_2	(Rutile structure)	Ge	4	0.718	5.571	4.366	0.000	(Haines et al., 2000)
GeO_2		O	-2	0.718	2.786	2.183	0.265	
HfO_2	(Flourite structure)	Hf	4	0.450	8.881	3.769	0.000	(Wyckoff, 1963)
HfO_2		O	-2	0.450	4.440	1.884	0.000	
$HfSiO_4$	Hafnon	Hf	4	0.555	7.206	4.042	0.000	(Speer and Cooper, 1982)
$HfSiO_4$		O	-2	0.972	2.057	2.034	0.446	
$HfSiO_4$		Si	4	0.972	4.113	4.095	0.000	
$HoPO_4$	Ho-Xenotime	Ho	3	0.445	6.735	3.369	0.000	(Ni et al., 1995)
$HoPO_4$		O	-2	1.225	1.633	2.110	0.788	
$HoPO_4$		P	5	1.225	4.083	5.070	0.000	
K_2CrO_4	Tarapacaite	Cr	6	1.462	4.103	5.880	0.012	(McGinnety, 1972)
K_2CrO_4		K	1	0.182	5.487	0.879	0.126	
K_2CrO_4		K	1	0.159	6.289	1.132	0.041	
K_2CrO_4		O	-2	1.462	1.368	1.943	1.462	
K_2CrO_4		O	-2	1.421	1.407	1.988	1.421	
K_2CrO_4		O	-2	1.443	1.386	1.980	1.443	
K_2O	N/A	K	1	0.144	6.957	0.580	0.000	(Wyckoff, 1963)
K_2O		O	-2	0.144	13.913	1.160	0.000	
K_2SO_4	Arcanite	K	1	0.167	6.004	1.009	0.092	(McGinnety, 1972)
K_2SO_4		K	1	0.165	6.065	1.173	0.038	
K_2SO_4		O	-2	1.515	1.320	1.989	1.515	
K_2SO_4		O	-2	1.468	1.362	2.068	1.468	
K_2SO_4		O	-2	1.470	1.361	2.042	1.470	
K_2SO_4		S	6	1.515	3.959	5.958	0.030	
α-KNO_3	N/A	K	1	0.131	7.649	1.096	0.012	(Nimmo and Lucas, 1973)

α-KNO_3		N	5	1.635	3.058	4.952	0.042	
α-KNO_3		O	-2	1.635	1.223	2.012	1.635	
α-KNO_3		O	-2	1.616	1.237	2.018	1.616	
$Li_2B_4O_7$	Diomignite	B	3	0.992	3.024	3.020	0.098	(Krogh-Moe, 1962)
$Li_2B_4O_7$		B	3	0.834	3.598	2.557	0.756	
$Li_2B_4O_7$		Li	1	0.394	2.539	1.066	0.247	
$Li_2B_4O_7$		O	-2	0.960	2.082	1.734	1.089	
$Li_2B_4O_7$		O	-2	0.865	2.313	1.880	0.882	
$Li_2B_4O_7$		O	-2	0.992	2.016	2.160	0.901	
$Li_2B_4O_7$		O	-2	0.739	2.706	1.739	0.854	
Li_2CO_3	Zabuyelite	C	4	1.340	2.984	4.012	0.065	(Idemoto et al., 1998)
Li_2CO_3		Li	1	0.244	4.101	1.030	0.029	
Li_2CO_3		O	-2	1.340	1.492	1.999	1.340	
Li_2CO_3		O	-2	1.276	1.568	2.036	1.276	
Li_2O_2	N/A	Li	1	0.201	4.987	0.878	0.000	(Wyckoff, 1963)
Li_2O_2		O	-2	0.201	9.974	1.756	0.000	
Li_3PO_4	Lithiophosphate	Li	1	0.240	4.170	1.035	0.039	(Baur, 1980)
Li_3PO_4		Li	1	0.220	4.539	0.986	0.097	
Li_3PO_4		O	-2	1.173	1.705	1.944	1.173	
Li_3PO_4		O	-2	1.165	1.717	1.958	1.165	
Li_3PO_4		O	-2	1.193	1.677	2.026	1.193	
Li_3PO_4		P	5	1.193	4.192	4.814	0.047	
$LuPO_4$	Lu-Xenotime	Lu	3	0.446	6.721	3.336	0.000	(Ni et al., 1995)
$LuPO_4$		O	-2	1.219	1.640	2.101	0.784	
$LuPO_4$		P	5	1.219	4.100	5.070	0.000	
$Mg_2B_2O_5$	Suanite	B	3	1.069	2.807	2.965	0.133	(G-C et al., 1995)
$Mg_2B_2O_5$		B	3	1.018	2.948	2.946	0.092	
$Mg_2B_2O_5$		Mg	2	0.353	5.667	2.034	0.048	
$Mg_2B_2O_5$		Mg	2	0.376	5.312	2.030	0.091	
$Mg_2B_2O_5$		O	-2	1.069	1.871	1.929	0.624	

$Mg_2B_2O_5$		O	-2	0.955	2.095	1.973	0.514	
$Mg_2B_2O_5$		O	-2	1.018	1.965	1.927	0.732	
$Mg_2B_2O_5$		O	-2	1.014	1.971	1.994	0.570	
$Mg_2B_2O_5$		O	-2	0.861	2.323	2.152	0.387	
Mg_2SiO_4	Forsterite	Mg	2	0.319	6.261	1.999	0.000	(Smyth and Hazen, 1973)
Mg_2SiO_4		Mg	2	0.330	6.056	1.879	0.031	
Mg_2SiO_4		O	-2	0.985	2.031	2.002	0.529	
Mg_2SiO_4		O	-2	0.901	2.219	1.997	0.718	
Mg_2SiO_4		O	-2	0.939	2.130	1.906	0.759	
Mg_2SiO_4		Si	4	0.985	4.063	3.933	0.211	
$Mg_3B_2O_6$	Kotoite	B	3	0.953	3.149	2.914	0.103	(Effenberger and Pertlik, 1984)
$Mg_3B_2O_6$		Mg	2	0.317	6.300	2.080	0.000	
$Mg_3B_2O_6$		Mg	2	0.332	6.029	1.995	0.025	
$Mg_3B_2O_6$		O	-2	0.953	2.100	1.990	0.547	
$Mg_3B_2O_6$		O	-2	0.914	2.188	1.979	0.689	
$Mg_3(PO_4)_2$	Farringtonite	Mg	2	0.394	5.074	1.917	0.139	(Nord and Kierkegaard, 1968)
$Mg_3(PO_4)_2$		Mg	2	0.342	5.848	1.892	0.000	
$Mg_3(PO_4)_2$		O	-2	1.216	1.645	1.937	0.951	
$Mg_3(PO_4)_2$		O	-2	1.295	1.545	2.021	1.040	
$Mg_3(PO_4)_2$		O	-2	1.217	1.643	1.909	1.235	
$Mg_3(PO_4)_2$		O	-2	1.237	1.616	2.070	0.771	
$Mg_3(PO_4)_2$		P	5	1.295	3.862	5.073	0.026	
$MgCO_3$	Magnesite	C	4	1.279	3.127	4.078	0.000	(Ross, 1997)
$MgCO_3$		Mg	2	0.300	6.667	2.112	0.000	
$MgCO_3$		O	-2	1.279	1.564	2.063	1.279	
MgO	Periclase	Mg	2	0.297	6.733	1.943	0.000	(Hazen, 1976)
MgO		O	-2	0.297	6.733	1.943	0.000	
$MgSiO_3$	Enstatite	Mg	2	0.362	5.523	2.095	0.091	(Hugh-Jones and Angel, 1994)

$MgSiO_3$		Mg	2	0.371	5.391	1.925	0.237	
$MgSiO_3$		O	-2	1.003	1.994	2.014	0.530	
$MgSiO_3$		O	-2	1.027	1.947	1.875	0.712	
$MgSiO_3$		O	-2	0.915	2.185	2.129	0.692	
$MgSiO_3$		O	-2	0.982	2.036	1.994	0.495	
$MgSiO_3$		O	-2	1.034	1.935	1.875	0.624	
$MgSiO_3$		O	-2	0.866	2.309	2.037	0.747	
$MgSiO_3$		Si	4	1.027	3.895	3.998	0.105	
$MgSiO_3$		Si	4	1.034	3.869	3.905	0.094	
$MgTiO_3$	Geikielite	Mg	2	0.353	5.670	1.983	0.056	(Liferovich and Mitchell, 2006)
$MgTiO_3$		O	-2	0.762	2.626	1.999	0.425	
$MgTiO_3$		Ti	4	0.762	5.246	4.016	0.035	
$MnCO_3$	Rhodochrosite	C	4	1.281	3.122	4.023	0.000	(Maslen et al., 1995)
$MnCO_3$		Mn	2	0.310	6.455	2.123	0.000	
$MnCO_3$		O	-2	1.281	1.561	2.049	1.281	
MnO_2	Pyrolusite	Mn	4	0.698	5.734	4.278	0.000	(Wyckoff, 1963)
MnO_2		O	-2	0.698	2.867	2.139	0.181	
$MnWO_4$	Hubnerite	Mn	2	0.371	5.388	2.143	0.073	(Macavei and Schulz, 1993)
$MnWO_4$		O	-2	0.988	2.025	2.020	0.667	
$MnWO_4$		O	-2	1.357	1.474	2.031	1.357	
$MnWO_4$		W	6	1.357	4.421	5.960	0.381	
MoO_2	N/A	Mo	4	0.682	5.864	4.194	0.165	(Wyckoff, 1963)
MoO_2		O	-2	0.682	2.932	2.215	0.307	
MoO_2		O	-2	0.621	3.219	1.978	0.104	
MoO_3	Molybdite	Mo	6	1.742	3.444	6.010	1.511	(Sitepu et al., 2005)
MoO_3		O	-2	1.051	1.903	2.355	0.435	
MoO_3		O	-2	1.258	1.590	1.852	0.729	
MoO_3		O	-2	1.742	1.148	1.803	1.742	
Na_2CO_3	Natrite	C	4	1.394	2.869	4.182	0.084	(Zubkova et al., 2002)

Na_2CO_3		Na	1	0.200	5.006	1.255	0.000	
Na_2CO_3		Na	1	0.211	4.736	1.273	0.000	
Na_2CO_3		Na	1	0.120	8.319	0.953	0.035	
Na_2CO_3		O	-2	1.394	1.434	2.157	1.394	
Na_2CO_3		O	-2	1.332	1.502	2.085	1.332	
Na_2O	N/A	Na	1	0.175	5.724	0.721	0.000	(Wyckoff, 1963)
Na_2O		O	-2	0.175	11.449	1.441	0.000	
Na_2SO_4	Thenardite	Na	1	0.202	4.956	1.124	0.068	(Hawthorne and Ferguson, 1975)
Na_2SO_4		O	-2	1.447	1.382	2.030	1.447	
Na_2SO_4		S	6	1.447	4.147	5.873	0.000	
$Na_2Ta_4O_{11}$	Natrotantite	Na	1	0.150	6.685	0.987	0.170	(Ercit et al., 1985)
$Na_2Ta_4O_{11}$		O	-2	0.848	2.359	1.948	0.637	
$Na_2Ta_4O_{11}$		O	-2	0.758	2.639	1.989	0.018	
$Na_2Ta_4O_{11}$		O	-2	0.747	2.677	2.419	0.379	
$Na_2Ta_4O_{11}$		Ta	5	0.848	5.897	5.268	0.030	
$Na_2Ta_4O_{11}$		Ta	5	0.746	6.706	4.717	0.000	
$NaNbO_3$	Lueshite	Na	1	0.173	5.766	1.203	0.237	(Seidel and Hoffmann, 1976)
$NaNbO_3$		Na	1	0.173	5.766	1.203	0.237	
$NaNbO_3$		Nb	5	1.005	4.974	4.956	0.313	
$NaNbO_3$		Nb	5	1.005	4.974	4.956	0.313	
$NaNbO_3$		O	-2	1.005	1.990	2.053	0.526	
$NaNbO_3$		O	-2	1.005	1.990	2.053	0.526	
$NaNbO_3$		O	-2	1.005	1.990	2.053	0.526	
$NaNbO_3$		O	-2	1.005	1.990	2.053	0.526	
$NaNO_3$	Nitratine	N	5	1.632	3.063	5.012	0.000	(Paul and Pryor, 1972)
$NaNO_3$		Na	1	0.175	5.725	1.205	0.000	
$NaNO_3$		O	-2	1.632	1.225	2.072	1.632	
NiO	Bunsenite	Ni	2	0.306	6.542	1.934	0.000	(Wyckoff, 1963)
NiO		O	-2	0.306	6.542	1.934	0.000	

OsO_2	(Rutile structure)	O	-2	0.659	3.036	2.033	0.073	(Baur and Khan, 1971)
OsO_2		Os	4	0.659	6.072	4.066	0.000	
P_2O_5	N/A	O	-2	1.132	1.766	2.322	0.684	(Stachel et al., 1995)
P_2O_5		O	-2	1.473	1.358	1.660	1.413	
P_2O_5		O	-2	1.521	1.315	1.629	1.519	
P_2O_5		O	-2	1.127	1.775	2.285	0.770	
P_2O_5		P	5	1.473	3.395	5.087	0.083	
P_2O_5		P	5	1.521	3.286	5.094	0.002	
$Pb_2As_2O_5$	Paulmooreite	As	3	1.050	2.856	3.023	1.466	(Araki et al., 1980)
$Pb_2As_2O_5$		As	3	1.088	2.756	2.986	1.426	
$Pb_2As_2O_5$		O	-2	1.042	1.919	2.081	0.718	
$Pb_2As_2O_5$		O	-2	1.050	1.904	2.026	0.679	
$Pb_2As_2O_5$		O	-2	0.864	2.314	1.940	0.808	
$Pb_2As_2O_5$		O	-2	0.988	2.024	1.983	0.663	
$Pb_2As_2O_5$		O	-2	1.088	1.838	1.925	0.735	
$Pb_2As_2O_5$		Pb	2	0.520	3.843	2.001	0.939	
$Pb_2As_2O_5$		Pb	2	0.573	3.492	1.946	0.890	
Pb_2OCrO_4	Phoenicochroite	Cr	6	1.448	4.144	5.618	0.205	(Williams et al., 1970)
Pb_2OCrO_4		O	-2	1.275	1.569	1.949	1.063	
Pb_2OCrO_4		O	-2	1.267	1.578	1.887	0.889	
Pb_2OCrO_4		O	-2	1.448	1.381	1.968	1.448	
Pb_2OCrO_4		O	-2	0.567	3.529	2.150	0.077	
Pb_2OCrO_4		Pb	2	0.567	3.529	2.236	0.912	
Pb_2OCrO_4		Pb	2	0.483	4.138	2.068	0.861	
Pb_2OSO_4	Lanarkite	O	-2	1.545	1.295	2.054	1.545	(Sahl, 1970)
Pb_2OSO_4		O	-2	1.420	1.409	1.892	1.420	
Pb_2OSO_4		O	-2	1.504	1.330	2.025	1.504	
Pb_2OSO_4		O	-2	0.524	3.814	2.101	0.006	
Pb_2OSO_4		Pb	2	0.524	3.814	2.095	0.883	
Pb_2OSO_4		Pb	2	0.515	3.887	1.930	0.820	

Pb_2OSO_4		S	6	1.545	3.884	5.939	0.089	
$Pb_2V_2O_7$	Chervetite	O	-2	1.157	1.729	1.922	1.055	(Kawahara, 1967)
$Pb_2V_2O_7$		O	-2	1.103	1.813	1.839	1.066	
$Pb_2V_2O_7$		O	-2	0.847	2.360	1.451	0.847	
$Pb_2V_2O_7$		O	-2	0.970	2.061	2.196	0.930	
$Pb_2V_2O_7$		O	-2	1.148	1.742	2.078	0.778	
$Pb_2V_2O_7$		O	-2	1.263	1.584	1.784	1.263	
$Pb_2V_2O_7$		O	-2	1.331	1.503	2.223	1.083	
$Pb_2V_2O_7$		Pb	2	0.399	5.012	1.876	0.401	
$Pb_2V_2O_7$		Pb	2	0.589	3.396	2.253	0.360	
$Pb_2V_2O_7$		V	5	1.157	4.322	4.348	0.109	
$Pb_2V_2O_7$		V	5	1.331	3.757	5.017	0.485	
$PbCO_3$	Cerussite	C	4	1.301	3.075	3.975	0.100	(Antao and Hassan, 2009)
$PbCO_3$		O	-2	1.274	1.570	1.938	1.274	
$PbCO_3$		O	-2	1.301	1.537	2.010	1.301	
$PbCO_3$		Pb	2	0.263	7.616	1.983	0.076	
$PbCrO_4$	Crocoite	Cr	6	1.548	3.875	5.999	0.290	(Quareni and De Pieri, 1965)
$PbCrO_4$		O	-2	1.548	1.292	2.206	1.548	
$PbCrO_4$		O	-2	1.360	1.470	1.978	1.360	
$PbCrO_4$		O	-2	1.396	1.433	1.953	1.396	
$PbCrO_4$		O	-2	1.381	1.449	1.997	1.381	
$PbCrO_4$		Pb	2	0.310	6.442	2.135	0.284	
$PbMoO_4$	Wulfenite	Mo	6	1.430	4.194	5.932	0.000	(Lugli et al., 1999)
$PbMoO_4$		O	-2	1.430	1.398	2.001	1.430	
$PbMoO_4$		Pb	2	0.254	7.863	2.071	0.000	
PbO	Litharge	Pb	2	0.507	3.948	2.066	1.025	(Boher et al., 1985)
PbO		O	-2	0.507	3.948	2.066	0.000	
PbO	Massicot	Pb	2	0.626	3.195	1.997	1.028	(Hill, 1985)
PbO		O	-2	0.626	3.195	1.997	0.386	
PbO_2	Plattnerite	O	-2	0.701	2.853	2.116	0.183	(Baur and Khan, 1971)

PbO_2		Pb	4	0.701	5.706	4.232	0.000	
PbO_2	Scrutinyite	O	-2	0.686	2.917	2.099	0.290	(Wyckoff, 1963)
PbO_2		Pb	4	0.686	5.834	4.198	0.466	
$PbSB_2O_6$	Rosiaite	O	-2	0.797	2.511	1.937	0.754	(Basso et al., 1996)
$PbSB_2O_6$		Pb	2	0.290	6.889	1.930	0.000	
$PbSB_2O_6$		Sb	5	0.797	6.277	4.843	0.001	
$PbSeO_3$	Molybdomenite	O	-2	1.346	1.486	1.818	1.346	(Pasero and Rotiroti, 2003)
$PbSeO_3$		O	-2	1.182	1.691	1.902	1.076	
$PbSeO_3$		Pb	2	0.305	6.563	1.742	0.366	
$PbSeO_3$		Se	4	1.346	2.973	3.880	1.698	
$PbSiO_3$	Alamosite	O	-2	0.950	2.106	2.056	0.000	(Boucher and Peacor, 1968)
$PbSiO_3$		O	-2	0.920	2.173	2.024	0.789	
$PbSiO_3$		O	-2	0.998	2.004	2.080	0.459	
$PbSiO_3$		O	-2	1.015	1.970	2.043	0.804	
$PbSiO_3$		O	-2	0.965	2.072	1.979	0.532	
$PbSiO_3$		O	-2	0.941	2.125	1.907	0.435	
$PbSiO_3$		O	-2	1.001	1.997	1.928	0.679	
$PbSiO_3$		O	-2	0.971	2.060	1.822	0.685	
$PbSiO_3$		O	-2	0.973	2.056	2.018	0.465	
$PbSiO_3$		O	-2	0.956	2.093	1.953	0.738	
$PbSiO_3$		Pb	2	0.551	3.628	1.867	0.856	
$PbSiO_3$		Pb	2	0.615	3.250	2.210	1.054	
$PbSiO_3$		Pb	2	0.517	3.870	1.998	0.858	
$PbSiO_3$		Si	4	0.965	4.144	3.798	0.107	
$PbSiO_3$		Si	4	1.001	3.994	3.871	0.116	
$PbSiO_3$		Si	4	1.015	3.940	4.026	0.118	
$PbSO_3$	Scotlandite	O	-2	1.375	1.454	1.909	1.375	(Pertlik and Zemann, 1985)
$PbSO_3$		O	-2	1.305	1.533	1.983	1.305	
$PbSO_3$		Pb	2	0.275	7.279	1.773	0.297	
$PbSO_3$		S	4	1.375	2.909	4.101	1.685	

$PbSO_4$	Anglesite	O	-2	1.508	1.326	1.969	1.508	(Jacobsen et al., 1998)
$PbSO_4$		O	-2	1.468	1.362	1.973	1.468	
$PbSO_4$		O	-2	1.424	1.404	2.006	1.424	
$PbSO_4$		Pb	2	0.256	7.820	1.992	0.195	
$PbSO_4$		S	6	1.508	3.978	5.961	0.018	
$PbTiO_3$	Macedonite	O	-2	0.919	2.176	1.891	0.653	(Glazer and Mabud, 1978)
$PbTiO_3$		O	-2	0.602	3.322	2.006	0.200	
$PbTiO_3$		Pb	2	0.315	6.359	2.198	0.684	
$PbTiO_3$		Ti	4	0.919	4.351	3.704	0.259	
$PbWO_4$	Raspite	O	-2	0.966	2.071	1.920	0.970	(Fujita et al., 1977)
$PbWO_4$		O	-2	0.855	2.340	2.084	0.424	
$PbWO_4$		O	-2	1.494	1.339	2.001	1.494	
$PbWO_4$		O	-2	1.217	1.644	1.931	0.963	
$PbWO_4$		Pb	2	0.506	3.955	2.157	0.505	
$PbWO_4$		W	6	1.494	4.017	5.780	0.543	
$PbWO_4$	Stolzite	O	-2	1.386	1.443	1.948	1.386	(Chipaux et al., 2001)
$PbWO_4$		Pb	2	0.253	7.903	2.018	0.000	
$PbWO_4$		W	6	1.386	4.330	5.776	0.000	
Rb_2O	N/A	O	-2	0.133	15.014	1.071	0.000	(Wyckoff, 1963)
Rb_2O		Rb	1	0.133	7.507	0.535	0.000	
ReO_2	N/A	O	-2	0.732	2.734	2.221	0.302	(Wyckoff, 1963)
ReO_2		Re	4	0.732	5.468	4.442	0.084	
RuO_2	(Rutile structure)	O	-2	0.718	2.787	2.155	0.097	(Baur and Khan, 1971)
RuO_2		Ru	4	0.718	5.574	4.310	0.000	
Sb_2O_3	Senarmontite	O	-2	0.874	2.289	1.972	0.705	(Svensson, 1975)
Sb_2O_3		Sb	3	0.874	3.433	2.958	1.348	
Sb_2O_5	N/A	Sb	5	1.009	4.956	5.050	0.306	(Jansen, 1979)
Sb_2O_5		O	-2	0.695	2.876	1.984	0.246	
Sb_2O_5		O	-2	1.009	1.982	2.062	0.684	
Sb_2O_5		O	-2	0.965	2.073	2.009	0.831	

Sb_2VO_5	Stibivanite	O	-2	1.383	1.447	1.580	1.383	(Merlino et al., 1989)
Sb_2VO_5		O	-2	0.796	2.512	2.078	0.528	
Sb_2VO_5		O	-2	0.852	2.347	1.975	0.614	
Sb_2VO_5		Sb	3	0.852	3.520	2.937	1.375	
Sb_2VO_5		V	4	1.383	2.893	3.811	0.674	
Sc_2O_3	Refined	O	-2	0.495	4.040	1.966	0.210	(Geller, 1967)
Sc_2O_3		Sc	3	0.454	6.605	2.906	0.000	
Sc_2O_3		Sc	3	0.495	6.059	2.962	0.049	
$ScPO_4$	Pretulite	O	-2	1.211	1.651	2.080	0.804	(Bernhard et al., 1998)
$ScPO_4$		P	5	1.211	4.129	5.083	0.000	
$ScPO_4$		Sc	3	0.420	7.149	3.237	0.000	
SeO_2	N/A	O	-2	1.020	1.961	2.089	0.992	(Stahl et al., 1992)
SeO_2		O	-2	1.518	1.317	1.841	1.518	
SeO_2		Se	4	1.518	2.635	3.930	1.865	
SeO_3	N/A	O	-2	1.126	1.777	2.134	1.012	(Mijlhoff, 1965)
SeO_3		O	-2	1.862	1.074	1.924	1.839	
SeO_3		O	-2	1.823	1.097	1.896	1.807	
SeO_3		Se	6	1.862	3.222	5.955	0.150	
SiO_2	Coesite	O	-2	1.030	1.941	2.112	0.000	(Levien and Prewitt, 1981)
SiO_2		O	-2	0.993	2.014	2.049	0.621	
SiO_2		O	-2	0.989	2.023	2.058	0.591	
SiO_2		O	-2	1.006	1.988	2.078	0.519	
SiO_2		O	-2	0.979	2.043	2.042	0.688	
SiO_2		Si	4	1.030	3.882	4.137	0.022	
SiO_2		Si	4	1.006	3.975	4.122	0.032	
SiO_2	Cristobalite	O	-2	1.013	1.974	2.065	0.583	(Downs and Palmer, 1994)
SiO_2		Si	4	1.013	3.949	4.131	0.037	
SiO_2	Quartz	O	-2	1.008	1.984	2.052	0.621	(Levien et al., 1980)
SiO_2		Si	4	1.008	3.967	4.105	0.028	
SiO_2	Stishovite	O	-2	0.709	2.819	2.195	0.301	(Ross et al., 1990)

SiO_2		Si	4	0.709	5.638	4.390	0.000	
SiO_2	Tridymite	O	-2	1.024	1.953	2.079	0.454	(Dollase and Baur, 1976)
SiO_2		O	-2	1.043	1.918	2.088	0.567	
SiO_2		O	-2	1.005	1.990	2.044	0.584	
SiO_2		O	-2	1.046	1.911	2.094	0.440	
SiO_2		O	-2	1.041	1.922	2.065	0.616	
SiO_2		O	-2	1.019	1.963	2.057	0.642	
SiO_2		O	-2	1.022	1.957	2.079	0.449	
SiO_2		O	-2	1.033	1.937	2.089	0.629	
SiO_2		O	-2	1.032	1.938	2.064	0.584	
SiO_2		O	-2	1.055	1.896	2.130	0.405	
SiO_2		O	-2	1.060	1.887	2.064	0.506	
SiO_2		O	-2	1.042	1.919	2.083	0.481	
SiO_2		O	-2	1.028	1.945	2.080	0.426	
SiO_2		O	-2	1.019	1.963	2.045	0.555	
SiO_2		O	-2	1.039	1.925	2.068	0.559	
SiO_2		O	-2	1.024	1.953	2.077	0.547	
SiO_2		O	-2	1.032	1.937	2.066	0.574	
SiO_2		O	-2	1.040	1.923	2.079	0.545	
SiO_2		O	-2	1.035	1.933	2.068	0.589	
SiO_2		O	-2	1.018	1.964	2.068	0.595	
SiO_2		O	-2	1.050	1.904	2.100	0.580	
SiO_2		O	-2	1.008	1.985	2.039	0.541	
SiO_2		O	-2	1.030	1.943	2.048	0.595	
SiO_2		O	-2	1.073	1.863	2.149	0.047	
SiO_2		Si	4	1.044	3.831	4.179	0.031	
SiO_2		Si	4	1.046	3.823	4.174	0.054	
SiO_2		Si	4	1.060	3.774	4.203	0.039	
SiO_2		Si	4	1.017	3.932	4.078	0.018	
SiO_2		Si	4	1.033	3.874	4.168	0.054	

SiO_2		Si	4	1.024	3.906	4.089	0.041	
SiO_2		Si	4	1.055	3.792	4.164	0.073	
SiO_2		Si	4	1.039	3.851	4.134	0.043	
SiO_2		Si	4	1.040	3.847	4.091	0.077	
SiO_2		Si	4	1.035	3.865	4.176	0.015	
SiO_2		Si	4	1.042	3.839	4.144	0.046	
SiO_2		Si	4	1.073	3.727	4.222	0.061	
SnO	Romarchite	O	-2	0.467	4.281	1.929	0.000	(Wyckoff, 1963)
SnO		Sn	2	0.467	4.281	1.929	0.969	
SnO_2	Cassiterite	O	-2	0.650	3.079	1.994	0.170	(Baur and Khan, 1971)
SnO_2		Sn	4	0.650	6.158	3.988	0.000	
$SnTa_2O_6$	Thoreaulite	O	-2	1.023	1.956	2.064	0.462	(Maksimova et al., 1975)
$SnTa_2O_6$		O	-2	0.892	2.242	1.891	0.341	
$SnTa_2O_6$		O	-2	1.090	1.834	2.073	0.584	
$SnTa_2O_6$		O	-2	0.935	2.139	1.955	0.508	
$SnTa_2O_6$		O	-2	0.832	2.402	2.054	0.151	
$SnTa_2O_6$		O	-2	0.683	2.927	2.059	0.145	
$SnTa_2O_6$		Sn	2	0.592	3.379	2.189	0.998	
$SnTa_2O_6$		Ta	5	1.090	4.586	5.035	0.332	
$SnTa_2O_6$		Ta	5	0.935	5.346	4.872	0.267	
$SrCO_3$	Strontianite	C	4	1.284	3.115	3.962	0.055	(Antao and Hassan, 2009)
$SrCO_3$		O	-2	1.281	1.561	1.968	1.281	
$SrCO_3$		O	-2	1.284	1.558	2.022	1.284	
$SrCO_3$		Sr	2	0.260	7.691	2.051	0.019	
$Sr(NO_3)_2$	N/A	N	5	1.616	3.095	4.989	0.019	(Howotny and Heger, 1983)
$Sr(NO_3)_2$		O	-2	1.616	1.238	2.003	1.616	
$Sr(NO_3)_2$		Sr	2	0.187	10.687	2.038	0.000	
$SrSO_4$	Celestite	O	-2	1.512	1.322	2.017	1.512	(Jacobsen et al., 1998)
$SrSO_4$		O	-2	1.474	1.357	1.966	1.474	
$SrSO_4$		O	-2	1.434	1.395	2.038	1.434	

$SrSO_4$		S	6	1.512	3.967	6.005	0.023	
$SrSO_4$		Sr	2	0.286	6.987	2.054	0.159	
$SrTiO_3$	Tausonite	O	-2	0.635	3.151	2.004	0.000	(Mitchell et al., 2000)
$SrTiO_3$		Sr	2	0.169	11.819	2.078	0.000	
$SrTiO_3$		Ti	4	0.635	6.303	3.933	0.000	
TbO_2	(Flourite structure)	O	-2	0.547	3.655	2.295	0.000	(Wyckoff, 1963)
TbO_2		Tb	4	0.547	7.310	4.590	0.000	
$TbPO_4$	Tb-Xenotime	O	-2	1.213	1.648	2.061	0.798	(Ni et al., 1995)
$TbPO_4$		P	5	1.213	4.121	5.015	0.000	
$TbPO_4$		Tb	3	0.422	7.115	3.230	0.000	
TeO_2	Paratellurite	O	-2	0.825	2.424	1.839	0.659	(Wyckoff, 1963)
TeO_2		Te	4	0.825	4.849	3.678	0.923	
TeO_2	Tellurite	O	-2	1.208	1.656	1.980	1.219	(Beyer, 1967)
TeO_2		O	-2	1.067	1.875	1.922	0.722	
TeO_2		Te	4	1.208	3.312	3.902	1.560	
TiO_2	Anatase	O	-2	0.659	3.035	2.035	0.329	(Horn et al., 1972)
TiO_2		Ti	4	0.659	6.069	4.069	0.000	
TiO_2	Brookite	O	-2	0.759	2.636	2.074	0.393	(Meagher and Lager, 1979)
TiO_2		O	-2	0.673	2.972	2.024	0.139	
TiO_2		Ti	4	0.759	5.271	4.098	0.161	
TiO_2	Rutile	O	-2	0.642	3.117	2.058	0.235	(Meagher and Lager, 1979)
TiO_2		Ti	4	0.642	6.235	4.115	0.000	
$TiTe_3O_8$	Winstanleyite	O	-2	1.237	1.617	2.037	0.873	(Bindi and Cipriani, 2003)
$TiTe_3O_8$		O	-2	0.670	2.984	2.094	0.359	
$TiTe_3O_8$		Te	4	1.237	3.233	4.147	1.818	
$TiTe_3O_8$		Ti	4	0.631	6.337	3.972	0.000	
Tl_2O_3	Avicennite	O	-2	0.672	2.975	2.202	0.162	(Otto et al., 1993)
Tl_2O_3		Tl	3	0.541	5.541	3.272	0.000	
Tl_2O_3		Tl	3	0.672	4.463	3.313	0.083	
$TmPO_4$	Tm-Xenotime	O	-2	1.163	1.720	2.088	0.703	(Ni et al., 1995)

$TmPO_4$		P	5	1.163	4.299	4.834	0.000	
$TmPO_4$		Tm	3	0.476	6.297	3.516	0.000	
VO	N/A	O	-2	0.405	4.939	2.623	0.000	(Wyckoff, 1963)
VO		V	2	0.405	4.939	2.623	0.000	
VO_2	N/A	O	-2	0.771	2.593	2.130	0.580	(Wyckoff, 1963)
VO_2		O	-2	0.971	2.060	2.133	0.314	
VO_2		V	4	0.971	4.119	4.263	0.332	
WO_3	N/A	O	-2	0.898	2.227	1.827	0.000	(Gerand et al., 1979)
WO_3		O	-2	1.050	1.904	2.127	0.535	
WO_3		W	6	1.050	5.712	6.080	0.000	
Y_2O_3	N/A	O	-2	0.490	4.081	1.880	0.181	(Baldinozzi et al., 1998)
Y_2O_3		Y	3	0.490	6.121	2.822	0.067	
Y_2O_3		Y	3	0.452	6.641	2.816	0.000	
YPO_4	Y-Xenotime	O	-2	1.202	1.664	2.082	0.783	(Ni et al., 1995)
YPO_4		P	5	1.202	4.160	4.976	0.000	
YPO_4		Y	3	0.429	6.997	3.351	0.000	
$YTaO_4$	Formanite	O	-2	0.721	2.775	2.066	0.377	(Wolten, 1967)
$YTaO_4$		O	-2	0.871	2.295	1.930	0.522	
$YTaO_4$		Ta	5	0.871	5.738	4.672	0.129	
$YTaO_4$		Y	3	0.484	6.194	3.321	0.103	
Zn_2SiO_4	Willemite	O	-2	0.932	2.147	1.977	0.379	(Klaska et al., 1978)
Zn_2SiO_4		O	-2	0.956	2.093	1.985	0.422	
Zn_2SiO_4		O	-2	0.922	2.168	1.891	0.418	
Zn_2SiO_4		O	-2	0.953	2.098	1.972	0.416	
Zn_2SiO_4		Si	4	0.956	4.186	3.846	0.082	
Zn_2SiO_4		Zn	2	0.484	4.130	2.013	0.096	
Zn_2SiO_4		Zn	2	0.490	4.084	1.967	0.061	
$Zn_3(AsO_3)_2$	Reinerite	As	3	1.036	2.895	3.060	1.465	(Ghose et al., 1977)
$Zn_3(AsO_3)_2$		As	3	0.992	3.025	3.018	1.499	
$Zn_3(AsO_3)_2$		O	-2	1.036	1.930	1.971	0.448	

$Zn_3(AsO_3)_2$		O	-2	0.986	2.029	1.956	0.593	
$Zn_3(AsO_3)_2$		O	-2	0.988	2.024	1.983	0.430	
$Zn_3(AsO_3)_2$		O	-2	0.991	2.019	1.996	0.482	
$Zn_3(AsO_3)_2$		Zn	2	0.499	4.006	1.911	0.076	
$Zn_3(AsO_3)_2$		Zn	2	0.480	4.162	1.949	0.024	
$ZnAl_2O_4$	Gahnite	Al	3	0.478	6.277	2.983	0.000	(Popovic et al., 2009)
$ZnAl_2O_4$		O	-2	0.478	4.184	2.013	0.247	
$ZnAl_2O_4$		Zn	2	0.476	4.198	2.084	0.000	
$ZnAs_2O_4$	Leiteite	As	3	1.074	2.792	3.028	1.488	(Ghose et al., 1987)
$ZnAs_2O_4$		As	3	1.113	2.696	3.068	1.503	
$ZnAs_2O_4$		O	-2	0.900	2.222	1.960	0.865	
$ZnAs_2O_4$		O	-2	0.901	2.220	1.952	0.883	
$ZnAs_2O_4$		O	-2	1.074	1.861	2.010	0.622	
$ZnAs_2O_4$		O	-2	1.113	1.797	2.027	0.655	
$ZnAs_2O_4$		Zn	2	0.468	4.273	1.853	0.057	
$ZnCO_3$	Smithsonite	C	4	1.285	3.112	4.092	0.000	(Graf, 1961b)
$ZnCO_3$		O	-2	1.285	1.556	2.061	0.968	
$ZnCO_3$		Zn	2	0.322	6.209	2.092	0.000	
$ZnCr_2O_4$	Zincochromite	Cr	3	0.507	5.914	3.155	0.000	(Levy et al., 2005)
$ZnCr_2O_4$		O	-2	0.507	3.943	1.992	0.369	
$ZnCr_2O_4$		Zn	2	0.381	5.255	1.658	0.000	
$ZnMn_2O_4$	Hetaerolite	Mn	3	0.571	5.255	3.000	0.000	(Nogues and Poix, 1972)
$ZnMn_2O_4$		O	-2	0.571	3.503	1.950	0.423	
$ZnMn_2O_4$		Zn	2	0.419	4.779	1.803	0.000	
ZnO	Zincite	O	-2	0.452	4.429	1.859	0.014	(Kihara and Donnay, 1985)
ZnO		Zn	2	0.452	4.429	1.859	0.014	
$ZnSB_2O_6$	Ordonezite	O	-2	0.822	2.433	2.053	0.666	(Ercit et al., 2002)
$ZnSB_2O_6$		O	-2	0.884	2.263	2.066	0.362	
$ZnSB_2O_6$		Sb	5	0.884	5.659	5.083	0.079	
$ZnSB_2O_6$		Zn	2	0.353	5.670	2.202	0.000	

ZrO_2	(Cubic Zirconia)	O	-2	0.489	4.088	2.054	0.000	(Wyckoff, 1963)
ZrO_2		Zr	4	0.489	8.176	4.109	0.000	
ZrO_2	(Orthorhombic zirconia)	O	-2	0.657	3.046	1.941	0.049	(Kisi, 1989)
ZrO_2		O	-2	0.582	3.437	2.084	0.182	
ZrO_2		Zr	4	0.657	6.091	4.025	0.152	
$ZrSiO_4$	N/A	O	-2	0.968	2.067	2.050	0.437	(Kolesov et al., 2001)
$ZrSiO_4$		Si	4	0.968	4.134	4.069	0.000	
$ZrSiO_4$		Zr	4	0.561	7.127	4.130	0.000	

REFERENCES

Åhman, J., Svensson, G., and Albertsson, J. (1996) A Reinvestigation of \b-Gallium Oxide. Acta Crystallographica C, 52, 1336-1338.

Antao, S.M. and Hassan, I. (2009) The orthorhombic structure of CaCO3, SrCO3, PbCO3 and BaCO3: Linear structural trends Note: HRPXRD. The Canadian Mineralogist 47, 1245-1255.

Antoa, S.M. and Hassan, I. (2009) The orthorhombic structure of CaCO3, SrCO3, PbCO3 and BaCO3: Linear structural trends. The Canadian Mineralogist, 47, 1245-1255.

Araki, T., Moore, P.B., and Brunton, G.D. (1980) The crystal structure of paulmooreite, Pb2[As2O5]: dimeric arsenite groups. American Mineralogist, 65, 340-345.

Baldinozzi, G., Berar, J.F., and Calvarin, G. (1998) Rietveld refinement of two-phase Zr-doped Y_2O_3. Materials Science Forum, 278, 680-685.

Basso, R., Lucchetti, G., Zefiro, L., and Palenzona, A. (1996) Rosiaite, PbSb2O6, a new mineral from the Cetine mine, Siena, Italy. European Journal of Mineralogy, 8, 487-492.

Baur, W.H. (1980) Solid solutions between octahedral and tetrahedral olivine types in Li-Zn-germanates Note: this is the quenchable high-temperature form. Inorganic and Nuclear Chemistry Letters, 16, 525-527.

Baur, W.H. and Khan, A.A. (1971) Rutile-type compounds. VI. SiO_2, GeO_2, and a comparison with other rutile-type structures. Acta Crystallographica, 27B, 2133-2139.

Bedlivy, D. and Mereiter, K. (1982) Structure of alpha-BiAsO4 (rooseveltite). Acta Crystallographica,, Section B, 1559-1561.

Bernhard, F., Walter, F., Ettinger, K., Taucher, J., and Mereiter, K. (1998) Pretulite, ScPO4, a new scandium mineral from the Styrian and Lower Austrian lazulite occurrences, Austria. American Mineralogist 83, 625-630.

Beyer, H. (1967) Verfeinerung der kristallstruktur von tellurit, dem rhomischen TeO_2. Zeitschrift für Kristallographie, 124, 228-237.

Bezou, C., Nonat, A., Mutin, J.C., Christensen, A.N., and Lehmann, M.S. (1995) Of the crystal structure of gamma-CaSO4, CaSO4*0.5(H2O), and CaSO4*0.6(H2O) by powder diffraction methods. Journal of Solid State Chemistry 117, 165-176.

Bindi, L. and Cipriani, C. (2003) The crystal structure of winstanleyite, TiTe3O8, from the Grand Central Mine, Tombstone, Arizona. The Canadian Mineralogist 41, 1469-1473.

Blake, R.L., Hessevick, R.E., Zoltai, T., and Finger, L.W. (1966) Refinement of the hematite structure. American Mineralogist, 51, 123-129.

Blower, S.K. and Greaves, C. (1988) The structure of beta-Bi_2O_3 from powder neutron diffraction data. Acta Crystallographica, C44, 587-589.

Bodenstein, D., Brehm, A., Jones, P.G., Schwarzmann, E., and Sheldrick, G.M. (1983) Darstellung und kristallstruktur von monoklinem arsen(III)antimon(III)oxid, AsSbO3. Zeitschrift fur Naturforschung, 901-904.

Boher, P., Garnier, P., Gavarri, J.R., and Hewat, A.W. (1985) Monoxyde quadratique PbO alpha(I): Description de la transition structurale ferroelastique Method: X-ray Diffraction; in the four-circle diffractometer T = 295 K. Journal of Solid State Chemistry, 57, 343-350.

Boucher, M.L. and Peacor, D.R. (1968) The crystal structure of alamosite, PbSiO3. Zeitschrift fur Kristallographie, 126, 98-111.

Brahim, A., Mongi, F.M., and Amor, H. (2002) Cerium arsenate, CeAsO4. Acta Crystallographica, Section E.

Bromiley, F.A., Boffa Ballaran, T., Langenhorst, F., and Seifert, F. (2007) Order and miscibility in the otavite - magnesite solid solution Sample: X_Mg = 0, synthesized at 600 C, 1 GPa, 3 h. American Mineralogist, 92, 829-836.

Chipaux, R., Andre, G., and Cousson, A. (2001) Crystal structure of lead tungstate at 1.4 and 300 K Sample: .Top. at T = 290 K Note: Scheelite structure. Journal of Alloys and Compounds, 325, 91-94.

Christidis, P.C. and Rentzeperis, P.J. (1976) The crystal structure of rhombohedral $Fe_2(SO_4)_3$ Sample: synthetic. Zeitschrift fur Kristallographie 144, 341-352.

Comodi, P., Zanazzi, P.F., Poli, S., and Schmidt, M.W. (1997) High-pressure behavior of kyanite: Compressibility and structural deformation Sample: P = 0.001 kbar, in air. American Mineralogist, 82, 452-459.

Dollase, W.A. and Baur, W.H. (1976) The superstructure of meteoritic low tridymite solved by computer simulation. American Mineralogist, 61, 971-978.

Downs, R.T. and Palmer, D.C. (1994) The pressure behavior of alpha cristobalite. American Mineralogist, 79, 9-14.

Dreyer, G. and Tillmanns, E. (1981) Dreyerite: ein naturliches, tetragonales wismutvanadat von Hirschhorn/Pfalz. Neues Jahrbuch fur Mineralogie, Monatshefte, 1981, 151-154.

Effenberger, H. and Pertlik, F. (1984) Verfeinerung der kristallstrukturen der isotypen verbindungen M3(BO3)2 mit M=Mg, Co und Ni (strukturtyp: kotoit). Zeitschrift fur Kristallographie, 166, 129-140.

Ercit, T.S., Hawthorne, F.C., and Cerny, P. (1985) The crystal structure of synthetic natrotantite. Bulletin de Mineralogie, 108, 541-549.

Ercit, T.S., Hawthorne, F.C., and Cerny, P. (1992) The crystal structure of alumotantite: Its relation to the structures of simpsonite and the (Al,Ga)(Ta,Nb)O4 compounds. The Canadian Mineralogist, 30, 653-662.
Ercit, T.S., Foord, E.E., and Fitzpatrick, J.J. (2002) Ordonezite from the Theodoso Soto Mine, Sapioris, Durango, Mexico: New data and structure refinement. The Canadian Mineralogist, 40, 1207-1210.
Fiquet, G., Richet, P., and Montagnac, G. (1999) High-temperature thermal expansion of lime, periclase, corundum, and spinel. Physics and Chemistry of Minerals, 27, 103-111.
Fischer, R. and Pertlik, F. (1975) Verfeinerung der kristallstruktur des schafarzikites, FeSb2O4. Tschermaks Mineralogische und Petrographische Mitteilungen, 22, 236-241.
Fujita, T., Kawada, I., and Kato, K. (1977) Raspite from Broken Hill. Acta Crystallographica, Section B, 162-164.
G-C, G., W-D, C., J-T, C., H-H, Z., J-S, H., and Q-E, Z. (1995) Monoclinic Mg2B2O5. Acta Crystallographica, Section C, 2469-2471.
Garcia-Munoz, J.L., Rodriguez-Carvajal, J., Sapina, F., Sanchis, M.J., Ibanez, R., and Beltran-Porter, D. (1990) Crystal and magnetic structures of Bi2CuO4 Sample: T = 290 K. Journal of Physics: Condensed Matter, 2, 2205-2214.
Geller, S.R., P.; Remeika, J. P. (1967) Refinement of the structure of scandium sesquioxide. Zeitschrift fur Kristallographie 124, 136-142.
Gerand, B., Nowogrocki, G., Guenot, J., and Figlarz, M. (1979) Structural study of a new hexagonal form of tungsten trioxide. Journal of Solid State Chemistry, 29, 429-434.
Ghose, S., Sen Gupta, P.K., and Schlemper, E.O. (1987) Leiteite, ZnAs2O4: A novel type of tetrahedral layer structure with arsenite chains. American Mineralogist, 72, 629-632.
Ghose, S., Boving, P., LaChapelle, W.A., and Wan, C. (1977) Reinerite, Zn3(AsO3)2: an arsenite with a novel type of Zn-tetrahedral double chain. American Mineralogist, 62, 1129-1134.
Glazer, A.M. and Mabud, S.A. (1978) Powder profile refinement of lead zirconate titanate at several temperatures. II. Pure PbTiO3 Sample: T = 25 C. Acta Crystallographica, Section B.
Goodwin, D.W. and Lindop, A.J. (1970) The crystal structure of CaO.2Al2O3. Acta Crystallographica, Section B.
Graf, D.L. (1961a) Crystallographic tables for the rhombohedral carbonates. American Mineralogist, 46.
Graf, D.L. (1961b) Crystallographic tables for the rhombohedral carbonates. American Mineralogist, 43, 1283-1316.
Haines, J., Leger, J.M., Chateau, C., and Pereira, A.S. (2000) Structural evolution of rutile-type and $CaCl_2$-type germanium dioxide at high pressure. Physics and Chemistry of Minerals, 27, 575-582.
Hanke, K., Kupcik, V., and Lindqvist, O. (1973) The crystal structure of CuTe2O5. Acta Crystallographica, Section B.
Hawthorne, F.C. and Ferguson, R.B. (1975) Anhydrous sulphates. I: Refinement of the crystal structure of celestite with an appendix on the structure of thenardite. The Canadian Mineralogist, 13, 181-187.
Hazen, R.M. (1976) Effects of temperature and pressure on the cell dimension and X-ray temperature factors of periclase. American Mineralogist, 61, 266-271.

Hazen, R.M. (1987) High-pressure crystal chemistry of chrysoberyl, Al2BeO4: insights on the origin of olivine elastic anisotropy Sample: P = 1 bar. Physics and Chemistry of Minerals 14, 13-20.
Hazen, R.M. and Au, A.Y. (1986) High-pressure crystal chemistry of phenakite (Be2SiO4) and bertrandite (Be4Si2O7(OH)2) Sample: P = 1 bar. Physics and Chemistry of Minerals, 13, 69-78.
Hazen, R.M., Finger, L.W., and Mariathasan, J.W.E. (1985) High-pressure crystal chemistry of scheelite-type tungstates and molybdates Note: P = 0.0001 GPa Note: B(2,2) altered from .0012 in order to match Biso. Journal of Physics and Chemistry of Solids, 46, 253-263.
Hill, R.J. (1984) X-ray powder diffraction profile refinement of synthetic hercynite inversion parameter = .163. American Mineralogist, 69, 937-942.
Hill, R.J. (1985) Refinement of the structure of orthorhombic PbO (massicot) by Rietveld analysis of neutron powder diffraction data. Acta Crystallographica C, 41, 1281-1284.
Horn, M., Schwerdtfeger, C.F., and Meagher, E.P. (1972) Refinement of the structure of anatase at several temperatures. Zeitschrift für Kristallographie, 136, 273-281.
Howotny, H. and Heger, G. (1983) Structure refinement of strontium nitrate, Sr(NO3)2, and barium nitrate, Ba(NO3)2 Locality: synthetic. Acta Crystallographica, Section C.
Hugh-Jones, D.A. and Angel, R.J. (1994) A compressional study of MgSiO3 orthoenstatite up to 8.5 GPa Sample: P = 0 GPa. American Mineralogist, 76, 405-410.
Husson, E. and Repelin, Y. (1996) Structural studies of transition aluminas. Theta alumina. European Journal of Solid State Inorganic Chemistry, 33, 1223-1231.
Idemoto, Y., Richardson, J.W., Koura, N., Kohara, S., and Loong, C.K. (1998) Crystal structure of (LixK1-x)2CO3 (x = 0,0.43,0.5,0.62,1) by neutron powder diffraction analysis Sample: neutron powder diffraction refinement of raw material. Journal of Physics and Chemistry of Solids, 59, 363-376.
Jacobsen, S.D., Smyth, J.R., Swope, R.J., and Downs, R.T. (1998) Rigid-body character of the SO4 groups in celestine, anglesite and barite. The Canadian Mineralogist, 36, 1053-1060.
Jansen, M. (1978) Die kristallstruktur von As_2O_5, eine neue raumnetzstruktur. Zeitschrift für Anorganische und Allgemeine Chemie, 441, 5-12.
Jansen, M. (1979) Die kristallstruktur von antimon(V)-oxid. Acta Crystallographica B, 35, 539-542.
Kanazawa, Y. and Sasaki, A. (1986) Structure of kamiokite Note: anisoB's taken from ICSD. Acta Crystallographica, Section C, 9-11.
Kawahara, A. (1967) La structure cristalline de la chervetite. Bulletin de la Societe Francaise de Mineralogie et de Cristallographie, 90, 279-284.
Kihara, K. and Donnay, G. (1985) Anharmonic thermal vibrations in ZnO Model: 2-c, at T = 293 K. The Canadian Mineralogist, 23, 647-654.

Kirfel, A. and Eichhorn, K. (1990) Accurate structure analysis with synchrotron radiation: The electron density in Al_2O_3 and Cu_2O. Acta Crystallographica, A46, 271-284.
Kisi, E.H.H., C.J.; Hill, R.J. (1989) Crystal structure of orthorhombic zirconia in partially stabilized zirconia. Journal of the American Ceramic Society, 72, 1757-1760.
Klaska, K.-H., Eck, J.C., and Pohl, D. (1978) New investigation of willemite Note: Anisotropic displacement parameters are from ICSD. Acta Crystallographica, Section B, 3324-3325.
Knight, K.S. (1992) The crystal structure of russellite;a re-determination using neutron powder diffraction of synthetic Bi2WO6. Mineralogical Magazine, 56, 399-409.
Kolesov, B.A., Geiger, C.A., and Armbruster, T. (2001) The dynamic properties of zircon studied by single-crystal X-ray diffraction and Raman spectroscopy. European Journal of Mineralogy, 13, 939-948.
Krogh-Moe, J. (1962) The crystal structure of lithium diborate, Li2O*2B2O3. Acta Crystallographica, 15, 190-193.
Lazic, B., Kahlenberg, V., and Konzett, J. (2007) Structural studies on a stuffed framework high pressure polymorph of CaAl2O4. Zeitschrift fur Kristallographie, 222, 690-695.
Lenaz, D., Skogby, H., Princivalle, F., and Halenius, U. (2004) Structural changes and valence states in the MgCr2O4-FeCr2O4 solid solution series Sample: Fe2-. Physics and Chemistry of Minerals, 31, 633-642.
Levien, L. and Prewitt, C.T. (1981) High-pressure crystal structure and compressibility of coesite P = 1 atm isotropic refinement. American Mineralogist, 66, 324-333.
Levien, L., Prewitt, C.T., and Weidner, D.J. (1980) Structure and elastic properties of quartz at pressure, P = 1 atm. American Mineralogist, 65, 920-930.
Levy, D., Diella, V., Pavese, A., Dapiaggi, M., and Sani, A. (2005) P-V equation of state, thermal expansion, and P-T stability of synthetic zincochromite (ZnCr2O4 spinel) Sample: T = 298 K. American Mineralogist, 90, 1157-1162.
Liferovich, R.P. and Mitchell, R.H. (2006) The pyrophanite-geikielite solid-solution series: crystal structures of the Mn1-xMgxTiO3 series ($0 < x < 0.7$) Sample: XMg = 1.0 Note: No bond lengths could be reproduced with the reported dataset. The Canadian Mineralogist, 44.
Lindqvist, O. (1972) The crystal structure of CuTeO3. Acta Chemica Scandinavica 26, 1423-1430.
Long, G.J., Cheetham, A.K., and Battle, P.D. (1983) Study of the iron-phosphorus-oxygen system by Mossbauer effect, neutron diffraction, magnetic susceptibility, and analytical electron microscopy: some pitfalls and solutions in the analysis of a complex mixture Locality: synthetic. Inorganic Chemistry, 22, 3012-3016.
Lugli, C., Medici, L., and Saccardo, D. (1999) Natural wulfenite: structural refinement by single-crystal X-ray diffraction. Neues Jahrbuch fur Mineralogie, Monatshefte, 1999, 281-288.
Macavei, J. and Schulz, H. (1993) The crystal structure of wolframite type tungstates at high pressure Note: P = 0.0001 GPa, in air. Zeitschrift fur Kristallographie 207, 193-208.

Maksimova, N.V., Ilyukhin, V.V., and Belov, N.V. (1975) Crystal structure of thoreaulite, SaTa2O6. Soviet Physics Doklady, 20, 528-529.
Markgraf, S.A. and Reeder, R.J. (1985) High-temperature structure refinements of calcite and magnesite Sample: T = 24 C. American Mineralogist, 70, 590-600.
Martinez-Ripoll, M., Martinez-Carrera, S., and Garcia-Blanco, S. (1971) The crystal structure of copper metaborate, CuB2O4. Acta Crystallographica, Section B, 677-681.
Maslen, E.N., Streltsov, V.A., Streltsova, N.R., and Ishizawa, N. (1995) Electron density and optical anisotropy in rhombohedral carbonates. III. Synchrotron X-ray studies of CaCO3, MgCO3 and MnCO3 Sample: Synchrotron data. Acta Crystallographica, Section B, 929-939.
McGinnety, J.A. (1972) Redetermination of the structures of potassium sulphate and potassium chromate: the effect of electrostatic crystal forces upon observed bond length. Acta Crystallographica, Section B.
Meagher, E.P. and Lager, G.A. (1979) Polyhedral thermal expansion in the TiO_2 polymorphs: Refinement of the crystal structures of rutile and brookite at high temperature. The Canadian Mineralogist, 17, 77-85.
Mereiter, K. and Preisinger, A. (1986) Kristallstrukturdaten der wismutminerale atelestit, mixit und pucherit. Anzeiger der Osterreichische Akademie der Wissenschaften 123, 79-81.
Merlino, S., Orlandi, P., Perchiazzi, N., Basso, R., and Palenzona, A. (1989) Polytypism in stibivanite. The Canadian Mineralogist, 27, 625-632.
Mijlhoff, F.C. (1965) The crystal structure of tetragonal selenium trioxide. Acta Crystallographica, 18, 795-798.
Mitchell, R.H., Chakhmouradian, A.R., and Woodward, P.M. (2000) Crystal chemistry of perovskite-type compounds in the tausonite-loparite series, (Sr1-2xNaxLax)TiO3 Sample: x = 0.00. Physics and Chemistry of Minerals 27, 583-589.
Mooney-Slater, R.C.L. (1962) Polymorphic forms of bismuth phosphate. Zeitschrift fur Kristallographie, 117, 371-385.
Muraoka, Y. and Kihara, K. (1997) The temperature dependence of the crystal structure of berlinite, a quartz-type form of AlPO4 Sample: T = 25 C. Physics and Chemistry of Minerals, 24, 243-253.
Ni, Y., Hughes, J.M., and Mariano, A.N. (1995) Crystal chemistry of the monazite and xenotime structures Dy(PO4). American Mineralogist, 80, 21-26.
Nimmo, J.K. and Lucas, B.W. (1973) A neutron diffraction determination of the crystal structure of alpha-phase potassium nitrate at 25 C and 100 C Sample: T = 25 C Locality: Synthetic. Journal of Physics C: Solid State Physics, 6, 201-211.
Nogues, M. and Poix, P. (1972) Effet Jahn-Teller cooperatif dans le systeme ZnMn2O4-Zn2SnO4. Annales de Chimie 1972, 301-314.
Nord, A.G. and Kierkegaard, P. (1968) The crystal structure of Mg3(PO4)2. Acta Chemica Scandinavica, 22, 1466-1474.
Nowotny, H. and Heger, G. (1983) Structure refinement of strontium nitrate, Sr(NO3)2, and barium nitrate, Ba(NO3)2 Locality: synthetic. Acta Crystallographica, Section C, 952-956.
Ohashi, Y. (1984) Polysynthetically-twinned structures of enstatite and wollastonite Sample: WO2M. Physics and Chemistry of Minerals 10, 217-229.

Ollivier, B., Retoux, R., Lacorre, P., Massiot, D., and Ferey, G. (1997) Crystal structure of kappa-alumina: An X-ray powder diffraction, TEM and NMR study. Journal of Materials Chemistry, 7, 1049-1056.
Otto, H.H., Baltrusch, R., and Brant, H.J. (1993) Further evidence for Tl3+ in Tl-based superconductors from improved bond strength parameters involving new structural data of cubic Tl2O3. Physica C, 215, 205-208.
Pasero, M. and Rotiroti, N. (2003) The crystal structure of molybdomenite, PbSeO3. Neues Jahrbuch fur Mineralogie, Monatshefte, 2003, 145-152.
Paul, G.L. and Pryor, A.W. (1972) The study of sodium nitrate by neutron diffraction Sample: T = 20 C Locality: synthetic. Acta Crystallographica, Section B, 2700-2702.
Pertlik, F. (1975) Verfeinerung der kristallstruktur von synthetischem trippkeit, CuAs2O4. Tschermaks Mineralogische und Petrographische Mitteilungen 22, 211-217.
Pertlik, F. and Zemann, J. (1985) The crystal structure of scotlandite, PbSO3. Tschermaks Mineralogische und Petrographische Mitteilungen, 34, 289-295.
Pohl, D. and Gross, T. (1993) Caesium nitrate (II) at 296 K. Acta Crystallographica, Section C, 316-318.
Popovic, J., Tkalcec, E., Grzeta, B., Kurajica, S., and Rakvin, B. (2009) Inverse spinel structure of Co-doped gahnite Note: Sample S0, inversion parameter = 0, ZnAl2O4. American Mineralogist, 97, 771-776.
Quareni, S. and De Pieri, R. (1965) A three-dimensional refinement of the structure of crocoite, PbCrO4. Acta Crystallographica 19, 287-289.
Reuter, B., Riedel, E., Hug, P., Arndt, D., Geisler, U., and Behnke, J. (1969) Zur kristallchemie der vanadin(III)-spinelle. Zeitschrift fur Anorganische und Allgemeine Chemie 369, 306-312.
Ross, N.L. (1997) The equation of state and high-pressure behaviour of magnesite Sample: at P = 0. American Mineralogist, 82.
Ross, N.L., Shu, J.F., Hazen, R.M., and T., G. (1990) High-pressure crystal chemistry of stishovite. American Mineralogist, 75, 739-747.
Sahl, K. (1970) Zur kristallstruktur von lanarkit, Pb2O(SO4). Zeitschrift fur Kristallographie, 132, 99-117.
Seidel, P. and Hoffmann, W. (1976) Verfeinerung der kristallstruktur von NaNbO3 N. Bestimmung der absoluten konfiguration und des zwillingsgesetzes Note T = 84 K. Zeitschrift fur Kristallographie, 143, 444-459.
Sitepu, H., O'Connor, B.H., and Li, D. (2005) Comparative evaluation of the March and generalized spherical harmonic preferred orientation models using X-ray diffraction data for molybdite and calcite powders Note: GSH model. Journal of Applied Crystallography, 38, 158-167.
Sleight, A.W., Chen, H.-Y., Ferretti, A., and Cox, D.E. (1979) Crystal growth and structure of BiVO4 Sample: T = 295 K. Materials Research Bulletin 14, 1571-1581.
Smith, G.S. and Isaacs, P.B. (1964) The crystal structure of quartz-like GeO2 Note: polymorph of argutite. Acta Crystallographica, 17, 842-846.
Smyth, J.R. (1975) High temperature crystal chemistry of fayalite T = 20 °C olivine. American Mineralogist, 60, 1092-1097.

Smyth, J.R. and Hazen, R.M. (1973) The crystal structures of forsterite and hortonolite at several temperatures up to 900 C T = 25 C. American Mineralogist, 58.
Sowa, H. (1991) The crystal structure of AlAsO4 at high pressure Note: P = 0 GPa, in the diamond anvil cell Locality: synthetic. Zeitschrift fur Kristallographie 194, 291-304.
Speer, J.A. and Cooper, B.J. (1982) Crystal structure of synthetic hafnon, HfSiO4, comparison with zircon and the actinide orthosilicates. American Mineralogist, 67, 804-808.
Stachel, D., Svoboda, I., and Fuess, H. (1995) Phosphorus pentoxide at 233 K. Acta Crystallographica C, 51, 1049-1050.
Stahl, K., Legros, J.P., and Galy, J. (1992) The crystal structure of SeO_2 at 139 and 286 K. Zeitschrift für Kristallographie, 202, 99-107.
Stephens, J.S. and Cruickshank, D.W.J. (1970) The crystal structure of (CrO3)inf. Acta Crystallographica B, 26, 222-226.
Sugiyama, K. and Tokonami, M. (1987) Structure and crystal chemistry of a dense polymorph of tricalcium phosphate Ca3(PO4)2: a host to accommodate large lithophile elements in the Earth's mantle. Physics and Chemistry of Minerals 15, 125-130.
Svensson, C. (1975) Refinement of the crystal structure of cubic antimony trioxide, Sb_2O_3. Acta Crystallographica B, 31, 2016-2018.
Teller, R.G., Brazdil, J.F., Grasselli, R.K., and Jorgensen, J.D. (1984) The structure of gamma-bismuth molybdate, Bi2MoO6, by powder neutron diffraction. Acta Crystallographica, Section C, 2001-2005.
Tsurumi, T., Hirano, Y., Kato, H., Kamiya, T., and Daimon, M. (1994) Crystal structure and hydration of belite. Ceramic Transactions, 40, 19-25.
Vegas, A., Cano, F.H., and Garcia-Blanco, S. (1975) The crystal structure of calcium orthoborate: a redetermination. Acta Crystallographica, Section B.
Wechsler, B.A. and Prewitt, C.T. (1984) Crystal structure of ilmenite (FeTiO3) at high temperature and high pressure 24 deg C. American Mineralogist, 69, 176-185.
Wildner, M. and Giester, G. (1988) Crystal structure refinements of synthetic chalcocyanite (CuSO4) and zincosite (ZnSO4). Mineralogy and Petrology 39, 201-209.
Williams, S.A., McLean, W.J., and Anthony, J.W. (1970) A study of phoenicochroite - its structure and properties. American Mineralogist 55, 784-792.
Winter, J.K. and Ghose, S. (1979) Thermal expansion and high-temperature crystal chemistry of the Al2SiO5 polymorphs T = 25 deg C. . American Mineralogist, 64, 573-586.
Wolten, G.M. (1967) The structure of the M'-phase of YTaO4, a third fergusonite polymorph. Acta Crystallographica, 23, 939-944.
Wyckoff, R.W.G. (1963) Crystal Structures, p. Interscience, New York, New York.
Xu, Y.N. and Ching, W.Y. (1993) Electronic, optical, and structural properties of some wurtzite crystals. Physical Review B, 48, 4335-4351.
Yamanaka, T., Hirai, M., and Komatsu, Y. (2002) Structure change of Ca1-xSrxTiO3 perovskite with composition and pressure Sample: CaTiO3, x = 0.0. American Mineralogist, 87, 1183-1189.

Zouari, S., Ranno, L., Cheikh-Rouhou, A., Isnard, O., Pernet, M., Wolfers, P., and Strobel, P. (2003) New model for the magnetic structure of the marokite-type oxide CaMn2O4 Sample: T = 280 K. Journal of Alloys and Compounds, 353, 5-11.

Zubkova, N.V., Pushcharovsky, D.Y., Ivaldi, G., Ferraris, G., Pekov, I.V., and Chukanov, N.V. (2002) Crystal structure of natrite, gamma-Na2CO3. Neues Jahrbuch fur Mineralogie, Monatshefte, 2002, 85-96.