

*Supporting Information For*

**Searching for Silicate Nonlinear Optical Materials in by  
Combining Calculation and Experiment**

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**Figure S1.** Rietveld refinement of PXRD of synthesized pure polycrystalline of  $\text{KNbSi}_2\text{O}_7$ .

**Figure S2.** Rietveld refinement of PXRD of synthesized pure polycrystalline of  $\text{PbZnSiO}_4$ .

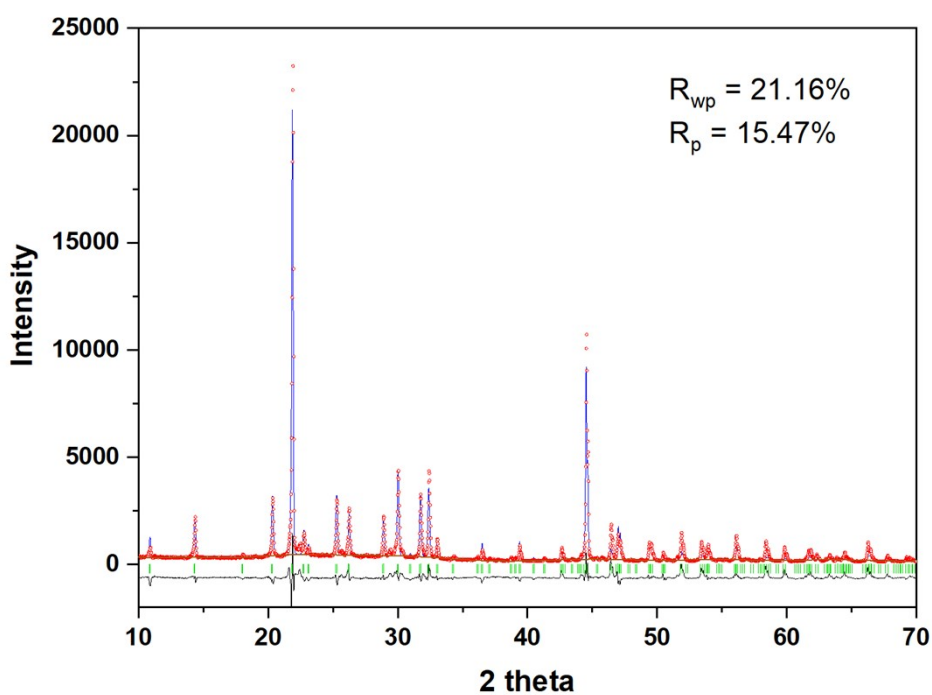
**Figure S3.** Rietveld refinement of PXRD of synthesized pure polycrystalline of  $\text{Na}_2\text{TiSiO}_5$ .

**Figure S4.** (a) Partial DOS of  $\text{PbZnSiO}_4$ , (b) Partial DOS of  $\text{Na}_2\text{TiSiO}_5$ .

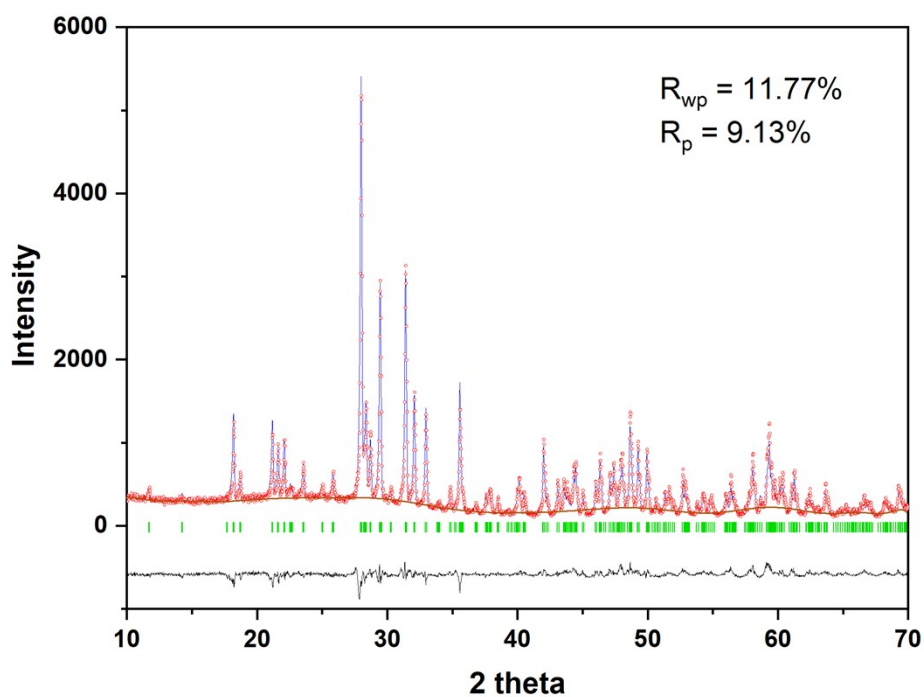
**Figure S5.** SHG density at (a) occupied state and (b) unoccupied state of  $\text{PbZnSiO}_4$ .

**Figure S6.** SHG density at (a) occupied state and (b) unoccupied state of  $\text{Na}_2\text{TiSiO}_5$ .

**Table S1.** Crystallographic data, details of the experiment and Rietveld refinement of PXRD.  
**Calculation results of 253 silicates**



**Figure S1.** Rietveld refinement of PXRD of synthesized pure polycrystalline of KNbSi<sub>2</sub>O<sub>7</sub>. Experimental (red circles) and calculated (blue line) PXRD patterns and their difference (black line) for the PXRD Rietveld refinement of KNbSi<sub>2</sub>O<sub>7</sub>. The short vertical green lines show the positions of Bragg reflections of the calculated pattern.



**Figure S2.** Rietveld refinement of PXRD of synthesized pure polycrystalline of PbZnSiO<sub>4</sub>.

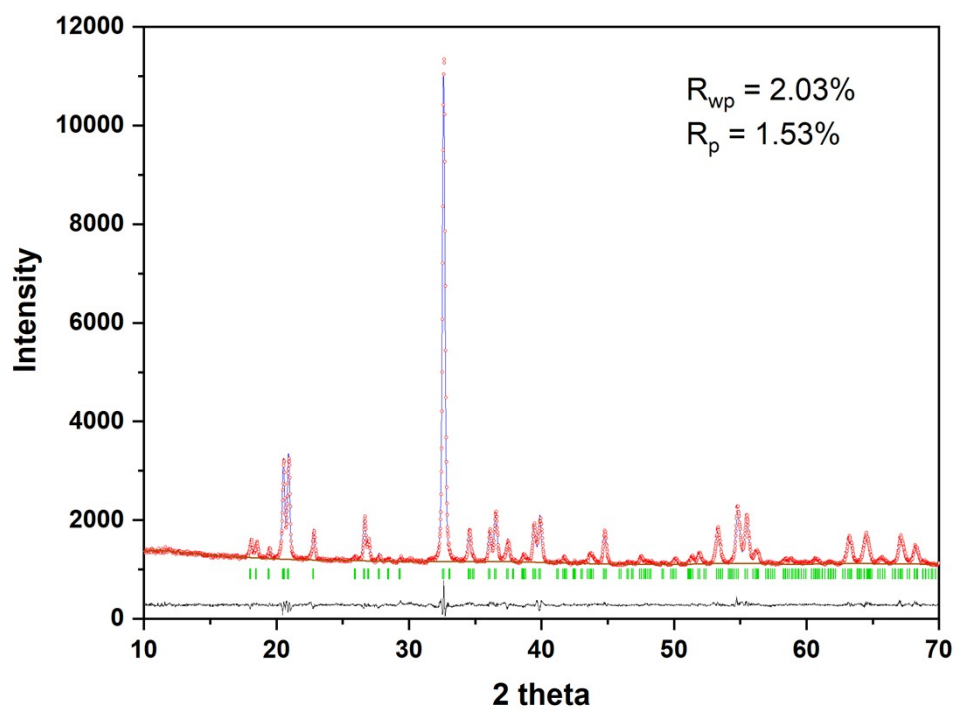


Figure S3. Rietveld refinement of PXR D of synthesized pure polycrystalline of  $\text{Na}_2\text{TiSiO}_5$ .

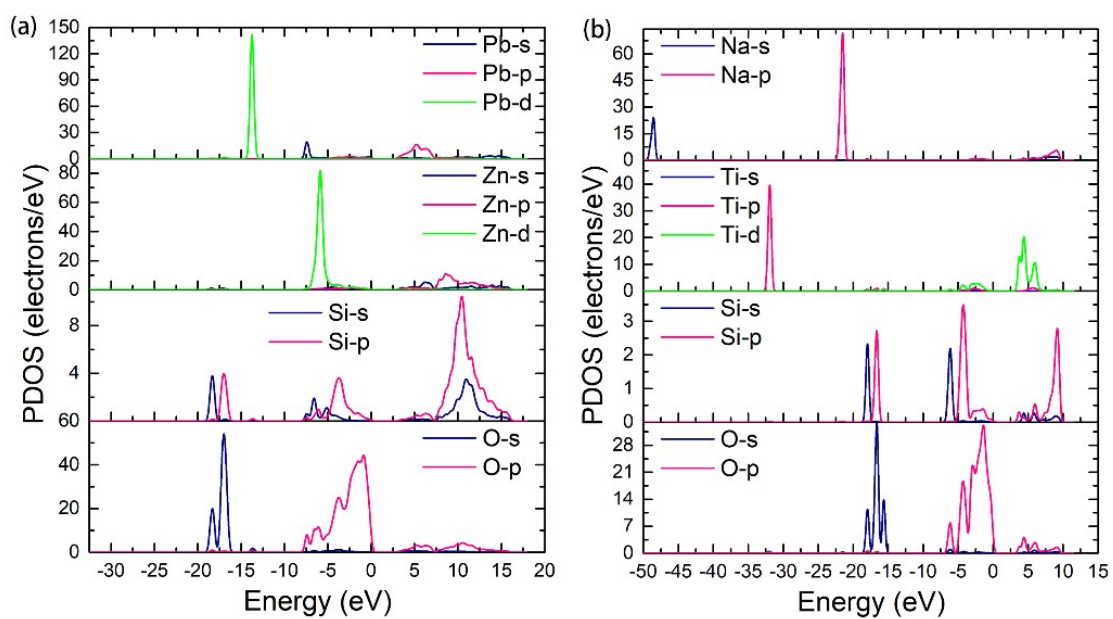


Figure S4. (a) Partial DOS of  $\text{PbZnSiO}_4$ , (b) Partial DOS of  $\text{Na}_2\text{TiSiO}_5$ .

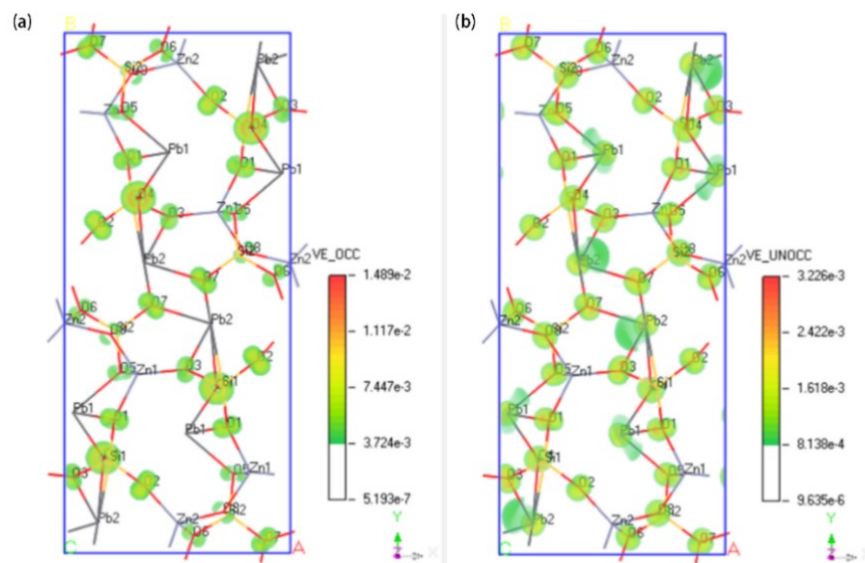


Figure S5. SHG density at (a) occupied state and (b) unoccupied state of  $\text{PbZnSiO}_4$ .

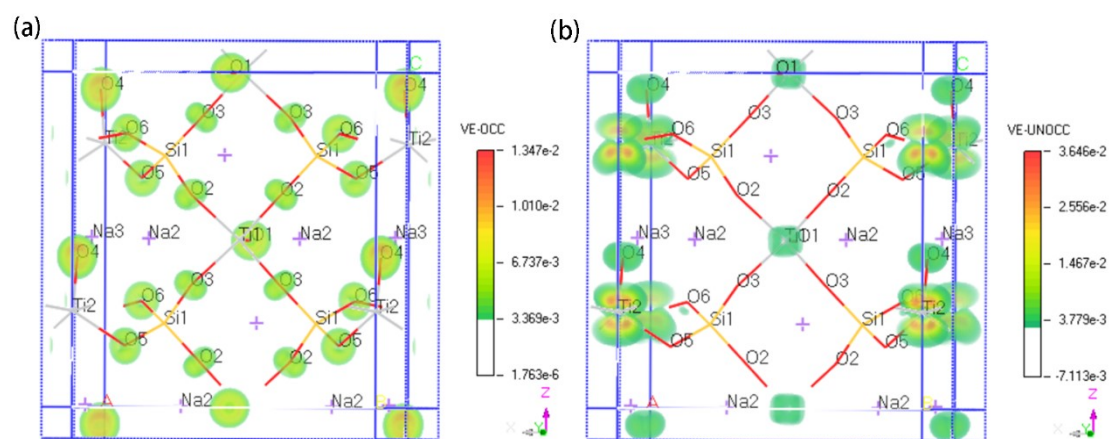


Figure S6. SHG density at (a) occupied state and (b) unoccupied state of  $\text{Na}_2\text{TiSiO}_5$ .

**Table S1.** Crystallographic data, details of the experiment and Rietveld refinement of PXRD.

Empirical formula	KNbSi <sub>2</sub> O <sub>7</sub>	PbZn(SiO <sub>4</sub> )	Na <sub>2</sub> TiSiO <sub>5</sub>
Crystal system	tetragonal	orthorhombic	orthorhombic
Space group (number)	<i>P4bm</i>	<i>Pna2</i> <sub>1</sub>	<i>Pmc2</i> <sub>1</sub>
<i>a</i> [Å]	8.7380	8.2319	9.12978
<i>b</i> [Å]	8.7380	18.9654	4.79649
<i>c</i> [Å]	8.1290	5.0439	9.824724
$\alpha$ (°)	90	90	90
$\beta$ (°)	90	90	90
$\gamma$ (°)	90	90	90
Volume [Å <sup>3</sup> ]	620.67	787.46	430.23
<i>Z</i>	4	8	4
$\rho_{\text{calc}}$ [gcm <sup>-3</sup> ]	3.21212	6.1516	3.11749
Radiation	CuK $\alpha$ ( $\lambda = 1.5408$ Å)		
Instrument type	Bragg-Brentano		
<i>R</i> <sub>wp</sub>	0.2116	0.1177	0.0203
<i>R</i> <sub>p</sub>	0.1547	0.0913	0.0153

The chemical formula, ICSD collection-code, space group, band gap ( $E_g$ ), birefringence ( $\Delta n$ ), second-order susceptibility ( $\chi^{(2)}$ ), and the maximum  $\chi^{(2)}$  tensor of all 253 structures.

Formula	ICSD	SG	$E_g$ -GGA	$\Delta n$	$\chi^{(2)}$ (pm/V)	$ \chi^{(2)} _{\max}$ (pm/V)
Ag <sub>2</sub> SiO <sub>3</sub>	36589	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	0.835	0.037	$\chi_{123}=3.926$	3.926
Ag <sub>6</sub> (Si <sub>2</sub> O <sub>7</sub> )	404355	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	0.394	0.149	$\chi_{112}=-22.530$ $\chi_{123}=-10.709$ $\chi_{222}=2.584$ $\chi_{233}=5.594$	22.53
Ba(Li <sub>2</sub> SiO <sub>4</sub> )	260259	<i>P6<sub>3</sub>cm</i>	4.444	0	$\chi_{113}=0.510$ $\chi_{223}=0.510$ $\chi_{333}=-7.386$	7.386
Ba(Si <sub>4</sub> O <sub>9</sub> )	80067	<i>P-6c2</i>	4.372	0.017	$\chi_{111}=1.115$ $\chi_{122}=-1.115$	1.115
BaBe(SiO <sub>4</sub> )	86792	<i>Cm</i>	4.742	0.02	$\chi_{111}=-5.791$ $\chi_{113}=-1.228$ $\chi_{122}=0.905$ $\chi_{133}=3.306$ $\chi_{223}=-2.249$ $\chi_{333}=4.410$	5.791
BaBe <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	250005	<i>Pm</i>	5.821	0.016	$\chi_{112}=-0.002$ $\chi_{113}=-0.638$ $\chi_{222}=-0.002$ $\chi_{223}=-1.092$ $\chi_{233}=0.001$ $\chi_{333}=2.961$	2.961
BaBe <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	151563	<i>Pmn2<sub>1</sub></i>	5.825	0.017	$\chi_{113}=0.655$ $\chi_{223}=1.093$ $\chi_{333}=-2.938$	2.938
BaBe <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	166582	<i>Pn2<sub>1</sub>a</i>	5.646	0.021	$\chi_{112}=0.024$ $\chi_{222}=0.024$ $\chi_{233}=0.004$	0.024
BaBe <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	22341	<i>Pn2<sub>1</sub>a</i>	5.651	0.021	$\chi_{222}=0.002$ $\chi_{233}=0.002$	0.002
BaBe <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	263133	<i>Pmn2<sub>1</sub></i>	5.827	0.017	$\chi_{113}=0.627$ $\chi_{223}=1.094$ $\chi_{333}=-2.962$	2.962
BaHf(SiO <sub>3</sub> ) <sub>3</sub>	183835	<i>P-6c2</i>	4.688	0.004	$\chi_{111}=0.221$ $\chi_{122}=-0.221$	0.221
BaMg(SiO <sub>4</sub> )	73776	<i>P6<sub>3</sub></i>	4.169	0.004	$\chi_{113}=1.765$ $\chi_{223}=1.765$ $\chi_{333}=-1.216$	1.765
BaN <sub>2</sub> (AlSiO <sub>4</sub> ) <sub>4</sub>	156658	<i>lba2</i>	4.913	0.006	$\chi_{113}=0.197$ $\chi_{223}=0.505$ $\chi_{333}=-0.605$	0.605
BaN <sub>2</sub> (AlSiO <sub>4</sub> ) <sub>4</sub>	156657	<i>lba2</i>	4.913	0.006	$\chi_{113}=0.192$ $\chi_{223}=0.504$ $\chi_{333}=-0.603$	0.603
BaSiO <sub>3</sub>	6245	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	4.69	0.014	$\chi_{123}=0.635$	0.635
BaSn(Si <sub>3</sub> O <sub>9</sub> )	10385	<i>P-6c2</i>	4.402	0.02	$\chi_{111}=0.939$ $\chi_{122}=-0.938$	0.939
BaTi(Si <sub>3</sub> O <sub>9</sub> )	290231	<i>P3c</i>	3.378	0.034	$\chi_{111}=0.005$ $\chi_{112}=-0.286$ $\chi_{113}=-0.003$ $\chi_{122}=0.001$ $\chi_{123}=-0.005$	0.290

					$\chi_{133}=0.006$ $\chi_{222}=0.290$ $\chi_{223}=0.003$ $\chi_{233}=0.003$ $\chi_{333}=-0.019$	
BaTi(Si <sub>3</sub> O <sub>9</sub> )	18100	<i>P-6c2</i>	3.366	0.033	$\chi_{111}=0.209$ $\chi_{122}=-0.209$	0.209
BaY <sub>6</sub> (Si <sub>3</sub> B <sub>6</sub> O <sub>24</sub> )F <sub>2</sub>	30674	<i>P3</i>	5.395	0.033	$\chi_{111}=-0.768$ $\chi_{112}=-0.002$ $\chi_{113}=4.106$ $\chi_{122}=0.768$ $\chi_{222}=0.002$ $\chi_{223}=4.106$ $\chi_{333}=-5.923$	5.923
BaZn(SiO <sub>4</sub> )	73777	<i>P6<sub>3</sub></i>	3.404	0.032	$\chi_{113}=0.632$ $\chi_{223}=0.632$ $\chi_{333}=1.771$	1.771
Ba <sub>2</sub> (TiO)(Si <sub>2</sub> O <sub>7</sub> )	4451	<i>P4bm</i>	4.059	0.060	$\chi_{113}=6.450$ $\chi_{223}=6.450$ $\chi_{333}=-21.409$	21.40
Ba <sub>2</sub> Ca(BSi <sub>2</sub> O <sub>7</sub> ) <sub>2</sub>	193536	<i>I-42m</i>	4.918	0.003	$\chi_{123}=-1.787$	1.787
Ba <sub>2</sub> In <sub>2</sub> Si <sub>3</sub> O <sub>10</sub> S	430641	<i>Pca2<sub>1</sub></i>	3.722	0.024	$\chi_{113}=-1.059$ $\chi_{223}=1.280$ $\chi_{333}=-0.504$	1.28
Ba <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	81117	<i>P-42<sub>1</sub>m</i>	4.559	0.023	$\chi_{123}=-0.657$	0.657
Ba <sub>2</sub> TiSi <sub>2</sub> O <sub>8</sub>	201844	<i>P4bm</i>	4.045	0.060	$\chi_{113}=-6.550$ $\chi_{223}=-6.550$ $\chi_{333}=21.424$	21.424
Ba <sub>2</sub> TiSi <sub>2</sub> O <sub>8</sub>	201845	<i>P4bm</i>	4.051	0.061	$\chi_{113}=-6.517$ $\chi_{223}=-6.517$ $\chi_{333}=21.460$	21.460
Ba <sub>2</sub> Y <sub>3</sub> (SiO <sub>4</sub> ) <sub>2</sub> F <sub>5</sub>	290289	<i>Pba2</i>	5.092	3.50E-02	$\chi_{113}=-0.756$ $\chi_{223}=0.704$ $\chi_{333}=-3.347$	3.347
Ba <sub>3</sub> (NbGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub> )	154215	<i>P321</i>	3.003	0.084	$\chi_{112}=-1.272$ $\chi_{222}=1.272$	1.272
Ba <sub>3</sub> Nb <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	15934	<i>P-62m</i>	1.996	0.315	$\chi_{112}=2.227$ $\chi_{222}=-2.227$	2.227
Ba <sub>3</sub> Si <sub>4</sub> Nb <sub>6</sub> O <sub>26</sub>	16029	<i>P-62m</i>	1.997	0.313	$\chi_{112}=2.385$ $\chi_{222}=-2.386$	2.386
Ba <sub>3</sub> Si <sub>4</sub> Ta <sub>6</sub> O <sub>26</sub>	18317	<i>P-62m</i>	3.261	0.148	$\chi_{112}=0.208$ $\chi_{222}=-0.208$	0.208
Ba <sub>3</sub> Si <sub>6</sub> O <sub>9</sub> N <sub>4</sub>	259431	<i>P3</i>	4.513	0.01	$\chi_{111}=1.003$ $\chi_{112}=-0.845$ $\chi_{113}=-0.031$ $\chi_{122}=-1.003$ $\chi_{222}=0.845$ $\chi_{223}=-0.031$ $\chi_{333}=0.757$	1.003
Ba <sub>3</sub> Si <sub>6</sub> O <sub>9</sub> N <sub>4</sub>	415918	<i>P3</i>	4.519	0.01	$\chi_{111}=0.991$ $\chi_{112}=-0.839$ $\chi_{113}=-0.034$ $\chi_{122}=-0.991$ $\chi_{222}=0.839$ $\chi_{223}=-0.034$ $\chi_{333}=0.709$	0.991

Ba <sub>3</sub> Si <sub>6</sub> O <sub>9</sub> N <sub>4</sub>	259432	<i>P3</i>	4.512	0.01	$\chi_{111}=0.988$ $\chi_{112}=-0.852$ $\chi_{113}=-0.048$ $\chi_{122}=-0.988$ $\chi_{222}=0.852$ $\chi_{223}=-0.048$ $\chi_{333}=0.665$	0.988
Ba <sub>3</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	15935	<i>P-62m</i>	3.265	0.149	$\chi_{112}=0.204$ $\chi_{222}=-0.204$	0.204
Ba <sub>4</sub> Si <sub>6</sub> O <sub>16</sub>	20038	<i>P2<sub>1</sub></i>	4.763	0.027	$\chi_{113}=0.211$ $\chi_{123}=0.046$ $\chi_{223}=0.331$ $\chi_{333}=-0.111$	0.331
Bi <sub>2</sub> O <sub>2</sub> (SiO <sub>3</sub> )	30995	<i>Cmc2<sub>1</sub></i>	3.055	0.06	$\chi_{113}=4.165$ $\chi_{223}=-0.565$ $\chi_{333}=3.212$	4.165
CaAl(AlSi)O <sub>6</sub>	239022	<i>P1</i>	4.993	0.044	$\chi_{111}=-0.194$ $\chi_{112}=-0.059$ $\chi_{113}=-0.007$ $\chi_{122}=0.127$ $\chi_{123}=-0.009$ $\chi_{133}=0.020$ $\chi_{222}=-0.467$ $\chi_{223}=-0.177$ $\chi_{233}=0.271$ $\chi_{333}=0.024$	0.467
CaAl(AlSi)O <sub>6</sub>	239023	<i>P1</i>	4.992	0.044	$\chi_{111}=0.191$ $\chi_{112}=-0.057$ $\chi_{113}=0.008$ $\chi_{122}=-0.127$ $\chi_{123}=-0.010$ $\chi_{133}=-0.021$ $\chi_{222}=-0.466$ $\chi_{223}=0.177$ $\chi_{233}=0.270$ $\chi_{333}=-0.027$	0.466
CaAl(AlSi)O <sub>6</sub>	239021	<i>P1</i>	4.976	0.034	-	0
CaBa(SiO <sub>4</sub> )	67092	<i>P6<sub>3</sub>mc</i>	4.507	0.04	$\chi_{113}=1.356$ $\chi_{223}=1.356$ $\chi_{333}=1.658$	1.658
CaNa(BeSi <sub>2</sub> O <sub>6</sub> )F	15314	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	5.539	0.009	$\chi_{123}=0.184$	0.184
CaSr(SiO <sub>4</sub> )	20544	<i>Pna2<sub>1</sub></i>	4.711	0.022	$\chi_{113}=0.293$ $\chi_{223}=0.023$ $\chi_{333}=-0.706$	0.706
CaZr(Si <sub>2</sub> O <sub>7</sub> )	203131	<i>C2</i>	4.54	0.062	$\chi_{112}=-0.532$ $\chi_{123}=-6.280$ $\chi_{222}=-3.299$ $\chi_{233}=2.472$	6.28
Ca <sub>14</sub> Mg <sub>2</sub> (SiO <sub>4</sub> ) <sub>8</sub>	254354	<i>P2nn</i>	4.898	0.021	$\chi_{111}=-1.658$ $\chi_{122}=0.041$ $\chi_{133}=0.149$	1.658
Ca <sub>14</sub> Mg <sub>2</sub> (SiO <sub>4</sub> ) <sub>8</sub>	254355	<i>P2nn</i>	4.9	0.021	$\chi_{111}=-1.560$ $\chi_{122}=-0.021$ $\chi_{133}=0.196$	1.56
Ca <sub>2</sub> (SiO <sub>3</sub> Cl <sub>2</sub> )	200221	<i>I4</i>	5.363	0.014	$\chi_{113}=0.030$ $\chi_{223}=0.030$ $\chi_{333}=-0.023$	0.03



Ca <sub>2</sub> (SiO <sub>4</sub> )	182054	<i>P6<sub>3</sub>mc</i>	3.546	0.078	χ <sub>113</sub> =-0.707 χ <sub>223</sub> =-0.708 χ <sub>333</sub> =-10.236	10.236
Ca <sub>2</sub> (SiO <sub>4</sub> )	182053	<i>P6<sub>3</sub>mc</i>	3.553	0.078	χ <sub>113</sub> =-0.724 χ <sub>223</sub> =-0.724 χ <sub>333</sub> =-10.191	10.191
Ca <sub>2</sub> (SiO <sub>4</sub> )	82996	<i>Pna2<sub>1</sub></i>	4.682	0.021	χ <sub>113</sub> =-0.282 χ <sub>223</sub> =-1.079 χ <sub>333</sub> =1.372	1.372
Ca <sub>2</sub> Al <sub>2</sub> (SiO <sub>4</sub> )O <sub>3</sub>	24588	<i>P-42<sub>1</sub>m</i>	4.743	0.009	χ <sub>123</sub> =-0.940	0.94
Ca <sub>2</sub> B <sub>2</sub> SiO <sub>7</sub>	263515	<i>P2<sub>1</sub>2<sub>1</sub>2</i>	6.03	0.015	χ <sub>123</sub> =0.632	0.632
Ca <sub>2</sub> Be(Si <sub>2</sub> O <sub>7</sub> )	31234	<i>P-42<sub>1</sub>m</i>	5.3	0.025	χ <sub>123</sub> =-0.293	0.293
Ca <sub>2</sub> Be(Si <sub>2</sub> O <sub>7</sub> )	94063	<i>P-42<sub>1</sub>m</i>	5.298	0.025	χ <sub>123</sub> =0.285	0.285
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	187931	<i>P-42<sub>1</sub>m</i>	4.722	0.014	χ <sub>123</sub> =-0.035	0.035
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	50065	<i>P-42<sub>1</sub>m</i>	4.721	0.014	χ <sub>123</sub> =-0.031	0.031
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	39924	<i>P-42<sub>1</sub>m</i>	4.722	0.014	χ <sub>113</sub> =-0.003 χ <sub>123</sub> =-0.024 χ <sub>223</sub> =0.003	0.024
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	26683	<i>P-42<sub>1</sub>m</i>	4.721	0.014	χ <sub>123</sub> =-0.022	0.022
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	92773	<i>P-42<sub>1</sub>m</i>	4.721	1.40E-02	χ <sub>123</sub> =0.021	0.021
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	160352	<i>P-42<sub>1</sub>m</i>	4.726	0.014	χ <sub>123</sub> =-0.018	0.018
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	158177	<i>P-42<sub>1</sub>m</i>	4.723	0.014	χ <sub>123</sub> =-0.016	0.016
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	192373	<i>P-42<sub>1</sub>m</i>	4.725	0.014	χ <sub>123</sub> =-0.013	0.013
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	34805	<i>P-42<sub>1</sub>m</i>	4.721	0.014	χ <sub>123</sub> =0.008	0.008
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	85088	<i>P-42<sub>1</sub>m</i>	4.725	0.014	χ <sub>113</sub> =-0.003 χ <sub>123</sub> =-0.004 χ <sub>223</sub> =0.003	0.004
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	67691	<i>P-42<sub>1</sub>m</i>	4.726	0.014	χ <sub>123</sub> =0.003	0.003
Ca <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	85089	<i>P-42<sub>1</sub>m</i>	4.725	0.014	χ <sub>113</sub> =-0.003 χ <sub>123</sub> =-0.002 χ <sub>223</sub> =0.003	0.003
Ca <sub>2</sub> MgSi <sub>2</sub> O <sub>7</sub>	100736	<i>P-42<sub>1</sub>m</i>	4.719	0.014	χ <sub>123</sub> =-0.007	0.007
Ca <sub>2</sub> SiB <sub>2</sub> O <sub>7</sub>	5244	<i>P-42<sub>1</sub>m</i>	6.028	0.015	χ <sub>123</sub> =0.636	0.636
Ca <sub>2</sub> Zn(Si <sub>2</sub> O <sub>7</sub> )	186944	<i>P-42<sub>1</sub>m</i>	4.288	0.011	χ <sub>123</sub> =-1.046	1.046
Ca <sub>2</sub> Zn(Si <sub>2</sub> O <sub>7</sub> )	18114	<i>P-42<sub>1</sub>m</i>	4.287	0.012	χ <sub>123</sub> =-0.982	0.982
Ca <sub>2</sub> ZnSi <sub>2</sub> O <sub>7</sub>	30262	<i>P-42<sub>1</sub>m</i>	4.284	0.011	χ <sub>123</sub> =-0.996	0.996
Ca <sub>3</sub> (SiO <sub>4</sub> )O	24625	<i>R3mH</i>	3.355	0	χ <sub>111</sub> =-1.242 χ <sub>113</sub> =2.238 χ <sub>122</sub> =1.242 χ <sub>223</sub> =2.238 χ <sub>333</sub> =-3.734	3.734
Ca <sub>3</sub> (SiO <sub>4</sub> )O	81100	<i>Cm</i>	3.384	0.002	χ <sub>111</sub> =-1.458 χ <sub>113</sub> =-0.484 χ <sub>122</sub> =1.393 χ <sub>133</sub> =0.022 χ <sub>223</sub> =-0.614 χ <sub>333</sub> =0.517	1.458
Ca <sub>3</sub> (SiO <sub>4</sub> )O	22501	<i>R3mH</i>	3.801	0.017	χ <sub>111</sub> =-0.649 χ <sub>113</sub> =-0.587 χ <sub>122</sub> =0.649 χ <sub>223</sub> =-0.587 χ <sub>333</sub> =1.354	1.354

Ca <sub>3</sub> (Si <sub>2</sub> O <sub>7</sub> )	424472	<i>Ima2</i>	4.828	0.002	$\chi_{113}=-0.409$ $\chi_{223}=-0.323$ $\chi_{333}=1.300$	1.3
Ca <sub>3</sub> TaGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub>	409728	<i>P321</i>	4.222	0.078	$\chi_{112}=0.006$ $\chi_{222}=-0.006$	0.006
Ca <sub>3</sub> TaGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub>	245381	<i>P321</i>	4.219	0.077	$\chi_{112}=0.017$ $\chi_{222}=-0.017$	0.017
Ca <sub>3</sub> TaGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub>	380525	<i>P321</i>	4.216	0.077	$\chi_{112}=0.033$ $\chi_{222}=-0.033$	0.033
Ca <sub>6</sub> (SiO <sub>4</sub> )(Si <sub>3</sub> O <sub>10</sub> )	190040	<i>I2cm</i>	4.817	1.00E-03	$\chi_{111}=1.279$ $\chi_{122}=-0.324$ $\chi_{133}=-0.408$	1.279
Ca <sub>6</sub> (SiO <sub>4</sub> )(Si <sub>3</sub> O <sub>10</sub> )	34354	<i>I2cm</i>	4.816	1.00E-03	$\chi_{111}=1.272$ $\chi_{122}=-0.337$ $\chi_{133}=-0.399$	1.272
Ca <sub>7</sub> K(SiO <sub>4</sub> ) <sub>3</sub> F <sub>3</sub>	380452	<i>P3c</i>	4.903	0.007	$\chi_{112}=1.542$ $\chi_{113}=0.148$ $\chi_{222}=-1.542$ $\chi_{223}=0.148$ $\chi_{333}=0.123$	1.542
Cr <sub>4</sub> Br <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	82687	<i>Pc</i>	1.304	0.227	$\chi_{111}=-12.492$ $\chi_{113}=-22.160$ $\chi_{122}=-21.107$ $\chi_{133}=-17.299$ $\chi_{223}=-20.997$ $\chi_{333}=4.104$	22.16
Cr <sub>4</sub> Cl <sub>2</sub> (Si <sub>2</sub> O <sub>7</sub> )	82686	<i>Pc</i>	1.348	0.166	$\chi_{111}=-10.118$ $\chi_{113}=-1.524$ $\chi_{122}=-2.905$ $\chi_{133}=-1.230$ $\chi_{223}=3.578$ $\chi_{333}=1.053$	10.118
Cs(AlSiO <sub>4</sub> )	160822	<i>Pc2<sub>1</sub>n</i>	4.491	0.008	$\chi_{112}=0.013$ $\chi_{222}=-0.023$ $\chi_{233}=-0.005$	0.023
Cs(SbO)(Si <sub>2</sub> O <sub>6</sub> )	66535	<i>Pna2<sub>1</sub></i>	5.014	0.02	$\chi_{113}=-0.032$ $\chi_{223}=0.039$ $\chi_{333}=-0.001$	0.039
CsSiB <sub>3</sub> O <sub>7</sub>	255774	<i>Pna2<sub>1</sub></i>	5.428	0.044	$\chi_{113}=-0.760$ $\chi_{223}=-2.035$ $\chi_{333}=2.228$	2.228
Cs <sub>2</sub> ((Al <sub>2</sub> Si <sub>3</sub> )O <sub>10</sub> )	180325	<i>Fdd2</i>	4.553	0.007	$\chi_{113}=0.843$ $\chi_{223}=-0.458$ $\chi_{333}=-0.161$	0.843
Cs <sub>2</sub> SnSi <sub>3</sub> O <sub>9</sub>	414425	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	4.762	0.005	$\chi_{123}=0.797$	0.797
Cs <sub>20</sub> (Sn <sub>4</sub> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	412509	<i>Cc</i>	1.554	0.091	$\chi_{111}=-15.187$ $\chi_{113}=5.623$ $\chi_{122}=12.937$ $\chi_{133}=-6.543$ $\chi_{223}=0.201$ $\chi_{333}=-17.563$	17.563
H <sub>2</sub> SiTi <sub>2</sub> O <sub>7</sub> (H <sub>2</sub> O) <sub>2</sub>	173578	<i>P1</i>	3.246	0.092	$\chi_{133}=-0.002$ $\chi_{222}=0.001$ $\chi_{223}=-0.002$ $\chi_{333}=-0.002$	0.002
K(AlSiO <sub>4</sub> )	95367	<i>P6<sub>3</sub></i>	4.667	0	$\chi_{113}=0.176$ $\chi_{223}=0.176$	0.331

					$\chi_{333}=-0.331$	
K(AlSiO <sub>4</sub> )	162489	<i>P2<sub>1</sub></i>	4.536	0.002	$\chi_{112}=-0.085$ $\chi_{123}=-0.007$ $\chi_{222}=-0.284$ $\chi_{233}=0.249$	0.284
K(SbO)(SiO <sub>4</sub> )	69429	<i>Pna2<sub>1</sub></i>	4.977	0.004	$\chi_{113}=-0.068$ $\chi_{223}=-0.103$ $\chi_{333}=-0.273$	0.273
KAl(SiO <sub>4</sub> )	83449	<i>P3c</i>	4.569	0.005	$\chi_{112}=1.231$ $\chi_{113}=0.464$ $\chi_{222}=-1.231$ $\chi_{223}=0.464$ $\chi_{333}=-0.828$	1.231
KAl(SiO <sub>4</sub> )	34350	<i>P6<sub>3</sub></i>	4.592	0.005	$\chi_{113}=0.436$ $\chi_{223}=0.436$ $\chi_{333}=-0.869$	0.869
KBSi <sub>2</sub> O <sub>6</sub>	380488	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	5.313	1.00E-03	$\chi_{123}=-0.584$	0.584
KLi(Si <sub>2</sub> O <sub>5</sub> )	82457	<i>P2<sub>1</sub></i>	4.709	0.018	$\chi_{112}=1.110$ $\chi_{123}=-0.142$ $\chi_{222}=-0.438$ $\chi_{233}=0.536$	1.11
KNa <sub>3</sub> (Al <sub>4</sub> Si <sub>4</sub> O <sub>16</sub> )	27596	<i>P6<sub>3</sub></i>	4.522	0.002	$\chi_{113}=-0.348$ $\chi_{223}=-0.347$ $\chi_{333}=0.637$	0.637
KNa <sub>3</sub> (Al <sub>4</sub> Si <sub>4</sub> O <sub>16</sub> )	27584	<i>P6<sub>3</sub></i>	4.521	0.002	$\chi_{113}=0.349$ $\chi_{223}=0.349$ $\chi_{333}=-0.632$	0.632
K <sub>2</sub> ((Al <sub>2</sub> Si <sub>3</sub> )O <sub>10</sub> )	180323	<i>Fdd2</i>	4.424	0.006	$\chi_{113}=0.495$ $\chi_{223}=0.007$ $\chi_{333}=-0.126$	0.495
K <sub>2</sub> (NbO) <sub>2</sub> (Si <sub>4</sub> O <sub>12</sub> )	72111	<i>P4bm</i>	2.926	0.125	$\chi_{113}=12.076$ $\chi_{223}=12.075$ $\chi_{333}=1.013$	12.076
K <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	280480	<i>Cc</i>	4.137	0.011	$\chi_{111}=0.185$ $\chi_{113}=-0.061$ $\chi_{122}=0.146$ $\chi_{133}=-0.455$ $\chi_{223}=-0.004$ $\chi_{333}=0.077$	0.455
K <sub>2</sub> (TiSi <sub>3</sub> O <sub>9</sub> )	412920	<i>R3H</i>	3.683	0.042	$\chi_{111}=-0.101$ $\chi_{112}=-3.471$ $\chi_{113}=-0.957$ $\chi_{122}=0.101$ $\chi_{222}=3.471$ $\chi_{223}=-0.956$ $\chi_{333}=1.666$	3.471
K <sub>2</sub> (ZnSi <sub>2</sub> O <sub>6</sub> )	79705	<i>C222<sub>1</sub></i>	3.657	0.005	$\chi_{123}=-2.130$	2.13
K <sub>2</sub> Be <sub>2</sub> Si <sub>6</sub> O <sub>15</sub>	60284	<i>Cmc2<sub>1</sub></i>	4.824	0.004	$\chi_{113}=-0.054$ $\chi_{223}=0.340$ $\chi_{333}=0.027$	0.34
K <sub>2</sub> Ca(Si <sub>2</sub> O <sub>5</sub> )(CO <sub>3</sub> )	429979	<i>P6<sub>3</sub>22</i>	3.942	0.058	-	0
K <sub>2</sub> Cd(SiO <sub>4</sub> )	83229	<i>Pca2<sub>1</sub></i>	2.703	0.002	$\chi_{113}=2.958$ $\chi_{223}=-3.256$ $\chi_{333}=0.015$	3.256
K <sub>2</sub> HfSi <sub>3</sub> O <sub>9</sub>	9253	<i>P-6</i>	4.634	0.03	$\chi_{111}=0.014$ $\chi_{112}=0.004$	0.014

					$\chi_{122}=-0.014$ $\chi_{222}=-0.004$	
$K_2Mg(SiO_4)$	83226	$Pca2_1$	3.741	1.00E-03	$\chi_{113}=-1.150$ $\chi_{223}=1.116$ $\chi_{333}=-0.221$	1.15
$K_2Ti(Si_3O_9)$	166627	$P6_3/m$	3.504	0.068	-	0
$K_2Zn(SiO_4)$	83227	$Pca2_1$	3.159	0.004	$\chi_{113}=2.874$ $\chi_{223}=-2.933$ $\chi_{333}=0.013$	2.933
$K_2Zn(Si_4O_{10})$	68499	$P2_12_12_1$	4.344	0.006	$\chi_{123}=-0.997$	0.997
$K_2Zn_2(Si_8O_{19})$	68904	$C2$	4.086	0.02	$\chi_{112}=-0.851$ $\chi_{123}=0.094$ $\chi_{222}=2.091$ $\chi_{233}=-0.662$	2.091
$K_2Zr(Si_3O_9)$	200082	$P3$	4.635	0.039	$\chi_{111}=-0.041$ $\chi_{112}=0.034$ $\chi_{113}=0.021$ $\chi_{122}=0.041$ $\chi_{222}=-0.034$ $\chi_{223}=0.021$ $\chi_{333}=0.187$	0.187
$K_2Zr(Si_3O_9)$	56898	$P-6$	4.633	0.039	$\chi_{111}=-0.084$ $\chi_{112}=0.079$ $\chi_{122}=0.084$ $\chi_{222}=-0.079$	0.084
$K_3(Nb_3O_6)(Si_2O_7)$	79734	$P-62c$	1.884	0.323	$\chi_{112}=-4.939$ $\chi_{222}=4.939$	4.939
$K_4(Sn_2Si_6O_{18})$	151543	$R3H$	4.715	0.005	$\chi_{111}=-0.221$ $\chi_{112}=1.304$ $\chi_{113}=-0.504$ $\chi_{122}=0.221$ $\chi_{222}=-1.304$ $\chi_{223}=-0.504$ $\chi_{333}=0.539$	1.304
$K_4Ba(Si_3O_9)$	246254	$Ama2$	4.061	0.008	$\chi_{113}=0.187$ $\chi_{123}=0.003$ $\chi_{223}=-0.051$ $\chi_{333}=-1.538$	1.538
$K_4SrSi_3O_9$	245304	$Ama2$	4.028	0.007	$\chi_{113}=0.036$ $\chi_{223}=-0.521$ $\chi_{333}=-0.415$	0.521
$K_5In_3Si_7O_{21}$	249478	$Pna2_1$	4.281	0.009	$\chi_{113}=1.133$ $\chi_{223}=0.192$ $\chi_{333}=-1.507$	1.507
$K_6(Ta_6Si_4O_{26})$	15937	$P-62m$	3.224	0.136	$\chi_{112}=0.770$ $\chi_{222}=-0.770$	0.770
$Li(AlSiO_4)$	66137	$Pa$	5.323	0.007	$\chi_{111}=0.461$ $\chi_{113}=0.543$ $\chi_{122}=-0.300$ $\chi_{133}=0.051$ $\chi_{223}=0.242$ $\chi_{333}=-0.880$	0.88
$Li(AlSiO_4)$	92708	$R3H$	5.475	0.008	$\chi_{111}=-0.036$ $\chi_{112}=-0.010$ $\chi_{113}=-0.165$ $\chi_{122}=0.036$ $\chi_{222}=0.010$	0.268

					$\chi_{223}=-0.165$ $\chi_{333}=0.268$	
Li(AlSi <sub>4</sub> O <sub>10</sub> )	15415	<i>Pa</i>	5.535	0.01	$\chi_{111}=0.018$ $\chi_{113}=0.005$ $\chi_{133}=-0.025$ $\chi_{223}=-0.006$ $\chi_{333}=-0.015$	0.025
Li(AlSi <sub>4</sub> O <sub>10</sub> )	64962	<i>Pa</i>	5.529	0.009	$\chi_{111}=0.005$ $\chi_{113}=-0.008$ $\chi_{122}=0.002$ $\chi_{133}=-0.012$ $\chi_{223}=-0.005$ $\chi_{333}=0.009$	0.012
LiB(SiO <sub>4</sub> )	67536	<i>I-4</i>	6.581	0.004	$\chi_{113}=-0.307$ $\chi_{123}=1.650$ $\chi_{223}=0.307$	1.65
LiGa(SiO <sub>4</sub> )	65125	<i>R3H</i>	4.175	0.018	$\chi_{111}=-0.804$ $\chi_{112}=0.047$ $\chi_{113}=-1.116$ $\chi_{122}=0.804$ $\chi_{222}=-0.047$ $\chi_{223}=-1.116$ $\chi_{333}=1.960$	1.96
Li <sub>2</sub> (SiO <sub>3</sub> )	853	<i>Cmc2<sub>1</sub></i>	5.329	0.012	$\chi_{113}=-0.596$ $\chi_{223}=0.007$ $\chi_{333}=-2.021$	2.021
Li <sub>2</sub> (SiO <sub>3</sub> )	16626	<i>Cmc2<sub>1</sub></i>	5.329	0.012	$\chi_{113}=-0.602$ $\chi_{223}=0.010$ $\chi_{333}=-2.018$	2.018
Li <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	78562	<i>Ccc2</i>	5.304	0.002	$\chi_{113}=-0.547$ $\chi_{223}=-0.781$ $\chi_{333}=-0.681$	0.781
Li <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	280481	<i>Ccc2</i>	5.301	0.003	$\chi_{113}=0.543$ $\chi_{223}=0.768$ $\chi_{333}=0.678$	0.768
Li <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	15414	<i>Cc</i>	5.3	0.002	$\chi_{111}=-0.005$ $\chi_{113}=0.541$ $\chi_{133}=-0.002$ $\chi_{223}=0.765$ $\chi_{333}=0.672$	0.765
Li <sub>2</sub> Ba(SiO <sub>4</sub> )	180289	<i>P6<sub>3</sub>cm</i>	4.441	0	$\chi_{113}=-0.545$ $\chi_{223}=-0.545$ $\chi_{333}=7.405$	7.405
Li <sub>2</sub> Be(SiO <sub>4</sub> )	28307	<i>Pn</i>	6.205	0.011	$\chi_{111}=-0.726$ $\chi_{113}=0.600$ $\chi_{122}=-0.183$ $\chi_{133}=-0.242$ $\chi_{223}=-0.487$ $\chi_{333}=-0.109$	0.726
Li <sub>2</sub> Be(SiO <sub>4</sub> )	193838	<i>Pn</i>	6.205	0.011	$\chi_{111}=-0.718$ $\chi_{113}=0.603$ $\chi_{122}=-0.185$ $\chi_{133}=-0.241$ $\chi_{223}=-0.488$ $\chi_{333}=-0.109$	0.718
Li <sub>2</sub> BeSiO <sub>4</sub>	2319	<i>C222<sub>1</sub></i>	5.885	0.017	$\chi_{123}=0.511$	0.511
Li <sub>2</sub> CaSiO <sub>4</sub>	19023	<i>I-42m</i>	5.429	0.015	$\chi_{123}=1.600$	1.6

Li <sub>2</sub> SiO <sub>3</sub>	100402	<i>Cmc2<sub>1</sub></i>	5.331	0.012	$\chi_{113}=-0.593$ $\chi_{223}=0.006$ $\chi_{333}=-2.019$	2.019
Li <sub>2</sub> SiO <sub>3</sub>	28192	<i>Cmc2<sub>1</sub></i>	5.326	0.011	$\chi_{113}=-0.594$ $\chi_{223}=0.010$ $\chi_{333}=-2.011$	2.011
Li <sub>3</sub> (GaSiO <sub>5</sub> )	72100	<i>P2<sub>1</sub>nb</i>	3.765	0.012	$\chi_{111}=0.455$ $\chi_{122}=1.608$ $\chi_{133}=0.886$	1.608
Li <sub>3</sub> AlSiO <sub>5</sub>	252215	<i>Pna2<sub>1</sub></i>	5.154	0.007	$\chi_{113}=0.026$ $\chi_{223}=0.363$ $\chi_{333}=-2.063$	2.063
Li <sub>4</sub> (B <sub>4</sub> Si <sub>8</sub> O <sub>24</sub> )	90849	<i>P2<sub>1</sub></i>	5.803	0.009	$\chi_{112}=-0.007$ $\chi_{222}=-0.001$ $\chi_{233}=-0.006$	0.007
Li <sub>6</sub> (Si <sub>2</sub> O <sub>7</sub> )	25752	<i>P-42<sub>1</sub>m</i>	4.997	0.003	$\chi_{123}=-0.133$	0.133
Li <sub>8</sub> O <sub>2</sub> (SiO <sub>4</sub> )	65176	<i>P6<sub>3</sub>cm</i>	4.662	1.00E-02	$\chi_{113}=-0.873$ $\chi_{223}=-0.873$ $\chi_{333}=3.340$	3.34
MgNa <sub>2</sub> (SiO <sub>4</sub> )	15619	<i>Pn</i>	3.73	0.006	$\chi_{111}=0.195$ $\chi_{113}=-0.409$ $\chi_{122}=-0.462$ $\chi_{133}=0.400$ $\chi_{223}=-0.229$ $\chi_{333}=0.431$	0.462
Mg <sub>2</sub> (SiO <sub>4</sub> )	189973	<i>Cmc2<sub>1</sub></i>	4.414	0.033	$\chi_{113}=-0.432$ $\chi_{223}=-0.161$ $\chi_{333}=-0.263$	0.432
Na(AlSiO <sub>4</sub> )	73511	<i>Pb2<sub>1</sub>a</i>	4.769	0	$\chi_{112}=-0.671$ $\chi_{222}=0.004$ $\chi_{233}=0.666$	0.671
Na(AlSiO <sub>4</sub> )	191581	<i>P6<sub>3</sub></i>	4.377	0.003	$\chi_{113}=-0.331$ $\chi_{223}=-0.331$ $\chi_{333}=0.612$	0.612
Na(AlSiO <sub>4</sub> )	85553	<i>P6<sub>1</sub></i>	4.62	0.004	$\chi_{113}=-0.305$ $\chi_{223}=-0.305$ $\chi_{333}=0.574$	0.574
Na(GaSiO <sub>4</sub> )	411328	<i>P6<sub>3</sub></i>	3.932	0.026	$\chi_{113}=0.167$ $\chi_{223}=0.167$ $\chi_{333}=-1.987$	1.987
Na(SbO)(SiO <sub>4</sub> )	66354	<i>Pna2<sub>1</sub></i>	4.73	0.004	$\chi_{113}=-0.048$ $\chi_{223}=-0.119$ $\chi_{333}=-0.102$	0.119
NaAl(SiO <sub>4</sub> )	36324	<i>P6<sub>3</sub></i>	4.397	0.003	$\chi_{113}=-0.327$ $\chi_{223}=-0.327$ $\chi_{333}=0.610$	0.61
NaAlSiO <sub>4</sub>	433181	<i>P3<sub>2</sub></i>	4.88	0.006	$\chi_{111}=0.588$ $\chi_{112}=-0.549$ $\chi_{113}=-0.312$ $\chi_{122}=-0.588$ $\chi_{222}=0.549$ $\chi_{223}=-0.312$ $\chi_{333}=0.681$	0.681
NaAlSiO <sub>4</sub>	8646	<i>P6<sub>3</sub></i>	4.392	0.003	$\chi_{113}=-0.331$ $\chi_{223}=-0.331$ $\chi_{333}=0.616$	0.616

NaAlSiO <sub>4</sub>	259567	<i>P6<sub>3</sub></i>	4.392	0.003	$\chi_{113}=-0.332$ $\chi_{223}=-0.332$ $\chi_{333}=0.615$	0.615
NaB(SiO <sub>4</sub> )	92822	<i>P6<sub>3</sub></i>	5.534	0.006	$\chi_{113}=-0.081$ $\chi_{223}=-0.081$ $\chi_{333}=-0.058$	0.081
NaBSiO <sub>4</sub>	39459	<i>P6<sub>3</sub></i>	5.546	0.008	$\chi_{113}=0.239$ $\chi_{223}=0.239$ $\chi_{333}=0.170$	0.239
NaCa <sub>3</sub> PSiO <sub>8</sub>	254593	<i>Pna2<sub>1</sub></i>	4.313	0.005	$\chi_{113}=-0.424$ $\chi_{223}=-0.280$ $\chi_{333}=-1.377$	1.377
NaCs(Si <sub>2</sub> O <sub>5</sub> )	92535	<i>Pna2<sub>1</sub></i>	4.666	0.006	$\chi_{113}=-0.007$ $\chi_{223}=0.009$ $\chi_{333}=-0.022$	0.022
NaY(SiO <sub>4</sub> )	30384	<i>Pbn2<sub>1</sub></i>	4.554	0.043	$\chi_{113}=0.001$ $\chi_{223}=0.001$ $\chi_{333}=0.022$	0.022
NaYSiO <sub>4</sub>	20161	<i>Pc2<sub>1</sub>n</i>	4.555	0.043	$\chi_{112}=0.006$ $\chi_{222}=-0.007$ $\chi_{233}=-0.006$	0.007
Na <sub>2</sub> (MgSiO <sub>4</sub> )	84562	<i>Pna2<sub>1</sub></i>	3.724	0.005	$\chi_{113}=-0.361$ $\chi_{223}=0.361$ $\chi_{333}=0.269$	0.361
Na <sub>2</sub> (MgSiO <sub>4</sub> )	84563	<i>Pna2<sub>1</sub></i>	3.724	0.005	$\chi_{113}=0.360$ $\chi_{223}=-0.361$ $\chi_{333}=-0.269$	0.361
Na <sub>2</sub> (SiO <sub>3</sub> )	15388	<i>Cmc2<sub>1</sub></i>	3.861	0.013	$\chi_{113}=-0.407$ $\chi_{223}=-0.479$ $\chi_{333}=0.363$	0.479
Na <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	80378	<i>Pbc2<sub>1</sub></i>	4.347	0.023	$\chi_{113}=-0.341$ $\chi_{223}=-0.239$ $\chi_{333}=-0.326$	0.341
Na <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> )	98564	<i>Pn2<sub>1</sub>a</i>	4.539	0.021	$\chi_{112}=-0.024$ $\chi_{222}=0.103$ $\chi_{233}=0.109$	0.109
Na <sub>2</sub> (TiSiO <sub>5</sub> )	82153	<i>Pmc2<sub>1</sub></i>	3.482	0.026	$\chi_{111}=0.001$ $\chi_{113}=-4.248$ $\chi_{223}=-0.564$ $\chi_{333}=11.670$	11.670
Na <sub>2</sub> (ZnSiO <sub>4</sub> )	83312	<i>Pna2<sub>1</sub></i>	3.021	0.014	$\chi_{113}=3.880$ $\chi_{223}=-3.099$ $\chi_{333}=0.311$	3.88
Na <sub>2</sub> (ZnSi <sub>3</sub> O <sub>8</sub> )	924	<i>P2<sub>1</sub></i>	4.03	0.009	$\chi_{112}=-0.638$ $\chi_{123}=0.143$ $\chi_{222}=1.085$ $\chi_{233}=-0.732$	1.085
Na <sub>2</sub> BaSi <sub>2</sub> O <sub>6</sub>	10217	<i>P2<sub>1</sub></i>	4.183	0.027	$\chi_{112}=-0.256$ $\chi_{123}=-0.003$ $\chi_{222}=0.137$ $\chi_{233}=-0.930$	0.93
Na <sub>2</sub> Be(SiO <sub>4</sub> )	69009	<i>Pca2<sub>1</sub></i>	4.688	1.00E-03	$\chi_{113}=0.708$ $\chi_{223}=-0.714$ $\chi_{333}=0.102$	0.714
Na <sub>2</sub> Be(SiO <sub>4</sub> )	202719	<i>Pca2<sub>1</sub></i>	4.693	0.002	$\chi_{113}=0.703$ $\chi_{223}=-0.710$ $\chi_{333}=0.104$	0.71

Na <sub>2</sub> Be(SiO <sub>4</sub> )	69010	<i>Pca2<sub>1</sub></i>	4.688	1.00E-03	$\chi_{113}=0.700$ $\chi_{223}=-0.707$ $\chi_{333}=0.115$	0.707
Na <sub>2</sub> Be(SiO <sub>4</sub> )	203149	<i>Pca2<sub>1</sub></i>	3.016	0.018	$\chi_{113}=0.324$ $\chi_{223}=0.207$ $\chi_{333}=-0.266$	0.324
Na <sub>2</sub> Mg(SiO <sub>4</sub> )	15618	<i>Pn</i>	3.73	0.006	$\chi_{111}=0.197$ $\chi_{113}=-0.415$ $\chi_{122}=-0.460$ $\chi_{133}=0.398$ $\chi_{223}=-0.237$ $\chi_{333}=0.423$	0.46
Na <sub>2</sub> Si(S <sub>2</sub> O <sub>7</sub> ) <sub>3</sub>	422034	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	5.547	0.013	$\chi_{123}=-0.167$	0.167
Na <sub>2</sub> SiO <sub>3</sub>	24664	<i>Cmc2<sub>1</sub></i>	3.863	0.013	$\chi_{113}=-0.421$ $\chi_{223}=-0.478$ $\chi_{333}=0.336$	0.478
Na <sub>2</sub> TiSiO <sub>5</sub>	259048	<i>Pmc2<sub>1</sub></i>	3.48	0.026	$\chi_{113}=-4.512$ $\chi_{223}=-0.607$ $\chi_{333}=11.660$	11.660
Na <sub>2</sub> Zn(SiO <sub>4</sub> )	27735	<i>Pn</i>	3.079	0.014	$\chi_{111}=4.924$ $\chi_{112}=-3.092$ $\chi_{122}=-2.351$ $\chi_{133}=-2.613$ $\chi_{222}=0.266$ $\chi_{233}=3.476$	4.924
Na <sub>2</sub> Zn(SiO <sub>4</sub> )	18314	<i>Pn</i>	3.08	0.013	$\chi_{111}=0.221$ $\chi_{113}=-2.375$ $\chi_{122}=3.449$ $\chi_{133}=-3.045$ $\chi_{223}=-2.587$ $\chi_{333}=4.903$	4.903
Na <sub>2</sub> Zn(SiO <sub>4</sub> )	34565	<i>Pn</i>	3.076	0.015	$\chi_{111}=4.886$ $\chi_{112}=-3.007$ $\chi_{122}=-2.331$ $\chi_{133}=-2.620$ $\chi_{222}=0.270$ $\chi_{233}=3.463$	4.886
Na <sub>2</sub> Zn(SiO <sub>4</sub> )	34068	<i>Pn</i>	3.078	0.014	$\chi_{111}=0.233$ $\chi_{113}=-2.367$ $\chi_{122}=3.517$ $\chi_{133}=-3.052$ $\chi_{223}=-2.579$ $\chi_{333}=4.853$	4.853
Na <sub>2</sub> Zn(Si <sub>2</sub> O <sub>6</sub> )	20837	<i>Fdd2</i>	3.656	0.01	$\chi_{113}=2.208$ $\chi_{223}=-3.125$ $\chi_{333}=-0.462$	3.125
Na <sub>2</sub> Zn(Si <sub>2</sub> O <sub>6</sub> )	16160	<i>Fdd2</i>	3.631	0.009	$\chi_{113}=2.121$ $\chi_{223}=-3.080$ $\chi_{333}=-0.370$	3.08
Na <sub>2</sub> Zn(Si <sub>3</sub> O <sub>8</sub> )	20114	<i>P2<sub>1</sub></i>	4.027	0.009	$\chi_{113}=0.641$ $\chi_{123}=-0.140$ $\chi_{223}=0.737$ $\chi_{333}=-1.091$	1.091
Na <sub>2</sub> Zn(Si <sub>3</sub> O <sub>8</sub> )	200440	<i>P2<sub>1</sub></i>	4.027	0.009	$\chi_{113}=0.651$ $\chi_{123}=-0.136$ $\chi_{223}=0.729$ $\chi_{333}=-1.071$	1.071



$\text{Na}_2\text{Zn}_2(\text{Si}_2\text{O}_7)$	20477	<i>C2cm</i>	3.289	0.05	$\chi_{111}=-5.402$ $\chi_{122}=5.218$ $\chi_{133}=0.443$	5.402
$\text{Na}_2\text{Zn}_2(\text{Si}_2\text{O}_7)$	34325	<i>C2cm</i>	3.286	0.049	$\chi_{111}=-5.395$ $\chi_{122}=5.199$ $\chi_{133}=0.407$	5.395
$\text{Na}_2\text{Zn}_3(\text{SiO}_4)_2$	4339	<i>P1</i>	2.667	0.027	$\chi_{111}=-1.245$ $\chi_{112}=-0.811$ $\chi_{113}=-0.075$ $\chi_{122}=1.242$ $\chi_{123}=-0.302$ $\chi_{133}=-0.042$ $\chi_{222}=0.112$ $\chi_{223}=-0.154$ $\chi_{233}=0.394$ $\chi_{333}=-0.313$	1.245
$\text{Na}_3(\text{Si}_2\text{PO}_8)$	161804	<i>P2_12_12_1</i>	3.608	0.008	$\chi_{123}=0.103$	0.103
$\text{Na}_3\text{AlBeSi}_2\text{O}_8$	4334	<i>P2_12_12</i>	4.561	0.003	$\chi_{123}=-0.372$	0.372
$\text{Na}_3\text{AlBeSi}_2\text{O}_8$	20495	<i>P2_12_12</i>	4.561	0.003	$\chi_{123}=-0.372$	0.372
$\text{Na}_3\text{YSi}_3\text{O}_9$	20774	<i>P2_12_12_1</i>	4.463	0	$\chi_{123}=-0.032$	0.032
$\text{Na}_4\text{Sc}_2(\text{Si}_4\text{O}_{13})$	200808	<i>Pna2_1</i>	4.679	0.028	$\chi_{113}=0.092$ $\chi_{223}=-0.343$ $\chi_{333}=0.128$	0.343
$\text{Na}_4\text{Sr}(\text{SiO}_3)_3$	33943	<i>C2</i>	4.084	0.005	$\chi_{112}=0.247$ $\chi_{123}=0.297$ $\chi_{222}=-0.908$ $\chi_{233}=0.578$	0.908
$\text{Na}_4\text{Zr}_2(\text{SiO}_4)_3$	20340	<i>R3cR</i>	4.338	0.032	$\chi_{111}=0.137$ $\chi_{113}=-0.069$ $\chi_{122}=-0.137$ $\chi_{223}=-0.069$ $\chi_{333}=-0.128$	0.137
$\text{Na}_6\text{Be}_3(\text{Si}_6\text{O}_{18})$	34075	<i>Fdd2</i>	4.845	0.002	$\chi_{113}=-0.424$ $\chi_{223}=0.479$ $\chi_{333}=0.054$	0.479
$\text{Na}_6\text{Cd}_3(\text{Si}_6\text{O}_{18})$	20475	<i>Pm2_1n</i>	3.244	1.30E-02	$\chi_{112}=-0.532$ $\chi_{222}=0.945$ $\chi_{233}=0.672$	0.945
$\text{Na}_8(\text{AlBeSi}_4\text{O}_{12})_2\text{Cl}_2$	69958	<i>I-4</i>	4.715	0.014	$\chi_{113}=-0.103$ $\chi_{123}=0.944$ $\chi_{223}=0.103$	0.944
$\text{Na}_8(\text{Be}_2\text{Al}_2\text{Si}_8\text{O}_{24})\text{Cl}_2$	34665	<i>I-4</i>	4.723	0.014	$\chi_{113}=-0.103$ $\chi_{123}=0.939$ $\chi_{223}=0.103$	0.939
$\text{NbCa}_7(\text{Si}_2\text{O}_7)_2\text{O}_3\text{F}$	31269	<i>Pa</i>	3.124	0.047	$\chi_{111}=3.219$ $\chi_{113}=3.158$ $\chi_{122}=1.082$ $\chi_{133}=-2.245$ $\chi_{223}=0.068$ $\chi_{333}=-4.164$	4.164
$\text{Nb}_2\text{Ca}_{14}(\text{Si}_2\text{O}_7)_4\text{O}_6\text{F}_2$	158915	<i>Pa</i>	3.121	0.047	$\chi_{111}=3.185$ $\chi_{113}=3.161$ $\chi_{122}=1.082$ $\chi_{133}=-2.246$ $\chi_{223}=0.080$ $\chi_{333}=-4.146$	4.146

PbZn(SiO <sub>4</sub> )	26840	<i>Pna2<sub>1</sub></i>	3.263	0.033	$\chi_{113}=-4.954$ $\chi_{223}=-3.024$ $\chi_{333}=15.160$	15.16
Pb <sub>2</sub> In <sub>2</sub> Si <sub>2</sub> O <sub>9</sub>	40857	<i>Pna2<sub>1</sub></i>	3.223	0.02	$\chi_{113}=5.923$ $\chi_{223}=3.693$ $\chi_{333}=2.454$	5.923
Pb <sub>2</sub> In <sub>2</sub> Si <sub>2</sub> O <sub>9</sub>	407263	<i>Pna2<sub>1</sub></i>	3.231	0.021	$\chi_{113}=5.787$ $\chi_{223}=3.770$ $\chi_{333}=2.357$	5.787
Pb <sub>4</sub> Zn <sub>2</sub> ((SO <sub>4</sub> )(SiO <sub>4</sub> (Si <sub>2</sub> O <sub>7</sub> ))	100296	<i>P2<sub>1</sub></i>	3.571	0.011	$\chi_{112}=-0.361$ $\chi_{123}=1.143$ $\chi_{222}=-11.660$ $\chi_{233}=1.570$	11.66
Rb(AlSiO <sub>4</sub> )	4335	<i>Pc2<sub>1</sub>n</i>	4.335	0.008	$\chi_{112}=-1.110$ $\chi_{222}=0.967$ $\chi_{233}=0.045$	1.11
Rb(AlSiO <sub>4</sub> )	160823	<i>Pc2<sub>1</sub>n</i>	4.335	0.009	$\chi_{112}=1.080$ $\chi_{222}=-0.967$ $\chi_{233}=-0.078$	1.08
RbNb(SiO <sub>3</sub> )O <sub>2</sub>	39594	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	2.81	0.023	$\chi_{123}=0.281$	0.281
Rb <sub>2</sub> ((Al <sub>2</sub> Si <sub>3</sub> )O <sub>10</sub> )	180324	<i>Fdd2</i>	4.512	0.004	$\chi_{113}=0.742$ $\chi_{223}=-0.200$ $\chi_{333}=0.110$	0.742
Rb <sub>2</sub> (Be <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> )	828	<i>P2nn</i>	4.382	0.005	$\chi_{111}=0.109$ $\chi_{122}=0.486$ $\chi_{133}=-0.337$	0.486
Rb <sub>2</sub> Ca <sub>2</sub> Si <sub>3</sub> O <sub>9</sub>	430223	<i>Pn</i>	4.247	0.009	$\chi_{111}=-0.208$ $\chi_{113}=0.321$ $\chi_{122}=0.164$ $\chi_{133}=-0.190$ $\chi_{223}=-2.201$ $\chi_{333}=1.141$	2.201
Rb <sub>2</sub> Cd(SiO <sub>4</sub> )	93879	<i>C222<sub>1</sub></i>	2.851	0.016	$\chi_{123}=-0.014$	0.014
Rb <sub>6</sub> (Si <sub>10</sub> O <sub>23</sub> )	250378	<i>Cm2m</i>	4.273	0.013	$\chi_{112}=-1.583$ $\chi_{222}=2.443$ $\chi_{233}=-0.755$	2.443
Rb <sub>6</sub> Si <sub>10</sub> O <sub>23</sub>	14023	<i>C2mm</i>	4.366	0.012	$\chi_{111}=1.132$ $\chi_{122}=-2.030$ $\chi_{133}=0.895$	2.03
Si(P <sub>2</sub> O <sub>7</sub> )	75116	<i>P6<sub>3</sub></i>	5.913	0.015	$\chi_{113}=-0.001$ $\chi_{223}=-0.001$ $\chi_{333}=-0.005$	0.005
SiO <sub>2</sub>	413210	<i>Cc</i>	5.669	0.006	$\chi_{111}=-1.746$ $\chi_{113}=-0.340$ $\chi_{122}=1.112$ $\chi_{133}=0.886$ $\chi_{223}=0.393$ $\chi_{333}=0.040$	1.746
SiO <sub>2</sub>	81382	<i>C1</i>	5.77	1.00E-03	$\chi_{111}=-1.458$ $\chi_{113}=-0.236$ $\chi_{122}=1.244$ $\chi_{123}=0.001$ $\chi_{133}=0.190$ $\chi_{222}=-0.002$ $\chi_{223}=0.188$ $\chi_{233}=-0.003$ $\chi_{333}=-0.025$	1.458

SiO <sub>2</sub>	27745	<i>P</i> 3 <sub>1</sub> 21	5.831	3.00E-03	$\chi_{112}=1.086$ $\chi_{222}=-1.086$	1.086
SiO <sub>2</sub>	62405	<i>P</i> 3 <sub>2</sub> 21	5.828	2.00E-03	$\chi_{112}=-1.061$ $\chi_{222}=1.061$	1.061
SiO <sub>2</sub>	67121	<i>P</i> 3 <sub>1</sub> 21	5.825	0.003	$\chi_{112}=-1.048$ $\chi_{222}=1.048$	1.048
SiO <sub>2</sub>	41414	<i>P</i> 3 <sub>1</sub> 21	5.823	0.002	$\chi_{112}=-1.038$ $\chi_{222}=1.038$	1.038
SiO <sub>2</sub>	69114	<i>Cmc</i> 2 <sub>1</sub>	5.737	4.00E-03	$\chi_{113}=0.021$ $\chi_{223}=0.671$ $\chi_{333}=-0.548$	0.671
SiO <sub>2</sub>	34867	<i>Cc</i>	5.643	0.004	$\chi_{111}=0.294$ $\chi_{113}=0.081$ $\chi_{122}=-0.084$ $\chi_{133}=-0.216$ $\chi_{223}=-0.040$ $\chi_{333}=-0.093$	0.294
SiO <sub>2</sub>	408281	<i>Cc</i>	5.634	0.003	$\chi_{111}=0.253$ $\chi_{113}=-0.080$ $\chi_{122}=-0.083$ $\chi_{133}=-0.172$ $\chi_{223}=0.025$ $\chi_{333}=0.111$	0.253
SiO <sub>2</sub>	153471	<i>Aa</i>	5.628	0.003	$\chi_{111}=-0.183$ $\chi_{113}=-0.082$ $\chi_{122}=-0.059$ $\chi_{133}=0.203$ $\chi_{223}=0.061$ $\chi_{333}=0.006$	0.203
SiO <sub>2</sub>	52371	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	5.869	0.004	$\chi_{123}=-0.021$	0.021
SiO <sub>2</sub>	171674	<i>Amm</i> 2	5.732	1.00E-03	$\chi_{113}=-0.015$ $\chi_{223}=0.014$ $\chi_{333}=0.012$	0.015
SiO <sub>2</sub>	47220	<i>P</i> 4 <sub>1</sub> 2 <sub>1</sub> 2	5.654	0.006	-	0
SiO <sub>2</sub>	29343	<i>P</i> 6 <sub>3</sub> 22	5.599	0.002	-	0
Si <sub>32</sub> O <sub>64</sub>	280624	<i>C</i> 222	5.882	0.002	$\chi_{123}=-0.024$	0.024
Si <sub>6</sub> O <sub>12</sub>	162441	<i>Cmc</i> 2 <sub>1</sub>	5.735	0.004	$\chi_{113}=-0.031$ $\chi_{223}=-0.634$ $\chi_{333}=0.543$	0.634
SrNa <sub>2</sub> (AlSiO <sub>4</sub> ) <sub>4</sub>	156656	<i>lba</i> 2	4.923	0.007	$\chi_{113}=0.206$ $\chi_{223}=0.468$ $\chi_{333}=-0.602$	0.602
SrSiAl <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	408170	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	4.173	1.50E-02	$\chi_{123}=-2.357$	2.357
Sr <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	261226	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.771	0.016	$\chi_{123}=-0.229$	0.229
Sr <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	155300	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.772	0.016	$\chi_{123}=-0.225$	0.225
Sr <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	183978	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.771	0.016	$\chi_{123}=-0.224$	0.224
Sr <sub>2</sub> Mg(Si <sub>2</sub> O <sub>7</sub> )	31308	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.772	0.016	$\chi_{123}=-0.216$	0.216
Sr <sub>2</sub> MgSi <sub>2</sub> O <sub>7</sub>	230649	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.769	0.016	$\chi_{123}=-0.218$	0.218
Sr <sub>2</sub> Zn(Si <sub>2</sub> O <sub>7</sub> )	247476	<i>P</i> -42 <sub>1</sub> <i>m</i>	4.184	0.004	$\chi_{123}=-1.413$	1.413
Sr <sub>3</sub> (Si <sub>3</sub> O <sub>9</sub> )	32542	<i>C</i> 2	4.714	0.039	$\chi_{112}=0.005$ $\chi_{123}=-0.006$ $\chi_{222}=0.007$ $\chi_{233}=-0.002$	0.007
Sr <sub>3</sub> (TaGa <sub>3</sub> Si <sub>2</sub> O <sub>14</sub> )	91779	<i>P</i> 321	3.988	0.066	$\chi_{112}=-0.198$	0.198

					$\chi_{222}=0.198$	
$\text{Sr}_3\text{Mg}(\text{SiO}_4)_2$	195459	<i>C2</i>	5.068	0.02	$\chi_{112}=0.043$ $\chi_{123}=-0.009$ $\chi_{222}=-0.042$ $\chi_{233}=0.015$	0.043
$\text{Sr}_3\text{TaGa}_3\text{Si}_2\text{O}_{14}$	421591	<i>P321</i>	3.987	0.066	$\chi_{112}=-0.193$ $\chi_{222}=0.193$	0.193
$\text{Sr}_3\text{TaGa}_3\text{Si}_2\text{O}_{14}$	380530	<i>P321</i>	3.986	0.066	$\chi_{112}=-0.190$ $\chi_{222}=0.190$	0.190
$\text{Sr}_3\text{Ta}_6\text{Si}_4\text{O}_{26}$	15936	<i>P-62m</i>	3.319	0.170	$\chi_{112}=-1.036$ $\chi_{222}=1.036$	1.036
$\text{Tl}(\text{AlSiO}_4)$	195357	<i>Pna2_1</i>	3.631	0.043	$\chi_{113}=0.329$ $\chi_{223}=0.064$ $\chi_{333}=0.276$	0.329
$\text{Y}_2(\text{SiP}_4\text{O}_{15})$	185335	<i>P22_12_1</i>	5.798	0.059	$\chi_{123}=0.203$	0.203
$\text{Y}_2(\text{Si}_2\text{O}_7)$	74778	<i>Pna2_1</i>	5.39	0.009	$\chi_{113}=0.005$ $\chi_{223}=-0.006$ $\chi_{333}=0.029$	0.029
$\text{Y}_2\text{Si}(\text{Be}_2\text{O}_7)$	95553	<i>P-421m</i>	5.628	0.034	$\chi_{123}=-0.447$	0.447
$\text{Y}_2\text{Si}(\text{Be}_2\text{O}_7)$	95552	<i>P-42_1m</i>	5.629	0.034	$\chi_{123}=-0.441$	0.441
$\text{Y}_2\text{SiBe}_2\text{O}_7$	23233	<i>P-42_1m</i>	5.628	0.034	$\chi_{123}=0.429$	0.429
$\text{Zn}_2(\text{SiO}_4)$	9147	<i>I-42d</i>	2.528	0.029	$\chi_{123}=2.465$	2.465