

AM-90-444

Crystal chemistry of synthetic pyroxenes on the join $\text{CaNiSi}_2\text{O}_6$ - $\text{CaMgSi}_2\text{O}_6$
(diopside): A Rietveld structure refinement study

Mati Raudsepp, Frank C. Hawthorne, Allan C. Turnock

For deposit: Unnumbered table

American Mineralogist, 75, 11-12, 1274-1281.

INTENSITY DATA

Raudsepp, M., Hawthorne, F.C. and Turnock, A.C. Crystal chemistry of synthetic pyroxenes on the join
CaNiSi₂O₆-CaMgSi₂O₆ (diopside): A Rietveld structure refinement study.

Sample No.		NiO (CaMgSi ₂ O ₆)		Yobs		Ycalc		2theta		Yobs		Ycalc		2theta		Yobs		Ycalc		2theta		Yobs		Ycalc		2theta		Yobs		Ycalc		2theta	
17.0000	85	80	23.0000	100	76	29.0000	126	132	35.0000	920	975	41.0000	506	465																			
17.1200	91	80	23.1200	69	76	29.1200	147	149	35.1200	792	801	41.1200	489	451																			
17.2400	81	80	23.2400	66	76	29.2400	177	175	35.2400	540	571	41.2400	321	310																			
17.3600	80	80	23.3600	79	76	29.3600	235	218	35.3600	728	770	41.3600	186	184																			
17.4800	70	80	23.4800	91	76	29.4800	358	314	35.4800	1506	1536	41.4800	134	138																			
17.6000	75	80	23.6000	99	77	29.6000	630	636	35.6000	2400	2365	41.6000	143	141																			
17.7200	100	79	23.7200	70	77	29.7200	1568	1641	35.7200	2301	2372	41.7200	172	198																			
17.8400	75	79	23.8400	77	78	29.8400	3061	3228	35.8400	1470	1512	41.8400	355	331																			
17.9600	78	79	23.9600	91	80	29.9600	3185	3289	35.9600	636	689	41.9600	444	430																			
18.0800	85	79	24.0800	95	89	30.0800	1880	1897	36.0800	288	322	42.0800	378	387																			
18.2000	72	79	24.2000	120	115	30.2000	1235	1256	36.2000	180	204	42.2000	399	418																			
18.3200	70	79	24.3200	145	154	30.3200	1282	1309	36.3200	127	158	42.3200	740	633																			
18.4400	80	79	24.4400	161	149	30.4400	994	1013	36.4400	115	134	42.4400	695	689																			
18.5600	78	79	24.5600	95	110	30.5600	546	594	36.5600	92	118	42.5600	453	462																			
18.6800	74	80	24.6800	98	87	30.6800	508	551	36.6800	84	108	42.6800	313	291																			
18.8000	79	80	24.8000	103	80	30.8000	891	945	36.8000	73	101	42.8000	319	303																			
18.9200	76	81	24.9200	83	78	30.9200	1216	1335	36.9200	57	95	42.9200	379	363																			
19.0400	84	82	25.0400	90	78	31.0400	978	997	37.0400	80	89	43.0400	304	296																			
19.1600	77	81	25.1600	87	77	31.1600	500	480	37.1600	90	86	43.1600	173	184																			
19.2800	72	81	25.2800	83	77	31.2800	263	240	37.2800	93	87	43.2800	117	126																			
19.4000	83	82	25.4000	88	77	31.4000	180	172	37.4000	82	90	43.4000	138	111																			
19.5200	93	84	25.5200	93	78	31.5200	157	154	37.5200	103	101	43.5200	135	117																			
19.6400	66	93	25.6400	113	80	31.6400	156	139	37.6400	123	111	43.6400	135	126																			
19.7600	120	122	25.7600	76	82	31.7600	126	120	37.7600	130	103	43.7600	130	122																			
19.8800	170	166	25.8800	94	83	31.8800	92	99	37.8800	91	86	43.8800	128	118																			
20.0000	184	167	26.0000	78	86	32.0000	99	89	38.0000	83	78	44.0000	155	133																			
20.1200	130	132	26.1200	97	91	32.1200	107	85	38.1200	71	78	44.1200	209	202																			
20.2400	122	109	26.2400	116	100	32.2400	110	83	38.2400	94	83	44.2400	372	393																			
20.3600	76	92	26.3600	126	127	32.3600	78	79	38.3600	96	94	44.3600	677	647																			
20.4800	80	84	26.4800	214	222	32.4800	96	76	38.4800	91	99	44.4800	602	616																			
20.6000	82	81	26.6000	429	413	32.6000	91	75	38.6000	73	97	44.6000	421	388																			
20.7200	69	79	26.7200	482	494	32.7200	93	74	38.7200	111	103	44.7200	318	275																			
20.8400	80	79	26.8400	377	328	32.8400	73	74	38.8400	141	134	44.8400	333	354																			
20.9600	85	78	26.9600	180	182	32.9600	90	71	38.9600	230	244	44.9600	492	516																			
21.0800	92	78	27.0800	141	135	33.0800	95	71	39.0800	488	482	45.0800	543	532																			
21.2000	60	78	27.2000	149	141	33.2000	78	72	39.2000	635	630	45.2000	427	456																			
21.3200	83	78	27.3200	216	206	33.3200	88	72	39.3200	435	451	45.3200	382	341																			
21.4400	75	77	27.4400	432	437	33.4400	75	73	39.4400	255	230	45.4400	233	215																			
21.5600	75	77	27.5600	880	846	33.5600	72	73	39.5600	157	132	45.5600	137	140																			
21.6800	80	77	27.6800	898	916	33.6800	80	78	39.6800	126	103	45.6800	124	116																			
21.8000	97	77	27.8000	546	523	33.8000	84	83	39.8000	148	93	45.8000	103	121																			
21.9200	93	77	27.9200	219	241	33.9200	69	81	39.9200	128	89	45.9200	179	169																			
22.0400	79	76	28.0400	144	146	34.0400	69	91	40.0400	106	89	46.0400	289	265																			
22.1600	70	76	28.1600	101	120	34.1600	82	97	40.1600	91	91	46.1600	314	296																			
22.2800	68	76	28.2800	108	111	34.2800	82	105	40.2800	89	99	46.2800	221	218																			
22.4000	89	76	28.4000	89	108	34.4000	106	116	40.4000	115	119	46.4000	153	141																			
22.5200	60	76	28.5200	96	108	34.5200	128	136	40.5200	157	172	46.5200	118	110																			
22.6400	76	76	28.6400	118	110	34.6400	197	181	40.6400	296	295	46.6400	99	94																			
22.7600	69	76	28.7600	100	113	34.7600	293	327	40.7600	417	433	46.7600	68	81																			
22.8800	79	76	28.8800	119	119	34.8800	639	669	40.8800	452	451	46.8800	57	74																			

2theta	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC	2theta	Yobs	YcalC
47.0000	71	69	87	86	59.0000	141	132	65.0000	151	114	71.0000	348	306												
47.1200	69	67	115	104	59.1200	213	168	65.1200	134	130	71.1200	299	291												
47.2400	43	66	107	123	59.2400	176	160	65.2400	198	180	71.2400	280	254												
47.3600	59	65	134	120	59.3600	144	142	65.3600	293	269	71.3600	198	211												
47.4800	63	64	75	108	59.4800	142	161	65.4800	410	409	71.4800	181	190												
47.6000	67	64	79	98	59.6000	223	211	65.6000	625	603	71.6000	191	190												
47.7200	72	66	84	86	59.7200	184	209	65.7200	625	601	71.7200	142	165												
47.8400	75	70	82	76	59.8400	182	166	65.8400	486	468	71.8400	131	135												
47.9600	66	75	63	72	59.9600	129	125	65.9600	376	311	71.9600	70	102												
48.0800	70	75	97	72	60.0800	117	109	66.0800	280	264	72.0800	90	83												
48.2000	62	70	63	75	60.2000	108	114	66.2000	336	340	72.2000	61	74												
48.3200	55	67	102	86	60.3200	158	148	66.3200	427	427	72.3200	71	70												
48.4400	63	68	118	106	60.4400	228	223	66.4400	410	403	72.4400	57	68												
48.5600	58	70	121	123	60.5600	278	286	66.5600	295	295	72.5600	63	68												
48.6800	78	75	134	153	60.6800	291	327	66.6800	163	191	72.6800	55	70												
48.8000	73	90	247	216	60.8000	361	350	66.8000	135	134	72.8000	74	75												
48.9200	123	119	256	256	60.9200	302	311	66.9200	105	114	72.9200	109	85												
49.0400	126	135	212	224	61.0400	242	234	67.0400	131	110	73.0400	101	99												
49.1600	126	121	170	191	61.1600	184	173	67.1600	141	122	73.1600	103	108												
49.2800	101	106	240	224	61.2800	184	166	67.2800	179	159	73.2800	123	125												
49.4000	116	120	256	264	61.4000	213	198	67.4000	212	191	73.4000	182	167												
49.5200	209	187	204	225	61.5200	295	285	67.5200	190	171	73.5200	234	226												
49.6400	311	300	128	157	61.6400	448	420	67.6400	128	133	73.6400	276	268												
49.7600	330	346	121	117	61.7600	438	423	67.7600	117	98	73.7600	326	325												
49.8800	304	293	121	107	61.8800	342	324	67.8800	91	88	73.8800	331	372												
50.0000	218	203	124	111	62.0000	225	219	68.0000	112	100	74.0000	393	329												
50.1200	154	151	153	127	62.1200	203	189	68.1200	157	120	74.1200	233	255												
50.2400	156	157	189	165	62.2400	226	215	68.2400	130	124	74.2400	181	172												
50.3600	175	173	311	272	62.3600	258	251	68.3600	113	106	74.3600	122	120												
50.4800	168	148	578	542	62.4800	213	231	68.4800	89	85	74.4800	105	97												
50.6000	123	115	999	944	62.6000	171	174	68.6000	64	69	74.6000	89	91												
50.7200	106	99	940	996	62.7200	125	121	68.7200	71	63	74.7200	97	96												
50.8400	89	89	732	734	62.8400	98	99	68.8400	58	60	74.8400	135	115												
50.9600	77	80	506	472	62.9600	110	95	68.9600	65	59	74.9600	148	151												
51.0800	75	76	344	308	63.0800	115	93	69.0800	57	59	75.0800	181	190												
51.2000	68	76	217	200	63.2000	95	94	69.2000	56	59	75.2000	247	237												
51.3200	68	81	113	136	63.3200	87	96	69.3200	57	60	75.3200	252	232												
51.4400	98	93	115	106	63.4400	83	97	69.4400	57	61	75.4400	201	204												
51.5600	123	102	157	156	63.5600	120	105	69.5600	82	63	75.5600	169	169												
51.6800	109	104	99	86	63.6800	120	116	69.6800	64	68	75.6800	129	136												
51.8000	116	117	94	86	63.8000	115	108	69.8000	83	80	75.8000	115	116												
51.9200	163	180	93	93	63.9200	109	96	69.9200	107	99															
52.0400	348	333	114	115	64.0400	101	94	70.0400	97	106															
52.1600	494	466	147	131	64.1600	125	113	70.1600	104	103															
52.2800	370	389	99	119	64.2800	157	149	70.2800	116	99															
52.4000	233	229	80	96	64.4000	150	165	70.4000	95	107															
52.5200	116	131	72	83	64.5200	151	154	70.5200	150	135															
52.6400	90	95	65	80	64.6400	142	142	70.6400	187	202															
52.7600	86	83	74	80	64.7600	133	129	70.7600	258	274															
52.8800	67	81	87	95	64.8800	154	118	70.8800	321	289															

2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc
77.0000	91	91	83.0000	47	56	89.0000	76	67	95.0000	93	97	95.0000	93	97
77.1200	119	93	83.1200	48	56	89.1200	57	67	95.1200	103	90	95.1200	103	90
77.2400	88	86	83.2400	49	56	89.2400	63	66	95.2400	82	94	95.2400	82	94
77.3600	71	77	83.3600	54	58	89.3600	66	64	95.3600	138	108	95.3600	138	108
77.4800	71	69	83.4800	63	62	89.4800	56	62	95.4800	117	125	95.4800	117	125
77.6000	81	67	83.6000	72	68	89.6000	53	60	95.6000	141	134	95.6000	141	134
77.7200	71	72	83.7200	54	75	89.7200	68	59	95.7200	132	118	95.7200	132	118
77.8400	58	78	83.8400	71	85	89.8400	64	61	95.8400	124	107	95.8400	124	107
77.9600	71	79	83.9600	123	105	89.9600	63	65	95.9600	97	92	95.9600	97	92
78.0800	93	83	84.0800	135	129	90.0800	50	68	96.0800	71	76	96.0800	71	76
78.2000	89	88	84.2000	147	155	90.2000	51	72	96.2000	62	68	96.2000	62	68
78.3200	89	91	84.3200	166	172	90.3200	80	81	96.3200	70	66	96.3200	70	66
78.4400	127	100	84.4400	152	151	90.4400	81	90	96.4400	61	67	96.4400	61	67
78.5600	103	114	84.5600	138	127	90.5600	119	100	96.5600	89	72	96.5600	89	72
78.6800	130	133	84.6800	99	99	90.6800	140	117	96.6800	68	80	96.6800	68	80
78.8000	140	136	84.8000	74	78	90.8000	125	115	96.8000	75	90	96.8000	75	90
78.9200	129	123	84.9200	91	68	90.9200	129	110	96.9200	94	105	96.9200	94	105
79.0400	102	101	85.0400	71	63	91.0400	142	110	97.0400	83	99	97.0400	83	99
79.1600	87	81	85.1600	61	61	91.1600	133	114	97.1600	93	90	97.1600	93	90
79.2800	74	69	85.2800	65	61	91.2800	156	141	97.2800	99	84	97.2800	99	84
79.4000	60	65	85.4000	62	66	91.4000	209	204	97.4000	71	74	97.4000	71	74
79.5200	47	68	85.5200	65	75	91.5200	307	283	97.5200	66	68	97.5200	66	68
79.6400	63	71	85.6400	86	82	91.6400	295	291	97.6400	65	67	97.6400	65	67
79.7600	74	71	85.7600	79	83	91.7600	291	291	97.7600	74	72	97.7600	74	72
79.8800	62	69	85.8800	78	77	91.8800	363	317	97.8800	92	84	97.8800	92	84
80.0000	71	68	86.0000	58	70	92.0000	312	302	98.0000	115	95	98.0000	115	95
80.1200	63	69	86.1200	54	63	92.1200	276	259	98.1200	116	93	98.1200	116	93
80.2400	60	72	86.2400	52	60	92.2400	249	244	98.2400	105	93	98.2400	105	93
80.3600	58	73	86.3600	63	60	92.3600	254	224	98.3600	93	99	98.3600	93	99
80.4800	72	76	86.4800	75	64	92.4800	263	232	98.4800	112	107	98.4800	112	107
80.6000	73	76	86.6000	82	67	92.6000	260	242	98.6000	124	118	98.6000	124	118
80.7200	76	71	86.7200	68	65	92.7200	216	216	98.7200	120	118	98.7200	120	118
80.8400	77	67	86.8400	57	63	92.8400	186	188	98.8400	98	105	98.8400	98	105
80.9600	68	65	86.9600	60	60	92.9600	185	160	98.9600	119	98	98.9600	119	98
81.0800	73	66	87.0800	64	58	93.0800	145	133	99.0800	92	88	99.0800	92	88
81.2000	68	68	87.2000	64	60	93.2000	124	118	99.2000	104	79	99.2000	104	79
81.3200	66	68	87.3200	65	65	93.3200	111	102	99.3200	78	76	99.3200	78	76
81.4400	77	70	87.4400	61	71	93.4400	107	94	99.4400	89	79	99.4400	89	79
81.5600	89	72	87.5600	59	69	93.5600	106	89	99.5600	83	84	99.5600	83	84
81.6800	63	73	87.6800	68	68	93.6800	85	88	99.6800	83	87	99.6800	83	87
81.8000	82	75	87.8000	50	65	93.8000	96	95	99.8000	87	90	99.8000	87	90
81.9200	74	83	87.9200	65	66	93.9200	106	104	99.9200	89	88	99.9200	89	88
82.0400	82	91	88.0400	76	74	94.0400	126	115	100.0400	97	90	100.0400	97	90
82.1600	113	104	88.1600	95	88	94.1600	127	139	100.1600	105	93	100.1600	105	93
82.2800	108	103	88.2800	68	87	94.2800	162	138	100.2800	99	104	100.2800	99	104
82.4000	99	91	88.4000	65	81	94.4000	142	128	100.4000	115	124	100.4000	115	124
82.5200	72	79	88.5200	67	76	94.5200	125	133	100.5200	155	134	100.5200	155	134
82.6400	60	66	88.6400	57	70	94.6400	122	133	100.6400	141	134	100.6400	141	134
82.7600	50	60	88.7600	61	69	94.7600	137	116	100.7600	137	127	100.7600	137	127
82.8800	37	57	88.8800	76	67	94.8800	102	103	100.8800	108	111	100.8800	108	111

2theta	Yca1c	2theta	Yca1c	Yobs	Yca1c	2theta	Yca1c	Yobs	Yca1c	2theta	Yca1c	Yobs	Yca1c	2theta	Yca1c	Yobs	Yca1c
107.0000	78	113.0000	123	138	119.0000	70	73	125.0000	100	91							
107.1200	71	113.1200	158	161	119.1200	64	79	125.1200	114	88							
107.2400	66	113.2400	158	155	119.2400	85	89	125.2400	68	82							
107.3600	63	113.3600	142	148	119.3600	92	90	125.3600	59	76							
107.4800	55	113.4800	156	156	119.4800	77	84	125.4800	68	71							
107.6000	60	113.6000	169	154	119.6000	82	84	125.6000	77	70							
107.7200	69	113.7200	157	145	119.7200	87	88	125.7200	83	71							
107.8400	48	113.8400	168	137	119.8400	107	89	125.8400	71	75							
107.9600	42	113.9600	106	126	119.9600	99	84	125.9600	88	81							
108.0800	50	114.0800	138	122	120.0800	78	80	126.0800	74	84							
108.2000	51	114.2000	146	130	120.2000	85	82	126.2000	76	84							
108.3200	47	114.3200	138	146	120.3200	87	88	126.3200	87	85							
108.4400	58	114.4400	195	159	120.4400	96	99	126.4400	71	88							
108.5600	45	114.5600	169	152	120.5600	84	106	126.5600	116	89							
108.6800	50	114.6800	165	142	120.6800	92	98	126.6800	100	87							
108.8000	62	114.8000	153	141	120.8000	79	89	126.8000	78	81							
108.9200	59	114.9200	127	130	120.9200	70	88	126.9200	76	77							
109.0400	75	115.0400	134	112	121.0400	87	89	127.0400	79	74							
109.1600	63	115.1600	114	98	121.1600	79	84	127.1600	74	72							
109.2800	88	115.2800	78	88	121.2800	68	80	127.2800	74	69							
109.4000	63	115.4000	85	80	121.4000	67	80	127.4000	70	67							
109.5200	90	115.5200	83	77	121.5200	91	77	127.5200	62	66							
109.6400	79	115.6400	75	76	121.6400	81	74	127.6400	56	66							
109.7600	90	115.7600	65	74	121.7600	80	73	127.7600	66	66							
109.8800	77	115.8800	54	72	121.8800	83	76	127.8800	71	67							
110.0000	106	116.0000	73	69	122.0000	76	78	128.0000	64	66							
110.1200	115	116.1200	62	66	122.1200	86	81	128.1200	72	65							
110.2400	101	116.2400	73	63	122.2400	93	90	128.2400	60	65							
110.3600	91	116.3600	60	61	122.3600	93	104	128.3600	79	66							
110.4800	86	116.4800	69	58	122.4800	108	108	128.4800	78	65							
110.6000	73	116.6000	63	56	122.6000	109	102	128.6000	57	64							
110.7200	69	116.7200	45	55	122.7200	101	103	128.7200	56	62							
110.8400	74	116.8400	62	55	122.8400	108	113	128.8400	60	61							
110.9600	69	116.9600	48	54	122.9600	132	116	128.9600	52	61							
111.0800	81	117.0800	47	54	123.0800	104	103	129.0800	58	60							
111.2000	63	117.2000	60	54	123.2000	93	92	129.2000	61	60							
111.3200	52	117.3200	60	56	123.3200	88	90	129.3200	81	60							
111.4400	58	117.4400	57	57	123.4400	86	89	129.4400	62	61							
111.5600	61	117.5600	53	58	123.5600	103	86	129.5600	57	63							
111.6800	58	117.6800	64	59	123.6800	105	84	129.6800	74	67							
111.8000	62	117.8000	68	61	123.8000	84	88	129.8000	74	70							
111.9200	69	117.9200	64	60	123.9200	110	94	129.9200	75	71							
112.0400	69	118.0400	62	60	124.0400	109	104	130.0400	59	69							
112.1600	64	118.1600	76	63	124.1600	104	113										
112.2800	75	118.2800	64	65	124.2800	108	114										
112.4000	76	118.4000	84	68	124.4000	106	114										
112.5200	79	118.5200	71	68	124.5200	111	118										
112.6400	93	118.6400	48	66	124.6400	131	121										
112.7600	77	118.7600	62	67	124.7600	137	111										
112.8800	114	118.8800	59	70	124.8800	112	99										

Sample No. Ni25 (CaMg75Ni25S1206)

2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc
17.0000	112	107	23.0000	86	107	29.0000	153	105	35.0000	1916	1814	41.0000	448	451			
17.1200	112	107	23.1200	95	107	29.1200	137	105	35.1200	697	740	41.1200	466	399			
17.2400	131	107	23.2400	92	107	29.2400	165	197	35.2400	446	457	41.2400	242	199			
17.3600	135	107	23.3600	110	107	29.3600	255	283	35.3600	696	664	41.3600	145	144			
17.4800	130	107	23.4800	115	106	29.4800	344	378	35.4800	2151	2111	41.4800	125	133			
17.6000	108	107	23.6000	100	106	29.6000	729	657	35.6000	3436	3545	41.6000	170	143			
17.7200	121	107	23.7200	84	108	29.7200	2067	1942	35.7200	2621	2723	41.7200	218	213			
17.8400	124	107	23.8400	118	109	29.8400	6998	7367	35.8400	744	783	41.8400	573	550			
17.9600	108	107	23.9600	113	110	29.9600	3208	3156	35.9600	310	320	41.9600	612	588			
18.0800	114	107	24.0800	102	114	30.0800	1046	1033	36.0800	201	200	42.0800	366	330			
18.2000	101	107	24.2000	135	141	30.2000	2185	2076	36.2000	142	144	42.2000	400	384			
18.3200	103	109	24.3200	150	179	30.3200	2022	1958	36.3200	124	110	42.3200	1262	1179			
18.4400	101	110	24.4400	120	121	30.4400	463	551	36.4400	120	101	42.4400	1101	1039			
18.5600	130	111	24.5600	79	110	30.5600	350	315	36.5600	94	101	42.5600	369	403			
18.6800	126	116	24.6800	99	108	30.6800	445	395	36.6800	101	101	42.6800	264	265			
18.8000	178	156	24.8000	102	107	30.8000	1209	1346	36.8000	118	101	42.8000	423	470			
18.9200	236	187	24.9200	111	106	30.9200	1750	1756	36.9200	119	101	42.9200	696	665			
19.0400	103	119	25.0400	106	106	31.0400	458	468	37.0400	79	101	43.0400	363	338			
19.1600	114	111	25.1600	114	106	31.1600	259	212	37.1600	98	101	43.1600	183	160			
19.2800	114	113	25.2800	102	106	31.2800	137	154	37.2800	114	102	43.2800	138	125			
19.4000	109	116	25.4000	97	106	31.4000	168	143	37.4000	100	103	43.4000	107	117			
19.5200	124	121	25.5200	108	106	31.5200	189	180	37.5200	127	109	43.5200	172	135			
19.6400	149	134	25.6400	110	106	31.6400	158	135	37.6400	163	120	43.6400	190	130			
19.7600	233	229	25.7600	131	106	31.7600	121	110	37.7600	114	110	43.7600	107	128			
19.8800	514	465	25.8800	110	106	31.8800	135	106	37.8800	109	104	43.8800	127	127			
20.0000	147	181	26.0000	135	110	32.0000	127	105	38.0000	110	104	44.0000	118	141			
20.1200	133	138	26.1200	113	114	32.1200	111	104	38.1200	89	106	44.1200	175	178			
20.2400	101	118	26.2400	119	118	32.2400	103	103	38.2400	107	120	44.2400	354	333			
20.3600	104	110	26.3600	145	128	32.3600	116	103	38.3600	190	158	44.3600	1120	1008			
20.4800	82	108	26.4800	189	171	32.4800	122	103	38.4800	146	138	44.4800	749	724			
20.6000	106	107	26.6000	485	447	32.6000	112	103	38.6000	108	129	44.6000	396	293			
20.7200	111	107	26.7200	321	295	32.7200	125	103	38.7200	111	137	44.7200	296	224			
20.8400	94	107	26.8400	135	140	32.8400	103	103	38.8400	128	167	44.8400	325	324			
20.9600	91	107	26.9600	138	142	32.9600	98	103	38.9600	256	296	44.9600	723	776			
21.0800	111	107	27.0800	150	158	33.0800	121	103	39.0800	956	915	45.0800	634	670			
21.2000	81	107	27.2000	141	181	33.2000	93	103	39.2000	614	623	45.2000	606	572			
21.3200	110	107	27.3200	237	247	33.3200	91	103	39.3200	230	219	45.3200	346	329			
21.4400	105	107	27.4400	665	624	33.4400	104	103	39.4400	141	141	45.4400	196	167			
21.5600	101	107	27.5600	2203	2037	33.5600	133	103	39.5600	114	119	45.5600	126	133			
21.6800	106	107	27.6800	692	753	33.6800	95	103	39.6800	111	109	45.6800	106	120			
21.8000	86	107	27.8000	247	242	33.8000	109	103	39.8000	108	102	45.8000	137	123			
21.9200	131	107	27.9200	139	158	33.9200	92	103	39.9200	133	99	45.9200	140	149			
22.0400	100	107	28.0400	109	129	34.0400	96	103	40.0400	131	106	46.0400	314	304			
22.1600	100	107	28.1600	108	116	34.1600	130	102	40.1600	107	112	46.1600	388	334			
22.2800	97	107	28.2800	101	105	34.2800	116	124	40.2800	111	119	46.2800	213	201			
22.4000	93	107	28.4000	104	105	34.4000	139	142	40.4000	138	138	46.4000	144	145			
22.5200	100	107	28.5200	115	105	34.5200	156	159	40.5200	148	180	46.5200	159	169			
22.6400	100	107	28.6400	128	105	34.6400	207	195	40.6400	408	406	46.6400	123	138			
22.7600	109	107	28.7600	128	105	34.7600	371	306	40.7600	596	562	46.7600	105	108			
22.8800	103	107	28.8800	145	105	34.8800	1015	1012	40.8800	352	341	46.8800	79	99			

2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs	2theta	Ycalc	Yobs
47.0000	98	98	53.0000	99	103	59.0000	204	226	65.0000	109	124	71.0000	124	459	77.0000	139	154	83.0000	154	169	89.0000	169	184
47.1200	92	95	53.1200	113	114	59.1200	298	239	65.1200	130	136	71.1200	136	364	77.1200	141	147	83.1200	147	162	89.1200	162	177
47.2400	84	95	53.2400	126	158	59.2400	261	209	65.2400	176	174	71.2400	174	288	77.2400	185	191	83.2400	191	206	89.2400	206	221
47.3600	84	95	53.3600	156	148	59.3600	167	147	65.3600	268	275	71.3600	268	220	77.3600	205	211	83.3600	211	226	89.3600	226	241
47.4800	98	95	53.4800	144	154	59.4800	152	169	65.4800	443	472	71.4800	443	149	77.4800	171	177	83.4800	177	192	89.4800	192	207
47.6000	85	95	53.6000	125	131	59.6000	368	337	65.6000	1020	1101	71.6000	1101	182	77.6000	202	208	83.6000	208	223	89.6000	223	238
47.7200	73	96	53.7200	101	106	59.7200	299	284	65.7200	626	701	71.7200	701	209	77.7200	221	227	83.7200	227	242	89.7200	242	257
47.8400	106	101	53.8400	81	97	59.8400	282	224	65.8400	540	517	71.8400	517	159	77.8400	193	199	83.8400	199	214	89.8400	214	229
47.9600	108	113	53.9600	83	95	59.9600	158	148	65.9600	274	277	71.9600	277	142	77.9600	137	143	83.9600	143	158	89.9600	158	173
48.0800	76	112	54.0800	102	94	60.0800	122	131	66.0800	240	234	72.0800	234	87	78.0800	106	112	84.0800	112	127	90.0800	127	142
48.2000	76	97	54.2000	84	98	60.2000	112	134	66.2000	260	287	72.2000	287	100	78.2000	90	96	84.2000	96	111	90.2000	111	126
48.3200	79	97	54.3200	113	106	60.3200	159	160	66.3200	544	601	72.3200	601	109	78.3200	85	91	84.3200	91	106	90.3200	106	121
48.4400	111	99	54.4400	132	139	60.4400	278	276	66.4400	545	578	72.4400	578	81	78.4400	82	88	84.4400	88	103	90.4400	103	118
48.5600	105	101	54.5600	164	154	60.5600	405	372	66.5600	440	442	72.5600	442	76	78.5600	79	85	84.5600	85	100	90.5600	100	115
48.6800	105	106	54.6800	176	155	60.6800	456	458	66.6800	283	258	72.6800	258	77	78.6800	79	85	84.6800	85	100	90.6800	100	115
48.8000	139	125	54.8000	218	198	60.8000	456	505	66.8000	168	161	72.8000	161	82	78.8000	82	88	84.8000	88	103	90.8000	103	118
48.9200	232	228	54.9200	349	314	60.9200	314	333	66.9200	133	143	72.9200	143	86	78.9200	86	92	84.9200	92	107	90.9200	107	122
49.0400	214	210	55.0400	252	248	61.0400	208	203	67.0400	110	130	73.0400	130	98	79.0400	98	104	85.0400	104	119	91.0400	119	134
49.1600	149	150	55.1600	185	160	61.1600	157	152	67.1600	131	133	73.1600	133	116	79.1600	116	122	85.1600	122	137	91.1600	137	152
49.2800	111	130	55.2800	181	173	61.2800	157	156	67.2800	171	176	73.2800	176	132	79.2800	132	138	85.2800	138	153	91.2800	153	168
49.4000	145	146	55.4000	296	312	61.4000	206	193	67.4000	273	269	73.4000	269	136	79.4000	136	142	85.4000	142	157	91.4000	157	172
49.5200	248	238	55.5200	223	238	61.5200	251	232	67.5200	179	204	73.5200	204	188	79.5200	188	194	85.5200	194	209	91.5200	209	224
49.6400	441	454	55.6400	143	148	61.6400	364	444	67.6400	151	149	73.6400	149	258	79.6400	258	264	85.6400	264	279	91.6400	279	294
49.7600	372	410	55.7600	123	110	61.7600	533	503	67.7600	101	111	73.7600	111	270	79.7600	270	276	85.7600	276	291	91.7600	291	306
49.8800	235	264	55.8800	102	108	61.8800	102	108	67.8800	104	103	73.8800	103	385	79.8800	385	391	85.8800	391	406	91.8800	406	421
50.0000	168	179	56.0000	138	122	62.0000	261	251	68.0000	124	112	74.0000	112	457	80.0000	457	463	86.0000	463	478	92.0000	478	493
50.1200	128	144	56.1200	126	138	62.1200	184	205	68.1200	164	139	74.1200	139	328	80.1200	328	334	86.1200	334	349	92.1200	349	364
50.2400	188	194	56.2400	171	168	62.2400	244	236	68.2400	142	152	74.2400	152	230	80.2400	230	236	86.2400	236	251	92.2400	251	266
50.3600	219	233	56.3600	269	246	62.3600	280	285	68.3600	144	130	74.3600	130	145	80.3600	145	151	86.3600	151	166	92.3600	166	181
50.4800	160	178	56.4800	504	470	62.4800	364	313	68.4800	109	117	74.4800	117	114	80.4800	114	120	86.4800	120	135	92.4800	135	150
50.6000	128	133	56.6000	1273	1337	62.6000	264	252	68.6000	79	93	74.6000	93	103	80.6000	103	109	86.6000	109	124	92.6000	124	139
50.7200	148	147	56.7200	1166	1268	62.7200	166	145	68.7200	75	86	74.7200	86	98	80.7200	98	104	86.7200	104	119	92.7200	119	134
50.8400	131	128	56.8400	807	859	62.8400	113	118	68.8400	90	83	74.8400	83	101	80.8400	101	106	86.8400	106	121	92.8400	121	136
50.9600	98	105	56.9600	685	575	62.9600	131	124	68.9600	84	81	74.9600	81	127	80.9600	127	133	86.9600	133	148	92.9600	148	163
51.0800	106	100	57.0800	396	367	63.0800	95	111	69.0800	90	80	75.0800	80	179	80.0800	179	185	86.0800	185	200	93.0800	200	215
51.2000	85	101	57.2000	212	210	63.2000	101	108	69.2000	81	80	75.2000	80	230	80.2000	230	236	86.2000	236	251	93.2000	251	266
51.3200	113	113	57.3200	153	149	63.3200	106	117	69.3200	92	79	75.3200	79	272	80.3200	272	278	86.3200	278	293	93.3200	293	308
51.4400	159	180	57.4400	117	111	63.4400	133	117	69.4400	71	80	75.4400	80	227	80.4400	227	233	86.4400	233	248	93.4400	248	263
51.5600	157	166	57.5600	114	100	63.5600	123	135	69.5600	69	81	75.5600	81	207	80.5600	207	213	86.5600	213	228	93.5600	228	243
51.6800	114	138	57.6800	135	95	63.6800	165	156	69.6800	105	83	75.6800	83	156	80.6800	156	162	86.6800	162	177	93.6800	177	192
51.8000	134	141	57.8000	112	95	63.8000	134	135	69.8000	85	88	75.8000	88	143	80.8000	143	149	86.8000	149	164	93.8000	164	179
51.9200	179	183	57.9200	112	100	63.9200	105	110	69.9200	106	107	75.9200	107	129	80.9200	129	135	86.9200	135	150	93.9200	150	165
52.0400	375	361	58.0400	122	131	64.0400	110	103	70.0400	132	133	76.0400	133	141	80.0400	141	147	86.0400	147	162	94.0400	162	177
52.1600	1173	883	58.1600	167	143	64.1600	126	113	70.1600	122	123	76.1600	123	190	80.1600	190	196	86.1600	196	211	94.1600	211	226
52.2800	739	621	58.2800	134	131	64.2800	164	156	70.2800	122	118	76.2800	118	365	80.2800	365	371	86.2800	371	386	94.2800	386	401
52.4000	215	296	58.4000	106	103	64.4000	202	193	70.4000	131	127	76.4000	127	309	80.4000	309	315	86.4000	315	330	94.4000	330	345
52.5200	135	154	58.5200	106	101	64.5200	161	175	70.5200	123	146	76.5200	146	294	80.5200	294	300	86.5200	300	315	94.5200	315	330
52.6400	107	124	58.6400	114	104	64.6400	183	172	70.6400	193	202	76.6400	202	174	80.6400	174	180	86.6400	180	195	94.6400	195	210
52.7600	104	113	58.7600	124	109	64.7600	148	142	70.7600	148	142	76.7600	142	161	80.7600	161	167	86.7600	167	182	94.7600	182	197
52.8800	88	100	58.8800	123	130	64.8800	126	127	70.8800	126	127	76.8800	127	107	80.8800	107	113	86.8800	113	128	94.8800	128	143

2theta	Ycalc	2theta	Ycalc	2theta	Ycalc	2theta	Ycalc	2theta	Ycalc	2theta	Ycalc	2theta	Ycalc	2theta	Ycalc
77.0000	107	83.0000	68	75	85	86	86	95.0000	132	101.0000	132	101.0000	129	136	136
77.1200	104	83.1200	75	75	86	86	86	95.1200	134	101.1200	134	101.1200	127	125	125
77.2400	155	83.2400	60	74	89.2400	101	87	95.2400	113	101.2400	113	101.2400	105	111	111
77.3600	118	83.3600	52	75	89.3600	113	87	95.3600	135	101.3600	135	101.3600	121	99	99
77.4800	108	83.4800	69	79	89.4800	92	81	95.4800	175	101.4800	175	101.4800	97	93	93
77.6000	115	83.6000	80	84	89.6000	80	81	95.6000	181	101.6000	181	101.6000	85	90	90
77.7200	99	83.7200	82	98	89.7200	86	76	95.7200	144	101.7200	144	101.7200	91	90	90
77.8400	90	83.8400	94	99	89.8400	82	76	95.8400	139	101.8400	139	101.8400	102	94	94
77.9600	112	83.9600	110	114	89.9600	93	77	95.9600	126	101.9600	126	101.9600	87	98	98
78.0800	113	84.0800	121	149	90.0800	88	81	96.0800	101	102.0800	101	102.0800	104	102	102
78.2000	134	84.2000	167	143	90.2000	90	82	96.2000	88	102.2000	88	102.2000	140	118	118
78.3200	114	84.3200	134	171	90.3200	104	84	96.3200	92	102.3200	92	102.3200	111	133	133
78.4400	116	84.4400	208	214	90.4400	115	93	96.4400	92	102.4400	92	102.4400	122	112	112
78.5600	134	84.5600	154	162	90.5600	129	104	96.5600	101	102.5600	101	102.5600	112	112	112
78.6800	147	84.6800	145	158	90.6800	131	117	96.6800	93	102.6800	93	102.6800	90	108	108
78.8000	197	84.8000	119	120	90.8000	179	160	96.8000	114	102.8000	114	102.8000	73	96	96
78.9200	152	84.9200	114	98	90.9200	123	141	96.9200	94	102.9200	94	102.9200	77	94	94
79.0400	156	85.0400	79	88	91.0400	141	138	97.0400	159	103.0400	159	103.0400	112	96	96
79.1600	122	85.1600	86	83	91.1600	129	139	97.1600	133	103.1600	133	103.1600	120	104	104
79.2800	82	85.2800	85	81	91.2800	143	138	97.2800	105	103.2800	105	103.2800	100	101	101
79.4000	84	85.4000	90	82	91.4000	153	164	97.4000	125	103.4000	125	103.4000	98	98	98
79.5200	80	85.5200	63	89	91.5200	231	223	97.5200	94	103.5200	94	103.5200	97	95	95
79.6400	92	85.6400	107	110	91.6400	437	396	97.6400	102	103.6400	102	103.6400	98	95	95
79.7600	92	85.7600	94	105	91.7600	301	363	97.7600	95	103.7600	95	103.7600	90	95	95
79.8800	83	85.8800	101	111	91.8800	380	368	97.8800	112	103.8800	112	103.8800	87	100	100
80.0000	83	86.0000	108	98	92.0000	558	499	98.0000	119	104.0000	119	104.0000	137	110	110
80.1200	90	86.1200	90	91	92.1200	289	335	98.1200	137	116.1200	137	116.1200	178	136	136
80.2400	78	86.2400	90	83	92.2400	293	322	98.2400	122	118.2400	122	118.2400	142	149	149
80.3600	97	86.3600	76	80	92.3600	257	276	98.3600	119	113.3600	119	113.3600	149	126	126
80.4800	103	86.4800	94	83	92.4800	228	240	98.4800	145	114.4800	145	114.4800	128	129	129
80.6000	82	86.6000	78	84	92.6000	260	272	98.6000	149	115.6000	149	115.6000	115	123	123
80.7200	106	86.7200	86	89	92.7200	323	311	98.7200	202	116.7200	202	116.7200	107	105	105
80.8400	101	86.8400	73	86	92.8400	230	238	98.8400	139	118.8400	139	118.8400	92	100	100
80.9600	85	86.9600	80	83	92.9600	243	232	98.9600	127	126.9600	127	126.9600	100	99	99
81.0800	86	87.0800	82	82	93.0800	191	189	99.0800	126	127.0800	126	127.0800	99	102	102
81.2000	86	87.2000	83	78	93.2000	150	164	99.2000	118	127.2000	118	127.2000	145	116	116
81.3200	79	87.3200	95	80	93.3200	117	126	99.3200	79	101.3200	79	101.3200	101	115	115
81.4400	99	87.4400	73	84	93.4400	124	118	99.4400	102	105.4400	102	105.4400	104	110	110
81.5600	92	87.5600	91	86	93.5600	104	105	99.5600	110	105.5600	110	105.5600	121	118	118
81.6800	98	87.6800	92	86	93.6800	100	99	99.6800	110	105.6800	110	105.6800	123	126	126
81.8000	94	87.8000	91	89	93.8000	100	101	99.8000	136	105.8000	136	105.8000	136	127	127
81.9200	113	87.9200	81	85	93.9200	129	117	99.9200	121	105.9200	121	105.9200	157	138	138
82.0400	130	88.0400	75	89	94.0400	112	126	100.0400	123	106.0400	123	106.0400	177	160	160
82.1600	142	88.1600	102	103	94.1600	139	128	100.1600	110	106.1600	110	106.1600	183	192	192
82.2800	149	88.2800	122	121	94.2800	157	158	100.2800	114	106.2800	114	106.2800	175	177	177
82.4000	139	88.4000	95	101	94.4000	162	187	100.4000	157	106.4000	157	106.4000	194	178	178
82.5200	104	88.5200	97	106	94.5200	152	159	100.5200	144	106.5200	144	106.5200	165	188	188
82.6400	93	88.6400	94	90	94.6400	190	183	100.6400	179	106.6400	179	106.6400	107	150	150
82.7600	85	88.7600	89	87	94.7600	180	171	100.7600	184	106.7600	184	106.7600	145	137	137
82.8800	79	88.8800	107	86	94.8800	153	157	100.8800	147	106.8800	147	106.8800	109	130	130

2theta	Yobs	Ycalc
107.0000	103	113
107.1200	121	116
107.2400	91	106
107.3600	105	97
107.4800	96	98
107.6000	98	92
107.7200	68	85
107.8400	94	84
107.9600	75	81
108.0800	86	80
108.2000	83	80
108.3200	100	80
108.4400	72	80
108.5600	84	82
108.6800	82	84
108.8000	80	88
108.9200	77	88
109.0400	108	90
109.1600	116	93
109.2800	92	101
109.4000	100	100
109.5200	119	99
109.6400	123	104
109.7600	104	112
109.8800	108	107
110.0000	93	109
110.1200	124	117
110.2400	151	128
110.3600	121	142
110.4800	121	129
110.6000	119	128
110.7200	113	126
110.8400	101	113
110.9600	111	109

Sample No.	Ni50 Yobs	2theta Ycalc	(CaMg5ONi5O5Si2O6) Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc	Yobs	2theta Ycalc
17.0000	107	118	107	115	143	112	143	112	1742	1878	1742	1878	1742	1878	1742	1878	1742	1878
17.1200	96	117	102	115	148	147	148	147	1376	1392	1376	1392	1376	1392	1376	1392	1376	1392
17.2400	137	117	118	115	160	176	160	176	436	480	436	480	436	480	436	480	436	480
17.3600	114	117	96	115	169	198	169	198	412	411	412	411	412	411	412	411	412	411
17.4800	129	117	102	115	224	251	224	251	1099	1177	1099	1177	1099	1177	1099	1177	1099	1177
17.6000	123	117	120	115	376	358	376	358	3759	3644	3759	3644	3759	3644	3759	3644	3759	3644
17.7200	134	117	119	115	1014	933	1014	933	4129	4201	4129	4201	4129	4201	4129	4201	4129	4201
17.8400	131	117	104	115	4259	4449	4259	4449	1673	1740	1673	1740	1673	1740	1673	1740	1673	1740
17.9600	121	117	135	115	5536	5543	5536	5543	453	442	453	442	453	442	453	442	453	442
18.0800	105	117	105	116	1559	1628	1559	1628	204	227	204	227	204	227	204	227	204	227
18.2000	135	119	123	122	1305	1336	1305	1336	160	173	160	173	160	173	160	173	160	173
18.3200	130	120	141	146	2287	2240	2287	2240	122	146	122	146	122	146	122	146	122	146
18.4400	122	120	124	135	844	951	844	951	110	127	110	127	110	127	110	127	110	127
18.5600	113	122	124	118	300	316	300	316	110	112	110	112	110	112	110	112	110	112
18.6800	155	128	114	115	282	268	282	268	120	109	120	109	120	109	120	109	120	109
18.8000	184	184	100	114	636	628	636	628	122	109	122	109	122	109	122	109	122	109
18.9200	320	333	103	114	1491	1574	1491	1574	119	109	119	109	119	109	119	109	119	109
19.0400	210	213	120	114	872	872	872	872	117	109	117	109	117	109	117	109	117	109
19.1600	119	133	116	114	232	245	232	245	110	109	110	109	110	109	110	109	110	109
19.2800	136	124	127	114	173	153	173	153	136	109	136	109	136	109	136	109	136	109
19.4000	104	123	116	114	126	136	126	136	116	109	116	109	116	109	116	109	116	109
19.5200	96	124	111	114	151	146	151	146	124	109	124	109	124	109	124	109	124	109
19.6400	110	129	129	114	143	143	143	143	101	111	101	111	101	111	101	111	101	111
19.7600	184	173	111	114	124	119	124	119	113	111	113	111	113	111	113	111	113	111
19.8800	359	371	114	114	125	112	125	112	112	110	112	110	112	110	112	110	112	110
20.0000	306	298	126	115	120	111	120	111	111	110	111	110	111	110	111	110	111	110
20.1200	157	152	127	116	126	111	126	111	123	113	123	113	123	113	123	113	123	113
20.2400	129	134	106	117	120	111	120	111	111	128	111	128	111	128	111	128	111	128
20.3600	121	122	116	119	132	111	132	111	175	192	175	192	175	192	175	192	175	192
20.4800	119	118	121	129	107	111	107	111	170	184	170	184	170	184	170	184	170	184
20.6000	116	117	206	209	89	111	89	111	133	135	133	135	133	135	133	135	133	135
20.7200	92	116	270	288	110	110	110	110	122	126	122	126	122	126	122	126	122	126
20.8400	113	116	165	172	103	110	103	110	121	135	121	135	121	135	121	135	121	135
20.9600	103	116	157	133	123	110	123	110	169	192	169	192	169	192	169	192	169	192
21.0800	122	116	122	131	135	110	135	110	703	698	703	698	703	698	703	698	703	698
21.2000	108	116	148	137	109	110	109	110	317	320	317	320	317	320	317	320	317	320
21.3200	110	116	163	155	108	110	108	110	155	149	155	149	155	149	155	149	155	149
21.4400	127	116	316	280	108	110	108	110	121	124	121	124	121	124	121	124	121	124
21.5600	111	115	961	932	113	110	113	110	107	113	107	113	107	113	107	113	107	113
21.6800	121	115	827	900	115	110	115	110	113	116	113	116	113	116	113	116	113	116
21.8000	126	115	290	274	117	110	117	110	107	113	107	113	107	113	107	113	107	113
21.9200	178	115	118	148	126	110	126	110	131	111	131	111	131	111	131	111	131	111
22.0400	139	115	109	129	115	110	115	110	133	113	133	113	133	113	133	113	133	113
22.1600	125	115	139	122	117	110	117	110	103	116	103	116	103	116	103	116	103	116
22.2800	134	115	117	118	95	126	95	126	116	122	116	122	116	122	116	122	116	122
22.4000	122	115	125	115	117	131	117	131	137	140	137	140	137	140	137	140	137	140
22.5200	125	115	113	112	137	140	137	140	147	163	147	163	147	163	147	163	147	163
22.6400	115	115	116	112	172	157	172	157	263	295	263	295	263	295	263	295	263	295
22.7600	124	115	135	112	252	207	252	207	775	754	775	754	775	754	775	754	775	754
22.8800	120	115	121	112	666	614	666	614	668	655	668	655	668	655	668	655	668	655

Sample No.	Ni80	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	
17.0000	131	116	23.0000	103	116	29.0000	120	116	35.0000	1518	1540	41.0000	493	456	41.0000	1518	1540	41.0000	493	456
17.1200	132	116	23.1200	127	116	29.1200	166	145	35.1200	2105	2220	41.1200	444	383	41.1200	2105	2220	41.1200	444	383
17.2400	138	116	23.2400	108	116	29.2400	145	168	35.2400	849	860	41.2400	417	395	41.2400	849	860	41.2400	417	395
17.3600	106	116	23.3600	107	116	29.3600	155	184	35.3600	377	389	41.3600	217	217	41.3600	377	389	41.3600	217	217
17.4800	108	116	23.4800	108	116	29.4800	176	214	35.4800	606	678	41.4800	142	143	41.4800	606	678	41.4800	142	143
17.6000	141	116	23.6000	109	116	29.6000	330	296	35.6000	2925	2872	41.6000	140	135	41.6000	2925	2872	41.6000	140	135
17.7200	123	116	23.7200	117	116	29.7200	650	563	35.7200	5207	5265	41.7200	137	147	41.7200	5207	5265	41.7200	137	147
17.8400	109	116	23.8400	88	116	29.8400	2819	2900	35.8400	2895	2960	41.8400	202	235	41.8400	2895	2960	41.8400	202	235
17.9600	130	116	23.9600	107	116	29.9600	6560	6665	35.9600	678	704	41.9600	527	507	41.9600	678	704	41.9600	527	507
18.0800	118	116	24.0800	105	116	30.0800	2857	2923	36.0800	256	268	42.0800	462	424	42.0800	256	268	42.0800	462	424
18.2000	130	120	24.2000	96	117	30.2000	1305	1355	36.2000	195	192	42.2000	267	253	42.2000	195	192	42.2000	267	253
18.3200	83	121	24.3200	121	122	30.3200	2649	2589	36.3200	145	160	42.3200	497	492	42.3200	145	160	42.3200	497	492
18.4400	126	122	24.4400	106	123	30.4400	1334	1352	36.4400	135	143	42.4400	1591	1435	42.4400	135	143	42.4400	1591	1435
18.5600	147	125	24.5600	125	117	30.5600	327	365	36.5600	140	119	42.5600	1223	1123	42.5600	140	119	42.5600	1223	1123
18.6800	143	135	24.6800	125	116	30.6800	236	242	36.6800	151	115	42.6800	422	387	42.6800	151	115	42.6800	422	387
18.8000	295	227	24.8000	113	116	30.8000	377	393	36.8000	139	115	42.8000	273	286	42.8000	139	115	42.8000	273	286
18.9200	515	549	24.9200	122	116	30.9200	1164	1201	36.9200	118	115	42.9200	788	700	42.9200	118	115	42.9200	788	700
19.0400	396	385	25.0400	106	116	31.0400	953	999	37.0400	132	115	43.0400	765	704	43.0400	132	115	43.0400	765	704
19.1600	154	158	25.1600	114	116	31.1600	289	289	37.1600	133	115	43.1600	381	304	43.1600	289	289	37.1600	381	304
19.2800	121	129	25.2800	106	116	31.2800	106	153	37.2800	138	115	43.2800	188	152	43.2800	106	153	37.2800	138	115
19.4000	113	125	25.4000	106	116	31.4000	133	135	37.4000	119	116	43.4000	142	130	43.4000	133	135	37.4000	119	116
19.5200	123	125	25.5200	122	116	31.5200	134	140	37.5200	108	117	43.5200	127	129	43.5200	122	116	37.5200	108	117
19.6400	139	128	25.6400	127	116	31.6400	194	153	37.6400	112	126	43.6400	155	138	43.6400	127	116	37.6400	112	126
19.7600	192	157	25.7600	135	116	31.7600	126	132	37.7600	116	135	43.7600	149	133	43.7600	135	132	37.7600	116	135
19.8800	333	361	25.8800	124	116	31.8800	102	117	37.8800	131	124	43.8800	127	124	43.8800	102	117	37.8800	131	124
20.0000	427	450	26.0000	141	116	32.0000	123	116	38.0000	98	114	44.0000	114	124	44.0000	123	116	38.0000	98	114
20.1200	188	205	26.1200	134	116	32.1200	135	116	38.1200	123	121	44.1200	120	129	44.1200	134	116	38.1200	123	121
20.2400	182	164	26.2400	129	116	32.2400	134	116	38.2400	129	140	44.2400	139	145	44.2400	182	164	26.2400	129	140
20.3600	128	135	26.3600	121	117	32.3600	114	116	38.3600	258	242	44.3600	278	284	44.3600	128	135	26.3600	121	117
20.4800	124	121	26.4800	126	118	32.4800	111	115	38.4800	245	253	44.4800	615	659	44.4800	124	121	26.4800	126	118
20.6000	110	118	26.6000	134	127	32.6000	125	115	38.6000	152	158	44.6000	561	507	44.6000	110	118	26.6000	134	127
20.7200	136	117	26.7200	174	155	32.7200	120	115	38.7200	119	131	44.7200	330	235	44.7200	136	117	26.7200	174	155
20.8400	114	116	26.8400	110	141	32.8400	116	115	38.8400	120	134	44.8400	202	196	44.8400	114	116	26.8400	110	141
20.9600	110	116	26.9600	124	126	32.9600	117	115	38.9600	154	160	44.9600	432	424	44.9600	110	116	26.9600	124	126
21.0800	112	116	27.0800	137	125	33.0800	115	115	39.0800	376	379	45.0800	928	988	45.0800	112	116	27.0800	137	125
21.2000	113	116	27.2000	137	129	33.2000	107	115	39.2000	670	656	45.2000	967	952	45.2000	113	116	27.2000	137	129
21.3200	113	116	27.3200	160	137	33.3200	104	115	39.3200	373	360	45.3200	849	773	45.3200	113	116	27.3200	160	137
21.4400	124	116	27.4400	210	187	33.4400	113	115	39.4400	135	158	45.4400	439	406	45.4400	124	116	27.4400	210	187
21.5600	121	116	27.5600	630	561	33.5600	114	115	39.5600	111	129	45.5600	167	183	45.5600	121	116	27.5600	630	561
21.6800	137	116	27.6800	767	827	33.6800	124	115	39.6800	103	122	45.6800	142	143	45.6800	137	116	27.6800	767	827
21.8000	113	116	27.8000	296	318	33.8000	116	115	39.8000	111	119	45.8000	135	135	45.8000	113	116	27.8000	296	318
21.9200	123	116	27.9200	148	148	33.9200	122	115	39.9200	111	118	45.9200	136	133	45.9200	123	116	27.9200	148	148
22.0400	111	116	28.0400	131	129	34.0400	128	115	40.0400	142	120	46.0400	152	153	46.0400	111	116	28.0400	131	129
22.1600	124	116	28.1600	102	123	34.1600	118	115	40.1600	128	123	46.1600	152	153	46.1600	124	116	28.1600	102	123
22.2800	128	116	28.2800	133	120	34.2800	118	126	40.2800	122	127	46.2800	152	153	46.2800	128	116	28.2800	133	120
22.4000	119	116	28.4000	116	118	34.4000	136	135	40.4000	114	140	46.4000	266	260	46.4000	119	116	28.4000	116	118
22.5200	98	116	28.5200	119	116	34.5200	129	142	40.5200	154	169	46.5200	195	190	46.5200	98	116	28.5200	119	116
22.6400	121	116	28.6400	120	116	34.6400	157	155	40.6400	211	235	46.6400	247	234	46.6400	121	116	28.6400	120	116
22.7600	91	116	28.7600	102	116	34.7600	194	184	40.7600	592	628	46.7600	178	184	46.7600	91	116	28.7600	102	116
22.8800	105	116	28.8800	138	116	34.8800	370	364	40.8800	955	884	46.8800	128	132	46.8800	105	116	28.8800	138	116

2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc
77.0000	126	129	83.0000	99	116	89.0000	111	123	95.0000	299	262	101.0000	235	237	101.0000	299	262	101.0000	235	237	101.0000	299	262	101.0000	235	237	101.0000	299	262	101.0000	235	237	101.0000	299	262	101.0000	235	237
77.1200	129	130	83.1200	109	115	89.1200	115	132	95.1200	202	176	101.1200	241	219	101.1200	202	176	101.1200	241	219	101.1200	202	176	101.1200	241	219	101.1200	202	176	101.1200	241	219	101.1200	202	176	101.1200	241	219
77.2400	151	161	83.2400	120	115	89.2400	141	133	95.2400	178	172	101.2400	175	166	101.2400	178	172	101.2400	175	166	101.2400	178	172	101.2400	175	166	101.2400	178	172	101.2400	175	166	101.2400	178	172	101.2400	175	166
77.3600	185	173	83.3600	109	115	89.3600	127	141	95.3600	169	155	101.3600	189	167	101.3600	169	155	101.3600	189	167	101.3600	169	155	101.3600	189	167	101.3600	169	155	101.3600	189	167	101.3600	169	155	101.3600	189	167
77.4800	152	152	83.4800	112	115	89.4800	131	138	95.4800	144	143	101.4800	169	152	101.4800	144	143	101.4800	169	152	101.4800	144	143	101.4800	169	152	101.4800	144	143	101.4800	169	152	101.4800	144	143	101.4800	169	152
77.6000	145	140	83.6000	112	116	89.6000	120	128	95.6000	168	180	101.6000	140	135	101.6000	168	180	101.6000	140	135	101.6000	168	180	101.6000	140	135	101.6000	168	180	101.6000	140	135	101.6000	168	180	101.6000	140	135
77.7200	129	122	83.7200	137	120	89.7200	137	125	95.7200	266	265	101.7200	136	127	101.7200	266	265	101.7200	136	127	101.7200	266	265	101.7200	136	127	101.7200	266	265	101.7200	136	127	101.7200	266	265	101.7200	136	127
77.8400	117	122	83.8400	129	127	89.8400	133	119	95.8400	185	210	101.8400	126	126	101.8400	185	210	101.8400	126	126	101.8400	185	210	101.8400	126	126	101.8400	185	210	101.8400	126	126	101.8400	185	210	101.8400	126	126
77.9600	120	135	83.9600	137	126	89.9600	124	116	95.9600	173	188	101.9600	134	128	101.9600	173	188	101.9600	134	128	101.9600	173	188	101.9600	134	128	101.9600	173	188	101.9600	134	128	101.9600	173	188	101.9600	134	128
78.0800	134	136	84.0800	140	143	90.0800	121	117	96.0800	204	188	102.0800	130	137	102.0800	204	188	102.0800	130	137	102.0800	204	188	102.0800	130	137	102.0800	204	188	102.0800	130	137	102.0800	204	188	102.0800	130	137
78.2000	149	144	84.2000	151	162	90.2000	112	117	96.2000	141	143	102.2000	123	144	102.2000	141	143	102.2000	123	144	102.2000	141	143	102.2000	123	144	102.2000	141	143	102.2000	123	144	102.2000	141	143	102.2000	123	144
78.3200	186	153	84.3200	131	159	90.3200	114	118	96.3200	119	126	102.3200	209	182	102.3200	119	126	102.3200	209	182	102.3200	119	126	102.3200	209	182	102.3200	119	126	102.3200	209	182	102.3200	119	126	102.3200	209	182
78.4400	157	140	84.4400	150	171	90.4400	110	120	96.4400	116	122	102.4400	188	199	102.4400	116	122	102.4400	188	199	102.4400	116	122	102.4400	188	199	102.4400	116	122	102.4400	188	199	102.4400	116	122	102.4400	188	199
78.5600	138	144	84.5600	192	254	90.5600	150	129	96.5600	120	120	102.5600	173	154	102.5600	120	120	102.5600	173	154	102.5600	120	120	102.5600	173	154	102.5600	120	120	102.5600	173	154	102.5600	120	120	102.5600	173	154
78.6800	133	143	84.6800	129	254	90.6800	150	151	96.6800	113	119	102.6800	147	159	102.6800	113	119	102.6800	147	159	102.6800	113	119	102.6800	147	159	102.6800	113	119	102.6800	147	159	102.6800	113	119	102.6800	147	159
78.8000	165	184	84.8000	276	202	90.8000	151	160	96.8000	104	121	102.8000	165	154	102.8000	104	121	102.8000	165	154	102.8000	104	121	102.8000	165	154	102.8000	104	121	102.8000	165	154	102.8000	104	121	102.8000	165	154
78.9200	263	245	84.9200	193	197	90.9200	205	220	96.9200	112	127	102.9200	144	131	102.9200	112	127	102.9200	144	131	102.9200	112	127	102.9200	144	131	102.9200	112	127	102.9200	144	131	102.9200	112	127	102.9200	144	131
79.0400	229	224	85.0400	142	147	91.0400	214	196	97.0400	145	132	103.0400	133	126	103.0400	145	132	103.0400	133	126	103.0400	145	132	103.0400	133	126	103.0400	145	132	103.0400	133	126	103.0400	145	132	103.0400	133	126
79.1600	194	200	85.1600	143	128	91.1600	179	170	97.1600	118	150	103.1600	146	133	103.1600	118	150	103.1600	146	133	103.1600	118	150	103.1600	146	133	103.1600	118	150	103.1600	146	133	103.1600	118	150	103.1600	146	133
79.2800	155	157	85.2800	129	125	91.2800	163	174	97.2800	201	190	103.2800	140	143	103.2800	201	190	103.2800	140	143	103.2800	201	190	103.2800	140	143	103.2800	201	190	103.2800	140	143	103.2800	201	190	103.2800	140	143
79.4000	130	130	85.4000	115	120	91.4000	146	149	97.4000	174	172	103.4000	144	137	103.4000	174	172	103.4000	144	137	103.4000	174	172	103.4000	144	137	103.4000	174	172	103.4000	144	137	103.4000	174	172	103.4000	144	137
79.5200	128	125	85.5200	114	119	91.5200	163	156	97.5200	143	151	103.5200	130	134	103.5200	143	151	103.5200	130	134	103.5200	143	151	103.5200	130	134	103.5200	143	151	103.5200	130	134	103.5200	143	151	103.5200	130	134
79.6400	127	128	85.6400	132	123	91.6400	202	214	97.6400	178	157	103.6400	140	134	103.6400	178	157	103.6400	140	134	103.6400	178	157	103.6400	140	134	103.6400	178	157	103.6400	140	134	103.6400	178	157	103.6400	140	134
79.7600	112	122	85.7600	137	133	91.7600	412	445	97.7600	139	134	103.7600	140	128	103.7600	139	134	103.7600	140	128	103.7600	139	134	103.7600	140	128	103.7600	139	134	103.7600	140	128	103.7600	139	134	103.7600	140	128
79.8800	118	123	85.8800	125	143	91.8800	480	455	97.8800	127	125	103.8800	113	125	103.8800	127	125	103.8800	113	125	103.8800	127	125	103.8800	113	125	103.8800	127	125	103.8800	113	125	103.8800	127	125	103.8800	113	125
80.0000	134	126	86.0000	119	133	92.0000	395	444	98.0000	125	124	104.0000	123	125	104.0000	125	124	104.0000	123	125	104.0000	125	124	104.0000	123	125	104.0000	125	124	104.0000	123	125	104.0000	125	124	104.0000	123	125
80.1200	140	129	86.1200	140	136	92.1200	552	567	98.1200	121	127	104.1200	132	129	104.1200	121	127	104.1200	132	129	104.1200	121	127	104.1200	132	129	104.1200	121	127	104.1200	132	129	104.1200	121	127	104.1200	132	129
80.2400	125	136	86.2400	133	124	92.2400	327	321	98.2400	133	144	104.2400	142	142	104.2400	133	144	104.2400	142	142	104.2400	133	144	104.2400	142	142	104.2400	133	144	104.2400	142	142	104.2400	133	144	104.2400	142	142
80.3600	140	159	86.3600	129	120	92.3600	314	330	98.3600	176	179	104.3600	200	200	104.3600	176	179	104.3600	200	200	104.3600	176	179	104.3600	200	200	104.3600	176	179	104.3600	200	200	104.3600	176	179	104.3600	200	200
80.4800	143	139	86.4800	134	118	92.4800	259	245	98.4800	199	192	104.4800	287	287	104.4800	199	192	104.4800	287	287	104.4800	199	192	104.4800	287	287	104.4800	199	192	104.4800	287	287	104.4800	199	192	104.4800	287	287
80.6000	131	139	86.6000	118	118	92.6000	214	206	98.6000	173	185	104.6000	205	213	104.6000	173	185	104.6000	205	213	104.6000	173	185	104.6000	205	213	104.6000	173	185	104.6000	205	213	104.6000	173	185	104.6000	205	213
80.7200	121	130	86.7200	127	120	92.7200	301	290	98.7200	249	255	104.7200	189	189	104.7200	249	255	104.7200	189	189	104.7200	249	255	104.7200	189	189												

2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc
107.0000	189	175	113.0000	139	142	119.0000	102	136	125.0000	243	256
107.1200	158	160	113.1200	163	155	119.1200	140	134	125.1200	217	227
107.2400	142	142	113.2400	210	175	119.2400	141	131	125.2400	178	191
107.3600	164	153	113.3600	210	190	119.3600	124	132	125.3600	187	
107.4800	164	162	113.4800	249	231	119.4800	150	135	125.4800	203	194
107.6000	126	141	113.6000	302	303	119.6000	152	144	125.6000	194	186
107.7200	146	141	113.7200	263	278	119.7200	200	164	125.7200	149	159
107.8400	142	145	113.8400	236	219	119.8400	163	176	125.8400	129	142
107.9600	110	130	113.9600	246	230	119.9600	149	158	125.9600	128	140
108.0800	137	124	114.0800	324	270	120.0800	146	150	126.0800	168	150
108.2000	107	121	114.2000	262	247	120.2000	167	158	126.2000	152	159
108.3200	108	119	114.3200	182	193	120.3200	145	160	126.3200	128	147
108.4400	95	118	114.4400	232	198	120.4400	131	147	126.4400	136	136
108.5600	110	119	114.5600	214	238	120.5600	133	139	126.5600	131	136
108.6800	121	121	114.6800	197	211	120.6800	135	139	126.6800	145	144
108.8000	134	124	114.8000	268	210	120.8000	165	146	126.8000	148	151
108.9200	138	127	114.9200	304	263	120.9200	194	171	126.9200	141	151
109.0400	121	123	115.0400	249	245	121.0400	207	206	127.0400	140	143
109.1600	118	124	115.1600	173	202	121.1600	168	182	127.1600	164	143
109.2800	124	132	115.2800	220	188	121.2800	152	152	127.2800	164	152
109.4000	142	133	115.4000	177	191	121.4000	150	152	127.4000	156	153
109.5200	127	129	115.5200	167	179	121.5200	146	167	127.5200	135	143
109.6400	121	128	115.6400	151	154	121.6400	159	158	127.6400	150	135
109.7600	127	133	115.7600	125	136	121.7600	155	147	127.7600	144	135
109.8800	162	142	115.8800	164	134	121.8800	151	153	127.8800	139	138
110.0000	117	142	116.0000	149	137	122.0000	146	146	128.0000	122	135
110.1200	151	132	116.1200	123	137	122.1200	126	135	128.1200	134	134
110.2400	127	136	116.2400	137	138	122.2400	126	133	128.2400	125	135
110.3600	151	153	116.3600	160	146	122.3600	126	139	128.3600	122	130
110.4800	220	194	116.4800	155	147	122.4800	137	141	128.4800	118	126
110.6000	226	213	116.6000	143	136	122.6000	137	139	128.6000	120	127
110.7200	155	163	116.7200	160	131	122.7200	152	140	128.7200	135	131
110.8400	164	156	116.8400	136	134	122.8400	179	151	128.8400	162	131
110.9600	168	172	116.9600	136	129	122.9600	211	183	128.9600	103	128
111.0800	140	147	117.0800	107	123	123.0800	213	216	129.0800	132	128
111.2000	135	129	117.2000	122	120	123.2000	174	191	129.2000	122	131
111.3200	138	127	117.3200	129	120	123.3200	195	175	129.3200	129	130
111.4400	125	130	117.4400	119	119	123.4400	179	185	129.4400	129	127
111.5600	144	133	117.5600	135	120	123.5600	186	188	129.5600	130	125
111.6800	132	126	117.6800	108	122	123.6800	172	169	129.6800	128	125
111.8000	157	126	117.8000	112	127	123.8000	129	152	129.8000	106	126
111.9200	102	127	117.9200	142	131	123.9200	176	151	129.9200	130	125
112.0400	127	123	118.0400	134	132	124.0400	137	148	130.0400	118	124
112.1600	142	122	118.1600	124	132	124.1600	140	140			
112.2800	128	122	118.2800	112	129	124.2800	148	137			
112.4000	118	122	118.4000	114	127	124.4000	118	138			
112.5200	136	123	118.5200	112	127	124.5200	160	144			
112.6400	143	132	118.6400	112	127	124.6400	171	160			
112.7600	160	142	118.7600	128	126	124.7600	205	193			
112.8800	148	139	118.8800	158	131	124.8800	267	236			

Sample No.	Ni100 (CaNiSi206)	2theta	YcaIc	Yobs	YcaIc	2theta	Yobs	YcaIc	2theta	Yobs	YcaIc	2theta	Yobs	YcaIc
17.0000	130	122	23.0000	125	124	29.0000	157	125	35.0000	1775	1766	41.0000	582	516
17.1200	119	122	23.1200	107	124	29.1200	125	125	35.1200	2915	2751	41.1200	313	335
17.2400	119	122	23.2400	118	124	29.2400	159	163	35.2400	986	948	41.2400	398	359
17.3600	116	122	23.3600	147	124	29.3600	173	197	35.3600	352	410	41.3600	226	217
17.4800	137	122	23.4800	134	124	29.4800	216	230	35.4800	635	585	41.4800	162	154
17.6000	123	122	23.6000	119	124	29.6000	265	316	35.6000	2592	2521	41.6000	149	144
17.7200	122	122	23.7200	141	124	29.7200	668	570	35.7200	5251	5601	41.7200	165	158
17.8400	136	122	23.8400	124	124	29.8400	2984	3047	35.8400	3276	3147	41.8400	220	238
17.9600	131	122	23.9600	160	124	29.9600	7333	7468	35.9600	753	691	41.9600	547	528
18.0800	115	122	24.0800	131	124	30.0800	2518	2677	36.0800	254	287	42.0800	457	430
18.2000	145	126	24.2000	123	125	30.2000	1422	1475	36.2000	194	209	42.2000	243	260
18.3200	117	130	24.3200	120	128	30.3200	3184	3078	36.3200	154	175	42.3200	507	514
18.4400	120	132	24.4400	126	128	30.4400	1087	1248	36.4400	151	150	42.4400	1644	1679
18.5600	138	138	24.5600	127	125	30.5600	314	345	36.5600	148	131	42.5600	1137	1269
18.6800	150	154	24.6800	109	124	30.6800	228	235	36.6800	143	126	42.6800	413	415
18.8000	320	314	24.8000	109	124	30.8000	366	355	36.8000	125	126	42.8000	317	324
18.9200	913	956	24.9200	123	124	30.9200	1138	1125	36.9200	135	126	42.9200	908	874
19.0400	447	450	25.0400	115	124	31.0400	845	784	37.0400	113	127	43.0400	880	822
19.1600	161	163	25.1600	125	124	31.1600	241	228	37.1600	175	127	43.1600	379	326
19.2800	141	141	25.2800	115	124	31.2800	132	154	37.2800	170	127	43.2800	252	169
19.4000	103	135	25.4000	147	124	31.4000	151	141	37.4000	141	128	43.4000	202	146
19.5200	129	135	25.5200	120	124	31.5200	125	143	37.5200	146	130	43.5200	162	142
19.6400	157	139	25.6400	122	124	31.6400	167	154	37.6400	143	151	43.6400	150	147
19.7600	196	166	25.7600	143	124	31.7600	154	134	37.7600	137	177	43.7600	126	139
19.8800	451	444	25.8800	115	124	31.8800	128	127	37.8800	149	147	43.8800	125	134
20.0000	476	519	26.0000	132	124	32.0000	127	126	38.0000	121	134	44.0000	113	135
20.1200	210	219	26.1200	125	124	32.1200	118	126	38.1200	131	137	44.1200	140	139
20.2400	272	243	26.2400	120	124	32.2400	125	126	38.2400	148	164	44.2400	154	151
20.3600	151	158	26.3600	125	125	32.3600	119	126	38.3600	283	325	44.3600	251	244
20.4800	147	130	26.4800	104	125	32.4800	141	126	38.4800	255	311	44.4800	626	595
20.6000	126	126	26.6000	120	125	32.6000	118	126	38.6000	164	173	44.6000	500	482
20.7200	135	124	26.7200	138	127	32.7200	126	126	38.7200	125	143	44.7200	259	239
20.8400	114	124	26.8400	129	126	32.8400	132	126	38.8400	144	144	44.8400	219	207
20.9600	131	123	26.9600	128	130	32.9600	136	126	38.9600	167	162	44.9600	366	425
21.0800	119	123	27.0800	132	132	33.0800	113	126	39.0800	319	339	45.0800	1107	1053
21.2000	127	123	27.2000	142	136	33.2000	114	126	39.2000	584	582	45.2000	975	948
21.3200	112	123	27.3200	155	145	33.3200	132	126	39.3200	352	315	45.3200	939	827
21.4400	139	123	27.4400	201	184	33.4400	129	126	39.4400	124	158	45.4400	465	457
21.5600	127	123	27.5600	614	559	33.5600	120	126	39.5600	138	138	45.5600	211	202
21.6800	115	123	27.6800	704	774	33.6800	139	126	39.6800	149	133	45.6800	158	158
21.8000	140	123	27.8000	224	260	33.8000	141	126	39.8000	118	131	45.8000	159	148
21.9200	124	123	27.9200	173	150	33.9200	150	126	39.9200	123	128	45.9200	117	144
22.0400	135	123	28.0400	135	136	34.0400	132	126	40.0400	148	128	46.0400	157	152
22.1600	114	124	28.1600	112	131	34.1600	110	126	40.1600	144	134	46.1600	260	262
22.2800	121	124	28.2800	138	129	34.2800	146	126	40.2800	124	141	46.2800	366	387
22.4000	105	124	28.4000	114	126	34.4000	122	142	40.4000	155	155	46.4000	281	264
22.5200	121	124	28.5200	121	125	34.5200	149	157	40.5200	191	196	46.5200	217	205
22.6400	137	124	28.6400	141	125	34.6400	150	173	40.6400	257	271	46.6400	326	282
22.7600	124	124	28.7600	125	125	34.7600	208	209	40.7600	634	658	46.7600	231	219
22.8800	136	124	28.8800	144	125	34.8800	410	365	40.8800	981	1040	46.8800	158	149

2theta	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	2theta	Yobs	Ycalc	
47.0000	131	53.0000	134	138	138	59.0000	247	262	65.0000	170	168	71.0000	464	497	71.0000	170	168	71.0000	464	497
47.1200	136	53.1200	130	135	133	59.1200	380	407	65.1200	182	153	71.1200	612	585	71.1200	182	153	71.1200	612	585
47.2400	128	53.2400	129	121	134	59.2400	283	315	65.2400	160	158	71.2400	380	392	71.2400	160	158	71.2400	380	392
47.3600	127	53.3600	129	147	143	59.3600	217	205	65.3600	207	180	71.3600	313	288	71.3600	207	180	71.3600	313	288
47.4800	105	53.4800	129	164	166	59.4800	168	167	65.4800	270	269	71.4800	207	196	71.4800	270	269	71.4800	207	196
47.6000	134	53.6000	129	220	230	59.6000	221	216	65.6000	712	696	71.6000	193	171	71.6000	712	696	71.6000	193	171
47.7200	118	53.7200	177	198	198	59.7200	444	498	65.7200	1052	1068	71.7200	181	207	71.7200	1052	1068	71.7200	181	207
47.8400	133	53.8400	153	151	151	59.8400	433	445	65.8400	729	741	71.8400	325	354	71.8400	729	741	71.8400	325	354
47.9600	177	53.9600	146	134	134	59.9600	415	392	65.9600	415	392	71.9600	264	275	71.9600	415	392	71.9600	264	275
48.0800	194	54.0800	130	132	60.0800	193	177	66.0800	215	209	72.0800	277	250	72.0800	215	209	72.0800	277	250	
48.2000	146	54.2000	111	131	60.2000	161	160	66.2000	198	192	72.2000	168	171	72.2000	161	160	72.2000	168	171	
48.3200	131	54.3200	124	133	60.3200	148	165	66.3200	258	233	72.3200	132	145	72.3200	148	165	72.3200	132	145	
48.4400	121	54.4400	146	137	60.4400	215	207	66.4400	556	557	72.4400	146	138	72.4400	215	207	72.4400	146	138	
48.5600	125	54.5600	184	170	60.5600	440	453	66.5600	901	817	72.5600	118	134	72.5600	440	453	72.5600	118	134	
48.6800	120	54.6800	188	201	60.6800	607	625	66.6800	715	696	72.6800	123	131	72.6800	607	625	72.6800	123	131	
48.8000	159	54.8000	227	182	60.8000	630	621	66.8000	520	415	72.8000	135	131	72.8000	227	182	72.8000	135	131	
48.9200	199	54.9200	199	200	60.9200	588	636	66.9200	201	219	72.9200	129	130	72.9200	199	200	72.9200	129	130	
49.0400	508	55.0400	448	385	61.0400	378	408	67.0400	185	188	73.0400	142	131	73.0400	508	448	73.0400	142	131	
49.1600	411	55.1600	343	329	61.1600	252	238	67.1600	205	206	73.1600	133	135	73.1600	411	390	73.1600	133	135	
49.2800	220	55.2800	247	217	61.2800	164	168	67.2800	185	187	73.2800	155	146	73.2800	220	205	73.2800	155	146	
49.4000	126	55.4000	179	162	61.4000	149	172	67.4000	204	203	73.4000	150	148	73.4000	126	151	73.4000	126	151	
49.5200	158	55.5200	239	227	61.5200	176	194	67.5200	384	371	73.5200	144	152	73.5200	158	156	73.5200	144	152	
49.6400	226	55.6400	276	258	61.6400	205	202	67.6400	326	331	73.6400	189	167	73.6400	226	227	73.6400	189	167	
49.7600	251	55.7600	241	205	61.7600	278	320	67.7600	277	282	73.7600	267	272	73.7600	251	246	73.7600	267	272	
49.8800	218	55.8800	165	146	61.8800	794	867	67.8800	204	174	73.8800	370	368	73.8800	218	223	73.8800	370	368	
50.0000	192	56.0000	127	140	62.0000	619	701	68.0000	165	149	74.0000	429	371	74.0000	192	200	74.0000	429	371	
50.1200	165	56.1200	135	148	62.1200	577	542	68.1200	161	161	74.1200	516	559	74.1200	165	164	74.1200	516	559	
50.2400	139	56.2400	155	155	62.2400	307	307	68.2400	150	157	74.2400	476	406	74.2400	139	145	74.2400	476	406	
50.3600	198	56.3600	167	177	62.3600	277	272	68.3600	165	173	74.3600	347	347	74.3600	198	175	74.3600	347	347	
50.4800	256	56.4800	215	236	62.4800	330	310	68.4800	218	227	74.4800	208	208	74.4800	256	229	74.4800	208	208	
50.6000	231	56.6000	630	577	62.6000	508	448	68.6000	191	189	74.6000	146	154	74.6000	231	194	74.6000	146	154	
50.7200	193	56.7200	1314	1172	62.7200	359	328	68.7200	151	171	74.7200	145	143	74.7200	193	187	74.7200	145	143	
50.8400	238	56.8400	1467	1474	62.8400	262	214	68.8400	154	139	74.8400	126	141	74.8400	238	236	74.8400	126	141	
50.9600	184	56.9600	1027	1080	62.9600	183	162	68.9600	121	133	74.9600	140	140	74.9600	184	194	74.9600	140	140	
51.0800	147	57.0800	785	757	63.0800	187	182	69.0800	125	131	75.0800	143	147	75.0800	147	146	75.0800	143	147	
51.2000	154	57.2000	375	389	63.2000	195	182	69.2000	117	131	75.2000	177	183	75.2000	154	138	75.2000	177	183	
51.3200	148	57.3200	223	215	63.3200	155	167	69.3200	130	130	75.3200	276	276	75.3200	148	141	75.3200	276	276	
51.4400	168	57.4400	174	166	63.4400	173	163	69.4400	129	130	75.4400	346	323	75.4400	168	192	75.4400	346	323	
51.5600	243	57.5600	147	149	63.5600	212	207	69.5600	137	130	75.5600	357	357	75.5600	243	227	75.5600	357	357	
51.6800	234	57.6800	162	138	63.6800	180	189	69.6800	113	130	75.6800	306	306	75.6800	234	227	75.6800	306	306	
51.8000	165	57.8000	165	139	63.8000	181	172	69.8000	142	130	75.8000	270	270	75.8000	165	164	75.8000	270	270	
51.9200	162	57.9200	150	145	63.9200	151	147	69.9200	120	131	75.9200	246	219	75.9200	162	159	75.9200	246	219	
52.0400	202	58.0400	124	151	64.0400	171	138	70.0400	131	133	76.0400	197	185	76.0400	202	185	76.0400	197	185	
52.1600	424	58.1600	218	189	64.1600	118	137	70.1600	155	147	76.1600	171	177	76.1600	424	405	76.1600	171	177	
52.2800	1207	58.2800	202	174	64.2800	157	146	70.2800	167	151	76.2800	201	208	76.2800	1207	1011	76.2800	201	208	
52.4000	804	58.4000	164	154	64.4000	194	201	70.4000	153	154	76.4000	389	366	76.4000	804	733	76.4000	389	366	
52.5200	318	58.5200	134	140	64.5200	226	220	70.5200	185	159	76.5200	453	468	76.5200	318	309	76.5200	453	468	
52.6400	187	58.6400	138	146	64.6400	241	214	70.6400	162	178	76.6400	345	334	76.6400	187	171	76.6400	345	334	
52.7600	141	58.7600	173	185	64.7600	207	224	70.7600	275	278	76.7600	278	271	76.7600	141	149	76.7600	278	271	
52.8800	140	58.8800	192	188	64.8800	190	184	70.8800	507	511	76.8800	192	166	76.8800	140	142	76.8800	507	511	

2theta	YcalC	2theta	YcalC	Yobs	2theta	YcalC	Yobs	2theta	YcalC	Yobs	2theta	YcalC	Yobs	2theta	YcalC	Yobs	2theta	YcalC	Yobs	
107.0000	191	113.0000	167	158	119.0000	151	150	125.0000	402	264	125.0000	151	150	125.0000	402	264	125.0000	151	150	
107.1200	201	113.1200	198	162	119.1200	140	140	125.1200	366	292	125.1200	140	140	125.1200	366	292	125.1200	140	140	
107.2400	161	113.2400	190	181	119.2400	140	140	125.2400	242	250	125.2400	140	140	125.2400	242	250	125.2400	140	140	
107.3600	160	113.3600	231	210	119.3600	153	149	125.3600	181	206	125.3600	153	149	125.3600	181	206	125.3600	153	149	
107.4800	212	113.4800	243	226	119.4800	141	149	125.4800	253	204	125.4800	141	149	125.4800	253	204	125.4800	141	149	
107.6000	177	113.6000	310	290	119.6000	162	153	125.6000	276	221	125.6000	162	153	125.6000	276	221	125.6000	162	153	
107.7200	168	113.7200	294	343	119.7200	168	164	125.7200	227	207	125.7200	168	164	125.7200	227	207	125.7200	168	164	
107.8400	161	113.8400	242	265	119.8400	195	188	125.8400	172	177	125.8400	195	188	125.8400	172	177	125.8400	195	188	
107.9600	157	113.9600	238	231	119.9600	162	165	125.9600	165	158	125.9600	162	165	125.9600	165	158	125.9600	162	165	
108.0800	138	114.0800	256	267	120.0800	137	168	126.0800	177	160	126.0800	137	168	126.0800	177	160	126.0800	137	168	
108.2000	153	114.2000	284	293	120.2000	162	165	126.2000	195	180	126.2000	162	165	126.2000	195	180	126.2000	162	165	
108.3200	124	114.3200	220	241	120.3200	195	177	126.3200	167	174	126.3200	195	177	126.3200	167	174	126.3200	195	177	
108.4400	141	114.4400	232	199	120.4400	179	176	126.4400	158	154	126.4400	179	176	126.4400	158	154	126.4400	179	176	
108.5600	129	114.5600	227	239	120.5600	143	160	126.5600	164	149	126.5600	143	160	126.5600	164	149	126.5600	143	160	
108.6800	153	114.6800	196	258	120.6800	150	153	126.6800	169	155	126.6800	150	153	126.6800	169	155	126.6800	150	153	
108.8000	156	114.8000	196	206	120.8000	160	154	126.8000	171	165	126.8000	160	154	126.8000	171	165	126.8000	160	154	
108.9200	149	114.9200	267	228	120.9200	184	161	126.9200	160	162	126.9200	184	161	126.9200	160	162	126.9200	184	161	
109.0400	149	115.0400	311	302	121.0400	248	196	127.0400	164	163	127.0400	248	196	127.0400	164	163	127.0400	248	196	
109.1600	121	115.1600	240	256	121.1600	265	251	127.1600	163	160	127.1600	265	251	127.1600	163	160	127.1600	265	251	
109.2800	148	115.2800	187	206	121.2800	180	201	127.2800	170	159	127.2800	180	201	127.2800	170	159	127.2800	180	201	
109.4000	148	115.4000	196	202	121.4000	149	165	127.4000	178	176	127.4000	149	165	127.4000	178	176	127.4000	149	165	
109.5200	142	115.5200	204	216	121.5200	164	170	127.5200	156	178	127.5200	164	170	127.5200	156	178	127.5200	164	170	
109.6400	134	115.6400	185	203	121.6400	173	198	127.6400	146	162	127.6400	173	198	127.6400	146	162	127.6400	173	198	
109.7600	148	115.7600	158	165	121.7600	173	178	127.7600	142	152	127.7600	173	178	127.7600	142	152	127.7600	173	178	
109.8800	149	115.8800	139	150	121.8800	162	167	127.8800	141	152	127.8800	162	167	127.8800	141	152	127.8800	162	167	
110.0000	148	116.0000	154	154	122.0000	161	180	128.0000	159	160	128.0000	161	180	128.0000	159	160	128.0000	161	180	
110.1200	139	116.1200	171	157	122.1200	154	162	128.1200	146	154	128.1200	154	162	128.1200	146	154	128.1200	154	162	
110.2400	176	116.2400	151	158	122.2400	167	148	128.2400	135	153	128.2400	167	148	128.2400	135	153	128.2400	167	148	
110.3600	169	116.3600	164	160	122.3600	143	150	128.3600	153	155	128.3600	164	160	128.3600	153	155	128.3600	164	160	
110.4800	192	116.4800	170	173	122.4800	150	161	128.4800	146	146	128.4800	170	173	122.4800	150	161	128.4800	170	173	
110.6000	283	116.6000	145	164	122.6000	157	160	128.6000	136	141	128.6000	145	164	122.6000	157	160	128.6000	145	164	
110.7200	218	116.7200	163	151	122.7200	155	156	128.7200	141	142	128.7200	163	151	122.7200	155	156	128.7200	163	151	
110.8400	152	116.8400	141	150	122.8400	156	156	128.8400	138	148	128.8400	141	150	122.8400	156	156	128.8400	141	150	
110.9600	179	116.9600	163	154	122.9600	189	172	128.9600	170	149	128.9600	179	172	122.9600	189	172	128.9600	179	172	
111.0800	213	117.0800	125	144	123.0800	244	216	129.0800	145	144	129.0800	213	144	123.0800	244	216	129.0800	213	144	
111.2000	151	117.2000	145	137	123.2000	235	247	129.2000	154	145	129.2000	151	137	123.2000	235	247	129.2000	151	137	
111.3200	165	117.3200	134	136	123.3200	187	200	129.3200	143	153	129.3200	165	136	123.3200	187	200	129.3200	165	136	
111.4400	149	117.4400	135	136	123.4400	185	197	129.4400	129	153	129.4400	149	136	123.4400	185	197	129.4400	149	136	
111.5600	166	117.5600	121	135	123.5600	210	210	129.5600	131	145	129.5600	166	135	123.5600	210	210	129.5600	166	135	
111.6800	155	117.6800	133	136	123.6800	198	208	129.6800	137	141	129.6800	155	136	123.6800	198	208	129.6800	155	136	
111.8000	128	117.8000	153	140	123.8000	165	178	129.8000	139	142	129.8000	128	153	123.8000	165	178	129.8000	128	153	
111.9200	150	117.9200	149	149	123.9200	168	165	129.9200	136	145	129.9200	150	149	123.9200	149	149	129.9200	150	149	
112.0400	135	118.0400	159	151	124.0400	158	171	130.0400	147	143	130.0400	135	151	124.0400	159	171	130.0400	135	151	
112.1600	108	118.1600	143	152	124.1600	157	163				112.1600	108	143	152	124.1600	157	163			
112.2800	127	118.2800	146	151	124.2800	141	151				112.2800	127	146	151	124.2800	141	151			
112.4000	139	118.4000	151	147	124.4000	155	149				112.4000	139	151	124.4000	155	149				
112.5200	139	118.5200	135	144	124.5200	165	153				112.5200	139	135	144	124.5200	165	153			
112.6400	149	118.6400	157	145	124.6400	179	159				112.6400	149	157	145	124.6400	179	159			
112.7600	173	118.7600	152	143	124.7600	171	173				112.7600	173	152	143	124.7600	171	173			
112.8800	159	118.8800	146	143	124.8800	275	211				112.8800	159	146	143	124.8800	275	211			