

TABLE 5:

**Observed and Calculated Step Intensities for Deposit**

Della Ventura, G., Robert, J.-L., Raudsepp, M. and Hawthorne, F.C.  
Quantitative characterization of site occupancies in synthetic monoclinic  
amphiboles. I. Rietveld structure refinement of (Ni-Mg-Co)-potassium-  
richterites.

Sample	KNiO														
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	
9.00	127	88	14.00	77	79	19.00	77	89	24.00	94	109	29.00	473	486	
9.10	97	88	14.10	84	79	19.10	80	92	24.10	74	80	29.10	261	265	
9.20	117	89	14.20	72	79	19.20	87	96	24.20	81	73	29.20	128	155	
9.30	127	89	14.30	81	78	19.30	104	104	24.30	83	71	29.30	121	127	
9.40	141	90	14.40	85	78	19.40	171	129	24.40	75	70	29.40	109	142	
9.50	123	130	14.50	68	78	19.50	294	264	24.50	66	70	29.50	112	159	
9.60	146	156	14.60	79	78	19.60	619	639	24.60	69	69	29.60	161	160	
9.70	212	238	14.70	65	78	19.70	757	678	24.70	87	69	29.70	180	178	
9.80	254	249	14.80	79	78	19.80	251	281	24.80	65	69	29.80	311	257	
9.90	237	173	14.90	77	78	19.90	105	124	24.90	68	69	29.90	660	640	
10.00	285	179	15.00	74	78	20.00	90	93	25.00	69	69	30.00	1527	1642	
10.10	450	353	15.10	89	78	20.10	61	80	25.10	83	69	30.10	2171	2043	
10.20	910	1062	15.20	75	77	20.20	65	74	25.20	94	69	30.20	1218	1197	
10.30	1515	1354	15.30	74	77	20.30	72	73	25.30	97	69	30.30	791	821	
10.40	526	468	15.40	86	77	20.40	94	73	25.40	126	119	30.40	710	673	
10.50	174	148	15.50	80	77	20.50	70	73	25.50	147	126	30.50	303	337	
10.60	119	98	15.60	92	77	20.60	82	73	25.60	139	134	30.60	135	159	
10.70	103	82	15.70	56	77	20.70	61	74	25.70	133	147	30.70	104	113	
10.80	97	82	15.80	66	77	20.80	59	73	25.80	180	169	30.80	97	101	
10.90	84	82	15.90	61	77	20.90	63	73	25.90	287	216	30.90	107	105	
11.00	113	82	16.00	61	77	21.00	63	73	26.00	494	424	31.00	161	125	
11.10	116	82	16.10	71	77	21.10	75	73	26.10	1131	1253	31.10	272	229	
11.20	96	82	16.20	85	77	21.20	59	73	26.20	2642	2771	31.20	524	578	
11.30	97	82	16.30	76	76	21.30	62	83	26.30	2421	2427	31.30	904	917	
11.40	93	82	16.40	62	76	21.40	55	84	26.40	698	958	31.40	586	622	
11.50	102	81	16.50	69	77	21.50	62	87	26.50	295	373	31.50	220	259	
11.60	94	81	16.60	83	77	21.60	92	94	26.60	339	284	31.60	118	144	
11.70	95	81	16.70	86	76	21.70	87	106	26.70	541	426	31.70	110	123	
11.80	88	81	16.80	93	76	21.80	89	109	26.80	1183	1207	31.80	120	124	
11.90	110	81	16.90	76	77	21.90	149	129	26.90	2432	2530	31.90	156	139	
12.00	103	81	17.00	64	77	22.00	250	276	27.00	2316	2057	32.00	289	204	
12.10	98	81	17.10	76	78	22.10	539	592	27.10	687	757	32.10	551	544	
12.20	78	81	17.20	79	90	22.20	588	544	27.20	192	280	32.20	1186	1286	
12.30	91	81	17.30	87	100	22.30	190	234	27.30	148	186	32.30	1437	1468	
12.40	89	80	17.40	77	98	22.40	114	124	27.40	125	164	32.40	675	779	
12.50	95	80	17.50	77	93	22.50	90	109	27.50	189	169	32.50	265	331	
12.60	81	80	17.60	64	94	22.60	126	124	27.60	303	213	32.60	232	236	
12.70	84	80	17.70	101	99	22.70	247	234	27.70	605	461	32.70	289	268	
12.80	85	80	17.80	118	111	22.80	461	535	27.80	1414	1371	32.80	596	517	
12.90	90	80	17.90	161	174	22.90	641	580	27.90	2499	2336	32.90	1412	1497	
13.00	83	80	18.00	337	386	23.00	231	262	28.00	1697	1495	33.00	2705	2879	
13.10	79	80	18.10	563	581	23.10	79	117	28.10	510	496	33.10	2569	2317	
13.20	78	80	18.20	530	486	23.20	87	87	28.20	213	196	33.20	884	901	
13.30	93	79	18.30	242	224	23.30	68	79	28.30	127	138	33.30	257	295	
13.40	64	79	18.40	98	109	23.40	50	75	28.40	122	114	33.40	119	154	
13.50	85	79	18.50	86	85	23.50	74	74	28.50	121	95	33.50	86	109	
13.60	87	79	18.60	81	78	23.60	63	76	28.60	92	89	33.60	95	86	
13.70	78	79	18.70	70	75	23.70	84	88	28.70	128	105	33.70	80	87	
13.80	73	79	18.80	74	83	23.80	92	127	28.80	214	188	33.80	84	89	
13.90	83	79	18.90	78	88	23.90	120	152	28.90	373	408	33.90	81	92	

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	90	97	39.00	401	329	44.00	588	602	49.00	300	335	54.00	108	106
34.10	99	108	39.10	736	797	44.10	763	647	49.10	262	272	54.10	145	139
34.20	124	132	39.20	1173	1155	44.20	569	531	49.20	208	232	54.20	215	228
34.30	218	191	39.30	908	836	44.30	533	551	49.30	153	182	54.30	363	374
34.40	355	334	39.40	404	408	44.40	584	598	49.40	152	136	54.40	488	483
34.50	787	806	39.50	233	220	44.50	531	492	49.50	104	106	54.50	521	441
34.60	1333	1390	39.60	129	137	44.60	350	293	49.60	93	93	54.60	385	324
34.70	1085	1117	39.70	108	99	44.70	209	163	49.70	77	91	54.70	336	271
34.80	520	541	39.80	102	91	44.80	149	139	49.80	55	85	54.80	427	395
34.90	331	329	39.90	83	103	44.90	155	160	49.90	62	74	54.90	709	711
35.00	539	476	40.00	124	113	45.00	152	142	50.00	51	67	55.00	978	1022
35.10	1065	1087	40.10	121	100	45.10	97	102	50.10	60	65	55.10	979	906
35.20	1894	1941	40.20	83	84	45.20	75	78	50.20	55	67	55.20	539	577
35.30	1909	1720	40.30	82	82	45.30	75	73	50.30	70	72	55.30	280	293
35.40	704	774	40.40	126	100	45.40	66	73	50.40	93	92	55.40	190	195
35.50	240	269	40.50	175	167	45.50	62	78	50.50	150	154	55.50	199	217
35.60	121	138	40.60	289	314	45.60	76	86	50.60	244	251	55.60	251	232
35.70	92	101	40.70	481	398	45.70	86	87	50.70	275	272	55.70	170	196
35.80	83	85	40.80	375	298	45.80	85	84	50.80	191	204	55.80	149	144
35.90	86	81	40.90	185	175	45.90	91	91	50.90	137	132	55.90	94	106
36.00	92	89	41.00	116	129	46.00	110	109	51.00	110	111	56.00	74	87
36.10	109	90	41.10	112	131	46.10	157	161	51.10	104	117	56.10	71	80
36.20	60	80	41.20	158	171	46.20	252	274	51.20	99	113	56.20	74	79
36.30	74	78	41.30	348	289	46.30	346	345	51.30	105	116	56.30	79	84
36.40	77	83	41.40	638	601	46.40	303	304	51.40	93	142	56.40	101	88
36.50	85	96	41.50	1171	1150	46.50	250	262	51.50	132	147	56.50	130	97
36.60	104	117	41.60	1338	1250	46.60	331	272	51.60	107	119	56.60	156	134
36.70	144	138	41.70	863	827	46.70	347	287	51.70	66	85	56.70	232	192
36.80	178	177	41.80	453	471	46.80	417	398	51.80	72	68	56.80	271	240
36.90	202	230	41.90	304	272	46.90	626	568	51.90	59	63	56.90	365	302
37.00	275	255	42.00	184	155	47.00	529	498	52.00	65	62	57.00	376	314
37.10	367	359	42.10	127	111	47.10	367	287	52.10	70	63	57.10	300	247
37.20	560	558	42.20	131	115	47.20	145	141	52.20	88	68	57.20	188	165
37.30	612	557	42.30	181	164	47.30	104	93	52.30	86	77	57.30	156	113
37.40	326	333	42.40	211	212	47.40	66	80	52.40	115	81	57.40	147	94
37.50	188	184	42.50	176	174	47.50	93	78	52.50	101	74	57.50	137	91
37.60	160	154	42.60	99	108	47.60	127	92	52.60	87	66	57.60	145	100
37.70	257	191	42.70	74	75	47.70	143	145	52.70	79	62	57.70	113	105
37.80	433	380	42.80	68	66	47.80	237	227	52.80	65	64	57.80	116	99
37.90	834	888	42.90	80	63	47.90	249	230	52.90	75	74	57.90	106	88
38.00	1303	1392	43.00	79	67	48.00	174	164	53.00	91	85	58.00	88	85
38.10	1346	1309	43.10	101	67	48.10	104	108	53.10	93	87	58.10	126	89
38.20	781	743	43.20	142	70	48.20	77	84	53.20	106	84	58.20	155	117
38.30	316	311	43.30	111	75	48.30	77	79	53.30	69	79	58.30	229	210
38.40	171	159	43.40	134	78	48.40	62	82	53.40	75	76	58.40	409	402
38.50	117	121	43.50	107	86	48.50	92	94	53.50	79	75	58.50	630	534
38.60	101	110	43.60	109	94	48.60	153	132	53.60	79	73	58.60	488	496
38.70	106	108	43.70	130	109	48.70	236	214	53.70	81	75	58.70	451	394
38.80	121	118	43.80	174	157	48.80	295	340	53.80	78	83	58.80	269	284
38.90	198	157	43.90	304	324	48.90	386	392	53.90	105	92	58.90	267	262

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	367	359	64.00	198	219	69.00	86	84	74.00	128	137	79.00	112	103
59.10	462	481	64.10	188	230	69.10	80	86	74.10	189	169	79.10	90	104
59.20	462	437	64.20	227	251	69.20	108	103	74.20	186	197	79.20	102	126
59.30	326	306	64.30	224	235	69.30	151	139	74.30	217	204	79.30	161	171
59.40	185	176	64.40	206	186	69.40	180	168	74.40	176	194	79.40	201	211
59.50	107	112	64.50	149	145	69.50	197	201	74.50	174	197	79.50	165	195
59.60	88	90	64.60	137	135	69.60	220	209	74.60	163	184	79.60	148	167
59.70	87	85	64.70	145	145	69.70	186	184	74.70	140	152	79.70	141	134
59.80	81	78	64.80	137	134	69.80	149	167	74.80	128	128	79.80	88	100
59.90	91	73	64.90	122	120	69.90	143	155	74.90	115	105	79.90	70	80
60.00	62	70	65.00	124	97	70.00	153	162	75.00	70	85	80.00	73	74
60.10	84	75	65.10	104	82	70.10	217	208	75.10	69	74	80.10	71	74
60.20	74	76	65.20	101	75	70.20	302	303	75.20	54	68	80.20	60	73
60.30	201	79	65.30	102	79	70.30	423	430	75.30	50	63	80.30	59	71
60.40	92	85	65.40	96	95	70.40	583	579	75.40	57	62	80.40	59	72
60.50	98	107	65.50	138	106	70.50	604	603	75.50	52	65	80.50	64	76
60.60	147	167	65.60	114	99	70.60	451	497	75.60	64	77	80.60	61	82
60.70	251	260	65.70	102	89	70.70	381	372	75.70	78	96	80.70	67	80
60.80	315	319	65.80	90	84	70.80	224	235	75.80	112	106	80.80	69	77
60.90	314	343	65.90	81	92	70.90	141	152	75.90	91	103	80.90	76	75
61.00	380	414	66.00	109	101	71.00	110	108	76.00	93	92	81.00	97	79
61.10	525	584	66.10	114	105	71.10	91	88	76.10	91	80	81.10	97	98
61.20	777	778	66.20	110	101	71.20	83	82	76.20	89	73	81.20	135	126
61.30	731	703	66.30	101	95	71.30	92	89	76.30	71	75	81.30	105	135
61.40	508	505	66.40	92	85	71.40	102	109	76.40	86	82	81.40	148	136
61.50	302	315	66.50	109	75	71.50	136	133	76.50	71	86	81.50	128	138
61.60	252	273	66.60	80	70	71.60	147	157	76.60	90	89	81.60	115	122
61.70	341	348	66.70	83	72	71.70	164	165	76.70	111	96	81.70	89	103
61.80	381	355	66.80	96	82	71.80	134	150	76.80	119	109	81.80	92	93
61.90	262	282	66.90	106	89	71.90	132	128	76.90	113	115	81.90	68	85
62.00	177	185	67.00	91	87	72.00	121	108	77.00	97	116	82.00	67	78
62.10	103	120	67.10	84	82	72.10	105	105	77.10	112	116	82.10	71	73
62.20	92	96	67.20	90	80	72.20	128	131	77.20	105	114	82.20	59	69
62.30	100	99	67.30	82	85	72.30	205	175	77.30	129	115	82.30	69	66
62.40	144	129	67.40	106	110	72.40	227	197	77.40	127	110	82.40	66	66
62.50	187	202	67.50	187	160	72.50	199	203	77.50	96	107	82.50	54	66
62.60	256	242	67.60	248	230	72.60	179	198	77.60	120	113	82.60	68	68
62.70	211	233	67.70	361	334	72.70	195	184	77.70	148	131	82.70	64	75
62.80	212	210	67.80	446	380	72.80	207	172	77.80	133	146	82.80	91	94
62.90	215	205	67.90	331	317	72.90	220	211	77.90	134	138	82.90	122	121
63.00	214	221	68.00	254	232	73.00	316	335	78.00	114	125	83.00	157	130
63.10	253	250	68.10	182	154	73.10	472	496	78.10	97	106	83.10	92	118
63.20	268	264	68.20	146	129	73.20	572	515	78.20	83	87	83.20	101	107
63.30	314	277	68.30	171	147	73.30	359	425	78.30	71	77	83.30	96	90
63.40	451	398	68.40	163	160	73.40	291	309	78.40	84	78	83.40	69	78
63.50	688	710	68.50	136	142	73.50	172	198	78.50	122	92	83.50	71	79
63.60	921	946	68.60	111	120	73.60	99	139	78.60	132	110	83.60	100	92
63.70	807	816	68.70	118	103	73.70	104	120	78.70	127	115	83.70	92	99
63.80	559	560	68.80	107	96	73.80	103	118	78.80	135	112	83.80	85	100
63.90	360	313	68.90	114	90	73.90	116	119	78.90	126	109	83.90	78	100

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	89	94	89.00	118	111	94.00	110	104	99.00	80	62			
84.10	89	93	89.10	120	113	94.10	98	86	99.10	78	64			
84.20	69	99	89.20	100	115	94.20	61	84	99.20	77	66			
84.30	83	95	89.30	111	115	94.30	111	99	99.30	66	63			
84.40	70	86	89.40	111	113	94.40	121	126	99.40	65	58			
84.50	58	80	89.50	125	116	94.50	158	144	99.50	53	57			
84.60	75	74	89.60	127	115	94.60	134	135	99.60	63	57			
84.70	76	78	89.70	101	107	94.70	142	124	99.70	69	56			
84.80	88	95	89.80	116	104	94.80	144	111	99.80	73	54			
84.90	128	112	89.90	114	108	94.90	125	91	99.90	56	52			
85.00	128	114	90.00	87	111	95.00	82	73	100.00	56	52			
85.10	120	112	90.10	104	113	95.10	83	61						
85.20	114	102	90.20	134	121	95.20	59	58						
85.30	83	87	90.30	129	137	95.30	63	59						
85.40	76	76	90.40	157	155	95.40	82	64						
85.50	81	70	90.50	186	166	95.50	82	67						
85.60	71	68	90.60	185	176	95.60	69	70						
85.70	72	69	90.70	155	188	95.70	83	77						
85.80	64	70	90.80	184	178	95.80	101	85						
85.90	59	75	90.90	170	151	95.90	100	89						
86.00	79	83	91.00	108	128	96.00	132	85						
86.10	69	89	91.10	84	107	96.10	88	77						
86.20	79	88	91.20	71	87	96.20	75	71						
86.30	78	85	91.30	69	73	96.30	69	65						
86.40	87	84	91.40	57	64	96.40	62	59						
86.50	88	83	91.50	66	58	96.50	71	55						
86.60	93	86	91.60	62	56	96.60	55	55						
86.70	99	96	91.70	58	55	96.70	59	59						
86.80	119	119	91.80	56	56	96.80	64	64						
86.90	130	140	91.90	61	58	96.90	55	72						
87.00	124	134	92.00	55	58	97.00	77	81						
87.10	100	119	92.10	67	58	97.10	91	95						
87.20	127	103	92.20	46	59	97.20	94	116						
87.30	86	82	92.30	46	61	97.30	145	142						
87.40	58	66	92.40	72	65	97.40	195	149						
87.50	47	57	92.50	64	68	97.50	141	138						
87.60	41	53	92.60	66	72	97.60	140	138						
87.70	58	51	92.70	69	83	97.70	164	151						
87.80	40	51	92.80	92	102	97.80	200	158						
87.90	52	52	92.90	112	123	97.90	174	159						
88.00	61	52	93.00	141	135	98.00	166	162						
88.10	59	52	93.10	142	155	98.10	183	163						
88.20	44	54	93.20	156	201	98.20	156	144						
88.30	63	57	93.30	251	247	98.30	136	122						
88.40	63	59	93.40	241	267	98.40	126	108						
88.50	50	60	93.50	258	279	98.50	88	92						
88.60	53	63	93.60	241	255	98.60	82	75						
88.70	74	70	93.70	198	208	98.70	68	67						
88.80	93	81	93.80	149	171	98.80	65	65						
88.90	102	98	93.90	141	134	98.90	72	64						



Sample KNi20

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	210	174	14.00	168	163	19.00	151	167	24.00	189	188	29.00	569	595
9.10	195	174	14.10	155	163	19.10	172	169	24.10	140	156	29.10	340	347
9.20	210	235	14.20	156	163	19.20	155	173	24.20	160	150	29.20	196	216
9.30	218	237	14.30	160	163	19.30	192	181	24.30	149	148	29.30	183	199
9.40	215	241	14.40	164	162	19.40	220	199	24.40	132	147	29.40	207	227
9.50	216	246	14.50	153	162	19.50	322	283	24.50	162	147	29.50	243	268
9.60	225	256	14.60	162	162	19.60	643	655	24.60	142	146	29.60	214	245
9.70	276	282	14.70	179	162	19.70	883	866	24.70	143	146	29.70	229	236
9.80	324	305	14.80	157	162	19.80	368	404	24.80	136	146	29.80	319	271
9.90	423	320	14.90	177	162	19.90	197	213	24.90	157	146	29.90	577	452
10.00	604	389	15.00	169	161	20.00	165	178	25.00	160	145	30.00	1268	1300
10.10	1023	714	15.10	163	161	20.10	171	165	25.10	171	164	30.10	2327	2329
10.20	2124	2380	15.20	179	161	20.20	159	159	25.20	152	175	30.20	1591	1477
10.30	3721	3520	15.30	141	161	20.30	153	156	25.30	151	178	30.30	710	731
10.40	1083	1165	15.40	166	161	20.40	173	154	25.40	164	181	30.40	610	595
10.50	351	383	15.50	172	160	20.50	159	157	25.50	179	186	30.50	313	356
10.60	255	246	15.60	163	160	20.60	159	170	25.60	179	193	30.60	216	218
10.70	219	196	15.70	163	160	20.70	194	192	25.70	180	204	30.70	152	183
10.80	200	171	15.80	148	160	20.80	169	174	25.80	219	247	30.80	153	172
10.90	193	169	15.90	156	160	20.90	151	157	25.90	285	283	30.90	166	171
11.00	189	169	16.00	152	160	21.00	159	158	26.00	426	373	31.00	227	181
11.10	169	169	16.10	160	159	21.10	184	160	26.10	952	822	31.10	302	249
11.20	184	169	16.20	171	159	21.20	161	160	26.20	2301	2407	31.20	466	523
11.30	193	168	16.30	140	159	21.30	150	161	26.30	3060	2944	31.30	960	953
11.40	172	168	16.40	138	159	21.40	191	162	26.40	1120	1315	31.40	722	701
11.50	178	168	16.50	170	159	21.50	158	165	26.50	433	506	31.50	277	316
11.60	188	168	16.60	162	159	21.60	183	175	26.60	347	357	31.60	203	206
11.70	176	168	16.70	145	159	21.70	194	202	26.70	463	422	31.70	174	187
11.80	166	167	16.80	169	158	21.80	193	203	26.80	994	942	31.80	211	209
11.90	155	167	16.90	158	158	21.90	218	206	26.90	2329	2437	31.90	229	234
12.00	177	167	17.00	125	163	22.00	321	293	27.00	2605	2325	32.00	312	278
12.10	165	167	17.10	163	164	22.10	638	650	27.10	761	870	32.10	523	505
12.20	165	167	17.20	163	167	22.20	812	798	27.20	273	362	32.20	1135	1274
12.30	150	166	17.30	173	173	22.30	345	387	27.30	239	271	32.30	1709	1597
12.40	178	166	17.40	162	169	22.40	185	221	27.40	209	250	32.40	787	834
12.50	180	166	17.50	157	166	22.50	210	197	27.50	230	257	32.50	280	378
12.60	186	166	17.60	160	167	22.60	207	204	27.60	338	300	32.60	240	299
12.70	141	166	17.70	146	171	22.70	327	287	27.70	658	488	32.70	312	322
12.80	166	165	17.80	169	179	22.80	599	651	27.80	1501	1477	32.80	552	452
12.90	166	165	17.90	230	218	22.90	854	857	27.90	3147	3124	32.90	1246	1184
13.00	193	165	18.00	339	398	23.00	410	417	28.00	2309	2088	33.00	2884	3314
13.10	139	165	18.10	509	518	23.10	194	212	28.10	611	671	33.10	3889	3643
13.20	176	165	18.20	364	307	23.20	178	174	28.20	285	302	33.20	1652	1574
13.30	180	165	18.30	212	196	23.30	157	162	28.30	226	227	33.30	434	507
13.40	169	164	18.40	189	169	23.40	165	156	28.40	171	197	33.40	245	288
13.50	161	164	18.50	176	161	23.50	189	154	28.50	187	179	33.50	187	229
13.60	174	164	18.60	157	167	23.60	155	153	28.60	174	171	33.60	183	199
13.70	167	164	18.70	151	165	23.70	178	161	28.70	248	176	33.70	208	182
13.80	174	164	18.80	161	165	23.80	210	199	28.80	282	236	33.80	171	173
13.90	172	163	18.90	160	166	23.90	207	237	28.90	474	482	33.90	145	170

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	182	185	39.00	385	318	44.00	521	617	49.00	431	462	54.00	169	171
34.10	201	201	39.10	715	776	44.10	941	955	49.10	370	359	54.10	195	186
34.20	202	218	39.20	1426	1473	44.20	896	877	49.20	277	302	54.20	259	255
34.30	226	250	39.30	1263	1195	44.30	883	845	49.30	235	250	54.30	403	410
34.40	379	342	39.40	511	551	44.40	972	868	49.40	205	217	54.40	565	563
34.50	787	798	39.50	264	286	44.50	852	812	49.50	205	194	54.50	637	574
34.60	1862	1940	39.60	221	208	44.60	629	551	49.60	170	178	54.60	489	440
34.70	1949	1986	39.70	175	170	44.70	509	309	49.70	161	183	54.70	349	319
34.80	966	985	39.80	166	157	44.80	331	223	49.80	185	185	54.80	391	342
34.90	431	483	39.90	176	164	44.90	234	254	49.90	147	163	54.90	642	627
35.00	486	470	40.00	212	185	45.00	252	251	50.00	129	141	55.00	1028	1130
35.10	999	993	40.10	193	179	45.10	224	196	50.10	139	132	55.10	1192	1272
35.20	2152	2352	40.20	163	156	45.20	164	155	50.20	127	131	55.20	843	912
35.30	2813	2554	40.30	149	156	45.30	149	144	50.30	154	134	55.30	506	481
35.40	1170	1204	40.40	162	167	45.40	154	142	50.40	160	143	55.40	256	270
35.50	318	422	40.50	234	208	45.50	119	150	50.50	191	184	55.50	243	268
35.60	234	240	40.60	364	346	45.60	158	177	50.60	311	303	55.60	321	319
35.70	180	192	40.70	564	514	45.70	177	185	50.70	407	398	55.70	276	288
35.80	156	170	40.80	497	434	45.80	163	168	50.80	338	341	55.80	211	226
35.90	129	162	40.90	298	266	45.90	152	159	50.90	229	230	55.90	159	172
36.00	156	174	41.00	207	197	46.00	176	169	51.00	171	166	56.00	124	148
36.10	193	183	41.10	179	193	46.10	192	184	51.10	157	158	56.10	146	140
36.20	151	164	41.20	220	224	46.20	268	247	51.20	146	162	56.20	128	143
36.30	162	149	41.30	345	329	46.30	422	341	51.30	169	180	56.30	162	154
36.40	172	151	41.40	649	575	46.40	355	339	51.40	207	235	56.40	200	159
36.50	179	168	41.50	1251	1205	46.50	320	306	51.50	230	249	56.50	186	161
36.60	174	186	41.60	1916	1781	46.60	401	335	51.60	178	206	56.60	203	197
36.70	208	193	41.70	1508	1339	46.70	376	327	51.70	157	156	56.70	279	276
36.80	231	248	41.80	805	752	46.80	388	358	51.80	135	134	56.80	342	316
36.90	280	365	41.90	455	445	46.90	508	502	51.90	125	128	56.90	339	379
37.00	336	344	42.00	242	271	47.00	545	474	52.00	114	127	57.00	470	476
37.10	376	323	42.10	193	196	47.10	367	309	52.10	135	128	57.10	423	428
37.20	497	512	42.20	200	181	47.20	193	187	52.20	153	133	57.20	341	315
37.30	671	632	42.30	199	210	47.30	119	150	52.30	157	146	57.30	205	211
37.40	397	424	42.40	314	288	47.40	167	143	52.40	167	157	57.40	177	168
37.50	187	251	42.50	285	278	47.50	140	143	52.50	169	149	57.50	149	158
37.60	237	216	42.60	219	198	47.60	188	157	52.60	127	136	57.60	161	160
37.70	277	242	42.70	154	148	47.70	224	221	52.70	136	127	57.70	132	162
37.80	477	393	42.80	153	138	47.80	345	368	52.80	131	126	57.80	140	158
37.90	908	920	42.90	136	137	47.90	443	400	52.90	133	131	57.90	154	154
38.00	1507	1593	43.00	144	138	48.00	305	293	53.00	159	146	58.00	138	151
38.10	1736	1753	43.10	140	138	48.10	192	189	53.10	142	155	58.10	152	151
38.20	1116	1080	43.20	146	142	48.20	153	151	53.20	167	153	58.20	180	160
38.30	470	466	43.30	143	145	48.30	139	143	53.30	126	147	58.30	257	206
38.40	301	255	43.40	139	147	48.40	159	142	53.40	131	144	58.40	421	378
38.50	213	201	43.50	148	151	48.50	154	148	53.50	144	145	58.50	697	663
38.60	195	183	43.60	148	157	48.60	200	172	53.60	154	141	58.60	761	709
38.70	169	179	43.70	159	168	48.70	273	238	53.70	132	142	58.70	652	619
38.80	177	186	43.80	211	191	48.80	355	372	53.80	119	148	58.80	543	475
38.90	235	211	43.90	320	286	48.90	476	505	53.90	181	160	58.90	405	384

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	448	472	64.00	235	262	69.00	141	140	74.00	184	183	79.00	172	172
59.10	700	655	64.10	259	261	69.10	138	140	74.10	217	224	79.10	181	162
59.20	661	598	64.20	299	315	69.20	152	149	74.20	274	273	79.20	156	171
59.30	466	431	64.30	343	347	69.30	183	179	74.30	320	303	79.30	220	218
59.40	254	253	64.40	327	308	69.40	221	214	74.40	307	306	79.40	250	288
59.50	177	172	64.50	247	246	69.50	272	241	74.50	273	301	79.50	289	301
59.60	132	150	64.60	212	211	69.60	313	281	74.60	313	302	79.60	247	263
59.70	146	145	64.70	219	216	69.70	287	274	74.70	293	260	79.70	225	227
59.80	145	144	64.80	221	206	69.80	237	248	74.80	202	217	79.80	173	181
59.90	144	140	64.90	197	186	69.90	203	225	74.90	205	184	79.90	116	148
60.00	131	139	65.00	214	163	70.00	228	205	75.00	136	157	80.00	128	135
60.10	143	139	65.10	231	144	70.10	237	220	75.10	136	139	80.10	144	133
60.20	138	143	65.20	176	134	70.20	348	309	75.20	127	132	80.20	140	134
60.30	162	149	65.30	187	134	70.30	491	487	75.30	145	127	80.30	127	131
60.40	154	150	65.40	172	148	70.40	699	708	75.40	117	123	80.40	108	130
60.50	176	158	65.50	151	171	70.50	803	852	75.50	130	123	80.50	117	134
60.60	191	190	65.60	188	170	70.60	683	739	75.60	123	132	80.60	146	144
60.70	271	278	65.70	161	157	70.70	562	566	75.70	150	150	80.70	151	152
60.80	353	381	65.80	159	143	70.80	359	374	75.80	165	162	80.80	128	149
60.90	421	392	65.90	169	144	70.90	226	237	75.90	153	162	80.90	134	143
61.00	477	423	66.00	150	158	71.00	190	176	76.00	146	155	81.00	136	143
61.10	599	573	66.10	171	168	71.10	137	149	76.10	137	141	81.10	151	156
61.20	896	917	66.20	164	169	71.20	151	138	76.20	131	134	81.20	165	185
61.30	1130	1033	66.30	156	168	71.30	137	138	76.30	162	135	81.30	222	196
61.40	685	799	66.40	163	163	71.40	150	151	76.40	161	141	81.40	182	192
61.50	511	502	66.50	118	151	71.50	177	179	76.50	157	143	81.50	196	198
61.60	285	326	66.60	168	140	71.60	206	211	76.60	160	144	81.60	185	189
61.70	389	384	66.70	122	134	71.70	225	236	76.70	162	143	81.70	167	166
61.80	524	499	66.80	117	138	71.80	222	228	76.80	168	151	81.80	154	154
61.90	412	440	66.90	184	143	71.90	211	210	76.90	168	168	81.90	142	144
62.00	349	328	67.00	140	140	72.00	203	182	77.00	167	174	82.00	128	134
62.10	180	215	67.10	122	135	72.10	172	163	77.10	181	177	82.10	145	130
62.20	153	164	67.20	124	132	72.20	189	170	77.20	171	177	82.20	126	129
62.30	140	153	67.30	143	136	72.30	245	221	77.30	177	176	82.30	120	127
62.40	167	161	67.40	150	157	72.40	298	284	77.40	198	178	82.40	142	126
62.50	204	206	67.50	217	205	72.50	317	293	77.50	179	171	82.50	116	129
62.60	302	282	67.60	269	254	72.60	282	279	77.60	196	169	82.60	128	130
62.70	332	309	67.70	329	333	72.70	251	253	77.70	191	176	82.70	116	131
62.80	321	311	67.80	462	471	72.80	233	218	77.80	200	194	82.80	152	139
62.90	312	300	67.90	501	477	72.90	225	209	77.90	207	200	82.90	165	161
63.00	293	288	68.00	346	387	73.00	276	275	78.00	178	190	83.00	197	197
63.10	293	306	68.10	325	285	73.10	411	461	78.10	222	180	83.10	221	215
63.20	353	364	68.20	193	214	73.20	686	641	78.20	242	160	83.20	169	197
63.30	405	385	68.30	210	225	73.30	577	593	78.30	181	144	83.30	172	179
63.40	497	468	68.40	257	256	73.40	456	479	78.40	172	142	83.40	146	157
63.50	766	800	68.50	238	233	73.50	352	342	78.50	189	157	83.50	125	138
63.60	1218	1199	68.60	200	200	73.60	205	229	78.60	198	187	83.60	156	135
63.70	1027	1078	68.70	146	164	73.70	181	184	78.70	204	198	83.70	143	145
63.80	728	772	68.80	149	146	73.80	153	175	78.80	159	189	83.80	168	151
63.90	442	426	68.90	144	143	73.90	191	171	78.90	189	182	83.90	129	153



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	138	152	89.00	190	171	94.00	189	194	99.00	149	133			
84.10	131	147	89.10	210	180	94.10	143	160	99.10	157	133			
84.20	139	150	89.20	167	177	94.20	148	142	99.20	139	136			
84.30	152	158	89.30	162	176	94.30	145	145	99.30	165	139			
84.40	114	156	89.40	194	175	94.40	142	169	99.40	159	137			
84.50	107	146	89.50	151	173	94.50	198	204	99.50	133	131			
84.60	146	140	89.60	163	178	94.60	253	218	99.60	147	128			
84.70	150	136	89.70	183	183	94.70	196	204	99.70	139	129			
84.80	133	144	89.80	170	178	94.80	199	194	99.80	126	127			
84.90	173	162	89.90	170	174	94.90	170	180	99.90	156	123			
85.00	174	170	90.00	186	184	95.00	151	156	100.00	132	120			
85.10	169	169	90.10	182	193	95.10	141	137						
85.20	159	168	90.20	212	196	95.20	119	126						
85.30	155	156	90.30	225	203	95.30	147	123						
85.40	134	144	90.40	232	216	95.40	121	124						
85.50	129	135	90.50	256	240	95.50	160	129						
85.60	118	129	90.60	252	257	95.60	126	134						
85.70	129	126	90.70	243	261	95.70	146	137						
85.80	124	126	90.80	277	270	95.80	174	143						
85.90	135	126	90.90	239	252	95.90	176	149						
86.00	121	132	91.00	208	216	96.00	171	152						
86.10	139	142	91.10	174	190	96.10	180	149						
86.20	146	146	91.20	132	166	96.20	161	140						
86.30	151	143	91.30	140	144	96.30	133	133						
86.40	139	141	91.40	137	131	96.40	133	128						
86.50	131	140	91.50	124	124	96.50	132	123						
86.60	143	142	91.60	131	120	96.60	119	119						
86.70	136	152	91.70	107	119	96.70	111	119						
86.80	177	172	91.80	132	120	96.80	113	122						
86.90	191	198	91.90	115	122	96.90	143	128						
87.00	202	200	92.00	114	123	97.00	142	136						
87.10	167	182	92.10	118	122	97.10	154	143						
87.20	162	167	92.20	94	121	97.20	162	157						
87.30	144	148	92.30	126	122	97.30	167	186						
87.40	139	129	92.40	125	125	97.40	258	220						
87.50	107	119	92.50	131	129	97.50	283	230						
87.60	110	115	92.60	117	133	97.60	170	216						
87.70	107	113	92.70	168	144	97.70	212	217						
87.80	89	113	92.80	181	167	97.80	255	237						
87.90	116	114	92.90	167	193	97.90	301	256						
88.00	108	115	93.00	208	200	98.00	246	265						
88.10	112	115	93.10	186	202	98.10	316	260						
88.20	120	115	93.20	219	236	98.20	246	239						
88.30	100	117	93.30	306	289	98.30	204	214						
88.40	115	119	93.40	311	321	98.40	180	192						
88.50	113	120	93.50	319	336	98.50	174	173						
88.60	133	121	93.60	355	355	98.60	162	153						
88.70	111	125	93.70	346	329	98.70	136	139						
88.80	115	135	93.80	231	271	98.80	152	133						
88.90	124	152	93.90	215	230	98.90	142	133						

Sample KNi40

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	270	296	14.00	243	209	19.00	204	217	24.00	228	253	29.00	546	586
9.10	286	299	14.10	224	209	19.10	219	219	24.10	213	221	29.10	555	555
9.20	263	302	14.20	216	209	19.20	201	223	24.20	218	206	29.20	330	349
9.30	289	307	14.30	208	209	19.30	254	230	24.30	233	202	29.30	263	266
9.40	274	314	14.40	226	209	19.40	210	243	24.40	225	201	29.40	283	270
9.50	279	322	14.50	189	209	19.50	293	286	24.50	211	200	29.50	311	330
9.60	314	335	14.60	197	209	19.60	498	465	24.60	213	200	29.60	345	361
9.70	343	355	14.70	201	208	19.70	810	849	24.70	202	199	29.70	332	311
9.80	422	386	14.80	218	208	19.80	824	771	24.80	212	199	29.80	332	294
9.90	525	436	14.90	192	208	19.90	399	402	24.90	197	199	29.90	445	341
10.00	804	536	15.00	217	208	20.00	253	266	25.00	201	211	30.00	655	589
10.10	1272	847	15.10	196	208	20.10	247	234	25.10	194	220	30.10	1291	1396
10.20	2340	2095	15.20	194	208	20.20	227	221	25.20	230	222	30.20	1988	1950
10.30	4452	4653	15.30	226	208	20.30	222	215	25.30	223	224	30.30	1198	1194
10.40	4179	3981	15.40	194	208	20.40	195	212	25.40	225	227	30.40	640	619
10.50	1165	1495	15.50	213	208	20.50	207	212	25.50	235	232	30.50	465	436
10.60	485	603	15.60	186	208	20.60	218	221	25.60	235	237	30.60	330	312
10.70	343	383	15.70	221	208	20.70	241	253	25.70	255	258	30.70	245	255
10.80	312	296	15.80	185	207	20.80	263	270	25.80	238	279	30.80	229	237
10.90	255	250	15.90	195	207	20.90	228	236	25.90	250	304	30.90	253	232
11.00	268	222	16.00	199	207	21.00	209	216	26.00	344	352	31.00	257	242
11.10	254	212	16.10	194	207	21.10	208	211	26.10	509	497	31.10	276	266
11.20	245	212	16.20	231	207	21.20	223	210	26.20	1140	1111	31.20	356	368
11.30	238	212	16.30	206	207	21.30	211	210	26.30	2370	2455	31.30	645	705
11.40	205	211	16.40	190	207	21.40	220	210	26.40	2472	2432	31.40	956	964
11.50	218	211	16.50	189	207	21.50	228	211	26.50	1136	1191	31.50	686	643
11.60	238	211	16.60	221	207	21.60	230	218	26.60	552	571	31.60	385	346
11.70	221	211	16.70	186	207	21.70	232	228	26.70	461	474	31.70	269	262
11.80	229	211	16.80	221	209	21.80	264	238	26.80	652	607	31.80	240	265
11.90	225	211	16.90	203	210	21.90	237	241	26.90	1202	1319	31.90	262	278
12.00	233	211	17.00	212	211	22.00	299	263	27.00	2429	2383	32.00	299	300
12.10	199	211	17.10	199	212	22.10	369	377	27.10	1943	1753	32.10	413	378
12.20	225	211	17.20	199	216	22.20	614	644	27.20	657	743	32.20	708	714
12.30	203	211	17.30	204	227	22.30	671	629	27.30	315	414	32.30	1283	1386
12.40	203	211	17.40	238	235	22.40	373	369	27.40	275	345	32.40	1321	1319
12.50	231	210	17.50	195	224	22.50	243	267	27.50	343	335	32.50	692	696
12.60	230	210	17.60	198	217	22.60	260	253	27.60	386	360	32.60	393	413
12.70	214	210	17.70	199	218	22.70	282	278	27.70	544	456	32.70	369	376
12.80	203	210	17.80	228	223	22.80	426	418	27.80	883	885	32.80	432	428
12.90	226	210	17.90	233	239	22.90	703	744	27.90	2247	2324	32.90	741	671
13.00	188	210	18.00	334	307	23.00	744	711	28.00	3679	3420	33.00	1566	1727
13.10	231	210	18.10	391	464	23.10	347	388	28.10	2243	1945	33.10	3402	3710
13.20	232	210	18.20	513	456	23.20	261	257	28.20	755	725	33.20	3521	3353
13.30	218	210	18.30	396	309	23.30	201	226	28.30	391	391	33.30	1549	1458
13.40	231	210	18.40	267	242	23.40	224	216	28.40	268	305	33.40	574	584
13.50	221	210	18.50	215	226	23.50	234	211	28.50	251	268	33.50	312	373
13.60	216	209	18.60	188	220	23.60	198	208	28.60	261	249	33.60	311	304
13.70	210	209	18.70	216	217	23.70	198	209	28.70	235	243	33.70	272	271
13.80	235	209	18.80	205	216	23.80	212	219	28.80	290	259	33.80	269	253
13.90	217	209	18.90	195	216	23.90	241	249	28.90	359	371	33.90	240	244

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	219	253	39.00	325	299	44.00	420	380	49.00	470	511	54.00	184	212
34.10	232	262	39.10	502	468	44.10	722	719	49.10	427	451	54.10	244	225
34.20	260	274	39.20	957	951	44.20	1048	1068	49.20	374	363	54.20	264	253
34.30	294	301	39.30	1446	1374	44.30	1041	1058	49.30	298	310	54.30	305	335
34.40	359	355	39.40	1035	1016	44.40	1021	1018	49.40	280	269	54.40	504	470
34.50	565	524	39.50	485	522	44.50	1058	1003	49.50	228	240	54.50	550	580
34.60	1157	1192	39.60	356	329	44.60	922	935	49.60	222	224	54.60	596	578
34.70	2232	2244	39.70	253	261	44.70	675	665	49.70	222	221	54.70	479	475
34.80	1970	1945	39.80	248	228	44.80	403	400	49.80	208	237	54.80	430	387
34.90	996	1010	39.90	218	219	44.90	319	295	49.90	216	240	54.90	484	433
35.00	543	587	40.00	223	233	45.00	329	291	50.00	186	220	55.00	766	738
35.10	608	620	40.10	262	251	45.10	272	271	50.10	182	197	55.10	1162	1236
35.20	1161	1267	40.20	242	236	45.20	253	233	50.20	204	188	55.20	1275	1371
35.30	2385	2512	40.30	231	221	45.30	224	208	50.30	165	187	55.30	938	1031
35.40	2574	2347	40.40	206	218	45.40	209	200	50.40	193	190	55.40	555	597
35.50	1070	1121	40.50	249	229	45.50	235	202	50.50	213	205	55.50	382	368
35.60	432	481	40.60	292	278	45.60	238	224	50.60	260	261	55.60	367	340
35.70	274	315	40.70	441	402	45.70	238	262	50.70	396	377	55.70	376	361
35.80	240	263	40.80	546	495	45.80	234	260	50.80	461	437	55.80	334	330
35.90	229	238	40.90	478	411	45.90	215	230	50.90	380	374	55.90	270	275
36.00	241	231	41.00	292	297	46.00	191	212	51.00	284	274	56.00	241	229
36.10	240	238	41.10	281	258	46.10	223	215	51.10	223	219	56.10	219	206
36.20	260	236	41.20	262	267	46.20	219	241	51.20	185	209	56.20	173	199
36.30	229	219	41.30	320	322	46.30	341	313	51.30	230	219	56.30	205	204
36.40	203	209	41.40	504	478	46.40	409	383	51.40	239	259	56.40	231	219
36.50	217	211	41.50	878	821	46.50	411	379	51.50	274	323	56.50	253	228
36.60	233	224	41.60	1553	1558	46.60	368	368	51.60	293	323	56.60	274	238
36.70	258	241	41.70	2066	1984	46.70	398	388	51.70	218	268	56.70	301	281
36.80	269	276	41.80	1519	1456	46.80	375	367	51.80	243	213	56.80	415	359
36.90	361	387	41.90	888	836	46.90	428	378	51.90	192	189	56.90	435	415
37.00	495	505	42.00	530	503	47.00	503	447	52.00	176	183	57.00	491	500
37.10	463	446	42.10	352	331	47.10	475	408	52.10	177	181	57.10	598	574
37.20	455	427	42.20	276	263	47.20	318	300	52.20	184	183	57.20	527	507
37.30	621	601	42.30	286	249	47.30	213	227	52.30	200	194	57.30	373	377
37.40	639	626	42.40	281	280	47.40	221	205	52.40	179	217	57.40	277	266
37.50	407	430	42.50	362	338	47.50	193	202	52.50	236	227	57.50	220	219
37.60	272	304	42.60	342	316	47.60	256	209	52.60	209	214	57.60	215	210
37.70	281	287	42.70	262	247	47.70	241	241	52.70	197	194	57.70	216	214
37.80	389	338	42.80	232	209	47.80	341	357	52.80	208	182	57.80	229	214
37.90	594	566	42.90	193	198	47.90	515	534	52.90	179	180	57.90	209	210
38.00	1093	1146	43.00	188	196	48.00	550	523	53.00	168	185	58.00	169	206
38.10	1672	1769	43.10	189	195	48.10	406	376	53.10	238	196	58.10	194	206
38.20	1763	1765	43.20	187	197	48.20	263	256	53.20	198	204	58.20	212	208
38.30	1108	1054	43.30	206	199	48.30	212	212	53.30	200	202	58.30	245	220
38.40	517	510	43.40	204	201	48.40	181	201	53.40	178	198	58.40	321	275
38.50	297	323	43.50	178	204	48.50	200	199	53.50	194	196	58.50	471	431
38.60	273	267	43.60	205	209	48.60	207	206	53.60	194	196	58.60	780	658
38.70	231	249	43.70	206	217	48.70	267	234	53.70	174	194	58.70	768	727
38.80	223	245	43.80	234	231	48.80	339	310	53.80	164	193	58.80	688	669
38.90	239	255	43.90	295	263	48.90	462	435	53.90	188	199	58.90	614	573

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	518	521	64.00	468	511	69.00	208	191	74.00	220	220	79.00	250	241
59.10	568	613	64.10	331	355	69.10	200	189	74.10	225	235	79.10	267	233
59.20	749	725	64.20	328	343	69.20	174	191	74.20	290	273	79.20	252	228
59.30	610	642	64.30	388	383	69.30	203	204	74.30	305	320	79.30	233	241
59.40	448	468	64.40	389	403	69.40	242	236	74.40	352	349	79.40	280	278
59.50	249	306	64.50	358	366	69.50	308	275	74.50	358	361	79.50	347	322
59.60	241	228	64.60	306	308	69.60	309	308	74.60	347	360	79.60	303	332
59.70	183	204	64.70	269	268	69.70	338	338	74.70	371	353	79.70	309	307
59.80	177	198	64.80	248	256	69.80	366	340	74.80	340	321	79.80	265	270
59.90	208	195	64.90	240	242	69.90	314	316	74.90	272	278	79.90	201	229
60.00	191	193	65.00	226	223	70.00	296	291	75.00	260	240	80.00	184	197
60.10	208	196	65.10	214	202	70.10	271	273	75.10	202	208	80.10	156	182
60.20	190	201	65.20	219	187	70.20	300	295	75.20	182	188	80.20	161	178
60.30	194	209	65.30	163	181	70.30	403	390	75.30	171	176	80.30	175	179
60.40	221	216	65.40	210	183	70.40	562	567	75.40	191	170	80.40	175	179
60.50	210	218	65.50	232	192	70.50	805	770	75.50	159	168	80.50	156	179
60.60	225	227	65.60	225	207	70.60	872	885	75.60	166	171	80.60	195	182
60.70	277	267	65.70	212	208	70.70	715	821	75.70	181	183	80.70	197	189
60.80	319	359	65.80	210	200	70.80	658	654	75.80	212	200	80.80	167	194
60.90	441	460	65.90	217	191	70.90	464	465	75.90	213	208	80.90	199	194
61.00	518	484	66.00	189	192	71.00	313	320	76.00	212	205	81.00	199	192
61.10	513	512	66.10	200	206	71.10	219	240	76.10	180	195	81.10	187	196
61.20	634	647	66.20	212	218	71.20	189	204	76.20	218	183	81.20	213	209
61.30	932	910	66.30	221	223	71.30	209	191	76.30	166	176	81.30	227	229
61.40	1028	1000	66.40	226	221	71.40	174	190	76.40	199	176	81.40	252	241
61.50	771	823	66.50	197	216	71.50	205	201	76.50	185	179	81.50	229	244
61.60	551	576	66.60	190	206	71.60	210	224	76.60	211	181	81.60	231	245
61.70	369	439	66.70	197	194	71.70	239	251	76.70	204	182	81.70	247	235
61.80	495	484	66.80	214	188	71.80	262	267	76.80	206	184	81.80	220	216
61.90	590	550	66.90	175	189	71.90	257	260	76.90	177	192	81.90	190	199
62.00	482	492	67.00	183	191	72.00	282	241	77.00	208	207	82.00	187	185
62.10	358	380	67.10	209	188	72.10	233	218	77.10	213	218	82.10	187	175
62.20	273	275	67.20	180	185	72.20	203	205	77.20	236	224	82.20	160	170
62.30	195	224	67.30	192	186	72.30	250	213	77.30	239	227	82.30	188	168
62.40	207	211	67.40	217	195	72.40	242	249	77.40	227	227	82.40	168	168
62.50	234	219	67.50	253	218	72.50	342	299	77.50	222	228	82.50	189	169
62.60	279	258	67.60	274	261	72.60	326	319	77.60	215	225	82.60	192	171
62.70	382	325	67.70	334	310	72.70	306	309	77.70	228	222	82.70	162	173
62.80	359	372	67.80	394	381	72.80	280	285	77.80	228	226	82.80	175	174
62.90	400	392	67.90	480	490	72.90	259	261	77.90	259	234	82.90	189	179
63.00	405	385	68.00	501	533	73.00	273	268	78.00	238	237	83.00	219	193
63.10	351	365	68.10	474	471	73.10	375	343	78.10	193	229	83.10	206	216
63.20	382	371	68.20	387	380	73.20	508	494	78.20	216	217	83.20	213	239
63.30	418	411	68.30	290	309	73.30	709	629	78.30	207	201	83.30	240	241
63.40	490	465	68.40	298	299	73.40	559	617	78.40	208	191	83.40	201	229
63.50	671	624	68.50	330	310	73.50	452	522	78.50	177	192	83.50	194	212
63.60	958	970	68.60	264	290	73.60	352	398	78.60	208	209	83.60	176	194
63.70	1280	1259	68.70	282	255	73.70	284	295	78.70	289	235	83.70	185	183
63.80	1097	1139	68.80	198	219	73.80	209	242	78.80	273	249	83.80	171	182
63.90	806	830	68.90	196	199	73.90	207	224	78.90	272	247	83.90	178	185



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	198	189	89.00	160	195	94.00	314	300	99.00	157	176			
84.10	174	189	89.10	220	210	94.10	250	262	99.10	187	175			
84.20	176	188	89.20	224	219	94.20	251	230	99.20	168	175			
84.30	193	188	89.30	225	221	94.30	194	210	99.30	158	175			
84.40	177	191	89.40	227	220	94.40	212	206	99.40	167	176			
84.50	175	192	89.50	212	218	94.50	231	218	99.50	178	177			
84.60	163	188	89.60	218	216	94.60	224	239	99.60	165	175			
84.70	184	184	89.70	233	217	94.70	260	255	99.70	158	174			
84.80	188	184	89.80	199	220	94.80	256	255	99.80	179	172			
84.90	178	191	89.90	228	222	94.90	261	246	99.90	176	171			
85.00	221	202	90.00	213	223	95.00	244	231	100.00	173	170			
85.10	220	210	90.10	217	227	95.10	231	212						
85.20	207	210	90.20	252	235	95.20	190	193						
85.30	199	206	90.30	249	244	95.30	177	180						
85.40	186	197	90.40	246	254	95.40	173	172						
85.50	186	186	90.50	273	268	95.50	161	171						
85.60	219	177	90.60	268	288	95.60	180	173						
85.70	186	170	90.70	338	305	95.70	204	176						
85.80	179	166	90.80	294	312	95.80	191	179						
85.90	141	165	90.90	308	311	95.90	199	182						
86.00	167	167	91.00	285	297	96.00	213	184						
86.10	156	171	91.10	286	271	96.10	187	184						
86.20	173	178	91.20	246	243	96.20	199	181						
86.30	163	183	91.30	208	218	96.30	176	176						
86.40	192	183	91.40	210	196	96.40	170	171						
86.50	174	182	91.50	202	181	96.50	178	167						
86.60	184	181	91.60	181	171	96.60	184	163						
86.70	177	184	91.70	166	165	96.70	143	162						
86.80	221	193	91.80	161	162	96.80	160	163						
86.90	205	208	91.90	166	162	96.90	172	166						
87.00	216	223	92.00	134	162	97.00	163	171						
87.10	219	227	92.10	140	163	97.10	190	180						
87.20	217	218	92.20	176	163	97.20	206	191						
87.30	201	204	92.30	167	163	97.30	185	208						
87.40	175	187	92.40	161	165	97.40	215	230						
87.50	164	172	92.50	167	169	97.50	298	251						
87.60	159	162	92.60	188	175	97.60	274	265						
87.70	176	156	92.70	178	184	97.70	283	269						
87.80	135	153	92.80	214	198	97.80	243	274						
87.90	155	152	92.90	234	217	97.90	311	283						
88.00	160	152	93.00	224	237	98.00	310	293						
88.10	147	153	93.10	260	253	98.10	350	300						
88.20	144	154	93.20	251	269	98.20	323	296						
88.30	157	154	93.30	278	295	98.30	300	283						
88.40	134	155	93.40	334	330	98.40	267	263						
88.50	164	156	93.50	343	361	98.50	247	242						
88.60	153	158	93.60	424	379	98.60	248	221						
88.70	155	162	93.70	413	388	98.70	196	203						
88.80	160	168	93.80	376	376	98.80	187	189						
88.90	155	179	93.90	319	341	98.90	174	181						



Sample	KNi60														
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	
9.00	263	239	14.00	236	231	19.00	222	240	24.00	245	243	29.00	566	610	
9.10	300	239	14.10	208	231	19.10	226	242	24.10	216	226	29.10	514	480	
9.20	292	239	14.20	222	231	19.20	230	247	24.20	212	221	29.20	279	303	
9.30	298	239	14.30	242	231	19.30	239	256	24.30	206	219	29.30	272	270	
9.40	298	238	14.40	215	231	19.40	277	273	24.40	228	219	29.40	313	303	
9.50	321	416	14.50	223	230	19.50	362	338	24.50	215	218	29.50	380	384	
9.60	330	435	14.60	242	230	19.60	573	607	24.60	227	218	29.60	341	383	
9.70	400	467	14.70	233	230	19.70	1032	1000	24.70	224	218	29.70	323	316	
9.80	552	516	14.80	236	230	19.80	753	707	24.80	211	218	29.80	318	304	
9.90	748	589	14.90	253	230	19.90	329	373	24.90	221	218	29.90	382	353	
10.00	1093	758	15.00	212	230	20.00	265	290	25.00	220	218	30.00	681	615	
10.10	1932	1404	15.10	210	230	20.10	287	259	25.10	227	217	30.10	1381	1393	
10.20	3644	3946	15.20	234	229	20.20	244	241	25.20	222	217	30.20	1676	1703	
10.30	7171	7175	15.30	225	229	20.30	238	233	25.30	238	217	30.30	980	937	
10.40	4222	3976	15.40	194	229	20.40	233	231	25.40	239	217	30.40	499	471	
10.50	973	1240	15.50	235	229	20.50	219	233	25.50	238	252	30.50	336	340	
10.60	512	560	15.60	211	229	20.60	251	252	25.60	223	262	30.60	259	281	
10.70	354	372	15.70	230	229	20.70	256	302	25.70	262	272	30.70	252	255	
10.80	309	284	15.80	238	229	20.80	289	300	25.80	277	287	30.80	264	247	
10.90	280	238	15.90	234	229	20.90	227	250	25.90	284	313	30.90	262	247	
11.00	249	235	16.00	240	228	21.00	245	230	26.00	389	366	31.00	235	254	
11.10	264	235	16.10	225	228	21.10	212	226	26.10	649	568	31.10	274	282	
11.20	252	235	16.20	223	228	21.20	229	225	26.20	1326	1362	31.20	463	423	
11.30	253	235	16.30	228	228	21.30	248	224	26.30	2711	2728	31.30	798	833	
11.40	258	235	16.40	241	228	21.40	212	232	26.40	2332	2271	31.40	971	1002	
11.50	249	235	16.50	231	229	21.50	227	235	26.50	910	1031	31.50	597	603	
11.60	266	235	16.60	222	228	21.60	235	243	26.60	477	531	31.60	353	341	
11.70	273	234	16.70	204	228	21.70	225	265	26.70	456	453	31.70	281	277	
11.80	268	234	16.80	231	229	21.80	274	272	26.80	689	636	31.80	265	266	
11.90	248	234	16.90	233	229	21.90	225	264	26.90	1377	1449	31.90	280	271	
12.00	229	234	17.00	251	229	22.00	301	292	27.00	2344	2213	32.00	331	295	
12.10	246	234	17.10	230	231	22.10	474	462	27.10	1353	1355	32.10	484	403	
12.20	259	234	17.20	222	241	22.20	693	753	27.20	522	593	32.20	886	879	
12.30	266	234	17.30	235	270	22.30	669	614	27.30	353	392	32.30	1440	1501	
12.40	247	233	17.40	286	271	22.40	342	354	27.40	288	355	32.40	1071	1162	
12.50	232	233	17.50	203	248	22.50	271	279	27.50	334	359	32.50	549	597	
12.60	250	233	17.60	203	242	22.60	283	272	27.60	422	399	32.60	372	419	
12.70	258	233	17.70	240	243	22.70	325	310	27.70	645	533	32.70	411	417	
12.80	244	233	17.80	222	250	22.80	446	500	27.80	1206	1164	32.80	515	498	
12.90	220	233	17.90	282	276	22.90	792	794	27.90	2812	2993	32.90	895	852	
13.00	228	233	18.00	367	381	23.00	600	598	28.00	3879	3575	33.00	2241	2319	
13.10	224	232	18.10	558	561	23.10	307	333	28.10	1818	1692	33.10	4337	4560	
13.20	233	232	18.20	528	539	23.20	224	256	28.20	627	637	33.20	3868	3553	
13.30	233	232	18.30	425	382	23.30	212	238	28.30	400	385	33.30	1415	1396	
13.40	252	232	18.40	233	274	23.40	210	230	28.40	303	312	33.40	500	570	
13.50	236	232	18.50	253	243	23.50	223	226	28.50	261	278	33.50	322	375	
13.60	225	232	18.60	229	234	23.60	251	224	28.60	252	260	33.60	301	305	
13.70	240	232	18.70	212	229	23.70	232	224	28.70	271	257	33.70	280	268	
13.80	236	231	18.80	202	227	23.80	234	233	28.80	266	285	33.80	292	268	
13.90	244	231	18.90	220	238	23.90	249	251	28.90	441	422	33.90	256	269	

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	239	268	39.00	373	370	44.00	450	428	49.00	523	516	54.00	253	232
34.10	293	268	39.10	644	639	44.10	800	823	49.10	421	439	54.10	248	245
34.20	281	291	39.20	1138	1245	44.20	1160	1247	49.20	338	358	54.20	273	280
34.30	359	339	39.30	1559	1489	44.30	1209	1277	49.30	289	318	54.30	396	375
34.40	475	442	39.40	1043	951	44.40	1201	1199	49.40	272	285	54.40	538	527
34.50	720	712	39.50	490	490	44.50	1156	1113	49.50	250	262	54.50	654	644
34.60	1700	1706	39.60	338	345	44.60	1103	1032	49.60	246	247	54.60	671	634
34.70	2847	2902	39.70	273	281	44.70	759	738	49.70	281	244	54.70	526	511
34.80	2285	2198	39.80	246	244	44.80	464	440	49.80	227	266	54.80	447	411
34.90	994	1078	39.90	226	236	44.90	352	322	49.90	296	273	54.90	491	445
35.00	683	669	40.00	274	247	45.00	334	313	50.00	258	249	55.00	764	739
35.10	871	817	40.10	235	256	45.10	299	288	50.10	224	222	55.10	1182	1270
35.20	1651	1829	40.20	260	239	45.20	247	247	50.20	250	211	55.20	1401	1465
35.30	3250	3158	40.30	233	223	45.30	225	224	50.30	211	210	55.30	1024	1117
35.40	2438	2365	40.40	236	221	45.40	233	218	50.40	203	214	55.40	660	653
35.50	877	984	40.50	254	234	45.50	250	225	50.50	243	232	55.50	395	399
35.60	356	449	40.60	351	295	45.60	273	259	50.60	335	298	55.60	430	367
35.70	299	319	40.70	463	435	45.70	292	310	50.70	444	436	55.70	385	388
35.80	296	274	40.80	630	511	45.80	277	298	50.80	497	496	55.80	336	356
35.90	245	252	40.90	444	411	45.90	258	256	50.90	421	415	55.90	297	298
36.00	252	249	41.00	295	308	46.00	213	234	51.00	315	301	56.00	243	251
36.10	278	266	41.10	280	283	46.10	231	238	51.10	234	241	56.10	233	230
36.20	252	260	41.20	302	301	46.20	276	267	51.20	211	227	56.20	209	225
36.30	226	231	41.30	366	376	46.30	328	347	51.30	248	242	56.30	233	228
36.40	220	224	41.40	609	579	46.40	448	419	51.40	320	306	56.40	287	245
36.50	225	237	41.50	1070	974	46.50	436	415	51.50	363	384	56.50	278	253
36.60	268	261	41.60	1941	1807	46.60	405	405	51.60	347	363	56.60	298	263
36.70	275	276	41.70	2308	2190	46.70	420	406	51.70	250	290	56.70	355	315
36.80	334	312	41.80	1646	1552	46.80	405	363	51.80	245	232	56.80	457	415
36.90	389	463	41.90	1003	865	46.90	409	350	51.90	200	211	56.90	527	478
37.00	588	584	42.00	498	515	47.00	465	391	52.00	195	206	57.00	580	580
37.10	548	489	42.10	313	345	47.10	394	356	52.10	171	205	57.10	720	681
37.20	470	462	42.20	262	278	47.20	310	281	52.20	210	210	57.20	625	596
37.30	587	605	42.30	279	266	47.30	247	236	52.30	205	230	57.30	406	439
37.40	588	572	42.40	307	301	47.40	233	223	52.40	284	263	57.40	315	303
37.50	367	396	42.50	407	352	47.50	227	224	52.50	256	268	57.50	295	249
37.60	314	311	42.60	311	314	47.60	229	234	52.60	265	245	57.60	256	243
37.70	305	310	42.70	273	250	47.70	303	281	52.70	203	218	57.70	230	247
37.80	440	377	42.80	218	217	47.80	433	444	52.80	217	205	57.80	248	245
37.90	666	646	42.90	238	208	47.90	646	657	52.90	219	203	57.90	224	239
38.00	1212	1272	43.00	202	205	48.00	626	605	53.00	232	207	58.00	227	236
38.10	1731	1923	43.10	208	204	48.10	438	412	53.10	211	220	58.10	214	238
38.20	1811	1754	43.20	222	203	48.20	288	279	53.20	253	227	58.20	265	239
38.30	980	955	43.30	203	210	48.30	231	235	53.30	211	225	58.30	295	253
38.40	434	475	43.40	226	215	48.40	175	224	53.40	229	221	58.40	328	311
38.50	331	331	43.50	233	223	48.50	240	222	53.50	204	218	58.50	532	499
38.60	247	285	43.60	227	230	48.60	231	229	53.60	217	217	58.60	893	788
38.70	286	271	43.70	209	244	48.70	256	260	53.70	230	213	58.70	890	855
38.80	302	272	43.80	248	262	48.80	355	343	53.80	219	212	58.80	788	775
38.90	323	292	43.90	334	297	48.90	494	465	53.90	217	217	58.90	709	672

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	574	622	64.00	531	535	69.00	203	214	74.00	240	258	79.00	277	281
59.10	717	735	64.10	378	373	69.10	232	211	74.10	271	268	79.10	292	273
59.20	761	820	64.20	343	363	69.20	217	211	74.20	288	311	79.20	241	267
59.30	697	688	64.30	395	410	69.30	250	223	74.30	371	371	79.30	273	275
59.40	490	486	64.40	495	443	69.40	252	255	74.40	363	409	79.40	301	314
59.50	286	321	64.50	391	407	69.50	304	300	74.50	422	428	79.50	375	370
59.60	245	250	64.60	318	347	69.60	358	335	74.60	462	433	79.60	363	385
59.70	207	228	64.70	279	305	69.70	385	369	74.70	390	423	79.70	317	355
59.80	213	218	64.80	282	292	69.80	348	380	74.80	364	379	79.80	298	315
59.90	251	216	64.90	298	267	69.90	362	357	74.90	293	323	79.90	266	268
60.00	214	215	65.00	233	244	70.00	349	328	75.00	265	277	80.00	205	233
60.10	225	219	65.10	213	223	70.10	312	305	75.10	248	240	80.10	205	216
60.20	213	226	65.20	206	209	70.20	336	319	75.20	205	218	80.20	187	210
60.30	249	244	65.30	198	204	70.30	450	417	75.30	179	207	80.30	180	212
60.40	257	261	65.40	234	204	70.40	648	623	75.40	214	202	80.40	197	212
60.50	263	258	65.50	225	212	70.50	896	865	75.50	185	199	80.50	204	211
60.60	273	257	65.60	231	225	70.60	1008	1006	75.60	203	202	80.60	224	214
60.70	315	283	65.70	253	229	70.70	875	945	75.70	231	213	80.70	193	223
60.80	375	372	65.80	217	222	70.80	704	755	75.80	224	233	80.80	218	232
60.90	509	494	65.90	236	215	70.90	518	539	75.90	227	243	80.90	222	235
61.00	533	532	66.00	222	216	71.00	352	371	76.00	277	237	81.00	217	230
61.10	542	569	66.10	206	231	71.10	274	279	76.10	234	226	81.10	212	230
61.20	736	740	66.20	267	251	71.20	237	238	76.20	206	213	81.20	239	240
61.30	1063	1076	66.30	268	258	71.30	237	222	76.30	180	204	81.30	242	259
61.40	1246	1165	66.40	255	257	71.40	236	218	76.40	224	204	81.40	270	271
61.50	888	936	66.50	259	253	71.50	238	226	76.50	206	207	81.50	247	275
61.60	648	633	66.60	247	243	71.60	252	247	76.60	231	209	81.60	298	279
61.70	427	469	66.70	219	228	71.70	273	271	76.70	245	211	81.70	275	272
61.80	534	531	66.80	236	220	71.80	306	287	76.80	264	214	81.80	261	251
61.90	629	625	66.90	238	217	71.90	276	282	76.90	236	223	81.90	239	234
62.00	576	558	67.00	236	218	72.00	283	265	77.00	240	237	82.00	229	218
62.10	472	429	67.10	200	215	72.10	270	247	77.10	263	249	82.10	193	206
62.20	292	307	67.20	227	213	72.20	234	234	77.20	255	256	82.20	155	200
62.30	240	248	67.30	230	215	72.30	254	246	77.30	239	258	82.30	180	198
62.40	258	231	67.40	237	224	72.40	289	295	77.40	256	257	82.40	210	199
62.50	258	229	67.50	223	247	72.50	399	370	77.50	261	261	82.50	204	201
62.60	275	263	67.60	300	292	72.60	412	397	77.60	275	263	82.60	205	205
62.70	313	325	67.70	330	338	72.70	359	374	77.70	247	258	82.70	225	208
62.80	411	393	67.80	367	389	72.80	328	334	77.80	253	260	82.80	177	208
62.90	440	432	67.90	475	501	72.90	294	295	77.90	249	267	82.90	217	210
63.00	446	432	68.00	571	590	73.00	269	286	78.00	274	270	83.00	234	221
63.10	408	402	68.10	492	538	73.10	337	350	78.10	285	261	83.10	236	245
63.20	422	405	68.20	434	450	73.20	474	511	78.20	283	251	83.20	248	280
63.30	458	457	68.30	420	370	73.30	692	687	78.30	216	237	83.30	287	295
63.40	556	515	68.40	377	358	73.40	687	687	78.40	239	225	83.40	276	282
63.50	716	670	68.50	395	366	73.50	561	589	78.50	226	225	83.50	249	263
63.60	1008	1035	68.60	298	334	73.60	478	459	78.60	252	241	83.60	285	241
63.70	1349	1350	68.70	303	290	73.70	297	344	78.70	305	272	83.70	231	222
63.80	1210	1202	68.80	258	246	73.80	238	286	78.80	313	292	83.80	216	214
63.90	878	874	68.90	210	222	73.90	281	265	78.90	265	288	83.90	217	214

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	223	218	89.00	224	226	94.00	340	362	99.00	225	215			
84.10	232	219	89.10	235	244	94.10	308	320	99.10	228	214			
84.20	199	217	89.20	281	257	94.20	279	281	99.20	224	214			
84.30	210	217	89.30	259	260	94.30	232	250	99.30	237	215			
84.40	183	222	89.40	259	257	94.40	226	234	99.40	227	216			
84.50	213	225	89.50	255	254	94.50	263	238	99.50	228	216			
84.60	211	222	89.60	263	251	94.60	252	260	99.60	247	214			
84.70	230	217	89.70	251	249	94.70	282	287	99.70	225	211			
84.80	203	214	89.80	234	253	94.80	315	298	99.80	200	209			
84.90	217	218	89.90	264	259	94.90	265	291	99.90	232	208			
85.00	247	229	90.00	260	261	95.00	296	278	100.00	221	205			
85.10	243	240	90.10	241	265	95.10	275	260						
85.20	232	240	90.20	247	278	95.20	251	239						
85.30	270	238	90.30	295	292	95.30	220	220						
85.40	221	232	90.40	315	300	95.40	229	209						
85.50	222	222	90.50	312	309	95.50	200	205						
85.60	163	213	90.60	323	329	95.60	195	205						
85.70	191	205	90.70	390	353	95.70	230	208						
85.80	202	200	90.80	365	365	95.80	219	212						
85.90	198	197	90.90	341	367	95.90	239	216						
86.00	215	196	91.00	386	358	96.00	254	219						
86.10	180	199	91.10	305	328	96.10	214	220						
86.20	177	205	91.20	310	294	96.20	263	218						
86.30	194	211	91.30	272	265	96.30	224	213						
86.40	226	213	91.40	242	239	96.40	192	207						
86.50	201	213	91.50	213	220	96.50	211	202						
86.60	217	212	91.60	201	208	96.60	182	197						
86.70	209	214	91.70	219	201	96.70	209	195						
86.80	241	224	91.80	207	197	96.80	176	195						
86.90	225	242	91.90	203	196	96.90	199	197						
87.00	240	259	92.00	227	197	97.00	172	201						
87.10	338	262	92.10	184	197	97.10	218	207						
87.20	245	252	92.20	187	197	97.20	200	216						
87.30	239	238	92.30	198	197	97.30	235	229						
87.40	233	221	92.40	188	199	97.40	199	252						
87.50	209	206	92.50	218	203	97.50	280	282						
87.60	190	195	92.60	215	210	97.60	315	307						
87.70	196	190	92.70	228	218	97.70	344	315						
87.80	170	188	92.80	204	232	97.80	311	318						
87.90	173	187	92.90	248	254	97.90	332	332						
88.00	204	187	93.00	299	277	98.00	361	353						
88.10	180	188	93.10	328	289	98.10	417	370						
88.20	179	189	93.20	290	295	98.20	387	370						
88.30	197	189	93.30	314	314	98.30	353	351						
88.40	203	190	93.40	374	351	98.40	331	324						
88.50	189	190	93.50	436	390	98.50	337	297						
88.60	174	191	93.60	397	413	98.60	265	271						
88.70	175	193	93.70	409	430	98.70	246	247						
88.80	195	199	93.80	413	438	98.80	235	231						
88.90	202	209	93.90	441	410	98.90	215	221						



Sample	KNi80														
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	
9.00	308	255	14.00	257	249	19.00	235	258	24.00	244	248	29.00	547	548	
9.10	286	255	14.10	247	249	19.10	240	259	24.10	245	241	29.10	503	495	
9.20	280	255	14.20	256	249	19.20	241	264	24.20	260	239	29.20	350	336	
9.30	353	255	14.30	219	249	19.30	248	272	24.30	237	238	29.30	282	289	
9.40	304	255	14.40	245	249	19.40	285	287	24.40	253	238	29.40	317	314	
9.50	332	449	14.50	235	248	19.50	373	343	24.50	237	237	29.50	364	396	
9.60	343	471	14.60	248	248	19.60	517	568	24.60	224	237	29.60	397	420	
9.70	423	507	14.70	249	248	19.70	959	948	24.70	248	237	29.70	368	349	
9.80	549	562	14.80	251	248	19.80	826	790	24.80	246	237	29.80	360	316	
9.90	802	647	14.90	243	248	19.90	447	446	24.90	245	237	29.90	414	338	
10.00	1307	840	15.00	236	248	20.00	344	347	25.00	232	237	30.00	566	490	
10.10	2122	1596	15.10	253	248	20.10	323	305	25.10	221	237	30.10	952	1007	
10.20	4126	4438	15.20	247	248	20.20	273	269	25.20	293	236	30.20	1449	1482	
10.30	8214	8441	15.30	258	247	20.30	236	256	25.30	255	236	30.30	1128	1014	
10.40	6190	5681	15.40	228	247	20.40	256	251	25.40	264	236	30.40	489	498	
10.50	1620	1893	15.50	242	247	20.50	214	251	25.50	270	269	30.50	373	335	
10.60	639	738	15.60	242	247	20.60	254	262	25.60	237	279	30.60	274	290	
10.70	400	460	15.70	252	247	20.70	293	298	25.70	257	287	30.70	283	272	
10.80	339	344	15.80	244	247	20.80	296	310	25.80	326	301	30.80	266	265	
10.90	293	280	15.90	217	247	20.90	245	272	25.90	344	325	30.90	248	265	
11.00	298	253	16.00	227	247	21.00	259	250	26.00	390	371	31.00	279	272	
11.10	297	252	16.10	247	247	21.10	227	245	26.10	621	534	31.10	290	294	
11.20	289	252	16.20	232	246	21.20	265	244	26.20	1203	1161	31.20	424	403	
11.30	296	252	16.30	252	246	21.30	250	244	26.30	2392	2472	31.30	735	753	
11.40	274	252	16.40	223	246	21.40	255	250	26.40	2579	2529	31.40	1077	1064	
11.50	253	252	16.50	265	247	21.50	250	253	26.50	1211	1303	31.50	679	757	
11.60	253	252	16.60	226	248	21.60	259	265	26.60	552	620	31.60	392	418	
11.70	255	252	16.70	257	248	21.70	292	296	26.70	455	463	31.70	291	310	
11.80	250	252	16.80	240	249	21.80	320	311	26.80	605	560	31.80	277	288	
11.90	278	251	16.90	218	250	21.90	277	289	26.90	1081	1109	31.90	278	289	
12.00	247	251	17.00	265	251	22.00	320	297	27.00	1836	1864	32.00	340	308	
12.10	262	251	17.10	224	256	22.10	408	411	27.10	1536	1421	32.10	479	392	
12.20	266	251	17.20	270	276	22.20	638	648	27.20	619	681	32.20	758	768	
12.30	272	251	17.30	325	336	22.30	625	628	27.30	341	421	32.30	1242	1377	
12.40	248	251	17.40	355	363	22.40	377	394	27.40	338	373	32.40	1237	1260	
12.50	276	251	17.50	304	305	22.50	298	298	27.50	362	376	32.50	639	704	
12.60	270	251	17.60	273	274	22.60	291	283	27.60	434	411	32.60	426	459	
12.70	277	251	17.70	252	270	22.70	315	308	27.70	596	524	32.70	389	432	
12.80	266	250	17.80	270	276	22.80	420	439	27.80	1097	1025	32.80	518	495	
12.90	258	250	17.90	301	302	22.90	657	674	27.90	2564	2615	32.90	865	764	
13.00	241	250	18.00	382	404	23.00	587	591	28.00	4074	3849	33.00	1874	1883	
13.10	284	250	18.10	598	625	23.10	340	362	28.10	2571	2299	33.10	3725	4099	
13.20	254	250	18.20	803	762	23.20	254	275	28.20	865	879	33.20	4375	4041	
13.30	244	250	18.30	652	616	23.30	241	255	28.30	430	459	33.30	1892	1911	
13.40	235	250	18.40	336	375	23.40	234	248	28.40	337	353	33.40	700	745	
13.50	258	250	18.50	277	284	23.50	225	244	28.50	310	309	33.50	400	438	
13.60	235	249	18.60	279	262	23.60	227	242	28.60	296	287	33.60	345	346	
13.70	247	249	18.70	241	254	23.70	236	241	28.70	303	279	33.70	311	302	
13.80	248	249	18.80	259	249	23.80	240	243	28.80	298	295	33.80	299	299	
13.90	271	249	18.90	265	258	23.90	275	249	28.90	365	385	33.90	272	298	



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	281	297	39.00	367	376	44.00	466	402	49.00	477	469	54.00	243	242
34.10	317	297	39.10	605	604	44.10	680	704	49.10	453	423	54.10	290	257
34.20	301	319	39.20	1038	1108	44.20	1130	1214	49.20	310	351	54.20	305	286
34.30	367	381	39.30	1589	1465	44.30	1324	1410	49.30	299	313	54.30	344	357
34.40	538	499	39.40	1081	1070	44.40	1411	1374	49.40	270	289	54.40	509	494
34.50	777	719	39.50	565	575	44.50	1279	1221	49.50	265	273	54.50	638	630
34.60	1574	1553	39.60	339	388	44.60	1179	1156	49.60	261	260	54.60	719	663
34.70	2914	2938	39.70	336	317	44.70	975	925	49.70	273	253	54.70	648	574
34.80	2675	2663	39.80	264	272	44.80	638	590	49.80	250	265	54.80	455	462
34.90	1369	1413	39.90	229	255	44.90	400	383	49.90	259	283	54.90	506	439
35.00	744	790	40.00	265	257	45.00	331	332	50.00	239	271	55.00	630	614
35.10	850	803	40.10	225	265	45.10	338	310	50.10	236	246	55.10	1007	1043
35.20	1460	1594	40.20	259	257	45.20	250	274	50.20	234	231	55.20	1368	1455
35.30	2916	2959	40.30	262	242	45.30	252	249	50.30	193	227	55.30	1246	1297
35.40	2789	2636	40.40	254	238	45.40	252	238	50.40	236	230	55.40	796	875
35.50	1118	1260	40.50	274	246	45.50	239	243	50.50	237	243	55.50	462	517
35.60	459	558	40.60	310	288	45.60	274	273	50.60	325	289	55.60	398	398
35.70	340	364	40.70	414	396	45.70	330	330	50.70	434	401	55.70	403	410
35.80	290	304	40.80	561	500	45.80	296	338	50.80	528	499	55.80	404	396
35.90	270	277	40.90	493	442	45.90	267	294	50.90	503	463	55.90	360	346
36.00	245	268	41.00	384	342	46.00	210	256	51.00	333	355	56.00	310	290
36.10	287	278	41.10	311	307	46.10	228	248	51.10	272	276	56.10	264	259
36.20	295	279	41.20	309	318	46.20	295	266	51.20	263	250	56.20	224	245
36.30	244	256	41.30	383	377	46.30	332	326	51.30	266	260	56.30	289	242
36.40	258	243	41.40	586	544	46.40	453	405	51.40	289	316	56.40	287	257
36.50	253	250	41.50	1033	887	46.50	437	428	51.50	370	409	56.50	313	265
36.60	246	266	41.60	1633	1601	46.60	418	419	51.60	382	416	56.60	307	273
36.70	295	283	41.70	2417	2313	46.70	431	418	51.70	296	346	56.70	316	304
36.80	360	320	41.80	2128	1918	46.80	365	374	51.80	245	270	56.80	426	388
36.90	419	456	41.90	1268	1133	46.90	365	331	51.90	256	236	56.90	520	480
37.00	660	642	42.00	697	651	47.00	389	339	52.00	228	226	57.00	596	571
37.10	587	598	42.10	408	419	47.10	381	333	52.10	241	224	57.10	746	702
37.20	491	503	42.20	324	320	47.20	309	292	52.20	213	227	57.20	704	682
37.30	528	547	42.30	299	289	47.30	265	255	52.30	255	243	57.30	526	539
37.40	534	543	42.40	309	305	47.40	236	241	52.40	274	278	57.40	366	375
37.50	433	418	42.50	366	349	47.50	241	241	52.50	292	299	57.50	293	286
37.60	303	333	42.60	356	338	47.60	255	251	52.60	287	280	57.60	238	266
37.70	356	323	42.70	301	279	47.70	326	287	52.70	260	248	57.70	279	270
37.80	404	369	42.80	265	239	47.80	433	418	52.80	218	227	57.80	241	273
37.90	599	554	42.90	237	227	47.90	669	651	52.90	214	220	57.90	267	270
38.00	1037	1058	43.00	212	223	48.00	669	687	53.00	236	222	58.00	220	263
38.10	1643	1766	43.10	226	222	48.10	543	516	53.10	248	231	58.10	282	262
38.20	1905	1931	43.20	237	221	48.20	340	341	53.20	231	242	58.20	274	265
38.30	1230	1220	43.30	253	228	48.30	274	267	53.30	250	240	58.30	249	271
38.40	604	610	43.40	241	233	48.40	214	245	53.40	242	233	58.40	348	309
38.50	345	389	43.50	230	241	48.50	221	240	53.50	237	229	58.50	460	444
38.60	278	320	43.60	238	249	48.60	238	243	53.60	230	230	58.60	780	710
38.70	285	297	43.70	240	263	48.70	248	263	53.70	254	230	58.70	972	880
38.80	300	294	43.80	290	280	48.80	322	322	53.80	230	229	58.80	822	823
38.90	318	310	43.90	337	310	48.90	399	414	53.90	221	232	58.90	785	725

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	670	663	64.00	726	709	69.00	226	233	74.00	275	284	79.00	311	306
59.10	669	723	64.10	468	462	69.10	213	227	74.10	263	287	79.10	312	303
59.20	753	838	64.20	376	385	69.20	216	226	74.20	305	318	79.20	307	299
59.30	724	759	64.30	418	407	69.30	216	232	74.30	350	379	79.30	323	302
59.40	542	578	64.40	439	453	69.40	275	254	74.40	422	434	79.40	336	328
59.50	380	391	64.50	478	452	69.50	313	296	74.50	465	460	79.50	352	378
59.60	275	290	64.60	427	400	69.60	341	338	74.60	467	474	79.60	407	414
59.70	259	254	64.70	392	348	69.70	380	365	74.70	465	464	79.70	382	397
59.80	227	240	64.80	318	320	69.80	410	386	74.80	436	431	79.80	302	358
59.90	221	240	64.90	306	294	69.90	421	381	74.90	417	371	79.90	339	311
60.00	218	238	65.00	296	271	70.00	369	358	75.00	322	318	80.00	256	266
60.10	234	238	65.10	275	247	70.10	349	338	75.10	250	272	80.10	226	239
60.20	268	244	65.20	239	232	70.20	337	338	75.20	239	243	80.20	243	227
60.30	276	262	65.30	230	223	70.30	435	398	75.30	233	227	80.30	206	226
60.40	258	279	65.40	241	222	70.40	601	561	75.40	209	219	80.40	219	228
60.50	314	284	65.50	243	226	70.50	863	799	75.50	223	215	80.50	224	228
60.60	291	280	65.60	263	233	70.60	892	998	75.60	224	216	80.60	222	229
60.70	327	289	65.70	228	239	70.70	984	1034	75.70	228	223	80.70	235	235
60.80	330	349	65.80	245	236	70.80	958	899	75.80	207	241	80.80	244	243
60.90	464	477	65.90	222	230	70.90	689	685	75.90	260	258	80.90	225	250
61.00	555	577	66.00	208	228	71.00	466	484	76.00	219	259	81.00	236	247
61.10	626	609	66.10	259	240	71.10	330	349	76.10	244	249	81.10	235	244
61.20	716	724	66.20	258	266	71.20	291	280	76.20	241	235	81.20	248	245
61.30	1001	1002	66.30	283	284	71.30	238	249	76.30	215	222	81.30	255	255
61.40	1298	1221	66.40	291	285	71.40	220	239	76.40	253	216	81.40	257	268
61.50	1031	1068	66.50	243	283	71.50	255	240	76.50	232	216	81.50	239	274
61.60	818	784	66.60	281	278	71.60	258	254	76.60	225	218	81.60	277	280
61.70	544	549	66.70	272	262	71.70	280	272	76.70	224	219	81.70	298	283
61.80	462	529	66.80	223	246	71.80	279	286	76.80	240	223	81.80	269	271
61.90	610	636	66.90	237	236	71.90	279	289	76.90	231	230	81.90	278	253
62.00	660	624	67.00	253	232	72.00	285	277	77.00	258	241	82.00	216	238
62.10	514	515	67.10	225	230	72.10	258	263	77.10	245	252	82.10	221	224
62.20	389	379	67.20	242	229	72.20	261	252	77.20	231	260	82.20	239	215
62.30	248	292	67.30	266	233	72.30	249	253	77.30	271	265	82.30	197	212
62.40	265	258	67.40	256	244	72.40	299	285	77.40	267	266	82.40	219	213
62.50	265	245	67.50	253	260	72.50	339	348	77.50	271	269	82.50	193	214
62.60	262	262	67.60	329	292	72.60	436	400	77.60	268	276	82.60	223	217
62.70	324	302	67.70	354	338	72.70	390	392	77.70	283	277	82.70	218	221
62.80	381	375	67.80	390	378	72.80	368	359	77.80	270	274	82.80	209	222
62.90	462	435	67.90	454	451	72.90	333	318	77.90	278	277	82.90	224	222
63.00	477	462	68.00	504	565	73.00	312	296	78.00	298	280	83.00	251	227
63.10	447	443	68.10	579	597	73.10	340	326	78.10	300	274	83.10	251	241
63.20	422	430	68.20	523	531	73.20	414	436	78.20	281	264	83.20	257	268
63.30	442	466	68.30	420	453	73.30	608	606	78.30	242	254	83.30	285	298
63.40	568	530	68.40	402	410	73.40	826	690	78.40	268	242	83.40	300	302
63.50	689	639	68.50	408	410	73.50	572	630	78.50	235	239	83.50	295	288
63.60	911	912	68.60	368	382	73.60	536	528	78.60	255	247	83.60	252	271
63.70	1206	1294	68.70	320	337	73.70	385	409	78.70	255	271	83.70	262	249
63.80	1320	1330	68.80	307	285	73.80	295	331	78.80	315	299	83.80	228	234
63.90	1055	1067	68.90	242	249	73.90	286	297	78.90	301	310	83.90	215	227

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	243	227	89.00	232	231	94.00	465	420	99.00	218	242			
84.10	228	230	89.10	227	248	94.10	400	375	99.10	232	239			
84.20	214	231	89.20	287	264	94.20	328	334	99.20	256	238			
84.30	209	229	89.30	292	273	94.30	301	297	99.30	246	238			
84.40	212	230	89.40	247	272	94.40	217	268	99.40	241	239			
84.50	206	232	89.50	255	269	94.50	264	256	99.50	270	239			
84.60	256	232	89.60	233	268	94.60	250	261	99.60	246	238			
84.70	253	228	89.70	281	265	94.70	272	280	99.70	260	234			
84.80	219	225	89.80	239	267	94.80	320	303	99.80	263	229			
84.90	244	227	89.90	273	272	94.90	289	311	99.90	239	226			
85.00	237	235	90.00	272	280	95.00	325	303	100.00	249	223			
85.10	262	248	90.10	307	283	95.10	303	290						
85.20	285	257	90.20	285	290	95.20	303	271						
85.30	258	258	90.30	282	305	95.30	242	251						
85.40	229	255	90.40	294	319	95.40	222	235						
85.50	222	247	90.50	335	326	95.50	231	224						
85.60	250	237	90.60	331	339	95.60	199	221						
85.70	218	228	90.70	323	362	95.70	230	222						
85.80	206	220	90.80	396	383	95.80	216	225						
85.90	217	214	90.90	420	391	95.90	235	229						
86.00	240	211	91.00	416	391	96.00	222	232						
86.10	188	210	91.10	372	373	96.10	263	234						
86.20	208	214	91.20	347	340	96.20	239	233						
86.30	224	220	91.30	316	308	96.30	247	230						
86.40	235	225	91.40	271	278	96.40	245	225						
86.50	221	226	91.50	249	252	96.50	253	218						
86.60	223	226	91.60	238	234	96.60	240	214						
86.70	250	227	91.70	204	223	96.70	234	212						
86.80	232	233	91.80	201	216	96.80	214	210						
86.90	249	247	91.90	205	213	96.90	221	211						
87.00	291	266	92.00	198	212	97.00	209	215						
87.10	282	275	92.10	225	214	97.10	195	220						
87.20	309	270	92.20	215	214	97.20	225	228						
87.30	258	258	92.30	231	213	97.30	224	239						
87.40	232	243	92.40	205	216	97.40	263	257						
87.50	211	227	92.50	225	219	97.50	264	284						
87.60	225	215	92.60	220	225	97.60	348	316						
87.70	205	207	92.70	244	234	97.70	369	339						
87.80	205	203	92.80	228	246	97.80	335	347						
87.90	200	202	92.90	263	263	97.90	331	354						
88.00	192	201	93.00	277	285	98.00	359	371						
88.10	181	202	93.10	319	303	98.10	388	389						
88.20	196	203	93.20	287	310	98.20	423	399						
88.30	202	204	93.30	296	320	98.30	398	389						
88.40	206	204	93.40	321	345	98.40	339	364						
88.50	203	204	93.50	396	383	98.50	349	337						
88.60	189	205	93.60	436	418	98.60	335	310						
88.70	193	206	93.70	439	437	98.70	291	284						
88.80	218	210	93.80	444	453	98.80	258	263						
88.90	176	218	93.90	481	455	98.90	271	250						

Sample	KNi100													
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	315	254	14.00	269	250	19.00	241	264	24.00	225	243	29.00	497	511
9.10	291	254	14.10	270	250	19.10	267	267	24.10	266	242	29.10	521	464
9.20	329	254	14.20	241	250	19.20	261	271	24.20	249	242	29.20	349	344
9.30	342	367	14.30	270	250	19.30	255	280	24.30	231	241	29.30	288	300
9.40	303	436	14.40	258	249	19.40	321	302	24.40	237	241	29.40	309	328
9.50	347	455	14.50	278	249	19.50	396	385	24.50	234	241	29.50	428	412
9.60	426	484	14.60	286	249	19.60	670	662	24.60	248	241	29.60	435	435
9.70	478	527	14.70	274	249	19.70	987	1031	24.70	214	241	29.70	356	370
9.80	641	596	14.80	250	249	19.80	908	840	24.80	254	241	29.80	342	339
9.90	1019	719	14.90	232	249	19.90	482	514	24.90	240	241	29.90	389	347
10.00	1516	1026	15.00	244	249	20.00	433	425	25.00	253	241	30.00	524	462
10.10	2732	2240	15.10	249	249	20.10	376	359	25.10	275	241	30.10	815	855
10.20	5233	5898	15.20	263	249	20.20	282	293	25.20	273	241	30.20	1254	1265
10.30	9682	9587	15.30	218	249	20.30	263	267	25.30	250	241	30.30	1044	967
10.40	6731	6060	15.40	274	249	20.40	248	258	25.40	246	270	30.40	510	518
10.50	1876	2149	15.50	239	249	20.50	220	256	25.50	291	278	30.50	339	340
10.60	748	863	15.60	253	248	20.60	258	263	25.60	255	284	30.60	296	293
10.70	487	535	15.70	245	248	20.70	253	284	25.70	263	295	30.70	269	279
10.80	343	401	15.80	243	248	20.80	243	290	25.80	300	311	30.80	275	274
10.90	330	326	15.90	214	248	20.90	254	267	25.90	356	338	30.90	280	276
11.00	303	279	16.00	231	248	21.00	228	252	26.00	447	403	31.00	323	285
11.10	302	253	16.10	241	248	21.10	241	248	26.10	658	591	31.10	354	315
11.20	277	252	16.20	263	248	21.20	267	247	26.20	1329	1274	31.20	508	438
11.30	291	252	16.30	270	248	21.30	240	252	26.30	2498	2573	31.30	799	806
11.40	259	252	16.40	251	251	21.40	257	254	26.40	2722	2667	31.40	1095	1168
11.50	289	252	16.50	253	251	21.50	267	259	26.50	1354	1445	31.50	883	888
11.60	269	252	16.60	248	252	21.60	274	280	26.60	647	685	31.60	464	494
11.70	257	252	16.70	234	253	21.70	300	324	26.70	544	486	31.70	369	342
11.80	230	252	16.80	245	254	21.80	359	337	26.80	601	565	31.80	341	308
11.90	277	252	16.90	245	256	21.90	295	301	26.90	943	1017	31.90	318	308
12.00	249	252	17.00	246	261	22.00	303	303	27.00	1618	1618	32.00	337	331
12.10	306	251	17.10	267	278	22.10	358	390	27.10	1335	1291	32.10	492	438
12.20	272	251	17.20	323	336	22.20	552	563	27.20	626	677	32.20	836	872
12.30	251	251	17.30	476	465	22.30	571	550	27.30	409	435	32.30	1441	1476
12.40	244	251	17.40	488	482	22.40	370	377	27.40	349	380	32.40	1401	1370
12.50	256	251	17.50	352	363	22.50	290	293	27.50	339	386	32.50	707	793
12.60	266	251	17.60	266	299	22.60	302	276	27.60	440	427	32.60	443	504
12.70	242	251	17.70	280	288	22.70	272	294	27.70	776	557	32.70	414	461
12.80	265	251	17.80	295	297	22.80	390	377	27.80	1269	1096	32.80	545	528
12.90	256	251	17.90	345	339	22.90	493	495	27.90	2532	2638	32.90	956	827
13.00	254	251	18.00	485	483	23.00	414	439	28.00	4085	3916	33.00	1913	1962
13.10	289	251	18.10	780	778	23.10	330	316	28.10	2834	2581	33.10	3886	4107
13.20	224	250	18.20	1008	1020	23.20	260	266	28.20	1075	1061	33.20	4519	4287
13.30	219	250	18.30	885	845	23.30	261	253	28.30	485	524	33.30	2258	2246
13.40	270	250	18.40	458	479	23.40	278	248	28.40	385	388	33.40	808	904
13.50	247	250	18.50	281	321	23.50	249	246	28.50	331	338	33.50	450	496
13.60	275	250	18.60	260	280	23.60	250	244	28.60	319	310	33.60	354	380
13.70	248	250	18.70	273	265	23.70	224	244	28.70	292	297	33.70	324	349
13.80	241	250	18.80	254	268	23.80	251	243	28.80	337	311	33.80	307	333
13.90	261	250	18.90	258	265	23.90	255	243	28.90	393	394	33.90	297	321



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	269	318	39.00	424	409	44.00	467	405	49.00	457	449	54.00	276	256
34.10	311	326	39.10	648	665	44.10	687	669	49.10	427	414	54.10	286	276
34.20	347	346	39.20	1060	1174	44.20	1117	1190	49.20	336	343	54.20	313	298
34.30	455	435	39.30	1574	1504	44.30	1478	1537	49.30	303	302	54.30	364	362
34.40	596	561	39.40	1181	1127	44.40	1509	1538	49.40	282	284	54.40	460	493
34.50	836	808	39.50	594	629	44.50	1336	1322	49.50	240	274	54.50	653	644
34.60	1667	1688	39.60	423	424	44.60	1262	1227	49.60	264	265	54.60	715	707
34.70	3044	3081	39.70	345	350	44.70	1061	1066	49.70	280	260	54.70	682	636
34.80	3073	2895	39.80	278	298	44.80	690	731	49.80	291	270	54.80	554	508
34.90	1562	1604	39.90	272	270	44.90	452	455	49.90	323	294	54.90	499	444
35.00	821	891	40.00	260	263	45.00	379	353	50.00	290	293	55.00	525	540
35.10	921	911	40.10	279	264	45.10	348	322	50.10	269	269	55.10	858	875
35.20	1671	1740	40.20	264	259	45.20	276	292	50.20	265	247	55.20	1214	1348
35.30	3020	3023	40.30	287	250	45.30	253	268	50.30	245	239	55.30	1452	1412
35.40	2899	2713	40.40	241	245	45.40	253	257	50.40	230	241	55.40	1048	1067
35.50	1250	1375	40.50	276	254	45.50	229	258	50.50	253	252	55.50	633	657
35.60	495	626	40.60	318	290	45.60	296	285	50.60	277	290	55.60	514	461
35.70	378	403	40.70	414	393	45.70	304	340	50.70	402	385	55.70	447	451
35.80	286	328	40.80	505	477	45.80	370	357	50.80	491	489	55.80	472	453
35.90	274	295	40.90	430	431	45.90	323	316	50.90	456	482	55.90	408	405
36.00	285	287	41.00	359	349	46.00	280	273	51.00	407	387	56.00	334	338
36.10	290	294	41.10	306	317	46.10	250	260	51.10	327	302	56.10	287	288
36.20	290	294	41.20	354	329	46.20	327	276	51.20	286	267	56.20	262	266
36.30	262	277	41.30	382	388	46.30	355	334	51.30	302	274	56.30	285	260
36.40	267	258	41.40	648	548	46.40	443	418	51.40	301	331	56.40	283	260
36.50	274	257	41.50	983	886	46.50	475	455	51.50	406	431	56.50	302	269
36.60	287	268	41.60	1613	1560	46.60	419	444	51.60	357	457	56.60	305	273
36.70	295	286	41.70	2340	2374	46.70	426	421	51.70	368	387	56.70	315	298
36.80	337	327	41.80	2301	2183	46.80	341	374	51.80	284	301	56.80	408	370
36.90	456	468	41.90	1497	1383	46.90	354	332	51.90	249	255	56.90	549	483
37.00	616	691	42.00	788	782	47.00	313	324	52.00	222	240	57.00	662	593
37.10	723	710	42.10	488	483	47.10	338	322	52.10	256	236	57.10	708	738
37.20	544	620	42.20	342	355	47.20	321	296	52.20	238	239	57.20	817	763
37.30	572	597	42.30	293	310	47.30	277	266	52.30	275	254	57.30	599	623
37.40	556	551	42.40	305	312	47.40	243	253	52.40	291	289	57.40	433	440
37.50	450	434	42.50	352	342	47.50	282	253	52.50	282	318	57.50	303	320
37.60	342	351	42.60	335	335	47.60	242	262	52.60	323	304	57.60	299	281
37.70	323	337	42.70	298	291	47.70	299	297	52.70	265	269	57.70	279	278
37.80	421	380	42.80	244	252	47.80	453	420	52.80	262	243	57.80	283	278
37.90	594	551	42.90	229	237	47.90	635	652	52.90	224	233	57.90	285	276
38.00	1048	1027	43.00	224	233	48.00	787	737	53.00	234	234	58.00	261	275
38.10	1624	1766	43.10	241	231	48.10	579	586	53.10	256	245	58.10	281	280
38.20	1985	2036	43.20	237	237	48.20	433	392	53.20	279	261	58.20	258	282
38.30	1420	1378	43.30	252	241	48.30	292	293	53.30	228	262	58.30	287	289
38.40	666	698	43.40	259	247	48.40	247	261	53.40	236	253	58.40	364	315
38.50	376	422	43.50	262	253	48.50	259	252	53.50	256	243	58.50	454	423
38.60	310	342	43.60	279	263	48.60	247	252	53.60	237	241	58.60	684	666
38.70	308	316	43.70	287	275	48.70	266	266	53.70	232	242	58.70	967	890
38.80	249	312	43.80	305	291	48.80	333	314	53.80	254	242	58.80	910	866
38.90	307	330	43.90	328	321	48.90	385	395	53.90	262	246	58.90	849	767



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	709	714	64.00	821	864	69.00	252	249	74.00	267	303	79.00	330	326
59.10	710	757	64.10	601	555	69.10	224	240	74.10	285	300	79.10	301	321
59.20	858	877	64.20	421	418	69.20	233	239	74.20	291	319	79.20	331	319
59.30	824	832	64.30	394	407	69.30	202	242	74.30	366	371	79.30	337	320
59.40	602	654	64.40	441	449	69.40	285	258	74.40	449	437	79.40	291	335
59.50	439	452	64.50	494	474	69.50	318	288	74.50	475	476	79.50	339	379
59.60	301	328	64.60	451	440	69.60	378	329	74.60	461	499	79.60	415	430
59.70	265	278	64.70	396	391	69.70	376	359	74.70	524	501	79.70	464	435
59.80	248	261	64.80	343	357	69.80	417	383	74.80	502	473	79.80	362	399
59.90	245	253	64.90	370	334	69.90	423	397	74.90	418	413	79.90	334	353
60.00	262	251	65.00	283	301	70.00	391	385	75.00	379	352	80.00	297	302
60.10	250	249	65.10	284	275	70.10	378	364	75.10	305	301	80.10	250	264
60.20	259	257	65.20	258	251	70.20	366	354	75.20	272	266	80.20	247	245
60.30	269	273	65.30	249	239	70.30	423	387	75.30	228	246	80.30	240	240
60.40	300	300	65.40	240	235	70.40	488	513	75.40	235	237	80.40	237	240
60.50	342	306	65.50	241	235	70.50	772	737	75.50	249	231	80.50	229	241
60.60	304	298	65.60	244	239	70.60	929	961	75.60	222	229	80.60	252	241
60.70	327	296	65.70	250	244	70.70	1049	1072	75.70	230	232	80.70	217	246
60.80	341	333	65.80	272	245	70.80	990	1005	75.80	242	243	80.80	238	253
60.90	432	433	65.90	251	242	70.90	813	810	75.90	283	260	80.90	247	261
61.00	479	565	66.00	242	242	71.00	577	592	76.00	238	270	81.00	258	264
61.10	655	629	66.10	262	253	71.10	437	422	76.10	265	264	81.10	263	260
61.20	751	730	66.20	306	282	71.20	333	323	76.20	247	253	81.20	242	257
61.30	918	969	66.30	295	310	71.30	264	277	76.30	256	241	81.30	217	260
61.40	1237	1224	66.40	301	312	71.40	254	259	76.40	254	232	81.40	272	270
61.50	1162	1137	66.50	291	304	71.50	243	256	76.50	244	229	81.50	278	279
61.60	889	873	66.60	304	295	71.60	255	265	76.60	230	230	81.60	275	285
61.70	622	606	66.70	297	284	71.70	279	282	76.70	264	232	81.70	296	291
61.80	459	531	66.80	259	269	71.80	287	295	76.80	232	234	81.80	317	287
61.90	612	620	66.90	289	259	71.90	295	300	76.90	234	240	81.90	283	271
62.00	669	651	67.00	248	252	72.00	298	295	77.00	264	249	82.00	270	255
62.10	500	561	67.10	242	250	72.10	335	284	77.10	252	259	82.10	250	241
62.20	422	430	67.20	271	247	72.20	287	271	77.20	256	266	82.20	220	230
62.30	291	326	67.30	267	248	72.30	282	267	77.30	288	272	82.30	219	224
62.40	262	279	67.40	242	255	72.40	268	284	77.40	281	272	82.40	195	224
62.50	248	264	67.50	279	267	72.50	325	335	77.50	284	273	82.50	241	225
62.60	282	273	67.60	302	289	72.60	450	397	77.60	274	280	82.60	222	228
62.70	313	296	67.70	322	332	72.70	402	408	77.70	281	289	82.70	230	232
62.80	344	355	67.80	409	376	72.80	357	381	77.80	300	292	82.80	236	236
62.90	455	431	67.90	425	419	72.90	358	340	77.90	279	293	82.90	244	236
63.00	505	482	68.00	479	508	73.00	336	308	78.00	326	298	83.00	218	237
63.10	519	483	68.10	540	600	73.10	322	315	78.10	298	297	83.10	237	244
63.20	461	463	68.20	634	585	73.20	362	389	78.20	265	287	83.20	261	261
63.30	507	491	68.30	484	523	73.30	520	535	78.30	266	276	83.30	259	290
63.40	601	556	68.40	454	467	73.40	719	662	78.40	264	264	83.40	306	315
63.50	708	640	68.50	449	450	73.50	671	645	78.50	266	255	83.50	324	312
63.60	853	847	68.60	437	420	73.60	494	561	78.60	273	257	83.60	296	298
63.70	1161	1211	68.70	363	372	73.70	464	449	78.70	278	271	83.70	266	279
63.80	1339	1402	68.80	339	316	73.80	352	361	78.80	313	298	83.80	263	257
63.90	1175	1206	68.90	285	271	73.90	308	318	78.90	319	323	83.90	248	243

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	24
84.00	230	237	89.00	235	237	94.00	500	455	99.00	316	259				
84.10	227	238	89.10	234	253	94.10	434	419	99.10	225	254				
84.20	220	240	89.20	267	270	94.20	343	375	99.20	256	253				
84.30	209	240	89.30	279	283	94.30	326	337	99.30	273	254				
84.40	246	239	89.40	314	286	94.40	321	302	99.40	275	256				
84.50	239	241	89.50	280	283	94.50	280	276	99.50	251	258				
84.60	268	244	89.60	284	280	94.60	253	265	99.60	264	258				
84.70	238	243	89.70	244	278	94.70	233	271	99.70	282	254				
84.80	228	239	89.80	286	276	94.80	285	292	99.80	256	248				
84.90	243	237	89.90	283	277	94.90	307	316	99.90	222	243				
85.00	226	239	90.00	275	284	95.00	323	324	100.00	242	239				
85.10	244	248	90.10	289	291	95.10	314	316							
85.20	259	259	90.20	276	296	95.20	312	303							
85.30	237	263	90.30	297	307	95.30	288	285							
85.40	247	262	90.40	312	326	95.40	266	265							
85.50	282	260	90.50	327	340	95.50	232	249							
85.60	238	251	90.60	365	347	95.60	254	240							
85.70	244	242	90.70	382	363	95.70	241	237							
85.80	232	233	90.80	403	388	95.80	259	238							
85.90	216	227	90.90	462	407	95.90	251	242							
86.00	241	223	91.00	422	412	96.00	274	247							
86.10	231	221	91.10	417	407	96.10	266	249							
86.20	224	222	91.20	371	381	96.20	270	250							
86.30	222	225	91.30	334	345	96.30	262	248							
86.40	215	230	91.40	313	312	96.40	276	244							
86.50	234	232	91.50	279	283	96.50	247	239							
86.60	209	233	91.60	258	259	96.60	233	233							
86.70	249	234	91.70	225	244	96.70	220	229							
86.80	233	238	91.80	215	236	96.80	209	225							
86.90	251	247	91.90	225	231	96.90	269	224							
87.00	252	265	92.00	237	229	97.00	222	225							
87.10	265	280	92.10	227	229	97.10	226	229							
87.20	311	281	92.20	238	230	97.20	251	234							
87.30	290	272	92.30	239	229	97.30	251	242							
87.40	250	260	92.40	212	229	97.40	245	254							
87.50	247	245	92.50	204	232	97.50	268	276							
87.60	235	232	92.60	221	236	97.60	287	306							
87.70	213	223	92.70	250	244	97.70	357	338							
87.80	189	218	92.80	255	256	97.80	390	358							
87.90	218	216	92.90	252	268	97.90	386	364							
88.00	223	216	93.00	285	287	98.00	348	374							
88.10	214	217	93.10	316	308	98.10	395	392							
88.20	233	219	93.20	331	319	98.20	426	409							
88.30	207	220	93.30	372	321	98.30	460	412							
88.40	222	220	93.40	328	332	98.40	439	394							
88.50	208	220	93.50	348	359	98.50	390	367							
88.60	202	221	93.60	360	397	98.60	312	340							
88.70	238	222	93.70	472	428	98.70	356	312							
88.80	239	223	93.80	468	443	98.80	268	286							
88.90	209	228	93.90	439	458	98.90	256	269							

Sample	KCoO														
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	
9.00	127	88	14.00	77	79	19.00	77	89	24.00	94	109	29.00	473	486	
9.10	97	88	14.10	84	79	19.10	80	92	24.10	74	80	29.10	261	265	
9.20	117	89	14.20	72	79	19.20	87	96	24.20	81	73	29.20	128	155	
9.30	127	89	14.30	81	78	19.30	104	104	24.30	83	71	29.30	121	127	
9.40	141	90	14.40	85	78	19.40	171	129	24.40	75	70	29.40	109	142	
9.50	123	130	14.50	68	78	19.50	294	264	24.50	66	70	29.50	112	159	
9.60	146	156	14.60	79	78	19.60	619	639	24.60	69	69	29.60	161	160	
9.70	212	238	14.70	65	78	19.70	757	678	24.70	87	69	29.70	180	178	
9.80	254	249	14.80	79	78	19.80	251	281	24.80	65	69	29.80	311	257	
9.90	237	173	14.90	77	78	19.90	105	124	24.90	68	69	29.90	660	640	
10.00	285	179	15.00	74	78	20.00	90	93	25.00	69	69	30.00	1527	1642	
10.10	450	353	15.10	89	78	20.10	61	80	25.10	83	69	30.10	2171	2043	
10.20	910	1062	15.20	75	77	20.20	65	74	25.20	94	69	30.20	1218	1197	
10.30	1515	1354	15.30	74	77	20.30	72	73	25.30	97	69	30.30	791	821	
10.40	526	468	15.40	86	77	20.40	94	73	25.40	126	119	30.40	710	673	
10.50	174	148	15.50	80	77	20.50	70	73	25.50	147	126	30.50	303	337	
10.60	119	98	15.60	92	77	20.60	82	73	25.60	139	134	30.60	135	159	
10.70	103	82	15.70	56	77	20.70	61	74	25.70	133	147	30.70	104	113	
10.80	97	82	15.80	66	77	20.80	59	73	25.80	180	169	30.80	97	101	
10.90	84	82	15.90	61	77	20.90	63	73	25.90	287	216	30.90	107	105	
11.00	113	82	16.00	61	77	21.00	63	73	26.00	494	424	31.00	161	125	
11.10	116	82	16.10	71	77	21.10	75	73	26.10	1131	1253	31.10	272	229	
11.20	96	82	16.20	85	77	21.20	59	73	26.20	2642	2771	31.20	524	578	
11.30	97	82	16.30	76	76	21.30	62	83	26.30	2421	2427	31.30	904	917	
11.40	93	82	16.40	62	76	21.40	55	84	26.40	698	958	31.40	586	622	
11.50	102	81	16.50	69	77	21.50	62	87	26.50	295	373	31.50	220	259	
11.60	94	81	16.60	83	77	21.60	92	94	26.60	339	284	31.60	118	144	
11.70	95	81	16.70	86	76	21.70	87	106	26.70	541	426	31.70	110	123	
11.80	88	81	16.80	93	76	21.80	89	109	26.80	1183	1207	31.80	120	124	
11.90	110	81	16.90	76	77	21.90	149	129	26.90	2432	2530	31.90	156	139	
12.00	103	81	17.00	64	77	22.00	250	276	27.00	2316	2057	32.00	289	204	
12.10	98	81	17.10	76	78	22.10	539	592	27.10	687	757	32.10	551	544	
12.20	78	81	17.20	79	90	22.20	588	544	27.20	192	280	32.20	1186	1286	
12.30	91	81	17.30	87	100	22.30	190	234	27.30	148	186	32.30	1437	1468	
12.40	89	80	17.40	77	98	22.40	114	124	27.40	125	164	32.40	675	779	
12.50	95	80	17.50	77	93	22.50	90	109	27.50	189	169	32.50	265	331	
12.60	81	80	17.60	64	94	22.60	126	124	27.60	303	213	32.60	232	236	
12.70	84	80	17.70	101	99	22.70	247	234	27.70	605	461	32.70	289	268	
12.80	85	80	17.80	118	111	22.80	461	535	27.80	1414	1371	32.80	596	517	
12.90	90	80	17.90	161	174	22.90	641	580	27.90	2499	2336	32.90	1412	1497	
13.00	83	80	18.00	337	386	23.00	231	262	28.00	1697	1495	33.00	2705	2879	
13.10	79	80	18.10	563	581	23.10	79	117	28.10	510	496	33.10	2569	2317	
13.20	78	80	18.20	530	486	23.20	87	87	28.20	213	196	33.20	884	901	
13.30	93	79	18.30	242	224	23.30	68	79	28.30	127	138	33.30	257	295	
13.40	64	79	18.40	98	109	23.40	50	75	28.40	122	114	33.40	119	154	
13.50	85	79	18.50	86	85	23.50	74	74	28.50	121	95	33.50	86	109	
13.60	87	79	18.60	81	78	23.60	63	76	28.60	92	89	33.60	95	86	
13.70	78	79	18.70	70	75	23.70	84	88	28.70	128	105	33.70	80	87	
13.80	73	79	18.80	74	83	23.80	92	127	28.80	214	188	33.80	84	89	
13.90	83	79	18.90	78	88	23.90	120	152	28.90	373	408	33.90	81	92	

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	90	97	39.00	401	329	44.00	588	602	49.00	300	335	54.00	108	106
34.10	99	108	39.10	736	797	44.10	763	647	49.10	262	272	54.10	145	139
34.20	124	132	39.20	1173	1155	44.20	569	531	49.20	208	232	54.20	215	228
34.30	218	191	39.30	908	836	44.30	533	551	49.30	153	182	54.30	363	374
34.40	355	334	39.40	404	408	44.40	584	598	49.40	152	136	54.40	488	483
34.50	787	806	39.50	233	220	44.50	531	492	49.50	104	106	54.50	521	441
34.60	1333	1390	39.60	129	137	44.60	350	293	49.60	93	93	54.60	385	324
34.70	1085	1117	39.70	108	99	44.70	209	163	49.70	77	91	54.70	336	271
34.80	520	541	39.80	102	91	44.80	149	139	49.80	55	85	54.80	427	395
34.90	331	329	39.90	83	103	44.90	155	160	49.90	62	74	54.90	709	711
35.00	539	476	40.00	124	113	45.00	152	142	50.00	51	67	55.00	978	1022
35.10	1065	1087	40.10	121	100	45.10	97	102	50.10	60	65	55.10	979	906
35.20	1894	1941	40.20	83	84	45.20	75	78	50.20	55	67	55.20	539	577
35.30	1909	1720	40.30	82	82	45.30	75	73	50.30	70	72	55.30	280	293
35.40	704	774	40.40	126	100	45.40	66	73	50.40	93	92	55.40	190	195
35.50	240	269	40.50	175	167	45.50	62	78	50.50	150	154	55.50	199	217
35.60	121	138	40.60	289	314	45.60	76	86	50.60	244	251	55.60	251	232
35.70	92	101	40.70	481	398	45.70	86	87	50.70	275	272	55.70	170	196
35.80	83	85	40.80	375	298	45.80	85	84	50.80	191	204	55.80	149	144
35.90	86	81	40.90	185	175	45.90	91	91	50.90	137	132	55.90	94	106
36.00	92	89	41.00	116	129	46.00	110	109	51.00	110	111	56.00	74	87
36.10	109	90	41.10	112	131	46.10	157	161	51.10	104	117	56.10	71	80
36.20	60	80	41.20	158	171	46.20	252	274	51.20	99	113	56.20	74	79
36.30	74	78	41.30	348	289	46.30	346	345	51.30	105	116	56.30	79	84
36.40	77	83	41.40	638	601	46.40	303	304	51.40	93	142	56.40	101	88
36.50	85	96	41.50	1171	1150	46.50	250	262	51.50	132	147	56.50	130	97
36.60	104	117	41.60	1338	1250	46.60	331	272	51.60	107	119	56.60	156	134
36.70	144	138	41.70	863	827	46.70	347	287	51.70	66	85	56.70	232	192
36.80	178	177	41.80	453	471	46.80	417	398	51.80	72	68	56.80	271	240
36.90	202	230	41.90	304	272	46.90	626	568	51.90	59	63	56.90	365	302
37.00	275	255	42.00	184	155	47.00	529	498	52.00	65	62	57.00	376	314
37.10	367	359	42.10	127	111	47.10	367	287	52.10	70	63	57.10	300	247
37.20	560	558	42.20	131	115	47.20	145	141	52.20	88	68	57.20	188	165
37.30	612	557	42.30	181	164	47.30	104	93	52.30	86	77	57.30	156	113
37.40	326	333	42.40	211	212	47.40	66	80	52.40	115	81	57.40	147	94
37.50	188	184	42.50	176	174	47.50	93	78	52.50	101	74	57.50	137	91
37.60	160	154	42.60	99	108	47.60	127	92	52.60	87	66	57.60	145	100
37.70	257	191	42.70	74	75	47.70	143	145	52.70	79	62	57.70	113	105
37.80	433	380	42.80	68	66	47.80	237	227	52.80	65	64	57.80	116	99
37.90	834	888	42.90	80	63	47.90	249	230	52.90	75	74	57.90	106	88
38.00	1303	1392	43.00	79	67	48.00	174	164	53.00	91	85	58.00	88	85
38.10	1346	1309	43.10	101	67	48.10	104	108	53.10	93	87	58.10	126	89
38.20	781	743	43.20	142	70	48.20	77	84	53.20	106	84	58.20	155	117
38.30	316	311	43.30	111	75	48.30	77	79	53.30	69	79	58.30	229	210
38.40	171	159	43.40	134	78	48.40	62	82	53.40	75	76	58.40	409	402
38.50	117	121	43.50	107	86	48.50	92	94	53.50	79	75	58.50	630	534
38.60	101	110	43.60	109	94	48.60	153	132	53.60	79	73	58.60	488	496
38.70	106	108	43.70	130	109	48.70	236	214	53.70	81	75	58.70	451	394
38.80	121	118	43.80	174	157	48.80	295	340	53.80	78	83	58.80	269	284
38.90	198	157	43.90	304	324	48.90	386	392	53.90	105	92	58.90	267	262



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	367	359	64.00	198	219	69.00	86	84	74.00	128	137	79.00	112	103
59.10	462	481	64.10	188	230	69.10	80	86	74.10	189	169	79.10	90	104
59.20	462	437	64.20	227	251	69.20	108	103	74.20	186	197	79.20	102	126
59.30	326	306	64.30	224	235	69.30	151	139	74.30	217	204	79.30	161	171
59.40	185	176	64.40	206	186	69.40	180	168	74.40	176	194	79.40	201	211
59.50	107	112	64.50	149	145	69.50	197	201	74.50	174	197	79.50	165	195
59.60	88	90	64.60	137	135	69.60	220	209	74.60	163	184	79.60	148	167
59.70	87	85	64.70	145	145	69.70	186	184	74.70	140	152	79.70	141	134
59.80	81	78	64.80	137	134	69.80	149	167	74.80	128	128	79.80	88	100
59.90	91	73	64.90	122	120	69.90	143	155	74.90	115	105	79.90	70	80
60.00	62	70	65.00	124	97	70.00	153	162	75.00	70	85	80.00	73	74
60.10	84	75	65.10	104	82	70.10	217	208	75.10	69	74	80.10	71	74
60.20	74	76	65.20	101	75	70.20	302	303	75.20	54	68	80.20	60	73
60.30	201	79	65.30	102	79	70.30	423	430	75.30	50	63	80.30	59	71
60.40	92	85	65.40	96	95	70.40	583	579	75.40	57	62	80.40	59	72
60.50	98	107	65.50	138	106	70.50	604	603	75.50	52	65	80.50	64	76
60.60	147	167	65.60	114	99	70.60	451	497	75.60	64	77	80.60	61	82
60.70	251	260	65.70	102	89	70.70	381	372	75.70	78	96	80.70	67	80
60.80	315	319	65.80	90	84	70.80	224	235	75.80	112	106	80.80	69	77
60.90	314	343	65.90	81	92	70.90	141	152	75.90	91	103	80.90	76	75
61.00	380	414	66.00	109	101	71.00	110	108	76.00	93	92	81.00	97	79
61.10	525	584	66.10	114	105	71.10	91	88	76.10	91	80	81.10	97	98
61.20	777	778	66.20	110	101	71.20	83	82	76.20	89	73	81.20	135	126
61.30	731	703	66.30	101	95	71.30	92	89	76.30	71	75	81.30	105	135
61.40	508	505	66.40	92	85	71.40	102	109	76.40	86	82	81.40	148	136
61.50	302	315	66.50	109	75	71.50	136	133	76.50	71	86	81.50	128	138
61.60	252	273	66.60	80	70	71.60	147	157	76.60	90	89	81.60	115	122
61.70	341	348	66.70	83	72	71.70	164	165	76.70	111	96	81.70	89	103
61.80	381	355	66.80	96	82	71.80	134	150	76.80	119	109	81.80	92	93
61.90	262	282	66.90	106	89	71.90	132	128	76.90	113	115	81.90	68	85
62.00	177	185	67.00	91	87	72.00	121	108	77.00	97	116	82.00	67	78
62.10	103	120	67.10	84	82	72.10	105	105	77.10	112	116	82.10	71	73
62.20	92	96	67.20	90	80	72.20	128	131	77.20	105	114	82.20	59	69
62.30	100	99	67.30	82	85	72.30	205	175	77.30	129	115	82.30	69	66
62.40	144	129	67.40	106	110	72.40	227	197	77.40	127	110	82.40	66	66
62.50	187	202	67.50	187	160	72.50	199	203	77.50	96	107	82.50	54	66
62.60	256	242	67.60	248	230	72.60	179	198	77.60	120	113	82.60	68	68
62.70	211	233	67.70	361	334	72.70	195	184	77.70	148	131	82.70	64	75
62.80	212	210	67.80	446	380	72.80	207	172	77.80	133	146	82.80	91	94
62.90	215	205	67.90	331	317	72.90	220	211	77.90	134	138	82.90	122	121
63.00	214	221	68.00	254	232	73.00	316	335	78.00	114	125	83.00	157	130
63.10	253	250	68.10	182	154	73.10	472	496	78.10	97	106	83.10	92	118
63.20	268	264	68.20	146	129	73.20	572	515	78.20	83	87	83.20	101	107
63.30	314	277	68.30	171	147	73.30	359	425	78.30	71	77	83.30	96	90
63.40	451	398	68.40	163	160	73.40	291	309	78.40	84	78	83.40	69	78
63.50	688	710	68.50	136	142	73.50	172	198	78.50	122	92	83.50	71	79
63.60	921	946	68.60	111	120	73.60	99	139	78.60	132	110	83.60	100	92
63.70	807	816	68.70	118	103	73.70	104	120	78.70	127	115	83.70	92	99
63.80	559	560	68.80	107	96	73.80	103	118	78.80	135	112	83.80	85	100
63.90	360	313	68.90	114	90	73.90	116	119	78.90	126	109	83.90	78	100



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	89	94	89.00	118	111	94.00	110	104	99.00	80	62			
84.10	89	93	89.10	120	113	94.10	98	86	99.10	78	64			
84.20	69	99	89.20	100	115	94.20	61	84	99.20	77	66			
84.30	83	95	89.30	111	115	94.30	111	99	99.30	66	63			
84.40	70	86	89.40	111	113	94.40	121	126	99.40	65	58			
84.50	58	80	89.50	125	116	94.50	158	144	99.50	53	57			
84.60	75	74	89.60	127	115	94.60	134	135	99.60	63	57			
84.70	76	78	89.70	101	107	94.70	142	124	99.70	69	56			
84.80	88	95	89.80	116	104	94.80	144	111	99.80	73	54			
84.90	128	112	89.90	114	108	94.90	125	91	99.90	56	52			
85.00	128	114	90.00	87	111	95.00	82	73	100.00	56	52			
85.10	120	112	90.10	104	113	95.10	83	61						
85.20	114	102	90.20	134	121	95.20	59	58						
85.30	83	87	90.30	129	137	95.30	63	59						
85.40	76	76	90.40	157	155	95.40	82	64						
85.50	81	70	90.50	186	166	95.50	82	67						
85.60	71	68	90.60	185	176	95.60	69	70						
85.70	72	69	90.70	155	188	95.70	83	77						
85.80	64	70	90.80	184	178	95.80	101	85						
85.90	59	75	90.90	170	151	95.90	100	89						
86.00	79	83	91.00	108	128	96.00	132	85						
86.10	69	89	91.10	84	107	96.10	88	77						
86.20	79	88	91.20	71	87	96.20	75	71						
86.30	78	85	91.30	69	73	96.30	69	65						
86.40	87	84	91.40	57	64	96.40	62	59						
86.50	88	83	91.50	66	58	96.50	71	55						
86.60	93	86	91.60	62	56	96.60	55	55						
86.70	99	96	91.70	58	55	96.70	59	59						
86.80	119	119	91.80	56	56	96.80	64	64						
86.90	130	140	91.90	61	58	96.90	55	72						
87.00	124	134	92.00	55	58	97.00	77	81						
87.10	100	119	92.10	67	58	97.10	91	95						
87.20	127	103	92.20	46	59	97.20	94	116						
87.30	86	82	92.30	46	61	97.30	145	142						
87.40	58	66	92.40	72	65	97.40	195	149						
87.50	47	57	92.50	64	68	97.50	141	138						
87.60	41	53	92.60	66	72	97.60	140	138						
87.70	58	51	92.70	69	83	97.70	164	151						
87.80	40	51	92.80	92	102	97.80	200	158						
87.90	52	52	92.90	112	123	97.90	174	159						
88.00	61	52	93.00	141	135	98.00	166	162						
88.10	59	52	93.10	142	155	98.10	183	163						
88.20	44	54	93.20	156	201	98.20	156	144						
88.30	63	57	93.30	251	247	98.30	136	122						
88.40	63	59	93.40	241	267	98.40	126	108						
88.50	50	60	93.50	258	279	98.50	88	92						
88.60	53	63	93.60	241	255	98.60	82	75						
88.70	74	70	93.70	198	208	98.70	68	67						
88.80	93	81	93.80	149	171	98.80	65	65						
88.90	102	98	93.90	141	134	98.90	72	64						

Sample	KCo2O														
	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
	9.00	118	121	14.00	105	111	19.00	101	113	24.00	107	127	29.00	345	380
	9.10	147	121	14.10	114	111	19.10	115	114	24.10	91	107	29.10	268	267
	9.20	147	121	14.20	107	111	19.20	103	117	24.20	107	100	29.20	159	157
	9.30	164	121	14.30	117	111	19.30	116	122	24.30	116	99	29.30	128	129
	9.40	156	153	14.40	96	111	19.40	133	134	24.40	94	98	29.40	127	138
	9.50	136	157	14.50	100	111	19.50	204	188	24.50	109	98	29.50	152	161
	9.60	165	165	14.60	112	111	19.60	379	384	24.60	111	97	29.60	159	159
	9.70	180	186	14.70	99	110	19.70	601	588	24.70	102	97	29.70	142	155
	9.80	230	215	14.80	130	110	19.80	412	393	24.80	92	97	29.80	215	180
	9.90	260	214	14.90	101	110	19.90	200	187	24.90	96	97	29.90	324	326
	10.00	278	227	15.00	105	110	20.00	120	129	25.00	108	97	30.00	764	850
	10.10	480	362	15.10	105	110	20.10	106	115	25.10	123	97	30.10	1385	1421
	10.20	827	905	15.20	102	110	20.20	106	110	25.20	116	96	30.20	1035	1039
	10.30	1670	1690	15.30	91	110	20.30	118	106	25.30	117	96	30.30	564	564
	10.40	1239	1207	15.40	111	109	20.40	104	105	25.40	108	118	30.40	479	458
	10.50	423	443	15.50	97	109	20.50	125	104	25.50	113	122	30.50	295	303
	10.60	203	205	15.60	112	109	20.60	96	106	25.60	113	127	30.60	177	172
	10.70	154	152	15.70	97	109	20.70	112	111	25.70	129	135	30.70	116	129
	10.80	139	131	15.80	102	109	20.80	115	109	25.80	147	147	30.80	111	119
	10.90	138	120	15.90	95	109	20.90	92	104	25.90	187	170	30.90	141	118
	11.00	123	116	16.00	117	108	21.00	114	103	26.00	264	247	31.00	126	126
	11.10	120	116	16.10	115	108	21.10	122	102	26.10	506	565	31.10	170	177
	11.20	134	116	16.20	109	108	21.20	113	102	26.20	1496	1482	31.20	397	380
	11.30	125	116	16.30	99	108	21.30	105	107	26.30	2116	2052	31.30	632	646
	11.40	128	116	16.40	99	108	21.40	122	107	26.40	1060	1196	31.40	522	521
	11.50	104	115	16.50	117	108	21.50	110	109	26.50	430	467	31.50	237	250
	11.60	110	115	16.60	123	108	21.60	97	114	26.60	263	268	31.60	128	146
	11.70	108	115	16.70	107	108	21.70	126	125	26.70	327	293	31.70	140	126
	11.80	121	115	16.80	112	108	21.80	139	131	26.80	586	640	31.80	140	124
	11.90	125	115	16.90	93	108	21.90	138	133	26.90	1463	1491	31.90	141	132
	12.00	117	115	17.00	110	108	22.00	160	182	27.00	1689	1643	32.00	154	162
	12.10	103	114	17.10	102	108	22.10	329	354	27.10	798	788	32.10	324	332
	12.20	126	114	17.20	115	114	22.20	520	500	27.20	280	302	32.20	806	798
	12.30	130	114	17.30	111	123	22.30	325	328	27.30	172	190	32.30	1018	1103
	12.40	117	114	17.40	112	122	22.40	184	172	27.40	157	169	32.40	659	702
	12.50	116	114	17.50	116	116	22.50	119	133	27.50	174	170	32.50	292	314
	12.60	114	114	17.60	101	114	22.60	117	132	27.60	200	196	32.60	204	209
	12.70	93	114	17.70	108	115	22.70	157	169	27.70	388	339	32.70	206	216
	12.80	134	113	17.80	107	120	22.80	322	321	27.80	1008	926	32.80	338	326
	12.90	126	113	17.90	130	139	22.90	503	495	27.90	1871	1791	32.90	895	870
	13.00	122	113	18.00	203	215	23.00	352	355	28.00	1477	1418	33.00	2052	2127
	13.10	99	113	18.10	326	337	23.10	187	177	28.10	597	557	33.10	2397	2408
	13.20	115	113	18.20	348	299	23.20	151	122	28.20	218	225	33.20	1206	1216
	13.30	130	113	18.30	186	183	23.30	108	110	28.30	167	154	33.30	429	412
	13.40	114	112	18.40	124	128	23.40	111	105	28.40	142	133	33.40	186	197
	13.50	125	112	18.50	106	113	23.50	106	103	28.50	99	121	33.50	131	145
	13.60	131	112	18.60	114	109	23.60	96	102	28.60	107	115	33.60	115	123
	13.70	109	112	18.70	87	107	23.70	116	104	28.70	110	118	33.70	93	118
	13.80	105	112	18.80	107	112	23.80	117	117	28.80	159	153	33.80	113	115
	13.90	95	112	18.90	112	112	23.90	131	136	28.90	274	275	33.90	96	112

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	109	109	39.00	218	216	44.00	436	462	49.00	300	306	54.00	124	109
34.10	95	113	39.10	531	510	44.10	644	625	49.10	238	243	54.10	133	131
34.20	131	123	39.20	989	930	44.20	592	556	49.20	197	190	54.20	213	196
34.30	159	143	39.30	847	841	44.30	572	542	49.30	152	148	54.30	289	307
34.40	204	230	39.40	477	448	44.40	580	599	49.40	111	125	54.40	396	398
34.50	584	539	39.50	239	224	44.50	543	529	49.50	128	114	54.50	416	394
34.60	1222	1173	39.60	122	144	44.60	405	332	49.60	96	112	54.60	306	304
34.70	1194	1255	39.70	100	112	44.70	270	184	49.70	111	115	54.70	268	240
34.80	682	696	39.80	100	104	44.80	146	144	49.80	91	108	54.80	359	320
34.90	313	336	39.90	113	111	44.90	156	156	49.90	100	95	54.90	593	619
35.00	301	298	40.00	119	123	45.00	159	144	50.00	82	85	55.00	899	896
35.10	564	582	40.10	103	116	45.10	103	113	50.10	89	82	55.10	762	782
35.20	1314	1345	40.20	117	100	45.20	88	94	50.20	81	82	55.20	446	482
35.30	1796	1805	40.30	117	94	45.30	80	89	50.30	73	85	55.30	214	243
35.40	1148	1128	40.40	102	99	45.40	77	88	50.40	99	98	55.40	163	172
35.50	402	426	40.50	151	128	45.50	110	95	50.50	161	147	55.50	227	198
35.60	192	189	40.60	227	220	45.60	104	109	50.60	254	237	55.60	216	207
35.70	137	135	40.70	380	329	45.70	108	111	50.70	250	269	55.70	195	175
35.80	100	117	40.80	340	301	45.80	85	101	50.80	210	211	55.80	122	130
35.90	111	111	40.90	222	194	45.90	89	97	50.90	154	138	55.90	107	102
36.00	107	118	41.00	140	135	46.00	106	103	51.00	111	105	56.00	94	90
36.10	101	122	41.10	118	127	46.10	122	128	51.10	99	103	56.10	95	84
36.20	107	108	41.20	144	151	46.20	195	194	51.20	95	104	56.20	97	88
36.30	89	97	41.30	212	231	46.30	251	248	51.30	112	117	56.30	100	96
36.40	94	96	41.40	503	448	46.40	219	227	51.40	122	148	56.40	120	103
36.50	108	102	41.50	1020	913	46.50	227	204	51.50	138	155	56.50	134	119
36.60	109	113	41.60	1166	1159	46.60	257	230	51.60	109	128	56.60	185	162
36.70	148	128	41.70	903	832	46.70	259	248	51.70	91	97	56.70	222	205
36.80	174	170	41.80	521	484	46.80	320	302	51.80	85	82	56.80	245	232
36.90	179	223	41.90	323	302	46.90	408	369	51.90	59	78	56.90	290	290
37.00	185	215	42.00	177	186	47.00	344	304	52.00	75	78	57.00	340	314
37.10	257	233	42.10	137	129	47.10	242	184	52.10	91	79	57.10	245	255
37.20	395	369	42.20	124	117	47.20	137	115	52.20	88	84	57.20	198	172
37.30	425	419	42.30	140	137	47.30	95	95	52.30	92	94	57.30	132	118
37.40	277	281	42.40	194	183	47.40	83	90	52.40	86	100	57.40	111	99
37.50	174	167	42.50	204	182	47.50	91	92	52.50	106	95	57.50	108	99
37.60	143	140	42.60	148	133	47.60	117	107	52.60	100	85	57.60	95	105
37.70	183	159	42.70	95	97	47.70	168	166	52.70	76	79	57.70	91	107
37.80	283	271	42.80	108	86	47.80	257	260	52.80	82	79	57.80	99	101
37.90	589	610	42.90	88	83	47.90	271	263	52.90	84	85	57.90	87	95
38.00	959	1040	43.00	72	82	48.00	209	187	53.00	103	96	58.00	89	93
38.10	1143	1147	43.10	87	84	48.10	99	120	53.10	116	98	58.10	100	94
38.20	740	747	43.20	98	86	48.20	87	95	53.20	82	94	58.20	98	108
38.30	336	337	43.30	94	87	48.30	73	90	53.30	89	88	58.30	182	165
38.40	186	173	43.40	103	90	48.40	93	90	53.40	72	87	58.40	344	316
38.50	117	131	43.50	97	94	48.50	84	97	53.50	98	87	58.50	495	489
38.60	110	119	43.60	97	99	48.60	136	123	53.60	86	85	58.60	513	508
38.70	102	116	43.70	109	107	48.70	181	183	53.70	74	85	58.70	471	429
38.80	117	120	43.80	123	129	48.80	279	279	53.80	93	90	58.80	314	307
38.90	152	137	43.90	199	223	48.90	346	339	53.90	99	99	58.90	251	268

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	339	354	64.00	187	173	69.00	104	88	74.00	152	137	79.00	113	104
59.10	432	438	64.10	180	197	69.10	116	94	74.10	172	169	79.10	104	111
59.20	352	376	64.20	213	227	69.20	121	115	74.20	209	192	79.20	132	140
59.30	258	253	64.30	222	222	69.30	161	144	74.30	184	203	79.30	167	181
59.40	142	148	64.40	173	180	69.40	178	168	74.40	175	200	79.40	185	198
59.50	100	104	64.50	168	142	69.50	210	194	74.50	191	199	79.50	184	179
59.60	95	93	64.60	143	130	69.60	179	193	74.60	174	195	79.60	155	152
59.70	97	90	64.70	144	135	69.70	146	171	74.70	128	168	79.70	111	121
59.80	102	86	64.80	128	130	69.80	160	153	74.80	137	142	79.80	103	96
59.90	82	83	64.90	128	116	69.90	146	141	74.90	128	118	79.90	87	84
60.00	102	82	65.00	111	100	70.00	170	147	75.00	93	97	80.00	73	81
60.10	87	83	65.10	98	88	70.10	188	194	75.10	91	85	80.10	80	82
60.20	80	87	65.20	111	85	70.20	305	299	75.20	75	79	80.20	95	82
60.30	96	92	65.30	119	93	70.30	450	443	75.30	75	75	80.30	86	81
60.40	108	96	65.40	124	105	70.40	521	564	75.40	84	75	80.40	69	84
60.50	129	114	65.50	108	106	70.50	518	541	75.50	82	81	80.50	70	89
60.60	146	163	65.60	98	97	70.60	428	431	75.60	79	93	80.60	90	93
60.70	249	234	65.70	91	88	70.70	309	301	75.70	93	101	80.70	62	91
60.80	282	260	65.80	97	86	70.80	205	189	75.80	118	102	80.80	87	88
60.90	251	260	65.90	95	95	70.90	121	127	75.90	105	97	80.90	109	89
61.00	298	299	66.00	113	104	71.00	101	99	76.00	97	88	81.00	75	99
61.10	413	435	66.10	107	108	71.10	94	86	76.10	104	82	81.10	120	118
61.20	673	647	66.20	95	108	71.20	81	84	76.20	90	82	81.20	156	129
61.30	674	657	66.30	94	105	71.30	104	91	76.30	108	85	81.30	125	129
61.40	479	498	66.40	100	96	71.40	105	111	76.40	93	87	81.40	124	132
61.50	286	320	66.50	102	87	71.50	141	137	76.50	92	88	81.50	126	126
61.60	248	263	66.60	78	82	71.60	158	154	76.60	94	89	81.60	94	112
61.70	306	322	66.70	67	83	71.70	147	149	76.70	99	94	81.70	94	100
61.80	328	328	66.80	85	88	71.80	140	133	76.80	121	104	81.80	72	92
61.90	264	261	66.90	113	88	71.90	116	114	76.90	113	111	81.90	85	86
62.00	178	174	67.00	94	85	72.00	92	98	77.00	117	116	82.00	78	82
62.10	120	116	67.10	70	83	72.10	88	97	77.10	118	121	82.10	78	80
62.20	88	96	67.20	93	86	72.20	135	118	77.20	121	122	82.20	64	78
62.30	126	98	67.30	96	98	72.30	182	161	77.30	133	120	82.30	74	77
62.40	134	124	67.40	125	126	72.40	193	196	77.40	110	113	82.40	85	78
62.50	166	176	67.50	185	163	72.50	206	206	77.50	127	109	82.50	91	78
62.60	232	209	67.60	205	218	72.60	214	195	77.60	116	115	82.60	73	79
62.70	232	211	67.70	294	302	72.70	165	167	77.70	141	127	82.70	74	85
62.80	207	205	67.80	355	324	72.80	157	150	77.80	112	134	82.80	97	100
62.90	185	201	67.90	248	270	72.90	169	183	77.90	120	127	82.90	98	123
63.00	193	204	68.00	179	197	73.00	278	295	78.00	104	118	83.00	137	137
63.10	221	226	68.10	158	138	73.10	423	430	78.10	137	104	83.10	112	131
63.20	259	251	68.20	128	125	73.20	473	447	78.20	95	93	83.20	123	118
63.30	277	290	68.30	143	146	73.30	346	372	78.30	97	92	83.30	102	102
63.40	441	454	68.40	152	158	73.40	298	273	78.40	99	104	83.40	80	90
63.50	724	738	68.50	153	143	73.50	158	181	78.50	141	121	83.50	78	87
63.60	779	814	68.60	118	121	73.60	122	130	78.60	135	127	83.60	94	93
63.70	621	642	68.70	101	102	73.70	103	114	78.70	108	122	83.70	101	98
63.80	444	397	68.80	93	95	73.80	119	110	78.80	129	116	83.80	104	100
63.90	202	220	68.90	88	91	73.90	107	115	78.90	122	109	83.90	86	98



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	79	95	89.00	130	119	94.00	96	99	99.00	78	82			
84.10	72	96	89.10	123	118	94.10	98	98	99.10	69	84			
84.20	115	99	89.20	104	117	94.20	117	111	99.20	99	85			
84.30	96	97	89.30	109	115	94.30	109	131	99.30	88	85			
84.40	77	91	89.40	106	114	94.40	162	142	99.40	70	83			
84.50	86	88	89.50	115	116	94.50	143	137	99.50	91	82			
84.60	95	90	89.60	135	118	94.60	124	129	99.60	83	81			
84.70	110	100	89.70	112	116	94.70	114	119	99.70	74	78			
84.80	101	111	89.80	107	118	94.80	127	105	99.80	99	75			
84.90	116	115	89.90	120	122	94.90	83	90	99.90	89	75			
85.00	125	113	90.00	104	124	95.00	77	80	100.00	95	79			
85.10	128	108	90.10	122	126	95.10	86	75						
85.20	107	98	90.20	130	137	95.20	70	73						
85.30	75	89	90.30	165	154	95.30	70	75						
85.40	84	83	90.40	167	169	95.40	79	79						
85.50	73	80	90.50	195	178	95.50	82	83						
85.60	81	79	90.60	213	181	95.60	102	87						
85.70	65	78	90.70	200	177	95.70	105	92						
85.80	82	80	90.80	171	159	95.80	110	97						
85.90	88	85	90.90	129	137	95.90	97	97						
86.00	86	91	91.00	117	117	96.00	102	94						
86.10	77	92	91.10	105	100	96.10	93	88						
86.20	99	90	91.20	103	86	96.20	84	82						
86.30	88	89	91.30	83	78	96.30	67	78						
86.40	81	88	91.40	65	73	96.40	79	74						
86.50	85	90	91.50	75	70	96.50	70	73						
86.60	99	95	91.60	68	69	96.60	81	73						
86.70	98	107	91.70	66	70	96.70	85	76						
86.80	98	124	91.80	70	72	96.80	94	81						
86.90	142	132	91.90	78	74	96.90	85	89						
87.00	128	124	92.00	74	74	97.00	104	101						
87.10	124	112	92.10	68	74	97.10	107	119						
87.20	109	98	92.20	76	75	97.20	122	139						
87.30	66	84	92.30	71	77	97.30	158	153						
87.40	54	74	92.40	81	79	97.40	191	152						
87.50	65	68	92.50	80	83	97.50	145	149						
87.60	69	66	92.60	90	93	97.60	162	153						
87.70	62	66	92.70	120	110	97.70	182	161						
87.80	70	66	92.80	144	129	97.80	168	169						
87.90	75	67	92.90	145	145	97.90	160	172						
88.00	68	68	93.00	133	164	98.00	191	170						
88.10	60	68	93.10	178	196	98.10	184	159						
88.20	68	70	93.20	237	228	98.20	146	143						
88.30	75	71	93.30	278	244	98.30	137	127						
88.40	68	72	93.40	257	251	98.40	124	111						
88.50	77	74	93.50	242	240	98.50	98	97						
88.60	76	78	93.60	190	207	98.60	82	87						
88.70	93	88	93.70	151	172	98.70	82	83						
88.80	96	101	93.80	146	141	98.80	71	81						
88.90	133	113	93.90	124	115	98.90	101	81						

Sample	KCo40													
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	155	131	14.00	123	123	19.00	146	123	24.00	127	123	29.00	305	289
9.10	170	131	14.10	120	123	19.10	133	124	24.10	121	114	29.10	207	180
9.20	153	131	14.20	115	123	19.20	108	127	24.20	118	112	29.20	121	139
9.30	177	168	14.30	102	123	19.30	117	132	24.30	114	111	29.30	137	137
9.40	152	172	14.40	105	123	19.40	144	147	24.40	100	111	29.40	154	160
9.50	182	177	14.50	134	122	19.50	222	216	24.50	111	111	29.50	161	178
9.60	169	186	14.60	128	122	19.60	356	392	24.60	115	111	29.60	143	162
9.70	226	203	14.70	136	122	19.70	458	443	24.70	110	110	29.70	157	159
9.80	231	223	14.80	113	122	19.80	271	259	24.80	112	110	29.80	233	193
9.90	325	244	14.90	116	122	19.90	171	156	24.90	118	110	29.90	356	385
10.00	408	318	15.00	110	122	20.00	140	132	25.00	138	110	30.00	832	864
10.10	728	641	15.10	117	122	20.10	131	124	25.10	146	110	30.10	1024	980
10.20	1410	1497	15.20	120	121	20.20	117	121	25.20	135	110	30.20	560	547
10.30	2045	1982	15.30	137	121	20.30	117	119	25.30	123	119	30.30	339	336
10.40	983	1051	15.40	127	121	20.40	141	118	25.40	129	125	30.40	309	279
10.50	356	405	15.50	105	121	20.50	132	121	25.50	140	129	30.50	184	189
10.60	197	225	15.60	108	121	20.60	146	129	25.60	127	133	30.60	133	140
10.70	178	174	15.70	102	121	20.70	108	135	25.70	128	140	30.70	122	128
10.80	153	151	15.80	119	121	20.80	130	125	25.80	147	151	30.80	143	125
10.90	160	137	15.90	116	121	20.90	106	118	25.90	146	174	30.90	131	128
11.00	159	128	16.00	127	120	21.00	123	116	26.00	234	264	31.00	172	146
11.10	138	127	16.10	109	120	21.10	134	115	26.10	615	635	31.10	218	245
11.20	146	127	16.20	119	120	21.20	120	115	26.20	1380	1395	31.20	440	482
11.30	154	127	16.30	110	120	21.30	108	118	26.30	1430	1392	31.30	522	530
11.40	149	127	16.40	112	120	21.40	117	119	26.40	618	678	31.40	330	304
11.50	137	127	16.50	113	120	21.50	104	120	26.50	293	307	31.50	184	166
11.60	155	127	16.60	139	120	21.60	115	126	26.60	205	234	31.60	132	134
11.70	126	126	16.70	109	120	21.70	137	135	26.70	343	322	31.70	130	129
11.80	135	126	16.80	119	120	21.80	141	136	26.80	765	747	31.80	128	130
11.90	129	126	16.90	103	120	21.90	151	141	26.90	1298	1272	31.90	156	141
12.00	139	126	17.00	112	120	22.00	199	200	27.00	927	915	32.00	198	189
12.10	142	126	17.10	115	121	22.10	307	340	27.10	355	382	32.10	384	417
12.20	136	126	17.20	94	127	22.20	366	364	27.20	205	207	32.20	744	797
12.30	156	126	17.30	115	131	22.30	215	222	27.30	149	174	32.30	689	722
12.40	157	125	17.40	111	128	22.40	152	149	27.40	160	171	32.40	355	367
12.50	109	125	17.50	101	124	22.50	132	135	27.50	178	185	32.50	190	209
12.60	115	125	17.60	119	124	22.60	150	141	27.60	317	249	32.60	158	190
12.70	124	125	17.70	123	126	22.70	198	188	27.70	652	569	32.70	226	220
12.80	132	125	17.80	138	131	22.80	283	325	27.80	1503	1393	32.80	383	394
12.90	137	125	17.90	116	155	22.90	369	389	27.90	1664	1615	32.90	1016	1107
13.00	132	125	18.00	233	230	23.00	233	244	28.00	829	797	33.00	2132	2117
13.10	122	124	18.10	278	292	23.10	154	149	28.10	336	300	33.10	1749	1695
13.20	119	124	18.20	235	218	23.20	120	125	28.20	162	179	33.20	670	682
13.30	116	124	18.30	130	149	23.30	114	119	28.30	128	148	33.30	287	264
13.40	129	124	18.40	123	128	23.40	114	117	28.40	142	135	33.40	176	171
13.50	134	124	18.50	123	122	23.50	122	115	28.50	139	128	33.50	133	143
13.60	100	124	18.60	133	120	23.60	128	115	28.60	132	126	33.60	101	128
13.70	137	124	18.70	103	119	23.70	133	118	28.70	124	135	33.70	106	126
13.80	105	123	18.80	108	122	23.80	129	128	28.80	206	187	33.80	133	125
13.90	113	123	18.90	119	123	23.90	129	135	28.90	267	298	33.90	116	123

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	121	121	39.00	259	259	44.00	517	491	49.00	212	235	54.00	115	126
34.10	146	125	39.10	564	545	44.10	524	539	49.10	170	186	54.10	154	161
34.20	118	137	39.20	812	756	44.20	491	500	49.20	160	146	54.20	238	232
34.30	178	171	39.30	571	551	44.30	562	565	49.30	114	126	54.30	329	310
34.40	268	279	39.40	293	281	44.40	624	597	49.40	135	125	54.40	330	337
34.50	695	675	39.50	189	165	44.50	451	444	49.50	116	127	54.50	318	301
34.60	1196	1175	39.60	127	127	44.60	315	254	49.60	131	134	54.60	257	239
34.70	882	949	39.70	114	114	44.70	207	163	49.70	140	132	54.70	293	245
34.80	441	460	39.80	123	113	44.80	177	159	49.80	106	118	54.80	397	425
34.90	248	260	39.90	97	121	44.90	161	160	49.90	91	104	54.90	690	708
35.00	249	285	40.00	110	125	45.00	137	137	50.00	94	98	55.00	716	736
35.10	603	598	40.10	116	115	45.10	120	113	50.10	99	97	55.10	465	522
35.20	1277	1278	40.20	114	106	45.20	101	105	50.20	88	98	55.20	308	284
35.30	1348	1372	40.30	125	104	45.30	88	103	50.30	111	102	55.30	166	176
35.40	717	715	40.40	97	110	45.40	110	108	50.40	121	124	55.40	188	173
35.50	279	280	40.50	151	135	45.50	116	122	50.50	220	184	55.50	198	187
35.60	145	162	40.60	230	203	45.60	116	133	50.60	239	243	55.60	178	170
35.70	139	134	40.70	304	253	45.70	121	124	50.70	245	228	55.70	132	140
35.80	129	123	40.80	200	211	45.80	118	112	50.80	153	169	55.80	122	115
35.90	130	124	40.90	149	151	45.90	102	111	50.90	124	124	55.90	107	104
36.00	123	131	41.00	142	129	46.00	138	120	51.00	92	111	56.00	120	100
36.10	102	127	41.10	145	136	46.10	168	152	51.10	105	112	56.10	94	99
36.20	111	112	41.20	163	172	46.20	194	206	51.20	109	121	56.20	101	103
36.30	119	107	41.30	262	281	46.30	216	215	51.30	129	147	56.30	122	113
36.40	107	111	41.40	640	563	46.40	187	185	51.40	142	167	56.40	145	131
36.50	118	119	41.50	1036	957	46.50	186	187	51.50	145	151	56.50	185	168
36.60	144	129	41.60	934	887	46.60	237	214	51.60	117	121	56.60	208	199
36.70	153	161	41.70	622	546	46.70	273	242	51.70	123	102	56.70	248	210
36.80	208	226	41.80	354	346	46.80	293	275	51.80	89	96	56.80	273	246
36.90	206	228	41.90	238	233	46.90	251	242	51.90	88	94	56.90	317	301
37.00	200	193	42.00	181	156	47.00	224	169	52.00	102	95	57.00	293	284
37.10	238	249	42.10	114	126	47.10	123	121	52.10	92	101	57.10	212	216
37.20	335	340	42.20	114	124	47.20	120	106	52.20	118	113	57.20	157	149
37.30	299	284	42.30	145	147	47.30	88	103	52.30	107	120	57.30	117	115
37.40	197	181	42.40	195	177	47.40	92	104	52.40	128	116	57.40	110	109
37.50	161	141	42.50	160	160	47.50	116	112	52.50	101	106	57.50	99	113
37.60	146	143	42.60	137	123	47.60	142	152	52.60	110	98	57.60	110	114
37.70	188	187	42.70	112	104	47.70	233	242	52.70	108	94	57.70	108	112
37.80	354	355	42.80	126	99	47.80	295	286	52.80	97	96	57.80	99	108
37.90	668	683	42.90	115	98	47.90	257	229	52.90	81	102	57.90	113	108
38.00	871	956	43.00	107	97	48.00	181	152	53.00	105	108	58.00	115	109
38.10	799	840	43.10	94	99	48.10	115	114	53.10	128	108	58.10	106	111
38.20	461	454	43.20	102	100	48.20	95	104	53.20	96	105	58.20	131	129
38.30	251	216	43.30	102	102	48.30	103	102	53.30	102	103	58.30	175	193
38.40	161	146	43.40	105	103	48.40	93	103	53.40	97	101	58.40	362	319
38.50	140	129	43.50	106	107	48.50	131	113	53.50	111	99	58.50	476	431
38.60	120	124	43.60	115	112	48.60	141	141	53.60	104	98	58.60	458	434
38.70	129	123	43.70	108	121	48.70	193	193	53.70	79	99	58.70	345	356
38.80	133	130	43.80	159	153	48.80	234	255	53.80	107	105	58.80	272	284
38.90	152	155	43.90	251	277	48.90	257	270	53.90	123	114	58.90	316	307

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	349	374	64.00	170	166	69.00	118	103	74.00	153	153	79.00	108	120
59.10	342	349	64.10	197	191	69.10	145	117	74.10	156	172	79.10	133	140
59.20	237	259	64.20	237	203	69.20	163	135	74.20	174	182	79.20	149	168
59.30	168	167	64.30	173	184	69.30	181	155	74.30	209	184	79.30	193	185
59.40	140	120	64.40	155	155	69.40	179	175	74.40	190	182	79.40	179	180
59.50	116	106	64.50	137	136	69.50	174	182	74.50	191	181	79.50	151	160
59.60	114	103	64.60	124	134	69.60	155	170	74.60	181	173	79.60	121	136
59.70	89	100	64.70	163	133	69.70	141	154	74.70	137	155	79.70	118	114
59.80	94	98	64.80	121	125	69.80	147	141	74.80	144	134	79.80	91	100
59.90	97	97	64.90	124	112	69.90	155	142	74.90	127	116	79.90	76	95
60.00	83	97	65.00	114	102	70.00	159	173	75.00	102	103	80.00	94	94
60.10	101	101	65.10	119	99	70.10	248	254	75.10	85	95	80.10	99	95
60.20	103	105	65.20	113	104	70.20	367	376	75.20	85	93	80.20	73	96
60.30	140	110	65.30	114	112	70.30	443	477	75.30	77	93	80.30	99	99
60.40	161	121	65.40	109	114	70.40	496	489	75.40	104	98	80.40	110	103
60.50	160	154	65.50	128	108	70.50	375	417	75.50	108	105	80.50	115	107
60.60	199	205	65.60	94	101	70.60	292	309	75.60	106	109	80.60	99	107
60.70	234	230	65.70	100	98	70.70	183	211	75.70	123	109	80.70	111	106
60.80	211	221	65.80	97	103	70.80	141	147	75.80	103	105	80.80	102	108
60.90	204	221	65.90	107	112	70.90	101	115	75.90	99	100	80.90	109	114
61.00	285	278	66.00	114	118	71.00	107	101	76.00	108	97	81.00	122	123
61.10	423	419	66.10	107	122	71.10	97	96	76.10	101	96	81.10	128	129
61.20	598	545	66.20	125	122	71.20	110	99	76.20	106	98	81.20	118	130
61.30	474	503	66.30	117	117	71.30	93	110	76.30	106	98	81.30	137	130
61.40	380	374	66.40	112	109	71.40	124	129	76.40	87	98	81.40	119	126
61.50	256	270	66.50	99	102	71.50	149	143	76.50	97	98	81.50	110	117
61.60	275	264	66.60	103	100	71.60	181	143	76.60	83	102	81.60	103	109
61.70	305	288	66.70	100	101	71.70	146	134	76.70	128	109	81.70	107	102
61.80	258	257	66.80	99	100	71.80	127	120	76.80	116	116	81.80	79	97
61.90	200	196	66.90	108	98	71.90	113	108	76.90	120	121	81.90	104	93
62.00	142	139	67.00	85	97	72.00	119	102	77.00	137	125	82.00	83	91
62.10	96	111	67.10	118	101	72.10	98	108	77.10	124	127	82.10	76	91
62.20	107	105	67.20	134	114	72.20	131	128	77.20	114	124	82.20	85	91
62.30	102	118	67.30	138	137	72.30	173	159	77.30	121	118	82.30	96	92
62.40	131	147	67.40	179	164	72.40	180	181	77.40	115	114	82.40	106	93
62.50	208	174	67.50	193	201	72.50	159	182	77.50	132	114	82.50	93	94
62.60	180	183	67.60	275	258	72.60	156	166	77.60	141	120	82.60	98	97
62.70	194	189	67.70	285	288	72.70	150	149	77.70	132	126	82.70	109	105
62.80	178	191	67.80	258	259	72.80	149	156	77.80	156	127	82.80	109	118
62.90	186	189	67.90	210	206	72.90	200	210	77.90	129	123	82.90	152	132
63.00	201	201	68.00	160	154	73.00	333	297	78.00	119	117	83.00	132	136
63.10	251	232	68.10	149	131	73.10	382	353	78.10	124	112	83.10	112	131
63.20	297	287	68.20	142	138	73.20	330	334	78.20	125	113	83.20	105	121
63.30	435	417	68.30	167	153	73.30	249	273	78.30	113	122	83.30	87	110
63.40	596	616	68.40	150	150	73.40	180	202	78.40	138	131	83.40	94	103
63.50	671	691	68.50	136	135	73.50	167	149	78.50	163	133	83.50	90	101
63.60	517	573	68.60	115	117	73.60	134	123	78.60	130	129	83.60	84	103
63.70	374	380	68.70	109	104	73.70	122	116	78.70	122	122	83.70	98	104
63.80	263	224	68.80	91	98	73.80	114	118	78.80	111	116	83.80	111	104
63.90	164	162	68.90	99	98	73.90	140	132	78.90	120	114	83.90	91	104



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	101	104	89.00	105	122	94.00	118	119	99.00	105	94			
84.10	88	106	89.10	118	121	94.10	136	126	99.10	86	95			
84.20	98	107	89.20	125	119	94.20	120	134	99.20	119	97			
84.30	99	106	89.30	123	119	94.30	166	136	99.30	92	98			
84.40	96	106	89.40	118	121	94.40	125	133	99.40	95	97			
84.50	114	107	89.50	131	124	94.50	99	126	99.50	100	96			
84.60	97	112	89.60	135	126	94.60	131	117	99.60	114	94			
84.70	116	115	89.70	111	129	94.70	112	107	99.70	111	93			
84.80	135	116	89.80	125	131	94.80	117	99	99.80	101	94			
84.90	124	114	89.90	131	133	94.90	114	93	99.90	118	98			
85.00	111	110	90.00	120	136	95.00	88	90	100.00	111	104			
85.10	101	104	90.10	138	143	95.10	75	89						
85.20	92	99	90.20	139	153	95.20	100	90						
85.30	90	95	90.30	173	164	95.30	80	92						
85.40	99	92	90.40	185	172	95.40	94	95						
85.50	80	90	90.50	192	173	95.50	118	97						
85.60	97	90	90.60	156	169	95.60	125	100						
85.70	106	91	90.70	157	157	95.70	106	102						
85.80	93	94	90.80	133	141	95.80	121	103						
85.90	100	97	90.90	127	125	95.90	114	102						
86.00	112	99	91.00	117	111	96.00	86	99						
86.10	102	99	91.10	92	101	96.10	97	95						
86.20	97	98	91.20	85	93	96.20	93	92						
86.30	86	98	91.30	101	89	96.30	102	89						
86.40	102	100	91.40	94	86	96.40	73	87						
86.50	89	104	91.50	95	85	96.50	95	87						
86.60	102	110	91.60	86	85	96.60	82	89						
86.70	102	118	91.70	93	86	96.70	78	93						
86.80	130	124	91.80	84	87	96.80	84	99						
86.90	128	122	91.90	98	89	96.90	106	109						
87.00	130	116	92.00	94	90	97.00	114	121						
87.10	118	107	92.10	96	91	97.10	151	133						
87.20	112	98	92.20	97	94	97.20	152	143						
87.30	91	91	92.30	90	97	97.30	167	148						
87.40	80	86	92.40	102	102	97.40	142	150						
87.50	77	84	92.50	112	111	97.50	154	152						
87.60	67	83	92.60	130	123	97.60	170	156						
87.70	81	83	92.70	135	139	97.70	179	160						
87.80	78	83	92.80	152	156	97.80	181	164						
87.90	80	84	92.90	156	176	97.90	147	163						
88.00	98	84	93.00	165	197	98.00	162	157						
88.10	84	85	93.10	219	216	98.10	162	147						
88.20	82	86	93.20	223	226	98.20	126	135						
88.30	92	87	93.30	239	227	98.30	102	122						
88.40	79	89	93.40	225	217	98.40	116	111						

Sample	KCo6O														
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	
9.00	180	153	14.00	145	142	19.00	145	142	24.00	119	129	29.00	267	259	
9.10	192	153	14.10	131	142	19.10	127	143	24.10	141	127	29.10	177	156	
9.20	206	153	14.20	150	142	19.20	128	145	24.20	116	126	29.20	142	134	
9.30	184	153	14.30	150	142	19.30	127	150	24.30	121	126	29.30	145	147	
9.40	199	153	14.40	117	142	19.40	186	161	24.40	123	126	29.40	178	188	
9.50	213	154	14.50	134	141	19.50	209	213	24.50	124	125	29.50	168	197	
9.60	215	267	14.60	161	141	19.60	419	435	24.60	155	125	29.60	161	167	
9.70	244	290	14.70	145	141	19.70	461	424	24.70	147	125	29.70	184	165	
9.80	319	315	14.80	160	141	19.80	210	204	24.80	148	125	29.80	206	190	
9.90	374	337	14.90	132	141	19.90	154	154	24.90	127	125	29.90	322	351	
10.00	571	418	15.00	129	140	20.00	142	144	25.00	149	125	30.00	804	868	
10.10	968	742	15.10	146	140	20.10	128	137	25.10	139	125	30.10	866	793	
10.20	2195	2311	15.20	136	140	20.20	155	134	25.20	131	125	30.20	363	337	
10.30	3091	2998	15.30	132	140	20.30	135	133	25.30	133	124	30.30	257	243	
10.40	720	875	15.40	134	140	20.40	143	134	25.40	151	124	30.40	228	204	
10.50	275	323	15.50	106	140	20.50	162	137	25.50	136	139	30.50	135	153	
10.60	187	199	15.60	116	139	20.60	150	156	25.60	138	150	30.60	162	137	
10.70	206	151	15.70	125	139	20.70	138	159	25.70	140	156	30.70	112	133	
10.80	172	149	15.80	138	139	20.80	143	138	25.80	127	165	30.80	146	134	
10.90	128	149	15.90	143	139	20.90	138	132	25.90	190	184	30.90	129	141	
11.00	144	148	16.00	136	139	21.00	136	131	26.00	247	235	31.00	195	164	
11.10	141	148	16.10	148	138	21.10	130	131	26.10	544	516	31.10	282	298	
11.20	145	148	16.20	123	138	21.20	147	131	26.20	1346	1375	31.20	573	602	
11.30	146	148	16.30	139	138	21.30	145	130	26.30	1089	1131	31.30	476	462	
11.40	165	148	16.40	112	138	21.40	135	130	26.40	451	447	31.40	233	210	
11.50	168	147	16.50	142	138	21.50	126	136	26.50	243	247	31.50	142	151	
11.60	160	147	16.60	126	138	21.60	149	141	26.60	241	222	31.60	164	143	
11.70	144	147	16.70	137	139	21.70	139	150	26.70	305	303	31.70	155	141	
11.80	158	147	16.80	110	139	21.80	148	147	26.80	803	804	31.80	161	144	
11.90	153	147	16.90	114	139	21.90	147	150	26.90	1233	1252	31.90	163	156	
12.00	122	146	17.00	137	140	22.00	171	186	27.00	627	574	32.00	230	204	
12.10	153	146	17.10	128	144	22.10	309	343	27.10	217	247	32.10	475	470	
12.20	171	146	17.20	147	167	22.20	374	347	27.20	169	198	32.20	824	874	
12.30	141	146	17.30	198	193	22.30	183	190	27.30	163	186	32.30	562	596	
12.40	144	146	17.40	150	159	22.40	164	150	27.40	164	190	32.40	246	269	
12.50	147	145	17.50	130	146	22.50	150	145	27.50	215	213	32.50	177	202	
12.60	160	145	17.60	139	144	22.60	158	148	27.60	381	291	32.60	202	204	
12.70	146	145	17.70	159	145	22.70	181	175	27.70	857	742	32.70	203	236	
12.80	151	145	17.80	127	149	22.80	277	311	27.80	2047	1991	32.80	379	383	
12.90	152	145	17.90	147	163	22.90	377	360	27.90	1556	1511	32.90	1080	1183	
13.00	164	144	18.00	212	239	23.00	203	196	28.00	563	475	33.00	2309	2301	
13.10	148	144	18.10	391	357	23.10	123	144	28.10	211	221	33.10	1456	1383	
13.20	145	144	18.20	221	245	23.20	125	134	28.20	172	169	33.20	448	437	
13.30	150	144	18.30	152	160	23.30	133	130	28.30	141	147	33.30	190	214	
13.40	150	144	18.40	141	143	23.40	137	128	28.40	137	136	33.40	124	162	
13.50	163	143	18.50	129	138	23.50	124	127	28.50	125	130	33.50	139	140	
13.60	167	143	18.60	144	135	23.60	126	127	28.60	147	131	33.60	142	127	
13.70	159	143	18.70	103	134	23.70	122	128	28.70	163	143	33.70	122	120	
13.80	141	143	18.80	144	134	23.80	135	133	28.80	185	206	33.80	109	127	
13.90	129	143	18.90	147	134	23.90	121	135	28.90	309	340	33.90	121	134	

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	104	138	39.00	267	262	44.00	561	524	49.00	211	204	54.00	126	132
34.10	130	146	39.10	519	525	44.10	546	528	49.10	149	157	54.10	156	169
34.20	149	165	39.20	677	669	44.20	482	500	49.20	124	130	54.20	204	232
34.30	217	205	39.30	494	429	44.30	624	609	49.30	127	122	54.30	290	288
34.40	312	292	39.40	247	222	44.40	598	606	49.40	122	127	54.40	303	285
34.50	793	762	39.50	152	153	44.50	388	385	49.50	108	137	54.50	253	254
34.60	1361	1298	39.60	130	128	44.60	275	205	49.60	151	149	54.60	226	217
34.70	774	832	39.70	115	120	44.70	192	150	49.70	129	140	54.70	270	268
34.80	324	358	39.80	112	122	44.80	184	151	49.80	111	122	54.80	527	523
34.90	235	239	39.90	130	133	44.90	155	141	49.90	112	111	54.90	731	765
35.00	237	263	40.00	129	132	45.00	153	124	50.00	96	108	55.00	631	640
35.10	434	486	40.10	110	121	45.10	102	115	50.10	107	109	55.10	377	387
35.20	1204	1220	40.20	93	115	45.20	103	113	50.20	117	110	55.20	210	208
35.30	1315	1277	40.30	130	115	45.30	114	114	50.30	136	116	55.30	159	171
35.40	521	561	40.40	112	119	45.40	122	121	50.40	132	145	55.40	215	195
35.50	205	224	40.50	147	138	45.50	130	142	50.50	240	217	55.50	200	192
35.60	135	157	40.60	221	192	45.60	142	145	50.60	260	255	55.60	176	168
35.70	124	136	40.70	291	233	45.70	139	130	50.70	218	213	55.70	159	138
35.80	128	127	40.80	218	192	45.80	130	120	50.80	167	153	55.80	125	121
35.90	125	128	40.90	144	149	45.90	120	124	50.90	101	123	55.90	107	112
36.00	158	136	41.00	137	143	46.00	112	134	51.00	109	120	56.00	120	110
36.10	127	129	41.10	154	155	46.10	170	177	51.10	124	124	56.10	111	110
36.20	118	120	41.20	197	201	46.20	224	232	51.20	165	144	56.20	116	117
36.30	103	119	41.30	338	326	46.30	233	211	51.30	167	189	56.30	152	133
36.40	112	124	41.40	703	681	46.40	162	168	51.40	162	195	56.40	194	169
36.50	139	132	41.50	1157	1078	46.50	200	168	51.50	132	160	56.50	235	216
36.60	153	149	41.60	778	793	46.60	195	191	51.60	117	125	56.60	278	218
36.70	228	219	41.70	430	436	46.70	216	236	51.70	136	111	56.70	256	219
36.80	290	299	41.80	331	311	46.80	285	239	51.80	90	108	56.80	297	272
36.90	246	234	41.90	242	214	46.90	206	185	51.90	86	107	56.90	331	312
37.00	203	190	42.00	169	153	47.00	168	135	52.00	117	110	57.00	233	262
37.10	279	274	42.10	121	134	47.10	121	118	52.10	110	123	57.10	194	186
37.20	308	320	42.20	120	128	47.20	118	115	52.20	134	136	57.20	149	134
37.30	239	225	42.30	169	142	47.30	110	115	52.30	138	132	57.30	136	117
37.40	156	159	42.40	168	166	47.40	117	118	52.40	142	122	57.40	108	115
37.50	136	149	42.50	161	149	47.50	122	133	52.50	121	113	57.50	113	118
37.60	155	159	42.60	123	122	47.60	229	201	52.60	107	108	57.60	128	117
37.70	203	212	42.70	113	112	47.70	270	318	52.70	100	106	57.70	117	113
37.80	363	417	42.80	119	110	47.80	285	299	52.80	118	108	57.80	107	112
37.90	712	725	42.90	135	109	47.90	227	207	52.90	120	116	57.90	104	111
38.00	939	992	43.00	119	108	48.00	153	142	53.00	123	123	58.00	117	114
38.10	740	713	43.10	119	108	48.10	113	122	53.10	123	123	58.10	136	119
38.20	333	314	43.20	108	112	48.20	101	115	53.20	135	118	58.20	151	135
38.30	183	170	43.30	113	114	48.30	110	114	53.30	140	113	58.30	156	185
38.40	179	142	43.40	104	115	48.40	102	115	53.40	96	110	58.40	337	304
38.50	135	134	43.50	104	120	48.50	128	124	53.50	101	108	58.50	532	433
38.60	136	131	43.60	152	128	48.60	145	154	53.60	88	108	58.60	432	437
38.70	142	131	43.70	119	137	48.70	215	210	53.70	109	109	58.70	332	350
38.80	166	138	43.80	172	164	48.80	234	261	53.80	135	113	58.80	264	297
38.90	170	168	43.90	264	288	48.90	223	249	53.90	110	120	58.90	367	353

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	330	376	64.00	175	184	69.00	134	120	74.00	154	167	79.00	148	141
59.10	291	304	64.10	199	203	69.10	131	133	74.10	170	174	79.10	154	170
59.20	199	205	64.20	218	202	69.20	179	148	74.20	160	176	79.20	193	198
59.30	144	140	64.30	165	176	69.30	187	168	74.30	175	175	79.30	210	200
59.40	125	118	64.40	131	148	69.40	216	186	74.40	163	173	79.40	186	181
59.50	125	113	64.50	143	133	69.50	181	182	74.50	202	177	79.50	144	156
59.60	111	111	64.60	153	133	69.60	167	166	74.60	161	173	79.60	120	131
59.70	103	109	64.70	142	131	69.70	142	152	74.70	172	157	79.70	110	113
59.80	111	108	64.80	132	123	69.80	142	143	74.80	153	139	79.80	106	106
59.90	97	108	64.90	127	113	69.90	144	152	74.90	118	123	79.90	92	104
60.00	128	108	65.00	120	108	70.00	253	203	75.00	94	112	80.00	88	105
60.10	109	110	65.10	138	109	70.10	331	313	75.10	107	107	80.10	107	107
60.20	132	118	65.20	131	118	70.20	413	430	75.20	122	106	80.20	106	110
60.30	132	127	65.30	126	122	70.30	479	469	75.30	108	109	80.30	101	114
60.40	169	147	65.40	127	119	70.40	432	435	75.40	90	115	80.40	129	119
60.50	217	195	65.50	118	112	70.50	280	344	75.50	115	118	80.50	119	121
60.60	268	241	65.60	121	106	70.60	244	247	75.60	113	117	80.60	97	119
60.70	251	230	65.70	112	107	70.70	161	176	75.70	93	114	80.70	107	119
60.80	197	204	65.80	106	112	70.80	159	135	75.80	100	110	80.80	112	124
60.90	201	199	65.90	115	120	70.90	84	116	75.90	105	108	80.90	135	133
61.00	226	250	66.00	136	127	71.00	102	109	76.00	114	108	81.00	151	139
61.10	397	382	66.10	151	133	71.10	114	108	76.10	111	110	81.10	130	139
61.20	556	490	66.20	115	131	71.20	118	113	76.20	97	109	81.20	148	139
61.30	403	434	66.30	111	123	71.30	140	127	76.30	100	109	81.30	129	137
61.40	280	327	66.40	146	116	71.40	132	146	76.40	115	108	81.40	137	129
61.50	218	262	66.50	132	114	71.50	149	151	76.50	109	109	81.50	125	121
61.60	333	284	66.60	121	117	71.60	143	144	76.60	119	114	81.60	99	113
61.70	320	281	66.70	116	117	71.70	123	132	76.70	104	121	81.70	94	107
61.80	276	232	66.80	130	114	71.80	127	120	76.80	135	126	81.80	92	102
61.90	178	170	66.90	101	111	71.90	100	111	76.90	152	131	81.90	85	100
62.00	124	130	67.00	135	112	72.00	104	109	77.00	161	135	82.00	99	99
62.10	112	116	67.10	133	123	72.10	98	113	77.10	125	135	82.10	90	100
62.20	131	115	67.20	136	147	72.20	127	130	77.20	140	129	82.20	111	101
62.30	139	128	67.30	179	169	72.30	202	159	77.30	111	122	82.30	108	103
62.40	174	154	67.40	193	186	72.40	191	178	77.40	105	118	82.40	111	103
62.50	172	169	67.50	226	232	72.50	180	174	77.50	134	121	82.50	103	103
62.60	170	176	67.60	347	293	72.60	166	158	77.60	149	128	82.60	104	104
62.70	186	187	67.70	269	292	72.70	150	145	77.70	148	132	82.70	110	110
62.80	191	188	67.80	248	245	72.80	144	160	77.80	114	133	82.80	127	122
62.90	171	184	67.90	218	186	72.90	222	225	77.90	123	129	82.90	149	136
63.00	213	202	68.00	166	143	73.00	309	309	78.00	139	125	83.00	111	140
63.10	287	252	68.10	127	136	73.10	344	332	78.10	130	126	83.10	121	134
63.20	390	358	68.20	158	157	73.20	271	291	78.20	149	135	83.20	141	125
63.30	549	576	68.30	191	172	73.30	249	230	78.30	145	143	83.30	108	116
63.40	673	736	68.40	175	162	73.40	162	171	78.40	185	144	83.40	96	110
63.50	641	648	68.50	113	143	73.50	130	138	78.50	154	140	83.50	89	109
63.60	431	454	68.60	115	124	73.60	134	127	78.60	135	133	83.60	101	110
63.70	292	266	68.70	113	112	73.70	135	125	78.70	137	128	83.70	87	110
63.80	220	176	68.80	125	109	73.80	151	132	78.80	131	125	83.80	82	110
63.90	156	166	68.90	122	110	73.90	144	149	78.90	131	127	83.90	117	110



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	130	112	89.00	130	125	94.00	142	138	99.00	108	102			
84.10	108	115	89.10	124	121	94.10	163	147	99.10	126	105			
84.20	99	116	89.20	99	118	94.20	149	148	99.20	124	108			
84.30	97	116	89.30	114	119	94.30	165	141	99.30	130	109			
84.40	108	117	89.40	122	123	94.40	123	131	99.40	101	107			
84.50	100	120	89.50	154	130	94.50	131	121	99.50	112	105			
84.60	143	121	89.60	122	136	94.60	103	111	99.60	109	103			
84.70	104	120	89.70	140	141	94.70	123	104	99.70	118	103			
84.80	120	117	89.80	136	144	94.80	106	99	99.80	126	107			
84.90	115	114	89.90	145	145	94.90	107	97	99.90	123	114			
85.00	110	109	90.00	145	150	95.00	102	97	100.00	129	124			
85.10	131	105	90.10	173	162	95.10	93	97						
85.20	107	102	90.20	161	175	95.20	100	99						
85.30	108	100	90.30	180	183	95.30	106	100						
85.40	101	99	90.40	175	186	95.40	119	102						
85.50	106	98	90.50	175	183	95.50	84	104						
85.60	115	99	90.60	192	171	95.60	113	106						
85.70	102	102	90.70	143	154	95.70	118	107						
85.80	107	106	90.80	127	137	95.80	108	107						
85.90	103	108	90.90	99	122	95.90	119	105						
86.00	101	108	91.00	133	111	96.00	107	103						
86.10	103	108	91.10	100	104	96.10	104	101						
86.20	102	106	91.20	102	99	96.20	80	99						
86.30	88	106	91.30	96	97	96.30	108	98						
86.40	95	107	91.40	107	96	96.40	99	97						
86.50	122	109	91.50	98	96	96.50	104	97						
86.60	112	115	91.60	93	97	96.60	91	99						
86.70	113	121	91.70	103	98	96.70	94	104						
86.80	115	124	91.80	105	99	96.80	108	112						
86.90	109	120	91.90	99	101	96.90	129	124						
87.00	112	114	92.00	114	102	97.00	137	138						
87.10	109	108	92.10	93	104	97.10	176	150						
87.20	105	102	92.20	102	105	97.20	152	154						
87.30	102	97	92.30	101	108	97.30	141	153						
87.40	75	95	92.40	105	116	97.40	173	151						
87.50	111	95	92.50	139	129	97.50	143	152						
87.60	98	94	92.60	143	145	97.60	163	155						
87.70	92	95	92.70	176	163	97.70	173	161						
87.80	103	95	92.80	199	183	97.80	167	163						
87.90	90	96	92.90	213	204	97.90	144	161						
88.00	85	96	93.00	204	220	98.00	154	153						
88.10	94	97	93.10	214	229	98.10	147	142						
88.20	92	98	93.20	213	232	98.20	122	130						
88.30	86	100	93.30	214	225	98.30	112	119						
88.40	117	104	93.40	195	206	98.40	117	109						
88.50	116	111	93.50	194	181	98.50	123	103						
88.60	114	119	93.60	165	158	98.60	115	100						
88.70	125	125	93.70	116	140	98.70	93	98						
88.80	118	129	93.80	152	129	98.80	81	98						
88.90	144	128	93.90	128	130	98.90	109	100						

Sample	KCo80													
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	174	152	14.00	148	144	19.00	131	144	24.00	134	132	29.00	220	202
9.10	180	152	14.10	141	144	19.10	155	145	24.10	138	131	29.10	144	145
9.20	176	152	14.20	150	143	19.20	144	147	24.20	142	131	29.20	140	137
9.30	187	151	14.30	135	143	19.30	138	152	24.30	140	131	29.30	150	148
9.40	200	151	14.40	133	143	19.40	165	163	24.40	134	131	29.40	200	210
9.50	189	151	14.50	132	143	19.50	250	217	24.50	146	131	29.50	184	206
9.60	201	265	14.60	128	143	19.60	447	441	24.60	142	131	29.60	183	165
9.70	229	280	14.70	149	143	19.70	409	392	24.70	129	130	29.70	176	162
9.80	296	303	14.80	177	143	19.80	184	195	24.80	132	130	29.80	228	177
9.90	374	338	14.90	118	142	19.90	167	157	24.90	133	130	29.90	308	299
10.00	598	424	15.00	120	142	20.00	151	150	25.00	145	130	30.00	711	741
10.10	1024	758	15.10	143	142	20.10	173	141	25.10	131	130	30.10	601	633
10.20	2267	2410	15.20	126	142	20.20	131	137	25.20	142	130	30.20	263	263
10.30	3284	3214	15.30	130	142	20.30	132	137	25.30	126	130	30.30	179	194
10.40	753	930	15.40	137	142	20.40	139	137	25.40	159	130	30.40	174	165
10.50	275	336	15.50	128	142	20.50	145	140	25.50	141	130	30.50	130	143
10.60	204	205	15.60	144	142	20.60	128	154	25.60	144	149	30.60	125	138
10.70	183	152	15.70	127	141	20.70	159	153	25.70	136	155	30.70	125	137
10.80	150	149	15.80	148	141	20.80	139	139	25.80	149	163	30.80	180	138
10.90	147	148	15.90	128	141	20.90	143	136	25.90	170	179	30.90	154	146
11.00	137	148	16.00	181	141	21.00	156	136	26.00	214	219	31.00	165	173
11.10	149	148	16.10	139	141	21.10	136	136	26.10	441	444	31.10	326	347
11.20	157	148	16.20	156	141	21.20	151	136	26.20	1196	1238	31.20	579	591
11.30	143	148	16.30	131	141	21.30	144	136	26.30	1075	1062	31.30	358	350
11.40	157	148	16.40	150	140	21.40	147	136	26.40	389	435	31.40	185	173
11.50	154	148	16.50	140	140	21.50	158	141	26.50	217	238	31.50	112	147
11.60	147	147	16.60	134	141	21.60	135	157	26.60	258	212	31.60	137	143
11.70	149	147	16.70	151	141	21.70	176	186	26.70	342	293	31.70	126	142
11.80	139	147	16.80	145	141	21.80	171	163	26.80	752	789	31.80	156	146
11.90	148	147	16.90	129	141	21.90	148	152	26.90	930	970	31.90	156	157
12.00	143	147	17.00	154	142	22.00	172	174	27.00	458	382	32.00	221	208
12.10	149	147	17.10	133	145	22.10	311	298	27.10	193	206	32.10	468	513
12.20	151	146	17.20	159	163	22.20	308	326	27.20	176	185	32.20	745	767
12.30	131	146	17.30	186	181	22.30	200	187	27.30	137	180	32.30	412	412
12.40	165	146	17.40	151	158	22.40	153	151	27.40	171	188	32.40	197	217
12.50	149	146	17.50	186	150	22.50	157	146	27.50	185	213	32.50	169	190
12.60	134	146	17.60	148	149	22.60	146	147	27.60	353	304	32.60	175	197
12.70	138	146	17.70	165	151	22.70	174	166	27.70	985	890	32.70	209	230
12.80	149	146	17.80	138	156	22.80	263	272	27.80	2035	2024	32.80	350	370
12.90	123	145	17.90	186	172	22.90	329	313	27.90	1259	1100	32.90	1145	1256
13.00	127	145	18.00	256	261	23.00	169	183	28.00	417	335	33.00	2438	2339
13.10	166	145	18.10	476	464	23.10	162	144	28.10	222	196	33.10	1239	1194
13.20	160	145	18.20	301	313	23.20	150	137	28.20	147	162	33.20	367	355
13.30	151	145	18.30	156	176	23.30	141	134	28.30	139	146	33.30	207	201
13.40	139	145	18.40	144	150	23.40	136	133	28.40	150	138	33.40	145	161
13.50	135	145	18.50	127	143	23.50	131	132	28.50	114	133	33.50	142	143
13.60	155	144	18.60	153	139	23.60	131	132	28.60	117	134	33.60	131	132
13.70	149	144	18.70	141	138	23.70	112	132	28.70	145	143	33.70	138	125
13.80	175	144	18.80	140	137	23.80	136	133	28.80	209	203	33.80	146	123
13.90	109	144	18.90	126	137	23.90	141	133	28.90	278	289	33.90	125	133

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	132	142	39.00	237	271	44.00	569	530	49.00	191	183	54.00	165	159
34.10	113	148	39.10	596	572	44.10	523	533	49.10	132	143	54.10	213	220
34.20	161	163	39.20	695	668	44.20	580	544	49.20	114	125	54.20	256	285
34.30	206	198	39.30	449	399	44.30	642	675	49.30	125	126	54.30	313	295
34.40	311	287	39.40	205	219	44.40	587	598	49.40	131	132	54.40	248	264
34.50	842	814	39.50	159	157	44.50	342	334	49.50	147	153	54.50	245	249
34.60	1295	1268	39.60	144	133	44.60	258	177	49.60	135	162	54.60	241	220
34.70	678	720	39.70	127	126	44.70	227	162	49.70	118	143	54.70	295	291
34.80	279	314	39.80	140	128	44.80	183	169	49.80	139	123	54.80	632	652
34.90	201	228	39.90	142	134	44.90	153	147	49.90	114	117	54.90	710	724
35.00	242	244	40.00	125	129	45.00	143	127	50.00	93	117	55.00	500	514
35.10	345	379	40.10	129	122	45.10	112	121	50.10	117	117	55.10	248	255
35.20	1050	1084	40.20	125	120	45.20	113	119	50.20	111	119	55.20	178	160
35.30	1207	1211	40.30	115	121	45.30	127	121	50.30	128	127	55.30	206	180
35.40	498	511	40.40	126	123	45.40	124	138	50.40	169	176	55.40	228	198
35.50	189	208	40.50	128	133	45.50	174	166	50.50	280	272	55.50	170	177
35.60	145	156	40.60	210	176	45.60	143	152	50.60	240	266	55.60	146	146
35.70	127	139	40.70	255	203	45.70	122	129	50.70	183	193	55.70	128	125
35.80	131	132	40.80	204	171	45.80	126	121	50.80	127	138	55.80	119	117
35.90	145	135	40.90	109	144	45.90	91	122	50.90	103	123	55.90	126	115
36.00	127	138	41.00	144	142	46.00	136	133	51.00	135	123	56.00	125	115
36.10	117	130	41.10	130	154	46.10	187	180	51.10	129	127	56.10	117	118
36.20	133	126	41.20	196	200	46.20	229	204	51.20	158	160	56.20	138	127
36.30	118	126	41.30	291	312	46.30	165	175	51.30	179	211	56.30	179	159
36.40	157	131	41.40	768	733	46.40	178	160	51.40	171	186	56.40	243	228
36.50	155	140	41.50	1019	1016	46.50	208	206	51.50	143	145	56.50	264	235
36.60	165	167	41.60	659	626	46.60	212	226	51.60	128	121	56.60	219	202
36.70	319	268	41.70	379	366	46.70	271	235	51.70	124	117	56.70	266	217
36.80	279	289	41.80	303	292	46.80	193	186	51.80	127	116	56.80	368	339
36.90	225	197	41.90	192	194	46.90	164	141	51.90	121	117	56.90	317	305
37.00	209	189	42.00	149	141	47.00	121	123	52.00	126	128	57.00	244	231
37.10	267	272	42.10	119	129	47.10	130	121	52.10	159	162	57.10	162	149
37.20	266	256	42.20	114	125	47.20	122	120	52.20	157	162	57.20	130	128
37.30	202	178	42.30	150	138	47.30	120	121	52.30	130	143	57.30	122	127
37.40	141	149	42.40	175	161	47.40	104	125	52.40	120	126	57.40	146	144
37.50	124	148	42.50	143	145	47.50	146	146	52.50	117	120	57.50	145	149
37.60	164	159	42.60	126	125	47.60	260	255	52.60	118	116	57.60	142	138
37.70	199	215	42.70	115	119	47.70	354	337	52.70	117	114	57.70	117	125
37.80	401	412	42.80	124	117	47.80	277	266	52.80	133	115	57.80	109	122
37.90	668	728	42.90	126	117	47.90	166	166	52.90	115	121	57.90	138	132
38.00	998	982	43.00	117	117	48.00	134	129	53.00	135	124	58.00	154	131
38.10	653	579	43.10	97	117	48.10	122	121	53.10	118	121	58.10	139	136
38.20	278	236	43.20	103	116	48.20	140	119	53.20	107	119	58.20	138	154
38.30	137	156	43.30	99	119	48.30	110	119	53.30	123	118	58.30	183	174
38.40	144	138	43.40	121	122	48.40	129	120	53.40	119	117	58.40	312	285
38.50	125	135	43.50	130	123	48.50	130	128	53.50	124	115	58.50	500	458
38.60	138	134	43.60	124	128	48.60	153	159	53.60	128	116	58.60	438	443
38.70	148	135	43.70	118	138	48.70	205	215	53.70	117	119	58.70	370	340
38.80	134	141	43.80	173	157	48.80	232	246	53.80	112	127	58.80	329	323
38.90	158	168	43.90	226	254	48.90	221	228	53.90	125	131	58.90	407	408

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	295	328	64.00	185	194	69.00	142	142	74.00	153	166	79.00	171	166
59.10	254	236	64.10	203	208	69.10	176	150	74.10	183	168	79.10	215	218
59.20	156	148	64.20	210	191	69.20	179	171	74.20	162	167	79.20	203	215
59.30	128	124	64.30	133	159	69.30	201	196	74.30	189	173	79.30	164	185
59.40	121	121	64.40	147	137	69.40	214	214	74.40	191	178	79.40	142	168
59.50	144	125	64.50	146	136	69.50	178	184	74.50	235	196	79.50	127	137
59.60	114	126	64.60	161	144	69.60	158	173	74.60	172	193	79.60	117	117
59.70	109	122	64.70	141	138	69.70	167	159	74.70	174	163	79.70	99	112
59.80	135	121	64.80	147	130	69.80	162	146	74.80	140	146	79.80	116	111
59.90	118	120	64.90	120	120	69.90	170	161	74.90	115	128	79.90	103	112
60.00	102	119	65.00	141	122	70.00	265	254	75.00	106	118	80.00	110	115
60.10	116	123	65.10	143	127	70.10	454	438	75.10	98	116	80.10	108	118
60.20	152	140	65.20	148	132	70.20	442	466	75.20	126	119	80.20	113	125
60.30	164	147	65.30	143	126	70.30	406	436	75.30	128	129	80.30	120	132
60.40	194	173	65.40	122	120	70.40	394	396	75.40	112	134	80.40	133	134
60.50	274	255	65.50	148	113	70.50	241	278	75.50	142	127	80.50	110	130
60.60	245	260	65.60	111	111	70.60	190	209	75.60	125	123	80.60	121	126
60.70	215	221	65.70	104	113	70.70	165	158	75.70	126	116	80.70	122	127
60.80	187	179	65.80	125	121	70.80	127	126	75.80	119	112	80.80	137	138
60.90	176	187	65.90	123	131	70.90	110	116	75.90	107	113	80.90	140	141
61.00	224	226	66.00	159	149	71.00	118	113	76.00	123	115	81.00	133	138
61.10	381	379	66.10	168	164	71.10	112	112	76.10	117	113	81.10	148	146
61.20	523	514	66.20	153	152	71.20	141	117	76.20	108	113	81.20	173	157
61.30	401	405	66.30	138	136	71.30	146	135	76.30	127	112	81.30	145	147
61.40	263	305	66.40	132	122	71.40	137	147	76.40	116	111	81.40	133	134
61.50	277	270	66.50	136	115	71.50	144	140	76.50	119	114	81.50	128	127
61.60	300	297	66.60	119	114	71.60	144	135	76.60	134	123	81.60	104	117
61.70	237	243	66.70	137	113	71.70	138	125	76.70	121	134	81.70	107	112
61.80	190	186	66.80	112	113	71.80	109	116	76.80	155	138	81.80	118	112
61.90	127	135	66.90	125	116	71.90	116	113	76.90	135	145	81.90	111	111
62.00	136	120	67.00	140	129	72.00	102	111	77.00	167	152	82.00	100	111
62.10	118	116	67.10	152	153	72.10	111	113	77.10	154	148	82.10	117	114
62.20	124	117	67.20	173	175	72.20	121	127	77.20	165	135	82.20	118	118
62.30	165	132	67.30	170	162	72.30	199	171	77.30	137	128	82.30	118	116
62.40	167	166	67.40	195	165	72.40	209	199	77.40	134	126	82.40	140	114
62.50	184	167	67.50	244	228	72.50	156	181	77.50	149	135	82.50	104	113
62.60	199	179	67.60	306	300	72.60	181	164	77.60	141	142	82.60	125	112
62.70	210	211	67.70	240	251	72.70	147	143	77.70	145	139	82.70	133	113
62.80	171	195	67.80	224	212	72.80	190	164	77.80	143	135	82.80	121	128
62.90	204	191	67.90	157	156	72.90	268	274	77.90	113	131	82.90	171	157
63.00	243	218	68.00	139	131	73.00	386	355	78.00	129	132	83.00	153	164
63.10	310	278	68.10	135	142	73.10	259	295	78.10	163	146	83.10	143	148
63.20	465	462	68.20	175	182	73.20	265	253	78.20	165	159	83.20	148	140
63.30	740	759	68.30	178	179	73.30	167	182	78.30	155	148	83.30	115	129
63.40	654	652	68.40	157	159	73.40	134	138	78.40	155	145	83.40	135	120
63.50	466	476	68.50	122	138	73.50	134	130	78.50	161	140	83.50	94	120
63.60	279	260	68.60	105	119	73.60	128	126	78.60	123	132	83.60	115	121
63.70	172	157	68.70	112	116	73.70	135	125	78.70	129	131	83.70	125	118
63.80	167	146	68.80	129	118	73.80	141	141	78.80	133	133	83.80	110	115
63.90	152	164	68.90	123	128	73.90	150	168	78.90	125	136	83.90	121	115



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	109	119	89.00	138	137	94.00	168	164	99.00	112	115			
84.10	118	124	89.10	134	130	94.10	143	154	99.10	146	123			
84.20	106	123	89.20	114	125	94.20	130	142	99.20	133	130			
84.30	130	126	89.30	119	125	94.30	162	137	99.30	131	129			
84.40	122	138	89.40	122	129	94.40	123	125	99.40	125	123			
84.50	128	142	89.50	134	138	94.50	112	113	99.50	141	121			
84.60	131	134	89.60	144	147	94.60	116	108	99.60	127	119			
84.70	135	132	89.70	141	153	94.70	115	109	99.70	135	118			
84.80	129	129	89.80	139	151	94.80	114	109	99.80	134	126			
84.90	131	124	89.90	142	149	94.90	100	107	99.90	167	141			
85.00	120	124	90.00	175	166	95.00	110	107	100.00	144	149			
85.10	116	124	90.10	189	191	95.10	115	110						
85.20	116	120	90.20	192	194	95.20	136	113						
85.30	114	117	90.30	202	190	95.30	115	117						
85.40	120	113	90.40	200	196	95.40	129	120						
85.50	114	111	90.50	186	183	95.50	126	123						
85.60	103	114	90.60	140	158	95.60	142	126						
85.70	125	122	90.70	118	142	95.70	152	125						
85.80	118	125	90.80	141	129	95.80	116	122						
85.90	91	121	90.90	109	117	95.90	107	119						
86.00	108	120	91.00	97	110	96.00	124	115						
86.10	112	117	91.10	109	108	96.10	112	111						
86.20	105	115	91.20	89	107	96.20	96	109						
86.30	109	120	91.30	105	106	96.30	92	107						
86.40	134	125	91.40	100	106	96.40	108	107						
86.50	121	127	91.50	115	107	96.50	112	108						
86.60	134	135	91.60	114	110	96.60	114	111						
86.70	126	143	91.70	121	115	96.70	125	116						
86.80	116	137	91.80	135	119	96.80	120	128						
86.90	121	129	91.90	128	122	96.90	140	150						
87.00	114	123	92.00	133	122	97.00	192	168						
87.10	117	115	92.10	106	120	97.10	159	166						
87.20	117	109	92.20	111	121	97.20	158	159						
87.30	98	106	92.30	112	123	97.30	162	160						
87.40	125	105	92.40	146	137	97.40	166	157						
87.50	107	105	92.50	182	159	97.50	170	154						
87.60	100	105	92.60	171	171	97.60	191	166						
87.70	112	105	92.70	194	190	97.70	190	185						
87.80	111	105	92.80	233	225	97.80	174	183						
87.90	119	106	92.90	207	232	97.90	156	169						
88.00	94	106	93.00	189	224	98.00	169	164						
88.10	93	107	93.10	244	239	98.10	153	158						
88.20	115	109	93.20	246	243	98.20	165	140						
88.30	116	114	93.30	189	207	98.30	118	128						
88.40	104	124	93.40	182	175	98.40	131	123						
88.50	127	133	93.50	175	160	98.50	115	118						
88.60	130	141	93.60	145	139	98.60	145	112						
88.70	147	147	93.70	118	123	98.70	107	111						
88.80	143	142	93.80	129	127	98.80	144	111						
88.90	130	137	93.90	169	148	98.90	103	112						

Sample	KCo100													
2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
9.00	155	124	14.00	99	117	19.00	109	116	24.00	112	107	29.00	144	141
9.10	179	124	14.10	131	117	19.10	121	117	24.10	104	107	29.10	110	114
9.20	153	124	14.20	122	117	19.20	105	118	24.20	111	107	29.20	123	111
9.30	157	123	14.30	110	117	19.30	126	121	24.30	110	107	29.30	130	122
9.40	167	123	14.40	116	117	19.40	140	129	24.40	110	106	29.40	160	169
9.50	148	200	14.50	116	116	19.50	167	170	24.50	78	106	29.50	127	157
9.60	171	207	14.60	109	116	19.60	309	307	24.60	94	106	29.60	119	128
9.70	177	219	14.70	108	116	19.70	267	261	24.70	108	106	29.70	133	125
9.80	242	237	14.80	114	116	19.80	143	150	24.80	103	106	29.80	188	133
9.90	330	266	14.90	105	116	19.90	131	139	24.90	109	106	29.90	221	208
10.00	543	339	15.00	114	116	20.00	163	143	25.00	100	106	30.00	461	450
10.10	802	658	15.10	117	116	20.10	111	122	25.10	105	106	30.10	376	351
10.20	1776	1922	15.20	119	116	20.20	106	113	25.20	96	106	30.20	167	167
10.30	2503	2415	15.30	116	115	20.30	117	111	25.30	115	106	30.30	165	137
10.40	706	816	15.40	106	115	20.40	105	111	25.40	101	106	30.40	123	121
10.50	232	287	15.50	106	115	20.50	99	112	25.50	128	106	30.50	125	112
10.60	146	176	15.60	127	115	20.60	116	117	25.60	124	118	30.60	115	111
10.70	145	132	15.70	108	115	20.70	91	115	25.70	121	123	30.70	77	111
10.80	138	121	15.80	107	115	20.80	107	111	25.80	155	128	30.80	112	113
10.90	138	121	15.90	115	115	20.90	109	110	25.90	143	140	30.90	105	121
11.00	120	121	16.00	96	115	21.00	106	110	26.00	185	169	31.00	147	150
11.10	118	121	16.10	117	115	21.10	113	110	26.10	342	328	31.10	290	320
11.20	126	121	16.20	106	114	21.20	125	110	26.20	808	857	31.20	433	434
11.30	138	120	16.30	111	114	21.30	97	111	26.30	778	714	31.30	239	225
11.40	138	120	16.40	113	114	21.40	113	111	26.40	293	312	31.40	132	130
11.50	130	120	16.50	106	114	21.50	104	116	26.50	185	179	31.50	109	117
11.60	129	120	16.60	111	115	21.60	118	131	26.60	162	161	31.60	94	115
11.70	124	120	16.70	100	115	21.70	140	156	26.70	210	220	31.70	115	115
11.80	122	120	16.80	119	115	21.80	119	132	26.80	494	529	31.80	126	118
11.90	113	120	16.90	105	116	21.90	125	120	26.90	583	524	31.90	132	127
12.00	148	120	17.00	119	117	22.00	137	130	27.00	203	215	32.00	180	172
12.10	130	119	17.10	115	122	22.10	177	191	27.10	136	146	32.10	386	413
12.20	147	119	17.20	141	144	22.20	219	207	27.20	119	139	32.20	482	492
12.30	115	119	17.30	164	165	22.30	144	137	27.30	130	139	32.30	274	248
12.40	127	119	17.40	145	144	22.40	112	118	27.40	136	146	32.40	111	159
12.50	116	119	17.50	103	127	22.50	112	115	27.50	165	168	32.50	127	149
12.60	115	119	17.60	106	123	22.60	115	116	27.60	339	251	32.60	141	158
12.70	111	119	17.70	105	124	22.70	120	127	27.70	826	751	32.70	163	187
12.80	134	119	17.80	134	129	22.80	187	183	27.80	1287	1323	32.80	274	307
12.90	130	118	17.90	136	144	22.90	221	201	27.90	652	589	32.90	991	1027
13.00	102	118	18.00	219	227	23.00	141	134	28.00	241	212	33.00	1686	1647
13.10	117	118	18.10	412	416	23.10	130	114	28.10	165	146	33.10	814	747
13.20	101	118	18.20	295	281	23.20	116	110	28.20	111	126	33.20	229	246
13.30	140	118	18.30	122	150	23.30	104	109	28.30	113	117	33.30	167	157
13.40	125	118	18.40	103	125	23.40	104	108	28.40	115	111	33.40	115	129
13.50	137	118	18.50	116	118	23.50	118	107	28.50	132	108	33.50	118	116
13.60	150	118	18.60	115	114	23.60	113	107	28.60	121	109	33.60	105	109
13.70	125	117	18.70	88	112	23.70	135	107	28.70	117	116	33.70	101	103
13.80	124	117	18.80	111	112	23.80	96	108	28.80	176	161	33.80	110	101
13.90	124	117	18.90	121	114	23.90	124	107	28.90	217	201	33.90	103	110

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
34.00	113	117	39.00	207	225	44.00	441	440	49.00	137	120	54.00	117	135
34.10	118	124	39.10	460	424	44.10	430	424	49.10	104	105	54.10	171	170
34.20	135	140	39.20	494	460	44.20	426	451	49.20	93	100	54.20	214	217
34.30	171	180	39.30	296	291	44.30	547	523	49.30	105	101	54.30	211	206
34.40	257	269	39.40	181	175	44.40	411	389	49.40	99	106	54.40	208	198
34.50	854	764	39.50	139	127	44.50	220	211	49.50	96	120	54.50	215	204
34.60	956	1006	39.60	106	109	44.60	124	131	49.60	116	117	54.60	219	199
34.70	485	513	39.70	108	104	44.70	117	118	49.70	98	107	54.70	258	294
34.80	243	236	39.80	111	103	44.80	129	112	49.80	96	98	54.80	496	518
34.90	183	181	39.90	110	102	44.90	96	105	49.90	101	97	54.90	447	445
35.00	198	189	40.00	100	100	45.00	117	101	50.00	87	97	55.00	313	300
35.10	269	292	40.10	106	99	45.10	98	99	50.10	95	98	55.10	170	168
35.20	806	848	40.20	111	99	45.20	99	99	50.20	112	101	55.20	124	138
35.30	900	926	40.30	107	100	45.30	104	102	50.30	90	111	55.30	182	158
35.40	380	386	40.40	103	102	45.40	103	123	50.40	163	161	55.40	150	150
35.50	165	168	40.50	130	112	45.50	139	137	50.50	213	203	55.50	109	137
35.60	136	129	40.60	160	148	45.60	122	121	50.60	183	178	55.60	119	114
35.70	114	116	40.70	162	162	45.70	105	104	50.70	126	131	55.70	99	104
35.80	117	110	40.80	144	136	45.80	87	101	50.80	109	107	55.80	111	98
35.90	125	114	40.90	111	118	45.90	111	103	50.90	108	103	55.90	113	97
36.00	123	111	41.00	128	119	46.00	104	118	51.00	95	105	56.00	123	99
36.10	118	105	41.10	139	132	46.10	154	162	51.10	101	112	56.10	106	102
36.20	93	103	41.20	187	178	46.20	154	159	51.20	145	150	56.20	131	114
36.30	120	103	41.30	275	278	46.30	138	134	51.30	153	171	56.30	163	154
36.40	114	106	41.40	704	664	46.40	132	129	51.40	129	146	56.40	186	198
36.50	120	114	41.50	711	725	46.50	155	153	51.50	110	112	56.50	196	176
36.60	166	147	41.60	410	407	46.60	149	158	51.60	94	100	56.60	175	159
36.70	231	241	41.70	264	260	46.70	160	150	51.70	90	98	56.70	221	207
36.80	236	213	41.80	192	203	46.80	144	124	51.80	86	98	56.80	243	269
36.90	140	148	41.90	131	140	46.90	127	104	51.90	91	101	56.90	205	219
37.00	153	172	42.00	124	113	47.00	106	100	52.00	98	120	57.00	156	156
37.10	225	210	42.10	106	106	47.10	111	100	52.10	143	147	57.10	125	114
37.20	189	177	42.20	110	102	47.20	83	101	52.20	124	132	57.20	89	105
37.30	125	133	42.30	114	110	47.30	93	103	52.30	120	113	57.30	112	107
37.40	131	119	42.40	132	121	47.40	101	108	52.40	110	103	57.40	104	116
37.50	111	121	42.50	126	111	47.50	138	138	52.50	85	100	57.50	114	113
37.60	127	131	42.60	116	100	47.60	275	247	52.60	100	98	57.60	100	106
37.70	210	182	42.70	112	98	47.70	246	250	52.70	77	96	57.70	121	101
37.80	286	320	42.80	111	97	47.80	195	181	52.80	84	98	57.80	110	101
37.90	584	593	42.90	94	97	47.90	113	121	52.90	103	106	57.90	101	107
38.00	664	666	43.00	109	96	48.00	134	104	53.00	112	107	58.00	118	108
38.10	353	345	43.10	100	96	48.10	100	100	53.10	94	103	58.10	122	115
38.20	188	160	43.20	106	96	48.20	98	99	53.20	98	99	58.20	113	126
38.30	126	122	43.30	105	96	48.30	89	99	53.30	101	99	58.30	142	147
38.40	107	111	43.40	102	100	48.40	111	100	53.40	90	98	58.40	281	249
38.50	103	109	43.50	93	103	48.50	125	106	53.50	101	98	58.50	429	387
38.60	102	110	43.60	113	107	48.60	143	131	53.60	100	98	58.60	354	356
38.70	129	111	43.70	118	117	48.70	154	163	53.70	99	100	58.70	294	288
38.80	118	117	43.80	145	135	48.80	186	168	53.80	112	104	58.80	267	294
38.90	132	141	43.90	207	216	48.90	140	147	53.90	113	110	58.90	232	282

2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
59.00	233	225	64.00	165	158	69.00	111	117	74.00	133	133	79.00	189	159
59.10	163	154	64.10	177	153	69.10	128	130	74.10	141	135	79.10	191	171
59.20	125	115	64.20	151	144	69.20	173	144	74.20	127	134	79.20	159	154
59.30	113	104	64.30	137	122	69.30	148	161	74.30	145	144	79.30	136	141
59.40	106	102	64.40	108	113	69.40	146	156	74.40	142	152	79.40	114	122
59.50	114	103	64.50	115	114	69.50	128	143	74.50	177	164	79.50	90	105
59.60	87	101	64.60	110	116	69.60	140	135	74.60	131	157	79.60	108	98
59.70	100	100	64.70	117	111	69.70	131	126	74.70	124	138	79.70	124	96
59.80	109	100	64.80	99	106	69.80	119	130	74.80	102	123	79.80	73	96
59.90	85	99	64.90	105	103	69.90	163	165	74.90	117	110	79.90	103	97
60.00	133	100	65.00	108	105	70.00	264	259	75.00	99	103	80.00	95	100
60.10	95	106	65.10	108	105	70.10	325	327	75.10	110	102	80.10	97	103
60.20	126	123	65.20	114	104	70.20	312	316	75.20	104	106	80.20	104	107
60.30	145	130	65.30	112	100	70.30	273	299	75.30	72	110	80.30	107	108
60.40	164	161	65.40	83	97	70.40	262	264	75.40	126	107	80.40	95	108
60.50	215	200	65.50	99	95	70.50	196	199	75.50	113	104	80.50	111	105
60.60	185	175	65.60	94	96	70.60	167	162	75.60	88	100	80.60	91	105
60.70	150	153	65.70	117	98	70.70	118	128	75.70	109	96	80.70	134	109
60.80	168	136	65.80	131	104	70.80	107	108	75.80	88	96	80.80	114	112
60.90	167	151	65.90	97	115	70.90	97	102	75.90	89	96	80.90	121	113
61.00	174	186	66.00	144	132	71.00	95	100	76.00	69	96	81.00	133	116
61.10	295	292	66.10	141	133	71.10	86	99	76.10	111	95	81.10	140	121
61.20	388	363	66.20	128	122	71.20	107	103	76.20	83	96	81.20	111	120
61.30	292	296	66.30	119	109	71.30	112	111	76.30	95	95	81.30	99	112
61.40	227	245	66.40	94	101	71.40	109	114	76.40	101	97	81.40	104	107
61.50	260	243	66.50	100	99	71.50	126	112	76.50	109	101	81.50	89	101
61.60	202	218	66.60	117	98	71.60	116	109	76.60	129	108	81.60	98	97
61.70	203	182	66.70	126	98	71.70	119	103	76.70	114	113	81.70	89	96
61.80	129	135	66.80	96	99	71.80	98	99	76.80	119	117	81.80	106	95
61.90	105	111	66.90	109	105	71.90	95	98	76.90	122	123	81.90	89	94
62.00	115	104	67.00	141	121	72.00	103	98	77.00	119	126	82.00	92	95
62.10	94	101	67.10	125	141	72.10	117	102	77.10	143	119	82.10	102	97
62.20	104	103	67.20	137	140	72.20	125	115	77.20	110	113	82.20	91	97
62.30	112	117	67.30	107	135	72.30	160	143	77.30	108	108	82.30	87	96
62.40	135	136	67.40	151	146	72.40	158	159	77.40	107	109	82.40	88	96
62.50	149	136	67.50	241	195	72.50	141	149	77.50	115	113	82.50	95	95
62.60	155	154	67.60	190	206	72.60	131	139	77.60	102	113	82.60	103	96
62.70	188	173	67.70	168	179	72.70	135	134	77.70	114	111	82.70	115	100
62.80	161	163	67.80	171	149	72.80	163	165	77.80	103	110	82.80	110	111
62.90	175	168	67.90	132	120	72.90	259	230	77.90	145	111	82.90	104	126
63.00	247	200	68.00	113	113	73.00	230	235	78.00	124	120	83.00	133	127
63.10	303	277	68.10	116	127	73.10	201	204	78.10	128	129	83.10	98	120
63.20	443	466	68.20	138	148	73.20	174	171	78.20	97	126	83.20	108	115
63.30	483	513	68.30	154	137	73.30	122	132	78.30	115	122	83.30	100	108
63.40	426	412	68.40	129	127	73.40	121	116	78.40	125	118	83.40	86	103
63.50	268	271	68.50	117	110	73.50	109	112	78.50	110	114	83.50	88	101
63.60	185	165	68.60	94	102	73.60	105	110	78.60	124	113	83.60	107	100
63.70	136	131	68.70	92	101	73.70	111	115	78.70	143	117	83.70	105	99
63.80	143	132	68.80	102	105	73.80	166	129	78.80	106	121	83.80	99	98
63.90	151	143	68.90	128	112	73.90	158	136	78.90	132	134	83.90	96	98



2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc	2theta	lobs	lcalc
84.00	96	100	89.00	107	107	94.00	113	123	99.00	114	101			
84.10	107	101	89.10	100	104	94.10	101	117	99.10	97	104			
84.20	99	103	89.20	109	103	94.20	81	112	99.20	109	105			
84.30	105	108	89.30	92	104	94.30	112	104	99.30	97	104			
84.40	108	111	89.40	115	108	94.40	112	97	99.40	131	102			
84.50	118	108	89.50	102	116	94.50	95	93	99.50	114	102			
84.60	89	106	89.60	107	122	94.60	103	92	99.60	112	104			
84.70	117	105	89.70	120	126	94.70	86	92	99.70	109	109			
84.80	112	103	89.80	121	129	94.80	88	92	99.80	122	116			
84.90	97	101	89.90	114	137	94.90	104	91	99.90	125	122			
85.00	103	100	90.00	167	151	95.00	99	92	100.00	131	126			
85.10	97	99	90.10	158	157	95.10	99	93						
85.20	89	97	90.20	152	157	95.20	114	95						
85.30	91	95	90.30	172	157	95.30	112	97						
85.40	112	94	90.40	155	150	95.40	119	100						
85.50	96	95	90.50	142	135	95.50	119	102						
85.60	89	97	90.60	111	122	95.60	104	103						
85.70	83	99	90.70	100	111	95.70	101	102						
85.80	116	98	90.80	102	102	95.80	116	101						
85.90	110	98	90.90	100	96	95.90	97	99						
86.00	95	97	91.00	93	94	96.00	88	97						
86.10	100	96	91.10	104	93	96.10	102	95						
86.20	98	97	91.20	80	92	96.20	102	93						
86.30	87	100	91.30	88	93	96.30	94	93						
86.40	85	102	91.40	121	93	96.40	104	94						
86.50	109	104	91.50	95	94	96.50	97	96						
86.60	102	108	91.60	80	97	96.60	107	100						
86.70	98	108	91.70	94	100	96.70	92	109						
86.80	113	104	91.80	96	102	96.80	134	121						
86.90	111	100	91.90	106	102	96.90	171	132						
87.00	104	97	92.00	104	102	97.00	144	135						
87.10	95	93	92.10	98	103	97.10	133	133						
87.20	79	91	92.20	93	107	97.20	139	132						
87.30	95	90	92.30	133	114	97.30	118	129						
87.40	89	90	92.40	115	128	97.40	113	127						
87.50	100	90	92.50	126	141	97.50	130	131						
87.60	91	90	92.60	183	154	97.60	165	140						
87.70	88	90	92.70	189	171	97.70	141	144						
87.80	84	91	92.80	194	176	97.80	125	139						
87.90	86	92	92.90	158	175	97.90	138	133						
88.00	91	92	93.00	163	178	98.00	125	127						
88.10	98	94	93.10	193	179	98.10	83	118						
88.20	117	98	93.20	171	164	98.20	109	110						
88.30	126	104	93.30	125	147	98.30	102	104						
88.40	106	110	93.40	152	134	98.40	98	99						
88.50	113	114	93.50	116	123	98.50	97	96						
88.60	103	118	93.60	122	114	98.60	99	95						
88.70	102	117	93.70	121	114	98.70	85	95						
88.80	119	113	93.80	148	121	98.80	98	96						
88.90	117	111	93.90	120	127	98.90	113	98						