Observed and Calculated Step Intensities for Deposit

Della Ventura, G., Robert, J.-L., Beny, J.-M., Raudsepp, M. and Hawthorne, F.C. The O–HF substitution in synthetic Ti-rich potassium-richterites: Rietveld structure refinement and FTIR and microraman spectroscopic studies of synthetic amphiboles in the system K_2O–Na_2O–CaO–MgO– SiO_2–TiO_2–H_2O–HF.

Sample Rich58

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
9.00	95	77	15.00	66	74	21.00	59	71	27.00	1726	1766
9.10	101	80	15.10	62	74	21.10	66	71	27.10	460	472
9.20	115	80	15.20	59	74	21.20	66	71	27.20	189	189
9.30	131	80	15.30	77	74	21.30	57	71	27.30	122	147
9.40	105	82	15.40	58	74	21.40	60	75	27.40	116	133
9.50	139	84	15.50	73	74	21.50	60	78	27.50	142	137
9.60	140	115	15.60	67	74	21.60	65	81	27.60	200	163
9.70	169	202	15.70	78	74	21.70	70	85	27.70	386	305
9.80	267	261	15.80	75	74	21.80	76	90	27.80	1203	1167
9.90	175	156	15.90	64	73	21.90	109	115	27.90	2453	2229
10.00	210	127	16.00	74	73	22.00	287	282	28.00	1263	1185
10.10	350	197	16.10	85	73	22.10	591	620	28.10	318	314
10.20	626	656	16.20	62	73	22.20	425	415	28.20	152	149
10.30	1140	1189	16.30	54	73	22.30	142	152	28.30	106	120
10.40	527	523	16.40	62	73	22.40	98	102	28.40	118	104
10.50	141	153	16.50	56	73	22.50	79	99	28.50	75	92
10.60	114	100	16.60	73	73	22.60	145	121	28.60	75	91
10.70	84	87	16.70	76	73	22.70	308	290	28.70	127	101
10.80	93	80	16.80	77	73	22.80	660	652	28.80	221	217
10.90	96	77	16.90	65	73	22.90	485	449	28.90	443	472
11.00	98	76	17.00	85	74	23.00	162	155	29.00	336	363
11.10	86	76	17.10	64	75	23.10	94	93	29.10	155	144
11.20	91	76	17.20	67	83	23.20	76	82	29.20	108	89
11.30	100	76	17.30	64	96	23.30	72	78	29.30	98	99
11.40	103	76	17.40	78	86	23.40	68	76	29.40	104	124
11.50	72	76	17.50	84	81	23.50	50	75	29.50	98	127
11.60	96	76	17.60	68	81	23.60	77	76	29.60	115	131
11.70	102	76	17.70	90	85	23.70	81	98	29.70	175	156
11.80	78	76	17.80	95	96	23.80	155	166	29.80	254	226
11.90	86	76	17.90	185	170	23.90	148	157	29.90	645	697
12.00	92	76	18.00	373	363	24.00	92	93	30.00	1954	2061
12.10	89	76	18.10	443	371	24.10	76	75	30.10	1878	1924
12.20	82	75	18.20	430	319	24.20	86	72	30.20	945	927
12.30	93	75	18.30	202	168	24.30	67	71	30.30	903	888
12.40	74	75	18.40	89	93	24.40	67	70	30.40	477	530
12.50	83	75	18.50	71	80	24.50	62	70	30.50	195	194
12.60	78	75	18.60	50	76	24.60	53	70	30.60	111	119
12.70	87	75	18.70	60	74	24.70	81	69	30.70	96	104
12.80	71	75	18.80	66	73	24.80	66	69	30.80	108	93
12.90	70	75	18.90	69	72	24.90	67	69	30.90	95	94
13.00	78	75	19.00	72	79	25.00	73	69	31.00	117	107
13.10	88	75	19.10	72	81	25.10	78	69	31.10	202	184
13.20	82	75	19.20	72	84	25.20	85	69	31.20	560	575
13.30	71	75	19.30	77	89	25.30	82	69	31.30	946	898
13.40	82	75	19.40	110	104	25.40	100	69	31.40	417	461
13.50	71	75	19.50	210	202	25.50	83	91	31.50	164	167
13.60	85	75	19.60	665	583	25.60	112	108	31.60	119	117
13.70	79	75	19.70	710	642	25.70	110	121	31.70	98	110
13.80	78	75	19.80	246	235	25.80	136	143	31.80	126	115
13.90	65	75	19.90	139	107	25.90	203	189	31.90	119	136
14.00	77	74	20.00	77	87	26.00	461	388	32.00	251	226
14.10	87	74	20.10	70	79	26.10	1482	1570	32.10	721	790
14.20	74	74	20.20	69	76	26.20	3425	3328	32.20	1748	1761
14.30	65	74	20.30	51	74	26.30	1866	1951	32.30	1198	1208
14.40	72	74	20.40	59	72	26.40	467	558	32.40	344	399
14.50	78	74	20.50	66	72	26.50	241	251	32.50	186	204
14.60	64	74	20.60	63	75	26.60	182	218	32.60	164	194
14.70	62	74	20.70	59	80	26.70	345	315	32.70	237	245
14.80	76	74	20.80	64	76	26.80	1003	1084	32.80	582	589
14.90	74	74	20.90	71	72	26.90	2641	2640	32.90	2096	2231

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
33.00	3435	3383	39.00	759	784	45.00	124	127	51.00	127	119
33.10	1619	1622	39.10	1587	1534	45.10	88	89	51.10	117	111
33.20	416	422	39.20	1152	1086	45.20	96	76	51.20	111	117
33.30	177	184	39.30	427	405	45.30	74	71	51.30	122	148
33.40	134	129	39.40	198	212	45.40	78	70	51.40	139	128

33.50	111	104	39.50	143	150	45.50	74	80	51.50	94	95
33.60	101	90	39.60	99	103	45.60	91	85	51.60	52	72
33.70	90	73	39.70	97	86	45.70	83	80	51.70	60	66
33.80	87	67	39.80	97	88	45.80	84	79	51.80	69	65
33.90	81	86	39.90	121	112	45.90	95	87	51.90	71	64
34.00	115	96	40.00	112	114	46.00	118	105	52.00	62	67
34.10	121	127	40.10	110	92	46.10	216	203	52.10	95	79
34.20	145	153	40.20	83	83	46.20	417	373	52.20	98	85
34.30	183	171	40.30	105	95	46.30	368	378	52.30	96	78
34.40	373	402	40.40	193	167	46.40	323	347	52.40	91	68
34.50	1373	1291	40.50	442	388	46.50	318	320	52.50	69	64
34.60	1567	1594	40.60	450	472	46.60	258	232	52.60	67	64
34.70	766	761	40.70	305	272	46.70	190	201	52.70	71	67
34.80	349	331	40.80	117	130	46.80	397	435	52.80	97	80
34.90	498	434	40.90	96	102	46.90	637	601	52.90	102	94
35.00	1241	1273	41.00	81	105	47.00	419	405	53.00	90	92
35.10	2499	2606	41.10	100	122	47.10	178	173	53.10	86	88
35.20	1888	1862	41.20	167	185	47.20	81	97	53.20	68	79
35.30	582	585	41.30	344	328	47.30	92	83	53.30	84	75
35.40	188	199	41.40	900	818	47.40	85	80	53.40	79	79
35.50	115	129	41.50	1482	1475	47.50	100	84	53.50	87	81
35.60	113	103	41.60	1177	1205	47.60	119	121	53.60	83	87
35.70	124	90	41.70	631	650	47.70	242	256	53.70	104	96
35.80	82	83	41.80	339	301	47.80	278	292	53.80	104	111
35.90	77	83	41.90	166	148	47.90	217	202	53.90	130	115
36.00	88	100	42.00	108	111	48.00	113	110	54.00	161	148
36.10	108	92	42.10	131	121	48.10	69	84	54.10	265	297
36.20	76	76	42.20	200	213	48.20	88	79	54.20	538	584
36.30	93	73	42.30	307	280	48.30	64	79	54.30	603	614
36.40	108	87	42.40	176	190	48.40	82	91	54.40	414	425
36.50	157	130	42.50	103	99	48.50	151	131	54.50	271	255
36.60	118	132	42.60	89	74	48.60	220	197	54.60	304	303
36.70	103	113	42.70	75	69	48.70	360	371	54.70	411	391
36.80	137	154	42.80	59	67	48.80	462	487	54.80	485	512
36.90	222	219	42.90	65	66	48.90	367	356	54.90	1041	1003
37.00	279	257	43.00	61	65	49.00	231	216	55.00	942	987
37.10	409	366	43.10	71	64	49.10	209	225	55.10	699	663
37.20	662	587	43.20	68	68	49.20	198	210	55.20	298	278
37.30	427	474	43.30	85	71	49.30	167	162	55.30	148	152
37.40	198	220	43.40	72	74	49.40	103	109	55.40	225	198
37.50	115	134	43.50	89	81	49.50	88	84	55.50	317	278
37.60	126	135	43.60	104	91	49.60	81	90	55.60	259	227
37.70	193	190	43.70	113	117	49.70	82	93	55.70	173	155
37.80	536	510	43.80	237	249	49.80	71	82	55.80	102	99
37.90	1095	1235	43.90	561	628	49.90	80	71	55.90	84	80
38.00	1585	1552	44.00	612	658	50.00	70	68	56.00	98	78
38.10	969	979	44.10	524	493	50.10	56	68	56.10	100	86
38.20	367	358	44.20	587	533	50.20	72	71	56.20	105	84
38.30	147	147	44.30	534	504	50.30	86	78	56.30	91	78
38.40	106	115	44.40	502	493	50.40	122	114	56.40	101	77
38.50	84	108	44.50	340	346	50.50	277	248	56.50	130	97
38.60	102	106	44.60	185	180	50.60	334	334	56.60	207	170
38.70	117	111	44.70	131	115	50.70	241	250	56.70	239	223
38.80	141	131	44.80	164	151	50.80	155	140	56.80	320	312
38.90	228	235	44.90	174	172	50.90	111	107	56.90	483	378

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
57.00	293	277	63.00	285	284	69.00	97	76	75.00	53	68
57.10	204	180	63.10	250	242	69.10	115	102	75.10	73	63
57.20	116	119	63.20	255	211	69.20	202	150	75.20	74	61
57.30	103	99	63.30	338	271	69.30	197	179	75.30	62	62
57.40	117	94	63.40	723	703	69.40	271	233	75.40	71	66
57.50	103	95	63.50	1054	1059	69.50	210	222	75.50	89	86
57.60	94	106	63.60	810	773	69.60	185	192	75.60	117	116
57.70	91	104	63.70	528	511	69.70	156	157	75.70	103	109
57.80	82	94	63.80	254	226	69.80	159	137	75.80	128	106
57.90	110	90	63.90	201	197	69.90	146	154	75.90	76	88
58.00	107	100	64.00	222	255	70.00	252	257	76.00	67	77
58.10	174	166	64.10	214	241	70.10	402	402	76.10	79	76

58.20	460	440	64.20	263	231	70.20	553	572	76.20	81	84
58.30	630	646	64.30	201	163	70.30	659	670	76.30	98	96
58.40	525	541	64.40	187	172	70.40	570	595	76.40	106	98
58.50	370	380	64.50	171	183	70.50	456	437	76.50	106	102
58.60	300	304	64.60	140	147	70.60	285	287	76.60	124	125
58.70	245	235	64.70	113	122	70.70	179	162	76.70	110	121
58.80	278	252	64.80	108	103	70.80	113	111	76.80	115	124
58.90	478	477	64.90	90	96	70.90	72	86	76.90	97	109
59.00	607	588	65.00	89	86	71.00	73	81	77.00	94	99
59.10	495	436	65.10	93	77	71.10	91	88	77.10	118	112
59.20	278	240	65.20	90	74	71.20	112	106	77.20	129	124
59.30	126	120	65.30	106	94	71.30	97	104	77.30	100	108
59.40	104	92	65.40	140	123	71.40	120	108	77.40	119	113
59.50	97	91	65.50	109	108	71.50	162	146	77.50	122	124
59.60	88	92	65.60	125	108	71.60	192	165	77.60	150	161
59.70	81	83	65.70	97	102	71.70	158	150	77.70	125	147
59.80	95	72	65.80	95	94	71.80	143	145	77.80	102	128
59.90	72	67	65.90	121	103	71.90	189	173	77.90	110	112
60.00	73	71	66.00	93	93	72.00	269	255	78.00	83	87
60.10	85	72	66.10	97	94	72.10	241	242	78.10	74	74
60.20	87	72	66.20	111	92	72.20	205	223	78.20	68	74
60.30	91	79	66.30	85	87	72.30	155	165	78.30	75	75
60.40	106	92	66.40	77	77	72.40	118	134	78.40	94	98
60.50	130	130	66.50	58	70	72.50	174	156	78.50	163	136
60.60	239	232	66.60	61	70	72.60	172	177	78.60	137	121
60.70	355	340	66.70	99	88	72.70	187	181	78.70	121	119
60.80	424	436	66.80	106	95	72.80	314	300	78.80	105	117
60.90	765	761	66.90	110	89	72.90	582	573	78.90	109	106
61.00	1056	1062	67.00	86	86	73.00	670	643	79.00	126	116
61.10	799	850	67.10	82	81	73.10	443	466	79.10	162	169
61.20	538	546	67.20	78	82	73.20	372	367	79.20	225	237
61.30	258	262	67.30	95	99	73.30	178	196	79.30	155	180
61.40	158	160	67.40	149	158	73.40	135	134	79.40	142	165
61.50	188	199	67.50	255	235	73.50	117	122	79.50	141	137
61.60	445	403	67.60	368	404	73.60	131	141	79.60	89	98
61.70	417	406	67.70	363	419	73.70	162	165	79.70	65	82
61.80	334	312	67.80	305	307	73.80	202	189	79.80	71	87
61.90	188	176	67.90	212	217	73.90	222	216	79.90	81	90
62.00	114	100	68.00	156	154	74.00	236	241	80.00	66	77
62.10	96	84	68.10	169	197	74.10	266	234	80.10	81	75
62.20	82	86	68.20	175	174	74.20	282	273	80.20	64	74
62.30	140	118	68.30	153	146	74.30	220	221	80.30	60	78
62.40	222	222	68.40	113	107	74.40	169	165	80.40	55	85
62.50	259	243	68.50	92	86	74.50	129	132	80.50	87	91
62.60	246	214	68.60	92	93	74.60	78	96	80.60	72	82
62.70	211	196	68.70	90	86	74.70	87	82	80.70	71	79
62.80	204	217	68.80	88	82	74.80	92	80	80.80	76	77
62.90	203	248	68.90	74	75	74.90	75	71	80.90	85	96

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
81.00	130	152	87.00	81	88	93.00	154	171	99.00	59	64
81.10	127	149	87.10	81	68	93.10	258	252	99.10	63	61
81.20	151	136	87.20	53	62	93.20	276	274	99.20	53	56
81.30	160	161	87.30	53	59	93.30	301	307	99.30	69	54
81.40	113	122	87.40	52	57	93.40	273	264	99.40	65	55
81.50	83	101	87.50	62	59	93.50	179	198	99.50	67	58
81.60	100	106	87.60	56	59	93.60	182	177	99.60	63	58
81.70	75	86	87.70	56	57	93.70	132	131	99.70	65	54
81.80	60	76	87.80	64	58	93.80	84	95	99.80	67	52
81.90	86	77	87.90	59	59	93.90	79	80	99.90	71	52
82.00	71	73	88.00	61	59	94.00	77	81	100.00	91	49
82.10	59	69	88.10	54	60	94.10	82	95			
82.20	64	74	88.20	75	68	94.20	140	136			
82.30	99	83	88.30	58	69	94.30	198	182			
82.40	87	86	88.40	60	67	94.40	166	153			
82.50	99	108	88.50	76	73	94.50	124	123			
82.60	153	168	88.60	74	85	94.60	112	125			
82.70	150	159	88.70	109	108	94.70	113	101			
82.80	105	123	88.80	126	121	94.80	83	77			

82.90	116	122	88.90	126	118	94.90	70	76
83.00	97	92	89.00	150	139	95.00	77	86
83.10	64	77	89.10	161	138	95.10	95	84
83.20	66	76	89.20	117	136	95.20	80	80
83.30	86	90	89.30	132	141	95.30	92	90
83.40	114	114	89.40	102	114	95.40	96	87
83.50	96	108	89.50	79	104	95.50	85	78
83.60	80	103	89.60	95	106	95.60	117	92
83.70	110	118	89.70	103	114	95.70	114	105
83.80	97	98	89.80	118	121	95.80	85	85
83.90	75	101	89.90	132	140	95.90	80	76
84.00	110	118	90.00	126	126	96.00	97	78
84.10	66	93	90.10	120	128	96.10	76	69
84.20	78	85	90.20	165	166	96.20	69	60
84.30	74	79	90.30	170	167	96.30	47	58
84.40	71	68	90.40	163	168	96.40	57	63
84.50	66	67	90.50	245	212	96.50	83	74
84.60	86	83	90.60	232	192	96.60	94	81
84.70	125	129	90.70	144	140	96.70	85	81
84.80	145	146	90.80	114	132	96.80	82	90
84.90	140	134	90.90	110	109	96.90	96	106
85.00	119	131	91.00	77	82	97.00	160	140
85.10	111	104	91.10	66	71	97.10	205	189
85.20	88	87	91.20	69	65	97.20	185	171
85.30	59	73	91.30	58	62	97.30	213	167
85.40	67	68	91.40	75	63	97.40	211	214
85.50	74	73	91.50	75	64	97.50	235	202
85.60	83	77	91.60	74	62	97.60	190	200
85.70	78	75	91.70	59	59	97.70	196	207
85.80	68	83	91.80	55	59	97.80	162	155
85.90	89	100	91.90	64	58	97.90	145	132
86.00	79	96	92.00	65	58	98.00	120	123
86.10	79	89	92.10	61	62	98.10	108	96
86.20	94	97	92.20	68	71	98.20	90	88
86.30	106	105	92.30	70	74	98.30	96	84
86.40	131	125	92.40	71	78	98.40	82	79
86.50	170	146	92.50	106	101	98.50	92	78
86.60	141	153	92.60	136	135	98.60	98	80
86.70	144	154	92.70	115	118	98.70	89	86
86.80	133	122	92.80	97	105	98.80	74	79
86.90	113	104	92.90	118	128	98.90	67	66

Sample Rich59

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
9.00	99	79	15.00	66	75	21.00	68	71	27.00	1967	1928
9.10	98	79	15.10	65	75	21.10	56	71	27.10	387	428
9.20	89	83	15.20	71	75	21.20	62	71	27.20	177	173
9.30	121	83	15.30	77	75	21.30	60	71	27.30	138	144
9.40	115	84	15.40	62	75	21.40	55	71	27.40	131	141
9.50	115	87	15.50	74	74	21.50	61	77	27.50	157	147
9.60	122	99	15.60	81	74	21.60	68	82	27.60	233	197
9.70	199	217	15.70	75	74	21.70	80	85	27.70	433	353
9.80	235	240	15.80	56	74	21.80	93	91	27.80	1081	1033
9.90	195	145	15.90	62	74	21.90	127	112	27.90	3084	2769
10.00	245	146	16.00	65	74	22.00	268	269	28.00	1750	1594
10.10	367	213	16.10	73	74	22.10	623	638	28.10	348	368
10.20	714	772	16.20	61	74	22.20	377	338	28.20	182	164
10.30	1451	1496	16.30	64	74	22.30	113	127	28.30	144	142
10.40	398	429	16.40	81	74	22.40	78	99	28.40	131	115
10.50	144	134	16.50	61	74	22.50	89	98	28.50	106	90
10.60	105	93	16.60	70	74	22.60	146	115	28.60	96	84
10.70	111	78	16.70	63	74	22.70	290	274	28.70	113	96
10.80	95	78	16.80	65	75	22.80	701	656	28.80	183	175
10.90	96	78	16.90	62	75	22.90	396	349	28.90	457	487
11.00	86	78	17.00	82	76	23.00	106	119	29.00	428	420
11.10	92	78	17.10	83	77	23.10	70	86	29.10	154	151
11.20	106	77	17.20	83	90	23.20	81	77	29.20	97	90
11.30	100	77	17.30	97	120	23.30	80	75	29.30	91	87
11.40	95	77	17.40	120	130	23.40	74	73	29.40	112	139
11.50	90	77	17.50	81	97	23.50	61	74	29.50	109	147

11.60	105	77	17.60	71	86	23.60	70	76	29.60	129	137
11.70	70	78	17.70	85	89	23.70	92	94	29.70	160	165
11.80	80	78	17.80	76	97	23.80	135	173	29.80	235	225
11.90	76	78	17.90	175	157	23.90	133	160	29.90	623	615
12.00	81	79	18.00	370	343	24.00	73	88	30.00	1987	2225
12.10	88	81	18.10	392	316	24.10	60	74	30.10	1895	2040
12.20	109	101	18.20	469	377	24.20	64	72	30.20	809	862
12.30	102	112	18.30	225	177	24.30	65	71	30.30	897	849
12.40	106	84	18.40	90	92	24.40	60	70	30.40	453	417
12.50	79	78	18.50	78	79	24.50	58	70	30.50	129	149
12.60	83	77	18.60	71	75	24.60	54	72	30.60	94	97
12.70	72	77	18.70	66	73	24.70	68	78	30.70	93	89
12.80	79	76	18.80	66	72	24.80	65	75	30.80	106	90
12.90	94	76	18.90	70	72	24.90	72	70	30.90	100	95
13.00	67	76	19.00	74	72	25.00	62	70	31.00	104	107
13.10	86	76	19.10	66	86	25.10	71	69	31.10	192	160
13.20	90	76	19.20	85	89	25.20	73	69	31.20	559	527
13.30	79	76	19.30	70	96	25.30	81	69	31.30	1154	1094
13.40	78	76	19.40	115	113	25.40	72	69	31.40	591	570
13.50	75	76	19.50	287	220	25.50	85	69	31.50	165	167
13.60	83	76	19.60	807	724	25.60	89	103	31.60	129	117
13.70	79	76	19.70	702	605	25.70	109	131	31.70	113	114
13.80	73	76	19.80	162	171	25.80	177	153	31.80	125	117
13.90	78	76	19.90	119	98	25.90	212	200	31.90	129	135
14.00	73	75	20.00	77	82	26.00	418	367	32.00	221	193
14.10	70	75	20.10	60	76	26.10	1434	1575	32.10	594	619
14.20	77	75	20.20	60	72	26.20	3354	3387	32.20	1838	1861
14.30	81	75	20.30	65	72	26.30	1468	1514	32.30	1301	1336
14.40	81	75	20.40	60	72	26.40	338	404	32.40	364	416
14.50	55	75	20.50	64	72	26.50	199	234	32.50	178	213
14.60	89	75	20.60	64	76	26.60	190	222	32.60	162	202
14.70	75	75	20.70	70	84	26.70	334	309	32.70	223	252
14.80	87	75	20.80	52	77	26.80	1073	1090	32.80	583	567
14.90	80	75	20.90	68	72	26.90	3224	3235	32.90	2170	2421

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
33.00	3462	3392	39.00	629	679	45.00	144	140	51.00	116	115
33.10	1285	1302	39.10	1495	1478	45.10	103	95	51.10	99	105
33.20	266	316	39.20	993	960	45.20	81	81	51.20	101	101
33.30	135	159	39.30	312	319	45.30	68	73	51.30	115	144
33.40	124	112	39.40	206	209	45.40	57	74	51.40	132	150
33.50	89	89	39.50	141	161	45.50	85	85	51.50	110	116
33.60	89	71	39.60	115	109	45.60	75	89	51.60	82	78
33.70	81	66	39.70	102	86	45.70	84	82	51.70	64	67
33.80	90	66	39.80	101	87	45.80	89	82	51.80	52	65
33.90	78	82	39.90	116	129	45.90	91	92	51.90	52	64
34.00	88	95	40.00	110	123	46.00	97	108	52.00	72	66
34.10	113	117	40.10	85	92	46.10	205	209	52.10	82	75
34.20	171	137	40.20	92	87	46.20	400	360	52.20	90	79
34.30	195	161	40.30	116	109	46.30	381	373	52.30	76	77
34.40	480	376	40.40	201	172	46.40	289	308	52.40	90	69
34.50	1506	1371	40.50	444	361	46.50	275	276	52.50	72	66
34.60	1325	1447	40.60	450	414	46.60	195	202	52.60	57	64
34.70	532	585	40.70	239	227	46.70	179	154	52.70	58	65
34.80	268	285	40.80	120	103	46.80	275	292	52.80	99	74
34.90	427	375	40.90	87	95	46.90	795	691	52.90	93	84
35.00	1010	1065	41.00	97	105	47.00	598	556	53.00	88	88
35.10	2249	2366	41.10	117	123	47.10	298	267	53.10	98	98
35.20	1589	1573	41.20	177	203	47.20	99	113	53.20	87	89
35.30	418	444	41.30	339	337	47.30	86	86	53.30	74	78
35.40	143	167	41.40	857	797	47.40	80	80	53.40	67	73
35.50	102	112	41.50	1651	1510	47.50	98	81	53.50	100	73
35.60	91	90	41.60	1077	1132	47.60	125	99	53.60	97	79
35.70	87	79	41.70	547	572	47.70	208	219	53.70	100	91
35.80	90	73	41.80	261	271	47.80	357	321	53.80	121	109
35.90	96	84	41.90	135	132	47.90	229	245	53.90	122	114
36.00	120	134	42.00	95	100	48.00	151	132	54.00	153	140
36.10	127	140	42.10	110	109	48.10	99	93	54.10	262	255
36.20	82	93	42.20	216	205	48.20	77	83	54.20	458	477

36.30	91	75	42.30	271	262	48.30	74	81	54.30	555	514
36.40	67	79	42.40	197	168	48.40	87	89	54.40	378	354
36.50	115	104	42.50	84	88	48.50	135	133	54.50	224	218
36.60	107	115	42.60	71	71	48.60	209	202	54.60	274	264
36.70	122	107	42.70	61	67	48.70	360	394	54.70	379	327
36.80	104	137	42.80	68	65	48.80	490	479	54.80	375	383
36.90	211	237	42.90	70	64	48.90	366	346	54.90	815	892
37.00	279	268	43.00	57	63	49.00	175	193	55.00	1220	1158
37.10	405	315	43.10	70	63	49.10	202	227	55.10	759	811
37.20	628	587	43.20	55	63	49.20	251	272	55.20	346	353
37.30	550	511	43.30	73	69	49.30	202	207	55.30	156	156
37.40	198	233	43.40	85	74	49.40	99	115	55.40	206	167
37.50	129	144	43.50	83	77	49.50	80	80	55.50	334	270
37.60	122	139	43.60	108	88	49.60	88	80	55.60	272	226
37.70	163	168	43.70	140	107	49.70	85	88	55.70	189	164
37.80	427	370	43.80	221	210	49.80	89	79	55.80	121	105
37.90	1043	1199	43.90	512	595	49.90	75	69	55.90	82	83
38.00	1690	1772	44.00	595	617	50.00	73	66	56.00	89	75
38.10	1179	1121	44.10	434	415	50.10	64	67	56.10	94	78
38.20	424	376	44.20	522	494	50.20	60	70	56.20	93	77
38.30	141	146	44.30	512	501	50.30	82	76	56.30	88	73
38.40	102	101	44.40	538	541	50.40	136	111	56.40	87	73
38.50	101	98	44.50	376	381	50.50	269	252	56.50	90	81
38.60	81	99	44.60	195	191	50.60	339	321	56.60	171	124
38.70	109	103	44.70	127	112	50.70	266	230	56.70	289	240
38.80	154	123	44.80	148	155	50.80	133	125	56.80	356	344
38.90	207	197	44.90	216	191	50.90	83	96	56.90	500	396

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
57.00	291	267	63.00	275	276	69.00	74	71	75.00	73	65
57.10	217	161	63.10	252	232	69.10	104	88	75.10	63	63
57.20	101	114	63.20	186	187	69.20	128	118	75.20	72	61
57.30	76	98	63.30	216	187	69.30	174	156	75.30	44	61
57.40	86	89	63.40	494	426	69.40	221	209	75.40	78	64
57.50	78	87	63.50	1153	1125	69.50	241	245	75.50	72	72
57.60	94	90	63.60	935	967	69.60	198	201	75.60	78	102
57.70	80	107	63.70	710	744	69.70	189	184	75.70	124	124
57.80	108	112	63.80	400	352	69.80	132	137	75.80	108	111
57.90	108	103	63.90	177	220	69.90	143	152	75.90	100	102
58.00	118	101	64.00	273	279	70.00	237	247	76.00	89	84
58.10	182	143	64.10	230	244	70.10	402	374	76.10	90	75
58.20	383	373	64.20	232	228	70.20	479	504	76.20	62	72
58.30	566	530	64.30	182	152	70.30	498	521	76.30	91	90
58.40	455	477	64.40	154	147	70.40	592	593	76.40	108	105
58.50	303	321	64.50	176	188	70.50	488	471	76.50	116	95
58.60	313	296	64.60	154	153	70.60	385	348	76.60	111	118
58.70	224	237	64.70	147	134	70.70	208	219	76.70	93	128
58.80	220	217	64.80	121	106	70.80	124	129	76.80	96	122
58.90	326	319	64.90	105	90	70.90	95	89	76.90	114	109
59.00	584	591	65.00	106	80	71.00	81	78	77.00	96	94
59.10	464	476	65.10	89	72	71.10	86	82	77.10	100	93
59.20	371	329	65.20	78	68	71.20	93	95	77.20	106	111
59.30	155	152	65.30	87	76	71.30	111	93	77.30	131	107
59.40	124	96	65.40	121	111	71.40	109	90	77.40	122	106
59.50	83	88	65.50	140	121	71.50	128	109	77.50	110	120
59.60	86	94	65.60	132	115	71.60	194	163	77.60	161	146
59.70	92	83	65.70	108	113	71.70	180	149	77.70	145	147
59.80	91	73	65.80	90	94	71.80	160	141	77.80	131	134
59.90	73	65	65.90	101	106	71.90	156	158	77.90	127	109
60.00	83	68	66.00	93	105	72.00	232	217	78.00	90	92
60.10	61	70	66.10	93	100	72.10	210	204	78.10	69	76
60.20	83	70	66.20	107	95	72.20	177	199	78.20	57	72
60.30	87	75	66.30	99	86	72.30	147	146	78.30	58	71
60.40	79	82	66.40	80	77	72.40	125	116	78.40	63	71
60.50	138	105	66.50	78	71	72.50	133	123	78.50	104	93
60.60	199	187	66.60	63	70	72.60	212	180	78.60	184	129
60.70	401	354	66.70	109	84	72.70	220	184	78.70	135	118
60.80	509	449	66.80	93	113	72.80	272	288	78.80	118	117
60.90	707	727	66.90	107	108	72.90	573	554	78.90	100	117

61.00	941	987	67.00	101	101	73.00	660	615	79.00	102	111
61.10	716	780	67.10	99	87	73.10	415	438	79.10	125	140
61.20	538	511	67.20	78	79	73.20	363	346	79.20	219	232
61.30	220	254	67.30	104	85	73.30	187	176	79.30	218	205
61.40	169	154	67.40	122	120	73.40	109	119	79.40	149	166
61.50	205	196	67.50	205	219	73.50	110	111	79.50	135	159
61.60	488	412	67.60	346	350	73.60	116	123	79.60	81	112
61.70	381	369	67.70	440	521	73.70	162	153	79.70	82	88
61.80	314	288	67.80	351	359	73.80	169	164	79.80	75	89
61.90	170	149	67.90	270	283	73.90	203	191	79.90	69	94
62.00	90	90	68.00	163	162	74.00	222	209	80.00	68	81
62.10	83	78	68.10	150	172	74.10	224	205	80.10	68	75
62.20	88	78	68.20	195	183	74.20	238	227	80.20	68	73
62.30	120	95	68.30	153	143	74.30	185	209	80.30	65	79
62.40	174	179	68.40	125	117	74.40	123	146	80.40	94	91
62.50	244	238	68.50	69	85	74.50	107	125	80.50	84	93
62.60	196	197	68.60	99	87	74.60	96	90	80.60	58	87
62.70	177	165	68.70	67	79	74.70	74	75	80.70	64	80
62.80	186	181	68.80	79	77	74.80	83	73	80.80	73	72
62.90	245	236	68.90	75	71	74.90	60	67	80.90	76	72

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
81.00	97	97	87.00	91	97	93.00	152	148	99.00	68	61
81.10	148	157	87.10	82	79	93.10	172	204	99.10	70	60
81.20	162	152	87.20	64	66	93.20	291	287	99.20	64	55
81.30	133	147	87.30	50	61	93.30	316	326	99.30	52	52
81.40	148	159	87.40	53	59	93.40	311	304	99.40	58	52
81.50	101	108	87.50	66	59	93.50	206	241	99.50	55	53
81.60	90	101	87.60	54	58	93.60	189	204	99.60	66	57
81.70	95	96	87.70	64	56	93.70	156	161	99.70	62	56
81.80	81	77	87.80	52	57	93.80	99	110	99.80	71	51
81.90	60	74	87.90	54	58	93.90	88	87	99.90	73	51
82.00	68	74	88.00	72	58	94.00	84	77	100.00	80	50
82.10	76	67	88.10	48	56	94.10	77	81			
82.20	54	69	88.20	48	60	94.20	118	94			
82.30	67	76	88.30	58	64	94.30	136	120			
82.40	57	77	88.40	72	63	94.40	169	174			
82.50	105	96	88.50	56	64	94.50	176	158			
82.60	161	147	88.60	91	74	94.60	108	116			
82.70	150	157	88.70	108	93	94.70	119	120			
82.80	107	116	88.80	121	114	94.80	125	105			
82.90	96	117	88.90	102	112	94.90	90	82			
83.00	83	89	89.00	133	128	95.00	76	84			
83.10	58	76	89.10	131	137	95.10	78	83			
83.20	79	77	89.20	101	125	95.20	90	73			
83.30	75	81	89.30	138	141	95.30	86	80			
83.40	86	106	89.40	117	120	95.40	73	83			
83.50	100	114	89.50	83	98	95.50	86	73			
83.60	95	102	89.60	92	100	95.60	92	82			
83.70	113	117	89.70	113	108	95.70	138	93			
83.80	90	99	89.80	126	113	95.80	108	78			
83.90	76	99	89.90	103	124	95.90	60	68			
84.00	94	120	90.00	129	145	96.00	67	70			
84.10	92	95	90.10	120	132	96.10	81	63			
84.20	59	84	90.20	156	162	96.20	68	56			
84.30	67	80	90.30	204	177	96.30	67	55			
84.40	56	66	90.40	165	149	96.40	61	58			
84.50	62	62	90.50	197	200	96.50	66	69			
84.60	67	66	90.60	256	222	96.60	77	85			
84.70	77	90	90.70	137	152	96.70	89	83			
84.80	174	139	90.80	107	135	96.80	86	84			
84.90	141	138	90.90	119	126	96.90	101	102			
85.00	148	126	91.00	79	89	97.00	113	126			
85.10	122	117	91.10	73	71	97.10	167	168			
85.20	95	93	91.20	57	66	97.20	180	163			
85.30	88	75	91.30	43	61	97.30	151	147			
85.40	58	66	91.40	58	60	97.40	202	182			
85.50	63	64	91.50	64	60	97.50	200	173			
85.60	54	71	91.60	74	58	97.60	176	154			

85.70	78	77	91.70	69	56	97.70	213	197
85.80	67	79	91.80	49	55	97.80	200	187
85.90	104	96	91.90	60	56	97.90	122	130
86.00	115	107	92.00	55	57	98.00	143	121
86.10	85	90	92.10	58	61	98.10	122	115
86.20	89	96	92.20	67	67	98.20	120	92
86.30	103	101	92.30	87	70	98.30	82	85
86.40	109	112	92.40	91	72	98.40	76	78
86.50	127	137	92.50	73	78	98.50	81	71
86.60	144	151	92.60	101	103	98.60	69	74
86.70	175	152	92.70	127	141	98.70	78	81
86.80	134	143	92.80	105	122	98.80	80	76
86.90	89	111	92.90	102	112	98.90	68	65

Sample Rich60

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
9.00	115	78	15.00	81	73	21.00	71	69	27.00	2391	2394
9.10	125	78	15.10	76	73	21.10	64	68	27.10	573	619
9.20	99	81	15.20	73	73	21.20	58	68	27.20	213	204
9.30	119	81	15.30	73	73	21.30	69	68	27.30	150	166
9.40	113	82	15.40	58	72	21.40	58	68	27.40	174	197
9.50	107	84	15.50	81	72	21.50	78	73	27.50	174	194
9.60	148	98	15.60	61	72	21.60	70	77	27.60	258	218
9.70	191	200	15.70	85	72	21.70	76	81	27.70	394	386
9.80	227	217	15.80	63	72	21.80	82	86	27.80	711	639
9.90	213	136	15.90	51	72	21.90	118	104	27.90	2328	2120
10.00	241	136	16.00	70	72	22.00	216	235	28.00	2680	2427
10.10	351	196	16.10	89	72	22.10	616	612	28.10	750	748
10.20	685	681	16.20	68	72	22.20	402	404	28.20	244	214
10.30	1429	1470	16.30	71	72	22.30	134	140	28.30	123	141
10.40	447	540	16.40	62	72	22.40	96	98	28.40	118	119
10.50	151	150	16.50	82	72	22.50	82	95	28.50	103	94
10.60	92	100	16.60	55	72	22.60	108	109	28.60	85	81
10.70	118	84	16.70	80	72	22.70	248	243	28.70	89	84
10.80	104	77	16.80	74	74	22.80	697	627	28.80	111	117
10.90	89	76	16.90	76	74	22.90	427	409	28.90	333	324
11.00	99	76	17.00	93	75	23.00	142	133	29.00	504	517
11.10	87	76	17.10	56	78	23.10	92	86	29.10	244	246
11.20	80	76	17.20	83	97	23.20	70	76	29.20	122	103
11.30	66	76	17.30	147	150	23.30	55	73	29.30	87	86
11.40	74	76	17.40	156	182	23.40	53	71	29.40	114	129
11.50	81	76	17.50	110	120	23.50	71	70	29.50	115	151
11.60	86	76	17.60	77	87	23.60	69	71	29.60	137	142
11.70	82	78	17.70	75	87	23.70	77	80	29.70	165	188
11.80	75	78	17.80	108	98	23.80	102	134	29.80	216	226
11.90	90	78	17.90	167	157	23.90	123	161	29.90	453	443
12.00	102	80	18.00	313	333	24.00	57	94	30.00	1606	1743
12.10	96	86	18.10	359	298	24.10	64	72	30.10	2206	2374
12.20	152	126	18.20	427	309	24.20	57	69	30.20	1155	1107
12.30	154	149	18.30	236	203	24.30	61	68	30.30	854	884
12.40	101	92	18.40	83	96	24.40	69	68	30.40	470	489
12.50	70	78	18.50	60	78	24.50	58	68	30.50	197	172
12.60	80	76	18.60	72	74	24.60	76	71	30.60	116	104
12.70	82	75	18.70	73	71	24.70	89	84	30.70	66	92
12.80	74	75	18.80	52	70	24.80	75	81	30.80	104	85
12.90	72	75	18.90	58	70	24.90	80	69	30.90	94	87
13.00	84	74	19.00	63	76	25.00	73	67	31.00	99	95
13.10	79	74	19.10	76	81	25.10	99	66	31.10	139	122
13.20	56	74	19.20	87	85	25.20	75	66	31.20	300	302
13.30	89	74	19.30	77	91	25.30	60	66	31.30	977	946
13.40	61	74	19.40	117	108	25.40	78	66	31.40	875	841
13.50	80	74	19.50	284	220	25.50	88	66	31.50	257	271
13.60	90	74	19.60	804	700	25.60	80	95	31.60	119	126
13.70	76	74	19.70	640	614	25.70	109	120	31.70	103	110
13.80	65	74	19.80	171	181	25.80	132	140	31.80	91	108
13.90	62	74	19.90	102	98	25.90	173	182	31.90	133	118
14.00	74	74	20.00	84	82	26.00	389	322	32.00	175	149
14.10	74	74	20.10	46	75	26.10	1274	1315	32.10	360	332
14.20	85	73	20.20	64	72	26.20	3120	3314	32.20	1261	1295
14.30	78	73	20.30	58	70	26.30	1832	1842	32.30	1640	1709

14.40	63	73	20.40	64	69	26.40	463	480	32.40	623	711
14.50	78	73	20.50	55	69	26.50	211	237	32.50	202	254
14.60	75	73	20.60	53	70	26.60	201	210	32.60	177	206
14.70	66	73	20.70	56	73	26.70	286	266	32.70	223	245
14.80	56	73	20.80	48	71	26.80	712	778	32.80	520	502
14.90	61	73	20.90	70	69	26.90	2783	2764	32.90	1895	2131

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
33.00	3637	3648	39.00	426	462	45.00	182	156	51.00	95	94
33.10	1723	1675	39.10	1364	1347	45.10	103	102	51.10	105	96
33.20	429	399	39.20	1266	1153	45.20	74	81	51.20	79	90
33.30	149	177	39.30	487	441	45.30	79	72	51.30	83	94
33.40	115	121	39.40	209	203	45.40	72	72	51.40	124	155
33.50	105	95	39.50	170	174	45.50	89	79	51.50	127	150
33.60	95	81	39.60	131	139	45.60	81	87	51.60	99	112
33.70	99	68	39.70	95	104	45.70	91	81	51.70	70	74
33.80	77	64	39.80	101	90	45.80	77	75	51.80	86	64
33.90	95	78	39.90	137	124	45.90	81	85	51.90	79	62
34.00	95	94	40.00	125	126	46.00	94	99	52.00	60	62
34.10	137	135	40.10	105	94	46.10	202	182	52.10	63	69
34.20	173	173	40.20	111	94	46.20	391	337	52.20	82	82
34.30	216	171	40.30	133	123	46.30	351	335	52.30	81	84
34.40	372	348	40.40	168	149	46.40	300	299	52.40	68	78
34.50	1350	1249	40.50	358	278	46.50	325	327	52.50	71	69
34.60	1452	1489	40.60	502	444	46.60	271	249	52.60	67	65
34.70	621	637	40.70	319	295	46.70	162	161	52.70	62	69
34.80	273	272	40.80	132	125	46.80	154	144	52.80	71	77
34.90	295	302	40.90	107	94	46.90	316	349	52.90	111	88
35.00	757	742	41.00	79	98	47.00	790	690	53.00	90	84
35.10	1866	1973	41.10	104	113	47.10	581	504	53.10	92	89
35.20	1862	1931	41.20	144	176	47.20	264	218	53.20	90	90
35.30	705	708	41.30	321	296	47.30	120	102	53.30	68	79
35.40	223	217	41.40	602	611	47.40	68	83	53.40	80	71
35.50	122	125	41.50	1538	1476	47.50	58	79	53.50	91	75
35.60	100	97	41.60	1274	1261	47.60	96	84	53.60	100	88
35.70	90	84	41.70	699	727	47.70	152	131	53.70	101	96
35.80	77	75	41.80	377	377	47.80	301	303	53.80	128	109
35.90	103	96	41.90	178	179	47.90	295	313	53.90	124	109
36.00	179	194	42.00	91	109	48.00	222	199	54.00	153	132
36.10	155	196	42.10	110	104	48.10	121	110	54.10	245	232
36.20	134	108	42.20	174	174	48.20	85	85	54.20	425	420
36.30	85	73	42.30	293	276	48.30	72	79	54.30	565	536
36.40	77	72	42.40	225	196	48.40	85	82	54.40	408	409
36.50	103	88	42.50	128	98	48.50	116	110	54.50	291	253
36.60	115	117	42.60	78	70	48.60	225	182	54.60	256	227
36.70	99	109	42.70	72	68	48.70	324	318	54.70	342	331
36.80	97	104	42.80	73	69	48.80	408	417	54.80	361	313
36.90	138	167	42.90	61	65	48.90	342	368	54.90	515	507
37.00	273	261	43.00	72	61	49.00	216	215	55.00	1185	1188
37.10	314	285	43.10	66	60	49.10	163	155	55.10	938	1003
37.20	492	449	43.20	67	62	49.20	197	243	55.20	677	639
37.30	611	575	43.30	81	68	49.30	246	254	55.30	239	235
37.40	359	325	43.40	79	68	49.40	168	173	55.40	140	146
37.50	110	165	43.50	75	73	49.50	91	92	55.50	288	224
37.60	115	136	43.60	104	86	49.60	66	73	55.60	303	280
37.70	118	142	43.70	123	111	49.70	96	84	55.70	233	227
37.80	193	206	43.80	156	162	49.80	77	83	55.80	152	139
37.90	522	636	43.90	409	437	49.90	73	73	55.90	98	95
38.00	1602	1655	44.00	632	665	50.00	53	65	56.00	92	78
38.10	1617	1594	44.10	463	461	50.10	60	65	56.10	87	74
38.20	700	659	44.20	419	379	50.20	60	68	56.20	81	74
38.30	229	203	44.30	532	545	50.30	68	77	56.30	92	70
38.40	113	115	44.40	622	591	50.40	108	109	56.40	97	69
38.50	92	102	44.50	492	496	50.50	244	239	56.50	75	71
38.60	90	100	44.60	297	280	50.60	367	343	56.60	99	82
38.70	85	99	44.70	161	129	50.70	270	258	56.70	157	136
38.80	120	111	44.80	144	126	50.80	130	142	56.80	356	332
38.90	144	157	44.90	198	190	50.90	81	89	56.90	538	459

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
57.00	359	338	63.00	268	297	69.00	75	67	75.00	86	67
57.10	240	197	63.10	290	281	69.10	73	76	75.10	63	68
57.20	121	123	63.20	218	218	69.20	109	102	75.20	53	63
57.30	99	110	63.30	174	164	69.30	122	107	75.30	57	60
57.40	90	96	63.40	247	190	69.40	174	157	75.40	67	60
57.50	99	85	63.50	525	476	69.50	230	226	75.50	64	60
57.60	90	88	63.60	1161	1129	69.60	241	251	75.60	76	68
57.70	102	105	63.70	1018	987	69.70	189	206	75.70	101	90
57.80	153	147	63.80	706	748	69.80	179	185	75.80	107	122
57.90	135	129	63.90	434	379	69.90	153	146	75.90	98	110
58.00	128	116	64.00	247	280	70.00	201	208	76.00	79	98
58.10	129	118	64.10	269	266	70.10	320	335	76.10	89	88
58.20	281	264	64.20	226	233	70.20	353	413	76.20	78	71
58.30	526	534	64.30	198	194	70.30	471	509	76.30	79	70
58.40	466	465	64.40	163	130	70.40	399	395	76.40	101	86
58.50	419	386	64.50	170	146	70.50	588	520	76.50	115	98
58.60	254	269	64.60	177	182	70.60	483	488	76.60	104	98
58.70	284	279	64.70	143	146	70.70	361	347	76.70	127	120
58.80	195	215	64.80	136	136	70.80	286	260	76.80	100	128
58.90	243	216	64.90	111	104	70.90	159	137	76.90	103	109
59.00	289	317	65.00	99	82	71.00	87	89	77.00	94	97
59.10	532	570	65.10	88	73	71.10	81	80	77.10	75	84
59.20	499	475	65.20	66	65	71.20	94	92	77.20	88	83
59.30	353	336	65.30	91	67	71.30	102	99	77.30	113	106
59.40	158	155	65.40	92	82	71.40	81	86	77.40	115	113
59.50	117	93	65.50	142	123	71.50	88	87	77.50	115	115
59.60	93	90	65.60	120	131	71.60	106	106	77.60	153	146
59.70	76	89	65.70	139	126	71.70	195	172	77.70	124	134
59.80	74	79	65.80	102	109	71.80	191	151	77.80	132	134
59.90	82	67	65.90	88	95	71.90	161	157	77.90	123	129
60.00	61	62	66.00	104	114	72.00	210	208	78.00	76	97
60.10	84	67	66.10	127	110	72.10	214	219	78.10	86	87
60.20	66	69	66.20	105	109	72.20	190	202	78.20	77	75
60.30	64	73	66.30	96	92	72.30	144	175	78.30	62	68
60.40	87	78	66.40	71	85	72.40	123	125	78.40	67	68
60.50	97	89	66.50	77	74	72.50	114	105	78.50	70	66
60.60	141	115	66.60	83	73	72.60	116	120	78.60	74	76
60.70	229	229	66.70	93	86	72.70	218	191	78.70	141	116
60.80	481	427	66.80	100	93	72.80	258	240	78.80	164	142
60.90	600	600	66.90	108	108	72.90	451	465	78.90	118	116
61.00	962	942	67.00	113	112	73.00	715	675	79.00	123	128
61.10	829	856	67.10	90	96	73.10	496	498	79.10	126	122
61.20	608	674	67.20	103	87	73.20	398	404	79.20	155	159
61.30	317	358	67.30	79	77	73.30	246	232	79.30	248	256
61.40	186	199	67.40	81	83	73.40	129	125	79.40	203	202
61.50	192	187	67.50	113	115	73.50	96	101	79.50	138	178
61.60	415	378	67.60	204	207	73.60	112	105	79.60	144	162
61.70	478	399	67.70	413	400	73.70	141	127	79.70	82	109
61.80	380	314	67.80	501	520	73.80	190	169	79.80	72	90
61.90	204	192	67.90	350	362	73.90	182	177	79.90	81	94
62.00	105	107	68.00	257	272	74.00	194	220	80.00	83	87
62.10	96	84	68.10	143	154	74.10	219	218	80.10	70	79
62.20	88	75	68.20	194	182	74.20	225	206	80.20	58	72
62.30	105	84	68.30	157	186	74.30	223	239	80.30	76	72
62.40	137	123	68.40	138	147	74.40	169	194	80.40	99	87
62.50	220	232	68.50	120	119	74.50	121	144	80.50	82	100
62.60	231	220	68.60	87	93	74.60	105	122	80.60	83	88
62.70	218	191	68.70	83	88	74.70	83	87	80.70	62	88
62.80	187	145	68.80	74	78	74.80	93	76	80.80	88	77
62.90	180	201	68.90	63	73	74.90	78	73	80.90	60	67

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
81.00	58	67	87.00	125	124	93.00	128	129	99.00	65	66
81.10	80	77	87.10	90	103	93.10	156	143	99.10	56	62
81.20	101	113	87.20	92	90	93.20	198	194	99.20	72	59
81.30	175	169	87.30	77	70	93.30	285	300	99.30	47	53
81.40	160	153	87.40	50	63	93.40	386	375	99.40	58	50
81.50	173	163	87.50	60	61	93.50	258	312	99.50	62	49

81.60	145	126	87.60	49	60	93.60	231	253	99.60	60	49
81.70	109	102	87.70	48	57	93.70	205	234	99.70	59	50
81.80	115	94	87.80	62	57	93.80	167	173	99.80	77	51
81.90	78	78	87.90	68	62	93.90	102	110	99.90	59	48
82.00	74	71	88.00	66	62	94.00	88	87	100.00	81	44
82.10	65	73	88.10	52	57	94.10	77	84			
82.20	68	69	88.20	49	56	94.20	78	81			
82.30	67	73	88.30	41	58	94.30	86	87			
82.40	60	73	88.40	62	61	94.40	107	94			
82.50	97	76	88.50	66	63	94.50	139	131			
82.60	117	110	88.60	61	64	94.60	233	184			
82.70	131	165	88.70	91	80	94.70	128	138			
82.80	119	139	88.80	113	102	94.80	104	109			
82.90	102	115	88.90	96	96	94.90	135	124			
83.00	108	110	89.00	104	113	95.00	106	104			
83.10	56	79	89.10	153	143	95.10	96	95			
83.20	55	70	89.20	104	124	95.20	102	92			
83.30	71	74	89.30	133	133	95.30	90	77			
83.40	75	85	89.40	140	149	95.40	85	84			
83.50	87	113	89.50	106	112	95.50	94	89			
83.60	105	117	89.60	89	96	95.60	105	79			
83.70	89	113	89.70	83	97	95.70	124	91			
83.80	116	113	89.80	97	103	95.80	104	89			
83.90	83	93	89.90	106	107	95.90	79	70			
84.00	93	108	90.00	112	109	96.00	74	69			
84.10	88	103	90.10	139	151	96.10	73	68			
84.20	58	81	90.20	131	158	96.20	60	60			
84.30	76	81	90.30	176	176	96.30	61	57			
84.40	54	71	90.40	216	177	96.40	46	57			
84.50	62	61	90.50	161	151	96.50	49	59			
84.60	51	60	90.60	198	195	96.60	65	68			
84.70	64	63	90.70	218	210	96.70	98	85			
84.80	91	81	90.80	153	159	96.80	79	84			
84.90	146	127	90.90	124	134	96.90	78	87			
85.00	181	152	91.00	116	128	97.00	99	113			
85.10	124	126	91.10	89	94	97.10	166	155			
85.20	117	118	91.20	74	71	97.20	193	166			
85.30	104	100	91.30	68	66	97.30	162	137			
85.40	85	80	91.40	67	63	97.40	185	168			
85.50	57	70	91.50	58	59	97.50	241	193			
85.60	58	69	91.60	58	60	97.60	153	145			
85.70	74	73	91.70	58	57	97.70	156	133			
85.80	78	80	91.80	52	56	97.80	172	162			
85.90	68	78	91.90	68	54	97.90	175	174			
86.00	88	96	92.00	58	53	98.00	165	155			
86.10	88	100	92.10	48	55	98.10	125	120			
86.20	79	83	92.20	70	61	98.20	108	111			
86.30	89	88	92.30	84	64	98.30	107	110			
86.40	95	91	92.40	70	62	98.40	88	97			
86.50	96	100	92.50	66	66	98.50	97	84			
86.60	105	121	92.60	88	73	98.60	59	72			
86.70	153	149	92.70	91	80	98.70	84	74			
86.80	117	139	92.80	104	113	98.80	102	84			
86.90	124	149	92.90	135	150	98.90	85	78			
86.90	135	138	92.90	94	80	98.90	82	82			

Sample Rich61

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
9.00	91	68	15.00	56	66	21.00	46	64	27.00	2683	2763
9.10	107	70	15.10	77	66	21.10	53	64	27.10	1306	1299
9.20	100	70	15.20	65	66	21.20	61	64	27.20	304	308
9.30	99	71	15.30	74	66	21.30	75	63	27.30	138	154
9.40	109	71	15.40	63	65	21.40	53	63	27.40	164	186
9.50	110	73	15.50	64	65	21.50	62	67	27.50	178	195
9.60	103	81	15.60	66	65	21.60	57	71	27.60	234	203
9.70	153	151	15.70	52	65	21.70	62	73	27.70	349	386
9.80	227	211	15.80	59	65	21.80	62	77	27.80	470	433
9.90	171	136	15.90	72	65	21.90	107	84	27.90	854	808
10.00	193	110	16.00	60	65	22.00	134	130	28.00	2471	2337
10.10	256	133	16.10	63	65	22.10	329	387	28.10	1977	1834

10.20	490	347	16.20	51	65	22.20	608	553	28.20	530	487
10.30	1003	1075	16.30	58	65	22.30	197	229	28.30	163	169
10.40	777	842	16.40	72	65	22.40	88	102	28.40	134	133
10.50	156	210	16.50	62	65	22.50	78	88	28.50	77	107
10.60	87	96	16.60	72	65	22.60	93	93	28.60	83	85
10.70	84	77	16.70	57	65	22.70	138	151	28.70	82	80
10.80	81	69	16.80	71	67	22.80	498	460	28.80	113	84
10.90	82	67	16.90	55	68	22.90	656	590	28.90	172	146
11.00	85	67	17.00	62	69	23.00	222	222	29.00	393	409
11.10	69	67	17.10	77	72	23.10	101	93	29.10	459	447
11.20	72	67	17.20	88	82	23.20	72	74	29.20	173	180
11.30	60	67	17.30	128	128	23.30	78	70	29.30	87	89
11.40	73	67	17.40	212	212	23.40	44	67	29.40	98	87
11.50	62	67	17.50	165	160	23.50	61	66	29.50	104	133
11.60	81	67	17.60	91	89	23.60	47	65	29.60	131	134
11.70	66	70	17.70	81	80	23.70	64	68	29.70	157	166
11.80	68	70	17.80	107	86	23.80	72	90	29.80	172	185
11.90	93	71	17.90	123	120	23.90	111	147	29.90	214	225
12.00	97	72	18.00	250	263	24.00	104	120	30.00	640	708
12.10	81	78	18.10	411	372	24.10	66	75	30.10	2065	2161
12.20	154	120	18.20	279	245	24.20	55	66	30.20	1806	1877
12.30	190	188	18.30	300	230	24.30	75	65	30.30	1022	1029
12.40	137	108	18.40	119	120	24.40	57	64	30.40	754	735
12.50	83	74	18.50	69	76	24.50	60	64	30.50	262	281
12.60	69	69	18.60	68	69	24.60	77	67	30.60	123	121
12.70	71	67	18.70	75	66	24.70	85	83	30.70	92	88
12.80	70	67	18.80	78	65	24.80	84	88	30.80	91	86
12.90	69	67	18.90	58	64	24.90	72	69	30.90	82	79
13.00	51	66	19.00	40	70	25.00	57	64	31.00	80	82
13.10	71	66	19.10	61	75	25.10	54	63	31.10	124	91
13.20	75	66	19.20	67	77	25.20	67	63	31.20	149	132
13.30	82	66	19.30	75	82	25.30	68	62	31.30	423	407
13.40	51	66	19.40	106	93	25.40	70	62	31.40	973	908
13.50	46	66	19.50	165	155	25.50	72	62	31.50	531	578
13.60	72	66	19.60	575	511	25.60	82	87	31.60	153	177
13.70	70	66	19.70	782	767	25.70	97	106	31.70	121	105
13.80	50	66	19.80	319	292	25.80	94	120	31.80	87	100
13.90	52	66	19.90	115	106	25.90	135	145	31.90	104	102
14.00	70	66	20.00	90	80	26.00	240	209	32.00	116	115
14.10	65	66	20.10	61	71	26.10	638	604	32.10	164	161
14.20	67	66	20.20	55	67	26.20	2390	2391	32.20	453	496
14.30	66	66	20.30	49	65	26.30	2894	2871	32.30	1605	1537
14.40	56	66	20.40	59	64	26.40	849	973	32.40	1304	1372
14.50	68	66	20.50	66	64	26.50	284	285	32.50	400	471
14.60	55	66	20.60	47	64	26.60	168	192	32.60	164	211
14.70	68	66	20.70	61	67	26.70	194	196	32.70	181	202
14.80	60	66	20.80	60	70	26.80	411	350	32.80	296	293
14.90	69	66	20.90	51	66	26.90	1327	1426	32.90	947	1013

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
33.00	3155	3215	39.00	252	238	45.00	193	173	51.00	87	80
33.10	2790	2771	39.10	801	852	45.10	142	130	51.10	97	93
33.20	893	827	39.20	1531	1473	45.20	87	89	51.20	90	96
33.30	267	231	39.30	943	917	45.30	81	76	51.30	91	86
33.40	140	134	39.40	335	310	45.40	85	74	51.40	84	88
33.50	77	100	39.50	205	190	45.50	86	77	51.50	125	141
33.60	88	83	39.60	217	182	45.60	59	83	51.60	117	144
33.70	91	73	39.70	162	134	45.70	77	83	51.70	102	110
33.80	89	62	39.80	157	95	45.80	87	77	51.80	64	74
33.90	85	74	39.90	134	109	45.90	86	78	51.90	44	63
34.00	82	86	40.00	138	137	46.00	97	87	52.00	62	61
34.10	110	109	40.10	124	109	46.10	136	124	52.10	54	63
34.20	140	164	40.20	111	91	46.20	284	271	52.20	77	76
34.30	201	172	40.30	148	125	46.30	371	314	52.30	90	91
34.40	270	230	40.40	176	142	46.40	296	286	52.40	102	86
34.50	775	783	40.50	212	183	46.50	276	299	52.50	83	76
34.60	1691	1697	40.60	424	375	46.60	344	339	52.60	75	67
34.70	1063	1090	40.70	476	433	46.70	235	236	52.70	62	66
34.80	370	380	40.80	283	237	46.80	137	138	52.80	66	73

34.90	278	251	40.90	136	113	46.90	145	123	52.90	78	80
35.00	412	425	41.00	72	94	47.00	297	281	53.00	86	85
35.10	1178	1214	41.10	94	99	47.10	615	591	53.10	79	81
35.20	2445	2557	41.20	124	127	47.20	496	460	53.20	95	86
35.30	1856	1781	41.30	216	222	47.30	275	217	53.30	97	89
35.40	525	525	41.40	318	337	47.40	90	100	53.40	78	81
35.50	180	178	41.50	863	869	47.50	84	80	53.50	78	76
35.60	103	117	41.60	1525	1416	47.60	76	78	53.60	113	88
35.70	82	95	41.70	1008	997	47.70	99	88	53.70	116	93
35.80	105	86	41.80	558	579	47.80	186	167	53.80	116	101
35.90	107	90	41.90	338	319	47.90	334	360	53.90	126	109
36.00	149	183	42.00	140	149	48.00	300	304	54.00	130	119
36.10	241	293	42.10	116	101	48.10	203	171	54.10	193	174
36.20	164	183	42.20	114	120	48.20	117	97	54.20	280	295
36.30	91	89	42.30	235	243	48.30	84	82	54.30	497	492
36.40	83	71	42.40	255	269	48.40	81	78	54.40	571	539
36.50	85	75	42.50	160	158	48.50	81	85	54.50	417	369
36.60	103	100	42.60	81	82	48.60	139	128	54.60	253	222
36.70	113	119	42.70	70	70	48.70	265	243	54.70	254	247
36.80	101	106	42.80	71	71	48.80	436	424	54.80	351	340
36.90	107	102	42.90	63	66	48.90	398	394	54.90	339	311
37.00	159	163	43.00	57	61	49.00	309	311	55.00	471	495
37.10	281	254	43.10	65	60	49.10	186	187	55.10	1067	1100
37.20	335	285	43.20	78	61	49.20	136	140	55.20	884	911
37.30	527	497	43.30	81	62	49.30	186	221	55.30	577	566
37.40	514	484	43.40	52	66	49.40	226	240	55.40	196	212
37.50	232	251	43.50	81	69	49.50	161	165	55.50	125	146
37.60	110	143	43.60	71	77	49.60	82	89	55.60	282	244
37.70	94	123	43.70	103	99	49.70	75	71	55.70	299	276
37.80	137	135	43.80	115	113	49.80	107	80	55.80	239	208
37.90	235	225	43.90	180	183	49.90	77	79	55.90	143	120
38.00	705	778	44.00	449	509	50.00	73	71	56.00	87	87
38.10	1688	1747	44.10	599	625	50.10	53	65	56.10	106	78
38.20	1312	1336	44.20	427	419	50.20	55	65	56.20	86	78
38.30	501	460	44.30	422	393	50.30	72	71	56.30	82	77
38.40	156	155	44.40	587	550	50.40	92	89	56.40	82	72
38.50	91	107	44.50	641	602	50.50	184	162	56.50	64	69
38.60	94	99	44.60	427	440	50.60	305	317	56.60	84	71
38.70	81	98	44.70	239	227	50.70	286	311	56.70	77	83
38.80	101	102	44.80	121	116	50.80	190	198	56.80	165	150
38.90	132	123	44.90	171	139	50.90	95	104	56.90	356	396

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
57.00	436	423	63.00	163	193	69.00	46	68	75.00	71	74
57.10	328	308	63.10	274	319	69.10	71	65	75.10	78	72
57.20	186	154	63.20	264	280	69.20	92	77	75.20	70	70
57.30	101	106	63.30	221	224	69.30	122	99	75.30	59	63
57.40	116	96	63.40	166	156	69.40	102	97	75.40	46	61
57.50	83	88	63.50	216	181	69.50	149	134	75.50	38	58
57.60	115	84	63.60	401	382	69.60	207	197	75.60	51	58
57.70	127	104	63.70	937	891	69.70	273	244	75.70	60	64
57.80	168	155	63.80	1100	998	69.80	187	206	75.80	78	77
57.90	162	167	63.90	701	720	69.90	196	192	75.90	101	106
58.00	162	144	64.00	460	446	70.00	134	164	76.00	133	114
58.10	127	115	64.10	319	317	70.10	241	242	76.10	94	96
58.20	153	137	64.20	271	254	70.20	336	345	76.20	112	93
58.30	389	357	64.30	213	227	70.30	400	416	76.30	75	73
58.40	612	599	64.40	193	171	70.40	398	471	76.40	95	73
58.50	445	494	64.50	136	121	70.50	298	348	76.50	75	82
58.60	328	366	64.60	171	132	70.60	384	378	76.60	93	82
58.70	245	245	64.70	160	171	70.70	475	473	76.70	100	96
58.80	266	271	64.80	160	154	70.80	348	340	76.80	127	106
58.90	215	221	64.90	133	140	70.90	316	278	76.90	129	132
59.00	231	235	65.00	100	102	71.00	205	165	77.00	129	111
59.10	282	262	65.10	85	78	71.10	105	93	77.10	93	98
59.20	470	473	65.20	82	67	71.20	87	82	77.20	88	85
59.30	484	493	65.30	76	64	71.30	101	97	77.30	71	76
59.40	354	355	65.40	95	72	71.40	106	98	77.40	86	90
59.50	193	185	65.50	99	86	71.50	93	86	77.50	127	116

59.60	108	98	65.60	99	101	71.60	83	83	77.60	132	130
59.70	102	91	65.70	132	129	71.70	105	92	77.70	151	151
59.80	94	95	65.80	125	121	71.80	155	144	77.80	120	128
59.90	77	83	65.90	118	111	71.90	172	148	77.90	115	125
60.00	89	70	66.00	94	99	72.00	148	152	78.00	110	115
60.10	71	65	66.10	104	105	72.10	193	221	78.10	74	93
60.20	82	70	66.20	94	106	72.20	261	250	78.20	83	82
60.30	68	74	66.30	123	100	72.30	247	222	78.30	78	76
60.40	70	78	66.40	98	85	72.40	182	199	78.40	61	70
60.50	77	78	66.50	97	81	72.50	138	135	78.50	62	65
60.60	97	87	66.60	116	74	72.60	106	110	78.60	57	64
60.70	109	114	66.70	103	92	72.70	91	109	78.70	68	66
60.80	241	217	66.80	92	106	72.80	201	174	78.80	73	81
60.90	475	455	66.90	90	90	72.90	330	298	78.90	121	123
61.00	668	670	67.00	99	92	73.00	569	557	79.00	160	125
61.10	1059	1052	67.10	91	99	73.10	700	671	79.10	100	117
61.20	901	859	67.20	96	90	73.20	479	476	79.20	138	129
61.30	616	646	67.30	92	86	73.30	367	381	79.30	153	151
61.40	332	329	67.40	96	76	73.40	181	194	79.40	244	235
61.50	195	198	67.50	99	76	73.50	116	117	79.50	194	197
61.60	273	273	67.60	98	93	73.60	98	97	79.60	135	164
61.70	494	467	67.70	165	139	73.70	99	103	79.70	143	156
61.80	376	362	67.80	313	300	73.80	125	122	79.80	86	106
61.90	290	272	67.90	469	504	73.90	155	169	79.90	88	88
62.00	143	140	68.00	387	394	74.00	160	181	80.00	84	93
62.10	89	91	68.10	307	311	74.10	220	233	80.10	73	84
62.20	81	77	68.20	183	181	74.20	207	228	80.20	74	78
62.30	70	73	68.30	173	172	74.30	193	197	80.30	69	71
62.40	91	86	68.40	186	195	74.40	242	234	80.40	79	70
62.50	138	117	68.50	144	149	74.50	187	212	80.50	80	86
62.60	223	209	68.60	133	127	74.60	122	149	80.60	95	97
62.70	236	212	68.70	86	94	74.70	108	135	80.70	78	83
62.80	196	179	68.80	69	81	74.80	76	95	80.80	68	83
62.90	157	141	68.90	73	73	74.90	83	79	80.90	88	74

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
81.00	53	63	87.00	161	143	93.00	109	119	99.00	94	93
81.10	74	63	87.10	145	144	93.10	142	152	99.10	90	79
81.20	72	67	87.20	95	112	93.20	146	135	99.20	72	64
81.30	99	79	87.30	94	101	93.30	164	144	99.30	65	64
81.40	120	126	87.40	80	79	93.40	214	219	99.40	69	60
81.50	180	170	87.50	63	68	93.50	336	333	99.50	54	52
81.60	151	157	87.60	70	64	93.60	312	329	99.60	56	49
81.70	138	142	87.70	58	62	93.70	206	243	99.70	46	48
81.80	110	113	87.80	46	61	93.80	191	231	99.80	58	47
81.90	102	95	87.90	57	63	93.90	203	197	99.90	48	44
82.00	82	84	88.00	57	62	94.00	128	126	100.00	80	42
82.10	56	72	88.10	60	62	94.10	69	88			
82.20	58	72	88.20	60	60	94.20	77	78			
82.30	66	73	88.30	56	56	94.30	90	81			
82.40	71	74	88.40	50	57	94.40	97	84			
82.50	64	70	88.50	51	59	94.50	105	87			
82.60	71	71	88.60	59	61	94.60	96	89			
82.70	83	91	88.70	69	66	94.70	118	120			
82.80	139	148	88.80	99	82	94.80	201	166			
82.90	143	160	88.90	131	101	94.90	121	131			
83.00	108	117	89.00	105	87	95.00	107	107			
83.10	119	122	89.10	84	96	95.10	112	119			
83.20	68	94	89.20	136	128	95.20	120	106			
83.30	61	70	89.30	100	121	95.30	118	99			
83.40	51	69	89.40	116	118	95.40	75	83			
83.50	85	80	89.50	139	152	95.50	74	78			
83.60	101	101	89.60	128	126	95.60	82	89			
83.70	97	127	89.70	84	97	95.70	113	88			
83.80	118	120	89.80	102	99	95.80	112	95			
83.90	118	108	89.90	96	94	95.90	97	88			
84.00	80	99	90.00	105	105	96.00	56	73			
84.10	112	105	90.10	98	102	96.10	84	73			
84.20	79	100	90.20	121	115	96.20	78	69			

84.30	71	83	90.30	151	166	96.30	68	63
84.40	72	81	90.40	177	178	96.40	67	62
84.50	51	70	90.50	194	169	96.50	57	59
84.60	49	61	90.60	123	157	96.60	57	59
84.70	53	57	90.70	198	177	96.70	59	68
84.80	62	59	90.80	216	184	96.80	75	78
84.90	72	69	90.90	170	166	96.90	120	83
85.00	88	96	91.00	168	140	97.00	81	87
85.10	155	146	91.10	103	120	97.10	142	115
85.20	139	135	91.20	76	102	97.20	187	162
85.30	126	115	91.30	85	78	97.30	162	155
85.40	123	113	91.40	56	65	97.40	137	122
85.50	66	88	91.50	70	63	97.50	147	154
85.60	63	75	91.60	67	62	97.60	239	196
85.70	74	69	91.70	51	59	97.70	162	154
85.80	56	68	91.80	50	57	97.80	140	126
85.90	68	78	91.90	76	58	97.90	161	144
86.00	84	79	92.00	72	59	98.00	152	141
86.10	102	89	92.10	50	53	98.10	146	154
86.20	93	99	92.20	61	55	98.20	145	154
86.30	88	81	92.30	70	61	98.30	124	112
86.40	65	81	92.40	60	61	98.40	90	104
86.50	82	84	92.50	56	59	98.50	110	113
86.60	97	91	92.60	66	62	98.60	107	99
86.70	116	112	92.70	70	66	98.70	88	83
86.80	123	138	92.80	87	69	98.80	83	74
86.90	135	138	92.90	94	80	98.90	82	82
86.90	133	136	92.90	74	72	98.90	87	83

Sample Rich63

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
9.00	93	67	15.00	58	65	21.00	54	64	27.00	2151	2302
9.10	103	69	15.10	59	65	21.10	63	64	27.10	2057	1994
9.20	82	69	15.20	65	65	21.20	55	64	27.20	651	631
9.30	106	69	15.30	58	65	21.30	69	64	27.30	370	374
9.40	81	70	15.40	55	65	21.40	51	64	27.40	735	768
9.50	123	71	15.50	65	65	21.50	42	67	27.50	570	606
9.60	111	76	15.60	61	65	21.60	63	70	27.60	257	238
9.70	128	121	15.70	50	65	21.70	50	73	27.70	184	165
9.80	168	177	15.80	54	65	21.80	61	78	27.80	285	179
9.90	164	140	15.90	58	65	21.90	79	82	27.90	381	341
10.00	147	110	16.00	60	65	22.00	99	99	28.00	1328	1256
10.10	228	126	16.10	57	65	22.10	203	213	28.10	2481	2243
10.20	370	251	16.20	66	65	22.20	535	517	28.20	1149	1097
10.30	761	799	16.30	41	65	22.30	402	405	28.30	293	297
10.40	877	1019	16.40	47	65	22.40	150	153	28.40	200	154
10.50	279	355	16.50	79	65	22.50	76	98	28.50	132	125
10.60	104	125	16.60	52	65	22.60	87	94	28.60	98	102
10.70	103	89	16.70	61	65	22.70	149	122	28.70	79	90
10.80	83	77	16.80	57	65	22.80	305	306	28.80	96	85
10.90	84	70	16.90	58	65	22.90	587	547	28.90	143	115
11.00	89	67	17.00	56	66	23.00	330	292	29.00	285	292
11.10	77	67	17.10	69	66	23.10	92	112	29.10	482	484
11.20	72	67	17.20	68	69	23.20	76	80	29.20	295	269
11.30	74	67	17.30	72	83	23.30	62	73	29.30	144	112
11.40	76	67	17.40	72	93	23.40	61	69	29.40	95	89
11.50	73	66	17.50	58	77	23.50	74	68	29.50	87	120
11.60	77	66	17.60	64	73	23.60	62	67	29.60	124	136
11.70	86	66	17.70	72	75	23.70	82	68	29.70	171	173
11.80	76	66	17.80	84	83	23.80	83	80	29.80	213	214
11.90	67	66	17.90	107	116	23.90	99	128	29.90	177	189
12.00	73	66	18.00	186	205	24.00	99	133	30.00	284	286
12.10	74	66	18.10	362	339	24.10	78	84	30.10	931	983
12.20	95	66	18.20	265	227	24.20	62	68	30.20	2033	2092
12.30	91	66	18.30	271	181	24.30	74	65	30.30	1431	1483
12.40	57	66	18.40	193	135	24.40	75	64	30.40	849	824
12.50	67	66	18.50	83	83	24.50	66	63	30.50	368	375
12.60	73	66	18.60	82	71	24.60	58	63	30.60	143	158
12.70	75	66	18.70	65	68	24.70	61	63	30.70	116	105
12.80	69	66	18.80	59	66	24.80	65	63	30.80	98	93

12.90	68	66	18.90	46	65	24.90	51	63	30.90	107	88
13.00	76	66	19.00	55	69	25.00	59	63	31.00	101	80
13.10	81	66	19.10	64	73	25.10	64	63	31.10	90	84
13.20	80	66	19.20	48	75	25.20	79	63	31.20	124	102
13.30	75	66	19.30	99	79	25.30	93	63	31.30	228	193
13.40	66	66	19.40	93	88	25.40	72	63	31.40	608	568
13.50	64	66	19.50	149	123	25.50	67	63	31.50	767	737
13.60	57	66	19.60	392	331	25.60	61	83	31.60	356	333
13.70	78	66	19.70	750	666	25.70	72	100	31.70	142	136
13.80	62	66	19.80	386	372	25.80	89	111	31.80	110	107
13.90	65	66	19.90	108	130	25.90	132	131	31.90	99	103
14.00	85	66	20.00	65	87	26.00	183	171	32.00	100	112
14.10	56	66	20.10	63	75	26.10	367	313	32.10	134	141
14.20	73	66	20.20	56	70	26.20	1128	1161	32.20	291	294
14.30	62	66	20.30	67	68	26.30	2840	2787	32.30	1071	1010
14.40	70	66	20.40	58	67	26.40	1714	1805	32.40	1397	1461
14.50	65	66	20.50	58	64	26.50	466	520	32.50	605	700
14.60	61	66	20.60	65	64	26.60	256	240	32.60	213	258
14.70	71	65	20.70	50	65	26.70	203	208	32.70	176	197
14.80	55	65	20.80	63	68	26.80	293	273	32.80	204	233
14.90	50	65	20.90	70	67	26.90	712	779	32.90	415	472

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
33.00	1556	1761	39.00	214	180	45.00	156	168	51.00	75	82
33.10	2955	3051	39.10	561	540	45.10	206	161	51.10	66	74
33.20	1716	1591	39.20	1300	1308	45.20	131	110	51.20	99	86
33.30	478	429	39.30	1224	1118	45.30	93	83	51.30	82	97
33.40	169	184	39.40	443	465	45.40	83	75	51.40	82	95
33.50	131	126	39.50	201	197	45.50	77	69	51.50	97	118
33.60	78	100	39.60	168	185	45.60	81	74	51.60	142	160
33.70	89	86	39.70	152	156	45.70	65	80	51.70	127	132
33.80	79	69	39.80	98	105	45.80	73	75	51.80	83	91
33.90	89	64	39.90	96	98	45.90	78	72	51.90	67	68
34.00	108	79	40.00	125	128	46.00	82	80	52.00	73	63
34.10	118	100	40.10	125	116	46.10	85	96	52.10	51	67
34.20	160	167	40.20	96	88	46.20	184	176	52.20	64	81
34.30	252	226	40.30	76	83	46.30	282	282	52.30	80	86
34.40	262	218	40.40	94	87	46.40	262	238	52.40	77	81
34.50	468	466	40.50	138	119	46.50	219	224	52.50	67	72
34.60	1358	1318	40.60	304	266	46.60	271	321	52.60	47	65
34.70	1300	1341	40.70	497	446	46.70	291	281	52.70	70	66
34.80	523	574	40.80	349	319	46.80	184	172	52.80	70	77
34.90	233	279	40.90	179	144	46.90	119	112	52.90	73	79
35.00	274	303	41.00	96	102	47.00	144	129	53.00	101	88
35.10	730	731	41.10	102	123	47.10	296	304	53.10	99	88
35.20	1848	1895	41.20	202	199	47.20	644	567	53.20	82	85
35.30	1944	1947	41.30	274	249	47.30	477	432	53.30	77	80
35.40	767	778	41.40	291	298	47.40	229	203	53.40	90	82
35.50	230	240	41.50	459	433	47.50	115	101	53.50	91	75
35.60	118	137	41.60	1234	1085	47.60	98	81	53.60	86	80
35.70	108	107	41.70	1417	1270	47.70	75	79	53.70	109	99
35.80	92	96	41.80	874	845	47.80	107	96	53.80	126	103
35.90	93	105	41.90	448	422	47.90	162	183	53.90	123	113
36.00	215	203	42.00	194	202	48.00	239	232	54.00	146	114
36.10	344	314	42.10	103	118	48.10	173	171	54.10	152	135
36.20	205	191	42.20	107	105	48.20	108	106	54.20	292	291
36.30	104	91	42.30	178	154	48.30	87	86	54.30	579	619
36.40	69	72	42.40	254	239	48.40	86	79	54.40	694	711
36.50	81	72	42.50	206	185	48.50	77	80	54.50	560	551
36.60	109	85	42.60	99	102	48.60	87	91	54.60	319	315
36.70	104	109	42.70	70	77	48.70	190	153	54.70	214	192
36.80	96	104	42.80	50	78	48.80	280	324	54.80	266	249
36.90	97	94	42.90	95	70	48.90	399	397	54.90	347	319
37.00	117	114	43.00	58	63	49.00	345	343	55.00	354	302
37.10	257	212	43.10	75	61	49.10	232	219	55.10	504	459
37.20	357	267	43.20	79	61	49.20	130	142	55.20	911	995
37.30	372	334	43.30	64	65	49.30	131	131	55.30	833	867
37.40	519	512	43.40	73	66	49.40	218	217	55.40	542	561
37.50	385	362	43.50	79	71	49.50	187	211	55.50	228	232

37.60	169	170	43.60	89	86	49.60	121	142	55.60	205	173
37.70	110	124	43.70	94	102	49.70	89	84	55.70	293	268
37.80	116	128	43.80	95	109	49.80	77	71	55.80	286	254
37.90	169	168	43.90	120	126	49.90	78	80	55.90	218	189
38.00	363	410	44.00	222	221	50.00	83	82	56.00	127	110
38.10	1066	1250	44.10	442	515	50.10	69	74	56.10	88	90
38.20	1431	1497	44.20	580	607	50.20	71	67	56.20	96	83
38.30	780	728	44.30	465	472	50.30	81	68	56.30	95	86
38.40	241	232	44.40	583	494	50.40	86	80	56.40	106	86
38.50	117	128	44.50	479	463	50.50	118	115	56.50	121	111
38.60	105	110	44.60	502	472	50.60	237	217	56.60	135	149
38.70	99	104	44.70	318	354	50.70	322	285	56.70	153	131
38.80	88	107	44.80	207	195	50.80	255	223	56.80	145	127
38.90	109	118	44.90	133	125	50.90	118	131	56.90	228	218

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
57.00	442	405	63.00	186	182	69.00	152	160	75.00	66	74
57.10	386	366	63.10	220	224	69.10	134	125	75.10	66	69
57.20	290	248	63.20	245	277	69.20	116	107	75.20	57	62
57.30	147	129	63.30	248	251	69.30	105	89	75.30	49	58
57.40	85	93	63.40	201	199	69.40	114	102	75.40	43	54
57.50	85	88	63.50	176	163	69.50	122	110	75.50	60	53
57.60	85	82	63.60	214	217	69.60	164	138	75.60	59	54
57.70	101	83	63.70	495	436	69.70	188	170	75.70	62	55
57.80	84	79	63.80	942	906	69.80	200	240	75.80	72	61
57.90	87	79	63.90	920	864	69.90	253	251	75.90	70	74
58.00	86	85	64.00	668	684	70.00	203	221	76.00	102	98
58.10	103	91	64.10	461	429	70.10	177	204	76.10	138	107
58.20	112	102	64.20	352	329	70.20	248	267	76.20	107	93
58.30	201	165	64.30	224	240	70.30	324	336	76.30	91	88
58.40	446	412	64.40	239	215	70.40	352	370	76.40	63	75
58.50	496	514	64.50	165	154	70.50	352	393	76.50	98	79
58.60	486	454	64.60	150	133	70.60	317	330	76.60	86	78
58.70	276	292	64.70	157	147	70.70	356	347	76.70	80	78
58.80	190	203	64.80	139	152	70.80	475	441	76.80	104	89
58.90	257	230	64.90	135	134	70.90	314	311	76.90	86	94
59.00	235	248	65.00	124	115	71.00	268	256	77.00	105	120
59.10	282	289	65.10	78	86	71.10	199	152	77.10	103	121
59.20	333	352	65.20	69	74	71.20	83	93	77.20	87	99
59.30	542	535	65.30	71	73	71.30	87	86	77.30	82	92
59.40	387	407	65.40	82	80	71.40	117	99	77.40	83	80
59.50	285	282	65.50	83	79	71.50	86	96	77.50	88	82
59.60	145	136	65.60	96	84	71.60	85	88	77.60	102	102
59.70	77	87	65.70	100	86	71.70	107	82	77.70	163	148
59.80	78	78	65.80	144	120	71.80	119	94	77.80	131	153
59.90	80	81	65.90	120	134	71.90	143	134	77.90	140	132
60.00	85	76	66.00	104	124	72.00	148	152	78.00	127	130
60.10	82	69	66.10	101	113	72.10	169	155	78.10	104	107
60.20	77	74	66.20	114	106	72.20	202	219	78.20	65	89
60.30	80	83	66.30	96	97	72.30	230	253	78.30	83	78
60.40	88	77	66.40	89	83	72.40	221	228	78.40	74	73
60.50	85	77	66.50	71	72	72.50	187	190	78.50	71	70
60.60	93	80	66.60	71	66	72.60	136	139	78.60	76	63
60.70	92	90	66.70	53	62	72.70	101	109	78.70	60	63
60.80	144	122	66.80	69	60	72.80	143	111	78.80	54	63
60.90	245	212	66.90	65	58	72.90	180	171	78.90	83	73
61.00	458	464	67.00	74	58	73.00	375	366	79.00	113	98
61.10	815	779	67.10	60	69	73.10	608	610	79.10	127	124
61.20	983	992	67.20	84	90	73.20	570	557	79.20	113	121
61.30	775	761	67.30	93	84	73.30	412	434	79.30	139	136
61.40	494	478	67.40	88	80	73.40	281	307	79.40	179	187
61.50	228	257	67.50	90	71	73.50	160	162	79.50	236	233
61.60	220	209	67.60	71	72	73.60	105	114	79.60	189	176
61.70	422	362	67.70	84	84	73.70	106	101	79.70	140	162
61.80	427	411	67.80	112	107	73.80	96	100	79.80	134	134
61.90	350	326	67.90	156	186	73.90	122	117	79.90	93	101
62.00	192	194	68.00	309	338	74.00	130	148	80.00	91	86
62.10	104	108	68.10	437	435	74.10	165	164	80.10	72	86
62.20	84	79	68.20	294	323	74.20	191	209	80.20	68	76

62.30	75	71	68.30	268	276	74.30	224	224	80.30	57	69
62.40	76	69	68.40	216	232	74.40	210	206	80.40	67	64
62.50	73	74	68.50	175	177	74.50	220	242	80.50	63	66
62.60	119	95	68.60	137	147	74.60	163	182	80.60	57	79
62.70	180	179	68.70	107	113	74.70	130	142	80.70	67	82
62.80	263	246	68.80	124	109	74.80	120	115	80.80	64	75
62.90	227	207	68.90	140	144	74.90	82	86	80.90	65	72

2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC	2THETA	YOBS	YCALC
81.00	54	66	87.00	116	130	93.00	79	83	99.00	73	73
81.10	64	63	87.10	149	144	93.10	115	113	99.10	84	79
81.20	59	63	87.20	124	129	93.20	112	130	99.20	90	71
81.30	81	69	87.30	94	98	93.30	116	121	99.30	63	61
81.40	76	84	87.40	98	90	93.40	130	126	99.40	61	57
81.50	136	125	87.50	62	71	93.50	151	157	99.50	48	52
81.60	152	162	87.60	56	59	93.60	266	227	99.60	41	46
81.70	146	150	87.70	57	58	93.70	310	284	99.70	50	43
81.80	135	131	87.80	65	61	93.80	262	267	99.80	64	42
81.90	127	109	87.90	59	61	93.90	182	220	99.90	57	41
82.00	107	91	88.00	57	63	94.00	203	196	100.00	64	39
82.10	86	80	88.10	64	60	94.10	149	157			
82.20	75	78	88.20	46	58	94.20	104	106			
82.30	88	87	88.30	56	58	94.30	94	82			
82.40	77	81	88.40	41	53	94.40	91	79			
82.50	101	79	88.50	70	51	94.50	81	83			
82.60	66	72	88.60	56	53	94.60	76	85			
82.70	66	68	88.70	48	56	94.70	65	79			
82.80	75	72	88.80	63	64	94.80	91	83			
82.90	86	96	88.90	99	84	94.90	108	112			
83.00	144	144	89.00	112	94	95.00	173	149			
83.10	123	133	89.10	102	85	95.10	154	147			
83.20	82	109	89.20	88	94	95.20	120	138			
83.30	106	104	89.30	115	118	95.30	138	136			
83.40	67	77	89.40	121	131	95.40	122	126			
83.50	61	67	89.50	132	134	95.50	96	103			
83.60	58	71	89.60	133	140	95.60	94	88			
83.70	63	80	89.70	138	137	95.70	103	88			
83.80	103	108	89.80	102	118	95.80	91	90			
83.90	135	128	89.90	95	96	95.90	152	104			
84.00	110	103	90.00	89	88	96.00	99	103			
84.10	99	107	90.10	88	89	96.10	93	82			
84.20	93	112	90.20	82	105	96.20	73	77			
84.30	78	103	90.30	111	120	96.30	88	73			
84.40	76	90	90.40	121	134	96.40	62	63			
84.50	73	82	90.50	151	164	96.50	63	59			
84.60	60	72	90.60	211	191	96.60	60	57			
84.70	56	61	90.70	170	175	96.70	58	59			
84.80	54	56	90.80	206	180	96.80	62	66			
84.90	51	56	90.90	201	204	96.90	84	75			
85.00	52	61	91.00	169	175	97.00	70	83			
85.10	70	77	91.10	154	142	97.10	97	93			
85.20	129	115	91.20	135	122	97.20	112	113			
85.30	148	135	91.30	80	100	97.30	170	151			
85.40	110	123	91.40	101	79	97.40	145	148			
85.50	105	114	91.50	66	65	97.50	117	124			
85.60	94	96	91.60	57	60	97.60	135	143			
85.70	53	76	91.70	52	59	97.70	218	173			
85.80	70	65	91.80	48	56	97.80	159	151			
85.90	55	59	91.90	59	53	97.90	113	123			
86.00	55	63	92.00	68	55	98.00	134	133			
86.10	80	75	92.10	62	53	98.10	158	144			
86.20	71	87	92.20	51	50	98.20	156	149			
86.30	81	95	92.30	65	52	98.30	149	138			
86.40	85	84	92.40	55	57	98.40	130	112			
86.50	84	80	92.50	61	60	98.50	88	99			
86.60	94	78	92.60	78	59	98.60	94	92			
86.70	85	81	92.70	61	59	98.70	95	81			
86.80	97	105	92.80	63	62	98.80	92	76			
86.90	129	137	92.90	61	68	98.90	77	70			