

# The synthesis and crystal structure of a magnesium-lithium-scandium protopyroxene

JOSEPH R. SMYTH

Geosciences Group, MS 978, Los Alamos Scientific Laboratory  
Los Alamos, New Mexico 87545

AND JUN ITO

James Frank Institute, University of Chicago  
Chicago, Illinois 60637

## Abstract

Crystals of protopyroxene solid solution,  $\text{Li}_x\text{Sc}_x\text{Mg}_{2-x}\text{Si}_2\text{O}_6$ ,  $0.1 \leq x \leq 0.35$ , were grown, in solvents of the system  $\text{Li}_2\text{O}-\text{V}_2\text{O}_5-\text{MoO}_3$ , by cooling from 1350 to 650° at 1.5°C per hour. The crystals are transparent, euhedral, and prismatic, elongate parallel to  $c$  and up to  $15 \times 4 \times 3$  mm in size, with well-developed {010}, {110}, and {121} faces. The cell edges used for structure analysis are:  $a = 9.251$ ,  $b = 8.773$ , and  $c = 5.377\text{\AA}$ . Long-exposure X-ray precession photographs showed no diffraction maxima inconsistent with space group  $Pbcn$  and no evidence of stack disorder. The crystal structure was refined from 1507 measured X-ray intensities, of which 826 were greater than  $3\sigma$  of the background intensity. Refinements of the structure in space groups  $P2_1cn$ ,  $Pb2n$ ,  $Pbc2_1$ , and  $P2/c$  yielded structures which did not differ significantly from that in space group  $Pbcn$ . The structure is ordered with all of the  $\text{Sc}^{3+}$  in  $M1$  and all of the  $\text{Li}^+$  in  $M2$ .

## Introduction

Protoenstatite is the stable form of  $\text{MgSiO}_3$  between approximately 1000° and 1540°C. On cooling below 1000°C it breaks down rapidly to a disordered mixture of ortho- and clinoenstatite (Brown and Smith, 1963; Smyth, 1973).

Due in part to its instability at lower temperature, single crystals of protopyroxene large enough for an X-ray structure determination have not been found in nature or made in the laboratory. Polysynthetically-twinned clinopyroxenes, which presumably originated by inversion from protopyroxene during rapid cooling, have been described in several meteorites (Binns, 1970; Dodd, 1974; Dodd *et al.*, 1975) and from a terrestrial porphyritic volcanic rock from Cape Vogel, Papua (Dallwitz *et al.*, 1966).

Atlas (1952) postulated that the space group is  $Pbcn$ , and the structure was determined by Smith (1959, 1969) from powder data. Sadanaga *et al.* (1969) reported a structure determination from 47 X-ray intensities measured from a single crystal at 1000°C. Smyth (1971) reported a structure refinement from 187 observed intensities measured from precession films taken at 1100°C, and noted numer-

ous violations of the  $b$ -glide diffraction symmetry. He reported the space group as  $P2_1cn$ ; however, the material studied showed significant stacking disorder, and he suggested that the violation of  $b$ -glide symmetry may have arisen from the stack disorder. Because of the difficulty of obtaining a well-crystallized specimen, the structure has never been refined from single-crystal intensity data obtained at room temperature, and the standard errors in all protopyroxene structures reported in the literature are relatively large. Further, as Thompson (1970) suggested that the ideal space group for the proto structure should be  $P2_1cn$ , there remains the question of the true space group of the protopyroxene structures.

## Crystal synthesis

During experiments of doping orthoenstatite with transition elements using a high-temperature solvent (Ito, 1975), it was found that  $\text{Sc}^{3+}$ , when coupled with  $\text{Li}^+$ , stabilizes protoenstatite structure at room temperature. Subsequent phase-equilibrium studies of the join  $\text{MgSiO}_3-\text{LiScSi}_2\text{O}_6$  showed that, using pure oxides as starting materials, a substantial field of stability for quenchable protopyroxene exists at sub-

## PROTO PBC21 F CALC

(1)

H	K	L	F(OBS)	F(CALC)
0	0	3	3.213	3.000
0	0	4	4.157	4.001
0	0	5	21.581	21.388
0	0	6	3.150 *	0.000
0	0	7	4.178 *	4.000
0	0	8	29.472	27.626
0	0	9	5.080 *	0.000
0	0	10	10.701	9.539
0	1	0	5.557 *	0.000
0	1	1	5.175 *	5.000
0	1	2	4.698 *	0.000
0	1	3	4.189 *	0.000
0	1	4	3.638 *	0.000
0	1	5	3.288 *	0.000
0	1	6	2.779 *	0.000
0	1	7	2.333 *	0.000
0	1	8	1.920 *	0.000
0	1	9	3.468	0.000
0	1	10	1.623 *	0.000
0	2	0	49.627	43.461
0	2	1	3.372	3.778
0	2	2	21.512	20.412
0	2	3	126.105	124.612
0	2	4	11.517	10.268
0	2	5	16.873	16.349
0	2	6	3.807 *	6.141
0	2	7	9.640	8.782
0	2	8	17.953	13.220
0	2	9	35.506	32.230
0	2	10	10.732	7.861
0	3	0	5.239 *	0.000
0	3	1	4.759 *	0.000
0	3	2	4.295 *	0.000
0	3	3	3.744 *	0.000
0	3	4	3.298 *	0.000
0	3	5	2.874 *	0.000
0	3	6	2.588 *	0.000
0	3	7	2.216 *	0.000
0	3	8	1.866 *	0.000
0	4	0	5.759	3.879
0	4	1	8.601	9.471
0	4	2	3.044 *	29.873
0	4	3	79.485	81.120
0	4	4	7.850	8.360
0	4	5	25.049	22.840
0	4	6	31.137	29.797
0	4	7	4.306 *	3.368
0	4	8	4.910 *	4.615
0	4	9	23.745	21.694
0	4	10	5.769 *	9.818
0	5	0	5.663 *	0.000
0	5	1	5.377 *	0.000
0	5	2	4.878 *	0.000
0	5	3	4.497 *	0.000
0	5	4	4.104 *	0.000
0	5	5	3.666 *	0.000

## PROTO PBC21 F CALC

(2)

H	K	L	F(OBS)	F(CALC)
0	0	3	3.151 *	0.000
0	0	4	2.310 *	0.000
0	0	5	2.588 *	0.000
0	0	6	2.344 *	0.000
0	0	7	2.323 *	0.000
0	0	8	125.353	131.390
0	0	9	3.447	33.839
0	0	10	18.421	19.343
0	1	0	7.349	5.661
0	1	1	8.770	7.158
0	1	2	73.133	71.877
0	1	3	4.772 *	7.532
0	1	4	11.114	12.503
0	1	5	15.749	13.317
0	1	6	5.451 *	0.000
0	1	7	5.271 *	0.000
0	1	8	4.709 *	0.000
0	1	9	4.359 *	0.000
0	2	0	3.881 *	0.000
0	2	1	3.606 *	0.000
0	2	2	3.245 *	0.000
0	2	3	3.075 *	0.000
0	2	4	2.916 *	0.000
0	2	5	2.863 *	0.000
0	2	6	34.329	33.699
0	2	7	9.651	12.640
0	2	8	18.474	19.830
0	2	9	74.215	74.533
0	2	10	12.853	13.749
0	3	0	10.255	10.141
0	3	1	8.420	7.666
0	3	2	13.299	16.764
0	3	3	5.313 *	2.892
0	3	4	33.724	34.500
0	3	5	5.684 *	0.000
0	3	6	5.451 *	0.000
0	3	7	5.037 *	0.000
0	3	8	4.751 *	0.000
0	3	9	4.327 *	0.000
0	3	10	4.062 *	0.000
0	4	0	5.366	0.000
0	4	1	3.595 *	0.000
0	4	2	3.478 *	0.000
0	4	3	3.362 *	0.000
0	4	4	43.842	47.362
0	4	5	29.450	29.529
0	4	6	3.881 *	3.290
0	4	7	14.052	15.266
0	4	8	4.316 *	7.891
0	4	9	17.721	18.170
0	4	10	21.645	23.782
0	4	11	5.281 *	8.397
0	4	12	5.706 *	6.697
0	4	13	5.727 *	0.000
0	4	14	5.154 *	0.001
0	4	15	4.857 *	0.000

## PROTO PBC21 F CALC

(3)

H	K	L	F(OBS)	F(CALC)
0	11	4	4.422 *	0.000
0	11	3	4.348 *	0.000
0	11	2	4.157 *	0.000
0	11	1	5.642	0.001
0	11	0	4.083 *	0.000
0	12	6	53.959	54.417
0	12	1	4.497 *	6.316
0	12	2	16.258	16.273
0	12	3	28.284	28.901
0	12	4	4.921 *	14.972
0	12	5	5.251 *	5.882
0	12	6	30.723	30.704
0	12	7	5.578 *	1.418
0	13	7	5.684 *	0.000
0	13	6	10.022	0.000
0	13	5	5.239 *	0.000
0	13	4	5.090 *	0.000
0	13	3	4.910 *	0.001
0	13	2	4.687 *	0.000
0	13	1	4.666 *	0.001
0	13	0	4.624 *	0.000
0	14	6	22.896	22.883
0	14	1	4.963 *	8.265
0	14	2	5.197 *	6.778
0	14	3	41.360	41.173
0	14	4	5.483 *	8.768
0	14	5	5.727 *	11.857
0	14	6	17.403	15.355
0	15	5	5.653 *	0.000
0	15	4	5.610 *	0.000
0	15	3	5.419 *	0.000
0	15	2	5.313 *	0.000
0	15	1	5.239 *	0.000
0	15	0	5.228 *	0.000
0	16	0	24.211	25.573
0	16	1	11.666	7.457
0	16	2	5.525 *	7.254
0	16	3	5.610 *	2.231
0	16	4	5.748 *	2.276
0	17	2	5.748 *	2.000
0	17	1	5.653 *	0.000
0	17	0	5.716 *	0.000
1	17	0	5.790 *	5.392
1	17	1	15.743	7.970
1	17	2	5.674 *	3.269
1	16	4	13.617	14.061
1	16	2	12.663	13.675
1	16	1	5.557 *	7.715
1	16	0	5.472 *	1.822
1	15	0	5.228 *	7.223
1	15	1	5.239 *	3.597
1	15	2	5.472 *	4.242
1	15	3	5.493 *	4.140
1	15	4	5.621 *	7.158
1	15	5	5.663 *	1.630
1	14	6	5.653 *	2.689

O PBC21 F CALC

(4)

	H	K	L	F(OBS)	F(CALC)
1	14	5	1	6.679	12.959
1	14	4	7	7.156 *	6.629
1	14	3	5	5.186 *	5.809
1	14	2	10	10.138	6.769
1	14	1	25	25.452	25.933
1	14	0	4	4.953 *	6.302
1	13	9	1	1.414	9.464
1	13	8	9	9.587	7.928
1	13	7	2	9.725	7.122
1	13	6	3	4.921 *	2.665
1	13	5	4	5.26 *	8.306
1	13	5	5	12.387	10.221
1	13	6	6	10.032	5.147
1	13	7	7	5.886 *	9.627
1	12	7	13	13.585	13.277
1	12	6	6	5.515 *	9.368
1	12	5	5	5.186 *	3.855
1	12	4	27	27.966	31.266
1	12	3	4	4.634 *	3.939
1	12	2	27	27.775	27.372
1	12	1	14	14.762	17.448
1	12	0	4	4.401 *	12.759
1	11	9	0	17.817	17.491
1	11	8	1	4.136 *	6.913
1	11	7	2	18.368	18.268
1	11	6	3	16.417	16.281
1	11	5	4	15.017	14.356
1	11	5	5	4.942 *	4.292
1	11	6	6	14.487	14.511
1	11	7	7	10.637	10.296
1	11	8	12	12.737	8.394
1	10	8	8	11.732	9.881
1	10	7	10	10.457	9.442
1	10	6	6	4.963 *	2.646
1	10	5	5	18.241	18.986
1	10	4	22	22.992	24.306
1	10	3	10	10.064	11.180
1	10	2	29	29.309	19.183
1	10	1	20	20.669	21.230
1	10	0	3	3.722 *	5.397
1	9	9	0	6.713	4.746
1	9	8	1	21.072	22.149
1	9	7	2	3.722 *	6.164
1	9	6	3	27.446	28.070
1	9	5	4	7.731	6.634
1	9	5	5	5.875 *	9.878
1	9	6	6	9.704	8.465
1	9	7	7	5.271 *	6.139
1	9	8	8	5.515 *	5.552
1	9	9	9	5.822 *	8.325
1	8	9	8	5.759 *	10.558
1	8	8	7	5.334 *	1.653
1	8	7	22	22.939	22.773
1	8	6	6	4.560 *	3.783
1	8	5	3	3.681	33.415
1	8	4	4	9.566	6.788

PROTO PBC21 F CALC

(5)

	H	K	L	F(OBS)	F(CALC)
●	1	8	3	14.518	15.724
●	1	8	2	3.468 *	7.426
●	1	8	1	45.315	47.545
●	1	8	0	3.107 *	1.304
●	1	7	0	9.226	8.915
●	1	7	1	23.246	24.596
●	1	7	2	6.766	8.261
●	1	7	3	3.319 *	6.383
●	1	7	4	3.553 *	1.026
●	1	7	5	15.993	15.468
●	1	7	6	4.284 *	1.355
●	1	7	7	4.783 *	4.596
●	1	7	8	5.281 *	1.248
●	1	7	9	5.536 *	3.644
●	1	6	9	5.462 *	4.595
●	1	6	8	18.050	20.127
●	1	6	7	4.645 *	4.362
●	1	6	6	17.117	21.756
●	1	6	5	15.335	13.958
●	1	6	4	5.750 *	49.204
●	1	6	3	8.930	9.334
●	1	6	2	68.148	74.309
●	1	6	1	14.253	15.739
●	1	6	0	2.619 *	5.182
●	1	5	0	66.282	65.129
●	1	5	2	44.785	48.593
●	1	5	3	29.769	31.709
●	1	5	4	26.269	29.144
●	1	5	5	3.680 *	6.978
●	1	5	6	17.095	17.189
●	1	5	7	4.645 *	3.974
●	1	5	8	11.814	9.362
●	1	5	9	5.451 *	4.217
●	1	5	10	5.801 *	5.312
●	1	4	10	10.743	9.655
●	1	4	9	5.472 *	9.009
●	1	4	8	11.785	11.726
●	1	4	7	28.655	24.286
●	1	4	6	13.150	12.399
●	1	4	5	21.051	24.008
●	1	4	4	11.719	12.295
●	1	4	3	2.704 *	2.522
●	1	4	2	37.383	41.004
●	1	4	1	63.503	66.587
●	1	4	0	2.068 *	4.411
●	1	3	0	36.651	35.547
●	1	3	1	35.177	37.345
●	1	3	2	19.333	19.845
●	1	3	3	65.232	67.783
●	1	3	4	3.065 *	6.562
●	1	3	5	24.816	25.361
●	1	3	6	3.318 *	1.441
●	1	3	7	21.507	20.482
●	1	3	8	4.794 *	3.165
●	1	3	9	16.852	19.027
●	1	3	10	5.515 *	1.856

## PROTO PBC21 F CALC

(5)

H	K	L	F(OBS)	F(CALC)
1	2	10	5.642 *	5.375
1	2	9	5.440 *	15.859
1	2	8	4.889 *	3.601
1	2	7	33.523	34.779
1	2	6	8.717	8.012
1	2	5	31.550	34.398
1	2	4	26.629	29.253
1	2	3	7.169	6.238
1	2	2	12.313	11.635
1	2	1	89.401	89.848
1	1	0	20.892	2.793
1	1	1	8.473	7.315
1	1	2	7.063	6.487
1	1	3	25.150	25.116
1	1	4	16.449	16.745
1	1	5	18.679	18.934
1	1	6	18.548	17.096
1	1	7	4.200 *	1.480
1	1	8	16.459	14.716
1	1	9	5.175 *	1.392
1	1	10	5.769 *	10.307
1	0	10	27.966	24.116
1	0	9	5.175 *	0.000
1	0	8	25.500	18.624
1	0	7	4.189 *	0.000
1	0	6	10.976	8.943
1	0	5	3.224 *	0.000
1	0	4	104.747	103.652
1	0	3	2.280 *	0.000
1	0	2	41.671	85.322
1	0	1	4.677	0.000
1	0	0	1.665 *	2.242
2	0	0	13.659	8.160
2	0	1	3.966	4.060
2	0	2	93.877	90.937
2	0	3	2.397 *	3.000
2	0	4	62.294	56.966
2	0	5	3.203 *	0.400
2	0	6	3.733 *	0.879
2	0	7	4.221 *	0.000
2	0	8	44.139	36.759
2	0	9	5.197 *	0.060
2	0	10	16.639	12.691
2	1	0	5.653 *	5.753
2	1	9	5.281 *	5.732
2	1	8	4.749 *	4.457
2	1	7	14.561	13.729
2	1	6	7.996	7.862
2	1	5	10.361	10.302
2	1	4	26.714	27.063
2	1	3	7.158	6.933
2	1	2	30.193	28.571
2	1	1	44.701	43.280
2	1	0	2.715	3.147
2	2	0	57.490	54.240

## PROTO PBC21 F CALC

(7)

H	K	L	F(CBS)	F(CALC)
2	2	3	11.560	12.429
2	2	4	3.001 *	3.784
2	2	5	44.573	47.398
2	2	6	14.964	14.401
2	2	7	18.623	18.505
2	2	8	8.749	8.594
2	2	9	5.154 *	2.554
2	2	10	5.578 *	1.972
2	3	10	5.684 *	1.816
2	3	9	5.260 *	3.895
2	3	8	4.836 *	4.957
2	3	7	4.337 *	2.084
2	3	6	10.849	10.182
2	3	5	12.053	9.903
2	3	4	16.077	17.233
2	3	3	9.142	10.302
2	3	2	17.785	18.632
2	3	1	36.757	37.126
2	3	0	1.951 *	3.131
2	4	6	17.011	16.070
2	4	2	30.787	35.203
2	4	3	23.681	26.279
2	4	4	14.487	15.330
2	4	5	26.237	27.863
2	4	6	13.744	13.201
2	4	7	9.173	9.505
2	4	8	6.618 *	12.199
2	4	9	5.409 *	5.357
2	4	10	5.642 *	2.734
2	5	10	5.759 *	2.716
2	5	9	5.409 *	7.388
2	5	8	4.931 *	5.972
2	5	7	12.429	14.710
2	5	6	11.390	11.429
2	5	5	3.797 *	2.947
2	5	4	6.437	5.478
2	5	3	2.948 *	2.987
2	5	2	15.112	16.533
2	5	1	30.649	32.950
2	5	0	2.460 *	8.477
2	6	0	2.556 *	0.952
2	6	1	16.480	17.532
2	6	2	58.540	66.286
2	6	3	3.150 *	2.212
2	6	4	30.712	37.818
2	6	5	10.170	11.295
2	6	6	4.295 *	6.699
2	6	7	4.666 *	4.178
2	6	8	18.304	23.969
2	6	9	5.472 *	1.120
2	7	9	5.695 *	5.793
2	7	8	5.292 *	2.819
2	7	7	9.014	6.083
2	7	6	4.550 *	9.413
2	7	5	13.394	16.435
2	7	4	3.659 *	3.793

## PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
2	7	2	10.361	12.353
2	7	1	15.282	19.938
2	7	0	2.810 *	2.967
2	8	0	20.012	20.882
2	8	1	5.292 *	50.539
2	8	2	10.170	10.786
2	8	3	3.648 *	5.675
2	8	4	10.287	9.879
2	8	5	28.347	36.728
2	8	6	13.193	13.284
2	8	7	14.094	15.087
2	8	8	5.430 *	4.155
2	8	9	5.621 *	2.791
2	9	9	5.684 *	6.123
2	9	8	5.472 *	0.934
2	9	7	5.292 *	9.235
2	9	6	4.868 *	5.500
2	9	5	4.359 *	4.447
2	9	4	7.869	6.085
2	9	3	3.977 *	6.834
2	9	2	3.648 *	7.299
2	9	1	9.481	10.750
2	9	0	3.489 *	2.622
2	10	0	14.901	14.521
2	10	1	3.881 *	6.991
2	10	3	16.491	15.697
2	10	4	12.663	15.588
2	10	5	4.666 *	5.963
2	10	6	5.133 *	4.713
2	10	7	5.313 *	5.025
2	10	8	8.527 *	15.199
2	11	8	5.748 *	1.443
2	11	7	5.546 *	4.781
2	11	6	5.197 *	4.829
2	11	5	12.461	12.332
2	11	4	8.527	6.163
2	11	3	9.110	13.404
2	11	2	4.136 *	7.247
2	11	1	9.417	8.407
2	11	0	5.653	2.392
2	12	0	13.299	13.873
2	12	1	9.969	10.464
2	12	2	14.571	19.119
2	12	3	4.825 *	3.623
2	12	4	10.817	12.674
2	12	5	11.199	11.581
2	12	6	5.462 *	7.076
2	12	7	5.674 *	7.149
2	13	7	5.896 *	7.944
2	13	6	5.546 *	2.619
2	13	5	5.430 *	2.501
2	13	4	5.133 *	3.176
2	13	3	5.027 *	4.113
2	13	2	4.804 *	1.893
2	13	1	13.490	11.276
2	13	0	4.751 *	12.959

## PROTO PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
2	14	1	10.966	9.675
2	14	1	16.692	17.146
2	14	2	11.135	9.911
2	14	3	5.292 *	6.970
2	14	4	5.515 *	9.457
2	14	5	9.216 *	17.438
2	14	6	5.831 *	6.512
2	15	5	5.737 *	6.731
2	15	4	5.546 *	6.297
2	15	3	5.515 *	4.518
2	15	2	5.409 *	2.357
2	15	1	5.334 *	2.595
2	15	0	5.250 *	9.139
2	16	0	5.621 *	5.889
2	16	1	5.653 *	7.209
2	16	2	7.540 *	12.954
2	16	3	7.604 *	12.873
2	16	4	5.896 *	8.396
2	17	2	5.684 *	2.875
2	17	1	5.875 *	8.817
2	17	0	5.727 *	8.451
3	17	0	15.250	13.002
3	17	1	5.812 *	8.239
3	16	3	5.546 *	5.920
3	16	2	5.706 *	6.698
3	16	1	5.600 *	4.010
3	16	0	5.515 *	1.583
3	15	0	11.432	19.844
3	15	1	5.313 *	5.062
3	15	2	5.377 *	5.449
3	15	3	5.546 *	6.317
3	15	4	5.504 *	9.255
3	15	5	5.684 *	2.521
3	14	6	5.600 *	6.441
3	14	5	5.621 *	4.715
3	14	3	5.334 *	2.957
3	14	2	5.197 *	7.583
3	14	1	5.271 *	6.200
3	14	0	4.942 *	5.191
3	13	0	4.731 *	0.615
3	13	1	8.728	8.756
3	13	2	11.581	17.116
3	13	3	19.768	25.260
3	13	4	5.334 *	13.617
3	13	5	5.377 *	3.648
3	13	6	5.642 *	3.276
3	12	7	5.631 *	0.616
3	12	6	5.345 *	6.690
3	12	5	5.239 *	4.916
3	12	4	4.921 *	2.264
3	12	3	4.719 *	2.829
3	12	2	4.624 *	3.582
3	12	1	4.539 *	4.864
3	12	0	4.433 *	0.936
3	11	0	36.153	38.018
3	11	1	21.910	25.107

## PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
3	11	2	8.908	1.737
3	11	3	4.518 *	7.780
3	11	4	9.576	11.972
3	11	5	6.819 *	14.434
3	11	6	8.739 *	17.843
3	11	7	5.568 *	8.813
3	11	8	5.674 *	1.385
3	10	8	5.600 *	4.413
3	10	7	5.398 *	6.386
3	10	6	5.037 *	4.945
3	10	5	4.719 *	3.504
3	10	4	12.175	13.016
3	10	3	4.168 *	4.919
3	10	2	15.218	15.148
3	10	1	8.240	10.296
3	10	0	3.839 *	2.340
3	9	0	18.145	21.047
3	9	1	3.722 *	7.073
3	9	2	7.943	1.634
3	9	3	16.523	20.055
3	9	4	4.178 *	5.902
3	9	5	8.325	7.921
3	9	6	4.889 *	7.257
3	9	7	7.922 *	12.127
3	9	8	5.568 *	6.879
3	8	9	5.642 *	1.816
3	8	8	5.387 *	4.311
3	8	7	6.702 *	8.925
3	8	6	4.719 *	5.724
3	8	5	4.327 *	5.702
3	8	4	12.694	13.493
3	8	3	3.595 *	3.603
3	8	2	10.361	9.562
3	8	1	16.258	17.153
3	8	0	3.277 *	9.822
3	7	0	3.139 *	4.028
3	7	1	18.966	12.274
3	7	2	14.582	20.504
3	7	4	3.659 *	4.673
3	7	5	8.569	7.451
3	7	6	6.787 *	13.382
3	7	7	6.512 *	10.148
3	7	8	5.260 *	1.079
3	7	9	9.799 *	16.779
3	6	9	5.504 *	0.423
3	6	8	5.143 *	2.140
3	6	7	4.730 *	3.272
3	6	6	4.221 *	2.083
3	6	5	3.892 *	2.634
3	6	4	10.032	10.454
3	6	3	3.224 *	4.222
3	6	2	2.959 *	2.747
3	6	1	5.653	5.062
3	6	0	2.779 *	5.776
3	5	0	40.066	44.494
3	5	2	6.671	6.286

## PROTO PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
3	5	3	12.223	13.310
1	6	3	8.940	9.334
3	5	4	21.595	19.564
3	5	5	21.030	21.997
3	5	6	38.019	36.385
3	5	7	10.319	7.284
3	5	8	11.572	9.631
3	4	8	5.016 *	4.887
3	4	7	8.325	7.814
3	4	6	4.168 *	4.047
3	4	5	10.192	10.376
3	4	4	27.064	27.236
3	4	3	6.321	8.019
3	4	2	18.389	20.114
3	4	1	13.129	13.180
3	4	0	2.344 *	0.439
3	3	0	28.135	27.215
3	3	1	67.173	68.803
3	3	2	16.989	18.332
3	3	3	56.122	59.229
3	3	4	3.086 *	2.470
3	3	5	22.981	22.268
3	3	6	10.393	9.564
3	3	7	14.195	16.766
3	3	8	10.796	8.768
3	2	8	4.889 *	5.707
3	2	7	11.952	10.131
3	2	6	10.828	10.962
3	2	5	12.037	11.973
3	2	4	15.780	15.901
3	2	3	7.222	6.202
3	2	2	2.959 *	3.547
3	2	1	12.864	13.879
3	2	0	1.888 *	8.273
3	1	0	98.416	99.022
3	1	1	16.268	16.398
3	1	2	40.946	41.659
3	1	4	18.676	19.797
3	1	5	19.142	17.810
3	1	6	23.893	23.322
3	1	7	4.221 *	1.067
3	1	8	10.637	8.743
3	0	8	4.772 *	4.345
3	0	7	4.215 *	0.000
3	0	6	8.802	6.609
3	0	5	3.341 *	0.000
3	0	4	2.959 *	2.325
3	0	3	2.513 *	0.000
3	0	2	3.892	5.278
3	0	1	3.807	6.000
3	0	0	4.231	4.317
4	0	0	23.565	20.034
4	0	1	4.284	0.000
4	0	2	55.539	56.296
4	0	3	2.662 *	0.000
4	0	4	17.011	41.127

## PROTO PBC21 F(CALC)

(12)

H	K	L	F(OBS)	F(CALC)
4	0	5	3.436 *	0.000
4	0	6	25.845	22.965
4	0	7	4.359 *	0.000
4	0	8	29.755	27.401
4	1	8	10.754	9.255
4	1	7	16.936	15.399
4	1	6	3.977 *	3.007
4	1	5	15.876	14.257
4	1	4	48.370	49.649
4	1	3	5.398	5.888
4	1	2	30.723	30.138
4	1	1	33.958	34.138
4	1	0	2.015 *	3.479
4	2	0	6.321	5.884
4	2	1	37.097	36.612
4	2	2	46.302	47.613
4	2	3	3.150	30.872
4	2	4	13.172	12.694
4	2	5	16.077	16.516
4	2	6	14.614	13.261
4	2	7	19.259	16.369
4	2	8	4.963 *	3.127
4	3	8	4.953 *	3.648
4	3	7	29.493	27.915
4	3	6	8.473	7.187
4	3	5	25.367	24.303
4	3	4	3.203 *	4.361
4	3	3	5.695	6.887
4	3	2	16.226	15.514
4	3	1	55.210	55.009
4	3	0	2.269 *	4.614
4	4	0	55.953	56.587
4	4	2	2.821 *	4.519
4	4	3	9.492	10.410
4	4	4	3.372 *	6.048
4	4	5	3.669 *	4.582
4	4	6	13.161	12.768
4	4	7	8.442	8.764
4	4	8	11.899	8.976
4	5	8	14.349	12.748
4	5	7	10.435	9.888
4	5	6	16.914	14.542
4	5	5	3.892 *	4.742
4	5	4	29.493	29.314
4	5	3	3.129 *	1.543
4	5	2	44.085	45.879
4	5	1	17.445	18.581
4	5	0	2.726 *	0.671
4	6	0	31.593	32.253
4	6	1	15.823	16.675
4	6	2	46.016	48.977
4	6	3	11.369	11.518
4	6	4	29.302	29.013
4	6	5	4.041 *	5.918
4	6	6	9.089	8.088

## PROTO PBC21 F CALC

(13)

H	K	L	F(OBS)	F(CALC)
4	6	8	13.818	11.686
4	7	7	14.667	12.995
4	7	6	14.292	10.569
4	7	5	19.047	19.254
4	7	4	16.608	17.187
4	7	3	11.061	9.233
4	7	2	26.523	28.183
4	7	1	25.717	28.108
4	7	0	3.075 *	2.294
4	8	0	9.672	8.815
4	8	1	34.424	34.320
4	8	2	19.047	18.767
4	8	3	30.850	31.243
4	8	4	14.879	14.415
4	8	5	14.890	15.113
4	8	6	4.709 *	2.997
4	8	7	13.596	13.446
4	9	6	4.825 *	2.881
4	9	5	21.051	20.716
4	9	4	13.564	13.123
4	9	3	9.916	12.219
4	9	2	8.845	7.643
4	9	1	27.764	27.764
4	9	0	3.585 *	2.773
4	10	0	23.724	20.917
4	10	1	7.551	4.383
4	10	2	4.083 *	2.209
4	10	3	4.189 *	3.309
4	10	4	8.346	9.588
4	10	5	8.749	6.284
4	10	6	18.644	15.355
4	11	5	5.080 *	4.787
4	11	4	25.219	23.699
4	11	3	4.523 *	6.373
4	11	2	20.988	2.492
4	11	1	4.242 *	1.825
4	11	0	4.210 *	7.641
4	12	0	4.507 *	2.286
4	12	1	4.550 *	2.814
4	12	2	14.382	19.188
4	12	3	4.942 *	3.865
4	12	4	10.554	9.972
4	13	3	5.069 *	0.271
4	13	2	8.940	7.548
4	13	1	19.386	18.783
4	13	0	4.794 *	9.319
4	14	0	4.995 *	0.351
4	14	1	5.250 *	5.313
4	14	2	14.518	16.486
5	14	1	5.265 *	3.479
5	14	0	5.165 *	2.159
5	13	0	21.422	20.821
5	13	1	19.757	18.686
5	13	2	5.080 *	3.093
5	13	3	12.917	10.830

## PBC21 F CALC

(14)

H	K	L	F(OBS)	F(CALC)
5	12	3	4.878 *	5.114
5	12	2	4.749 *	5.967
5	12	1	4.709 *	3.807
5	12	0	4.528 *	5.339
5	11	0	21.921	20.919
5	11	1	15.420	13.609
5	11	2	36.429	37.047
5	11	3	8.516	6.051
5	11	4	24.880	24.737
5	11	5	15.006	11.293
5	10	6	5.398 *	4.515
5	10	5	5.027 *	7.604
5	10	4	4.666 *	3.708
5	10	2	10.298	9.062
5	10	1	3.998 *	7.616
5	10	0	4.041 *	8.094
5	9	0	11.626	10.703
5	9	1	40.331	41.147
5	9	2	17.021	17.185
5	9	3	29.387	29.731
5	9	4	12.026	10.628
5	9	5	37.828	37.440
5	9	6	5.133 *	4.660
5	8	7	5.250 *	4.122
5	8	6	4.878 *	1.356
5	8	5	9.216	8.094
5	8	4	14.815	14.523
5	8	3	7.424	8.093
5	8	2	3.744 *	2.352
5	8	1	6.915	6.843
5	8	0	3.510 *	6.784
5	7	0	38.613	39.233
5	7	1	23.056	25.498
5	7	2	19.333	22.477
5	7	3	19.227	18.527
5	7	4	11.008	11.277
5	7	5	22.674	23.067
5	7	6	20.489	21.572
5	7	7	11.899	10.098
5	6	7	4.889 *	3.904
5	6	6	9.248	9.215
5	6	5	7.742	7.083
5	6	4	3.754 *	2.077
5	6	3	8.134	9.175
5	6	2	18.007	18.640
5	6	1	3.203 *	8.255
5	6	0	3.044 *	5.555
5	5	0	33.883	33.288
5	5	1	10.732	10.247
5	5	2	65.678	67.912
5	5	3	17.700	18.302
5	5	4	38.284	40.152
5	5	5	3.998 *	3.915
5	5	6	18.570	18.138
5	5	7	4.762 *	2.940
5	5	8	33.883	32.137

## PROTO PBC21 F CALC

(15)

H	K	L	F(OBS)	F(CALC)
5	4	8	5.165 *	2.172
5	4	7	4.730 *	4.618
5	4	6	4.348 *	5.729
5	4	5	3.831 *	4.524
5	4	4	21.772	24.741
5	4	3	7.995	8.000
5	4	2	2.768 *	5.257
5	3	0	2.651 *	3.913
5	3	1	6.936	5.851
5	3	2	92.360	94.301
5	3	3	10.828	11.431
5	3	3	38.125	38.850
5	3	4	3.447 *	5.782
5	3	5	67.650	67.534
5	3	6	4.200 *	2.519
5	3	7	29.802	25.675
5	2	8	5.101 *	5.189
5	2	8	5.059 *	5.554
5	2	7	4.518 *	3.547
5	2	6	14.508	14.793
5	2	5	3.638 *	1.857
5	2	4	3.362 *	4.928
5	2	3	5.812	4.695
5	2	2	28.634	28.282
5	2	1	5.949	5.724
5	1	0	4.253	2.837
5	1	1	51.509	50.653
5	1	1	12.853	12.310
5	1	2	63.620	63.852
5	1	3	24.742	24.542
5	1	4	35.294	35.102
5	1	5	13.023	13.483
5	1	6	25.017	22.24
2	1	7	4.539 *	5.132
5	1	8	32.950	29.765
5	0	8	4.942 *	1.305
5	0	7	4.475 *	0.000
5	0	6	8.442	8.449
5	0	5	3.574 *	0.000
5	0	4	30.840	29.962
5	0	3	2.874 *	0.000
5	0	2	2.524 *	2.547
5	0	1	2.376 *	0.000
5	0	0	2.301 *	5.889
6	0	0	74.034	77.310
6	0	1	2.630 *	0.000
6	0	2	60.152	60.514
6	0	3	3.012 *	0.000
6	0	4	38.974	37.286
6	0	5	3.722 *	0.000
6	0	6	20.075	19.082
6	0	7	4.581 *	0.000
6	0	8	12.726	9.105
6	1	8	19.545	18.706
6	1	7	11.857	10.893
6	1	6	17.875	17.900

## PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
0	1	5	15.537	15.512
0	1	4	39.143	39.713
0	1	3	3.477 *	4.463
0	1	2	62.114	63.014
0	1	1	17.435	18.911
0	1	0	2.636 *	6.771
0	2	2	11.751	11.151
0	2	3	11.813	35.016
0	2	2	6.263	7.357
0	2	3	26.953	27.934
0	2	4	3.413 *	2.937
0	2	6	7.911	6.221
0	2	7	14.553	12.184
0	2	8	10.173	6.331
0	3	2	5.133 *	3.360
0	3	7	44.679	4.334
0	3	6	4.337 *	3.523
0	3	5	45.082	44.685
0	3	4	16.924	14.956
0	3	3	16.133	18.050
0	3	2	4.313 *	1.484
0	3	1	86.103	38.854
0	3	0	2.715 *	1.133
0	4	6	11.264	10.624
0	4	1	16.972	17.382
0	4	2	3.129 *	3.941
0	4	3	13.893	13.193
0	4	4	3.712 *	3.449
0	4	5	4.072 *	7.053
0	4	6	9.045	8.159
0	4	7	4.921 *	5.148
0	4	8	16.529	10.503
0	5	7	4.879 *	2.274
0	5	6	8.354	8.781
0	5	5	4.221 *	7.083
0	5	4	52.752	52.351
0	5	3	3.513 *	5.185
0	5	2	43.258	45.092
0	5	1	3.012 *	5.722
0	5	0	3.012 *	7.737
0	6	9	21.304	21.822
0	6	8	3.266 *	3.786
0	6	7	21.567	18.975
0	6	6	3.506 *	3.702
0	6	5	21.231	21.797
0	6	4	4.295 *	6.382
0	6	3	19.503	18.005
0	6	2	5.133 *	6.567
0	6	1	18.145	17.618
0	6	0	4.740 *	5.380
0	7	5	13.331	11.138
0	7	4	33.332	32.799
0	7	3	3.871 *	1.820
0	7	2	25.484	26.694
0	7	1	27.107	26.520
0	7	0	3.425 *	6.369

(16)

## PROTO PBC21 F CALC

H	K	L	F(OBS)	F(CALC)
0	8	1	18.373	19.713
0	8	2	18.845	16.821
0	8	3	17.103	16.912
0	8	4	16.293	16.655
0	8	5	9.714	1.321
0	8	6	18.527	16.678
0	8	7	4.984 *	4.451
0	9	6	5.165 *	6.210
0	9	7	23.469	24.167
0	9	8	4.306 *	7.456
0	9	9	12.952	11.230
0	9	10	4.306 *	7.456
0	10	2	17.651	15.798
0	10	3	48.062	5.359
0	10	4	3.913 *	2.646
0	10	5	12.791	13.356
0	10	6	13.712	13.353
0	10	7	4.634 *	7.407
0	10	8	5.440 *	1.406
0	10	9	17.414	13.825
0	10	10	5.875 *	5.718
0	10	11	5.451 *	3.384
0	10	12	17.456	13.684
0	10	13	5.854 *	7.417
0	10	14	5.759 *	6.470
0	10	15	5.356 *	3.722
0	10	16	10.494	8.932
0	10	17	5.642 *	2.354
0	10	18	5.515 *	1.497
0	10	19	5.239 *	0.662
0	10	20	5.292 *	5.089
0	10	21	18.665	16.113
0	10	22	12.725	12.060
0	10	23	5.313 *	4.847
0	10	24	14.784	10.999
0	10	25	5.769 *	7.463
0	10	26	5.663 *	2.517
0	10	27	5.600 *	9.184
0	10	28	5.495 *	7.452
0	10	29	5.674 *	1.945
0	10	30	5.483 *	3.383
0	10	31	5.557 *	0.738
0	10	32	5.759 *	6.382
0	10	33	5.398 *	8.462
0	10	34	16.396	15.133
0	10	35	5.737 *	3.476
0	10	36	5.610 *	3.546
0	10	37	5.493 *	4.505
0	10	38	5.631 *	4.154
0	10	39	5.462 *	1.676
0	10	40	5.377 *	5.803
0	10	41	5.303 *	8.291
0	10	42	5.377 *	2.431
0	10	43	5.865 *	7.351
0	10	44	5.525 *	3.699
0	10	45	5.578 *	7.338
0	10	46	5.303 *	8.811

(17)

H	K	L	F(OBS)	F(CALC)
4	14	3	5.431 *	7.83
4	14	4	10.616	9.97
4	14	5	5.727 *	7.963
4	15	4	5.833 *	8.476
4	15	3	5.515 *	5.134
4	15	2	5.578 *	8.469
4	15	1	14.115	13.583
4	15	0	5.271 *	4.609
4	16	0	13.564	9.538
4	16	1	13.564	12.267
4	16	2	5.610 *	4.038
4	16	3	5.812 *	6.099
4	17	3	5.621 *	1.295
5	16	3	5.695 *	5.035
5	16	2	5.716 *	5.268
5	16	1	5.684 *	5.981
5	16	0	5.589 *	4.967
5	15	0	5.631 *	8.196
5	15	1	12.525	13.966
5	15	2	13.458	14.160
5	15	3	19.185	19.595
5	15	4	10.743	9.299
5	14	5	5.695 *	4.166
5	14	4	5.493 *	5.925
5	14	3	5.440 *	4.617
5	14	2	5.334 *	7.458
5	13	4	5.462 *	4.207
5	13	5	17.170	18.399
5	13	6	15.250	12.830
5	12	7	5.759 *	5.513
5	12	6	5.525 *	1.525
5	12	5	5.387 *	5.221
5	11	6	14.073	13.566
5	11	7	5.727 *	6.051
5	10	8	5.563 *	3.056
5	10	7	5.536 *	4.776
5	9	7	14.009	15.644
5	9	8	11.761	11.583
5	8	8	5.557 *	3.012
5	7	6	16.300	14.234
5	7	9	5.854 *	6.258
5	6	9	5.653 *	2.565
5	6	8	5.281 *	5.347
5	5	9	5.748 *	5.476
5	4	9	5.472 *	2.768
5	3	9	13.394	13.986
5	3	10	5.684 *	1.588
5	2	10	5.812 *	5.832
5	2	9	5.398 *	2.538
5	1	9	5.440 *	6.773
5	1	10	5.875 *	8.999
5	0	10	5.663 *	4.832
5	0	9	5.440 *	0.000
6	0	9	5.440 *	0.000
6	0	10	5.896 *	6.653
6	1	10	21.062	18.114

H	K	L	F(OBS)	F(CALC)
0	1	9	5.356 *	2.789
6	2	9	10.626	7.010
0	3	9	15.502	17.022
6	4	9	5.536 *	1.537
6	5	9	5.514 *	1.918
6	5	8	16.077	15.837
6	6	8	16.247	14.816
6	7	9	5.759 *	5.569
6	7	8	10.616	1.151
6	8	7	16.046	13.952
6	8	8	5.621 *	1.649
6	9	8	5.695 *	5.092
6	9	7	29.419	32.219
0	10	6	5.260 *	5.480
0	10	7	5.515 *	2.497
6	11	7	5.695 *	2.960
6	11	6	5.578 *	12.073
6	12	5	5.446 *	6.292
5	12	6	5.631 *	4.524
6	13	6	5.674 *	4.347
0	13	5	14.359	14.514
6	13	4	10.552	16.845
6	14	0	5.472 *	8.354
6	14	1	15.399	13.833
6	14	2	5.493 *	9.286
6	14	3	10.605	10.049
6	14	4	5.631 *	10.446
6	14	5	5.886 *	7.607
0	15	4	14.444	11.567
6	15	3	5.759 *	15.825
6	15	2	11.719	12.093
6	15	1	20.213	21.512
6	15	0	5.536 *	6.512
6	16	0	5.716 *	6.245
6	16	1	5.790 *	4.046
6	16	2	5.822 *	7.903
7	16	1	5.769 *	2.539
7	16	0	5.748 *	4.585
7	15	0	17.265	15.204
7	15	1	11.740	12.728
7	15	2	5.684 *	3.881
7	15	3	16.703	16.238
7	14	4	5.759 *	5.825
7	14	3	5.515 *	4.232
7	14	2	5.419 *	4.819
7	14	1	5.366 *	1.070
7	14	0	5.345 *	8.842
7	13	3	16.852	18.193
7	13	4	5.610 *	7.397
7	13	5	5.610 *	2.300
7	12	6	5.557 *	4.191
7	12	5	5.462 *	2.864
7	12	4	5.271 *	3.653
7	11	5	5.366 *	5.583
7	11	6	29.790	29.846
7	11	7	16.732	8.967

BC21 F CALC

(20)

K	L	F(OBS)	F(CALC)
10	7	5.589 *	1.429
10	6	5.366 *	3.472
9	7	5.472 *	2.532
9	8	5.748 *	1.517
8	8	5.610 *	3.628
8	7	5.356 *	2.999
7	8	14.338	13.435
6	9	5.748 *	2.914
6	8	5.440 *	5.219
5	8	10.541	11.238
5	9	5.642 *	3.077
4	9	5.589 *	1.311
4	8	5.303 *	2.293
3	8	5.451 *	6.842
3	9	36.545	32.455
2	9	5.610 *	3.084
1	9	10.690	9.156
3	9	5.504 *	0.000
0	8	12.302	9.487
0	9	5.578 *	0.000
1	9	5.600 *	2.554
1	8	10.425	10.147
2	8	5.313 *	5.607
2	9	5.812 *	7.146
3	9	11.772	6.099
3	8	5.334 *	2.466
4	8	14.147	12.998
4	9	5.653 *	2.378
5	9	5.674 *	2.635
5	8	5.610 *	4.175
3	6	5.228 *	5.632
3	6	12.652	8.107
3	7	5.684 *	4.364
3	7	15.537	12.438
3	8	11.634	11.230
3	8	5.727 *	5.084
3	9	13.564	14.448
3	9	5.313 *	4.358
3	10	5.440 *	1.780
3	10	5.695 *	1.226
3	11	5.568 *	4.427
3	11	5.621 *	5.564
3	12	5.377 *	4.061
3	12	5.610 *	6.023
3	12	5.812 *	6.593
3	13	11.782	10.129
3	13	5.695 *	6.395
3	13	5.504 *	5.540
3	13	5.398 *	9.160
3	13	5.472 *	7.764
3	13	5.303 *	1.727
3	14	15.727	16.096
3	14	12.578	10.597
3	14	5.525 *	7.758
3	14	5.737 *	7.117
3	14	5.737 *	7.016

PROTO	PBC21	F CALC	H	K	L	F(OBS)	F(CALC)
●			8	15	2	5.727 *	5.746
●			8	15	1	5.769 *	6.801
●			9	15	1	5.748 *	5.614
●			9	15	1	5.748 *	3.683
●			9	14	3	5.737 *	5.762
●			9	14	2	5.674 *	7.436
●			9	14	1	10.701	7.127
●			9	14	0	5.462 *	5.571
●			9	13	1	1.531	4.957
●			9	13	1	12.472	13.275
●			9	13	2	5.447 *	6.772
●			9	13	3	5.525 *	3.388
●			9	13	4	5.78 *	3.961
●			9	12	5	5.833 *	7.808
●			9	12	4	5.493 *	3.961
●			9	12	3	5.430 *	5.492
●			9	12	2	5.324 *	7.001
●			9	11	4	10.486	11.222
●			9	11	5	5.514 *	6.856
●			9	11	6	5.716 *	5.561
●			9	10	6	5.61 *	7.351
●			9	10	5	5.356 *	5.375
●			9	9	0	5.515 *	3.171
●			9	9	7	10.743	9.156
●			9	8	7	15.155	12.405
●			9	8	6	5.223 *	2.834
●			9	7	7	5.535 *	8.069
●			9	7	8	5.875 *	6.077
●			9	6	8	5.610 *	1.558
●			9	6	7	5.446 *	5.949
●			9	5	7	5.345 *	6.307
●			9	5	8	19.174	14.731
●			9	4	8	5.568 *	7.888
●			9	3	8	5.525 *	5.463
●			9	3	9	12.726	7.908
●			9	2	9	5.801 *	5.158
●			9	2	8	5.54 *	6.972
●			9	1	8	5.610 *	6.457
●			9	1	9	5.568 *	2.674
●			9	0	9	5.653 *	6.000
●			9	0	8	5.546 *	6.737
●			10	0	8	5.653 *	2.729
●			10	1	8	5.589 *	3.868
●			10	2	7	5.387 *	10.801
●			10	2	8	5.600 *	1.922
●			10	3	8	5.621 *	6.792
●			10	3	7	5.356 *	6.395
●			10	4	7	5.409 *	8.995
●			10	4	8	11.772	11.509
●			10	5	8	5.642 *	4.100
●			10	5	7	5.409 *	6.844
●			10	6	7	5.493 *	2.430
●			10	6	8	5.822 *	1.477
●			10	7	7	5.780 *	4.318
●			10	7	6	5.398 *	2.323
●			10	8	6	5.430 *	3.933

PBC21	F CALC			
H	K	L	F(OBS)	F(CALC)
10	8	7	5.621 *	4.91
10	9	7	5.759 *	5.066
11	9	6	5.462 *	5.248
10	10	4	5.373 *	2.535
11	10	5	5.614 *	11.619
12	10	6	22.112	21.643
13	11	5	5.663 *	5.551
14	11	4	5.566 *	1.225
15	11	3	5.292 *	5.625
16	12	7	21.817	21.571
17	12	1	5.393 *	4.593
18	12	2	5.387 *	10.831
19	12	3	5.695 *	11.016
20	12	4	5.589 *	3.355
21	12	5	5.634 *	1.945
22	13	4	5.621 *	1.323
23	13	3	5.695 *	1.208
24	13	2	5.536 *	2.371
25	13	1	5.716 *	4.278
26	13	0	5.398 *	4.143
27	14	6	5.769 *	7.645
28	14	1	5.706 *	7.648
29	14	2	5.589 *	5.966
30	14	0	5.769 *	5.442
31	13	5	5.737 *	5.068
32	13	1	5.822 *	7.998
33	13	2	5.557 *	4.632
34	13	3	11.782	10.670
35	12	4	18.697	2.103
36	12	3	5.663 *	5.690
37	12	2	18.485	22.219
38	12	1	5.610 *	9.462
39	12	0	5.441 *	6.304
40	11	0	14.667	10.906
41	11	1	13.193	12.924
42	11	2	10.525	10.619
43	11	3	5.451 *	4.885
44	11	4	10.711	9.458
45	11	5	10.732	8.790
46	11	5	5.578 *	6.697
47	10	4	10.455	13.503
48	10	3	5.271 *	2.589
49	9	4	5.441 *	5.441
50	9	5	12.588	11.682
51	9	6	5.695 *	3.196
52	8	6	5.462 *	3.752
53	8	5	15.547	16.312
54	7	6	5.546 *	1.843
55	7	7	5.790 *	7.656
56	6	7	5.780 *	8.754
57	6	6	5.515 *	9.714
58	5	6	14.699	11.631
59	5	7	5.600 *	3.145
60	4	8	5.822 *	6.360
61	4	7	17.785	16.182
62	3	7	14.211	11.243

PROTO	PBC21	F CALC			
H	K	L	F(OBS)	F(CALC)	
●	11	3	8	5.716 *	4.98
●	11	2	8	5.769 *	6.563
●	11	2	7	22.069	21.967
●	11	1	7	5.440 *	2.541
●	11	1	8	5.684 *	4.047
●	11	0	8	19.853	20.845
●	11	1	7	5.356 *	0.00
●	12	0	6	18.464	19.947
●	12	0	7	5.493 *	1.00
●	12	0	8	29.747	28.814
●	12	1	8	5.684 *	3.052
●	12	1	7	5.589 *	2.582
●	12	2	6	5.493 *	6.756
●	12	2	7	15.855	13.728
●	12	3	7	5.557 *	3.065
●	12	3	6	5.472 *	6.436
●	12	5	6	5.515 *	5.197
●	12	4	6	5.727 *	9.621
●	12	4	7	5.631 *	3.103
●	12	5	7	5.589 *	6.413
●	12	5	6	11.43	8.488
●	12	6	5	17.859	16.896
●	12	6	6	5.748 *	4.292
●	12	6	7	5.653 *	4.045
●	12	7	5	5.472 *	6.11
●	12	8	4	5.536 *	5.33
●	12	8	5	27.785	26.468
●	12	8	6	5.727 *	2.042
●	12	9	5	5.790 *	6.461
●	12	9	4	5.515 *	4.751
●	12	9	3	5.356 *	7.861
●	12	10	0	5.398 *	6.643
●	12	10	1	5.186 *	4.135
●	12	10	2	16.905	16.218
●	12	10	3	19.545	16.496
●	12	10	4	12.694	12.908
●	12	10	5	5.886 *	7.218
●	12	11	4	5.737 *	3.153
●	12	11	2	5.504 *	0.20
●	12	11	1	5.356 *	5.599
●	12	11	0	5.419 *	5.899
●	12	12	0	23.024	20.183
●	12	12	1	12.705	11.626
●	12	12	2	19.863	20.011
●	12	12	3	5.674 *	4.264
●	12	13	1	5.759 *	6.129
●	12	13	0	5.674 *	4.180
●	13	12	1	11.772	6.618
●	13	12	0	5.663 *	5.121
●	13	11	0	5.727 *	5.799
●	13	11	1	5.727 *	5.506
●	13	11	2	11.761	8.244
●	13	11	3	5.674 *	3.641
●	13	10	4	11.782	8.439
●	13	10	3	5.483 *	4.972
●	13	10	2	16.679	7.888

H	K	L	F(OBS)	F(CALC)
13	10	1	11.634	9.486
13	10	0	5.504 *	3.819
13	9	0	5.292 *	3.617
13	9	1	15.473	16.189
13	9	2	5.387 *	3.075
13	9	3	5.695 *	6.505
13	9	4	5.665 *	6.779
13	9	5	10.722	8.974
13	8	5	13.596	13.089
13	8	4	5.546 *	1.659
13	8	3	5.493 *	6.725
13	8	2	5.154 *	1.392
13	7	4	5.377 *	2.213
13	7	5	5.536 *	4.770
13	7	6	5.674 *	1.101
13	6	6	5.833 *	8.694
13	6	5	5.619 *	5.105
13	6	4	22.239	21.502
13	5	5	5.611 *	6.400
13	5	6	5.785 *	5.516
13	4	7	15.250	12.496
13	4	6	5.589 *	3.949
13	4	5	12.366	9.825
13	3	5	16.692	16.111
13	3	6	5.483 *	1.665
13	3	7	14.465	12.585
13	2	7	18.039	14.507
13	2	6	5.589 *	2.800
13	1	6	12.535	9.757
13	1	7	5.621 *	2.416
13	0	7	5.695 *	0.000
13	0	6	5.493 *	6.777
14	0	5	5.440 *	0.000
14	0	6	18.591	16.465
14	1	6	5.653 *	5.461
14	1	5	5.462 *	6.230
14	2	5	5.483 *	2.961
14	2	6	5.589 *	3.378
14	3	6	7.424 *	4.154
14	3	5	5.366 *	1.126
14	4	4	5.398 *	1.358
14	4	5	5.642 *	2.437
14	4	6	11.782	9.809
14	5	6	5.737 *	3.795
14	5	5	5.695 *	7.072
14	5	4	5.515 *	8.284
14	6	3	5.462 *	3.977
14	6	4	10.626	6.477
14	6	5	5.504 *	4.528
14	7	5	5.663 *	2.807
14	7	4	5.748 *	6.653
14	7	3	5.469 *	3.491
14	7	2	5.313 *	2.247
14	7	1	5.451 *	11.081
14	8	0	10.510	5.402
14	8	1	5.377 *	2.850

H	K	L	F(OBS)	F(CALC)
14	8	2	11.605	9.413
14	8	3	18.506	15.119
14	8	4	5.705 *	6.328
14	9	4	5.674 *	2.116
14	9	3	5.684 *	4.245
14	9	2	5.525 *	2.981
14	9	1	5.483 *	1.624
14	9	0	5.462 *	5.926
14	1		18.623	13.265
14	10	1	18.732	9.120
14	10	2	5.621 *	4.468
14	10	3	5.822 *	2.549
14	11	1	5.822 *	7.588
14	11	0	5.748 *	4.684
15	10	0	5.695 *	5.002
15	9	0	5.536 *	5.827
15	9	1	12.737	10.326
15	9	2	18.732	6.643
15	8	3	5.790 *	4.781
15	8	2	5.663 *	7.664
15	8	1	5.546 *	3.534
15	8	0	5.525 *	3.651
15	7	0	5.653 *	7.735
15	7	1	13.426	11.909
15	7	2	5.589 *	6.893
15	7	3	5.737 *	6.652
15	7	4	5.663 *	5.693
15	6	4	5.822 *	6.798
15	6	2	5.493 *	2.884
15	6	1	5.430 *	2.677
15	6	0	5.324 *	5.981
15	5	0	5.228 *	2.934
15	5	1	5.271 *	2.437
15	5	2	24.892	18.176
15	5	3	11.613	10.785
15	5	4	15.897	12.660
15	5	5	5.727 *	4.652
15	4	5	5.706 *	2.331
15	4	4	5.504 *	2.751
15	4	3	5.356 *	4.505
15	4	2	5.462 *	9.031
15	3	3	5.313 *	3.121
15	3	4	5.451 *	2.545
15	3	5	17.997	15.377
15	2	6	5.684 *	4.427
15	2	5	5.546 *	1.683
15	2	4	13.384	13.156
15	2	3	5.271 *	5.523
15	1	3	12.270	10.029
15	1	4	11.560	9.988
15	1	5	11.729	10.391
15	1	6	5.833 *	3.180
15	0	6	5.748 *	9.535
15	0	5	5.536 *	5.000
15	0	4	5.525 *	6.132
15	0	3	5.303 *	6.000

PBC21	F	CALC		
H	K	L	F(OBS)	F(CALC)
16	0	0	16.77	12.859
16	0	1	5.185 *	3.890
16	0	2	5.431 *	3.825
16	0	3	5.525 *	3.600
16	0	4	10.711	7.576
16	0	5	5.737 *	3.603
16	1	5	5.890 *	6.793
16	1	4	23.045	19.592
16	1	3	5.451 *	4.785
16	1	2	15.579	12.772
16	1	1	13.213	11.429
16	1	0	5.356 *	7.603
16	2	0	16.141	12.880
16	2	1	5.483 *	7.301
16	2	2	5.451 *	2.804
16	2	3	11.655	8.461
16	2	4	5.580 *	1.527
16	2	5	5.833 *	6.671
16	3	4	5.684 *	2.060
16	3	3	5.514 *	19.581
16	3	2	5.564 *	5.060
16	3	1	23.915	19.948
16	3	0	5.345 *	3.258
16	4	0	5.546 *	4.448
16	4	1	5.334 *	1.441
16	4	2	12.578	11.586
16	4	3	5.684 *	2.919
16	4	4	5.799 *	5.741
16	5	4	15.250	13.874
16	5	3	5.589 *	5.928
16	5	2	21.952	17.664
16	5	1	5.695 *	6.502
16	5	0	5.536 *	1.394
16	6	0	20.939	19.761
16	6	1	5.695 *	6.271
16	6	2	12.694	8.493
16	6	3	5.791 *	5.998
16	7	3	5.684 *	9.072
16	7	2	12.737	11.291
16	7	1	13.606	12.468
16	7	0	5.600 *	7.626
16	8	0	5.801 *	6.414
16	8	1	16.003	11.300
17	6	1	5.600 *	1.828
17	6	0	5.653 *	2.506
17	5	0	26.364	25.136
17	5	1	5.716 *	0.814
17	5	2	5.886 *	10.621
17	4	3	5.684 *	3.556
17	4	2	5.706 *	4.749
17	4	1	5.589 *	0.263
17	4	0	5.589 *	4.120
17	3	0	5.546 *	1.578
17	3	1	5.557 *	9.823
17	3	2	5.663 *	5.043
17	3	3	37.722	35.852

PROTO	PBC21	F	CALC	
H	K	L	F(OBS)	F(CALC)
			5.716 *	3.704
			5.568 *	7.211
			5.525 *	3.879
			5.681 *	3.655
			37.521	34.119
			5.515 *	3.679
			5.631 *	3.656
			12.772	11.553
			5.536 *	5.517
			5.769 *	3.244
			5.462 *	3.693
			5.504 *	1.600
			5.631 *	4.533
			11.782	9.658
			5.578 *	3.703
			11.761	8.132
			13.617	14.392
			5.737 *	5.947
			5.578 *	1.113
			5.663 *	1.227
			5.886 *	6.854
			25.590	23.036
			5.611 *	6.297
			15.346	14.121
			5.716 *	6.193
			5.483 *	5.005
			5.313 *	6.591
			5.653 *	4.294
			5.387 *	5.076
			5.663 *	3.829
			5.631 *	3.000
			5.610 *	1.556
			9.629	9.083
			5.059 *	6.865
			5.334 *	7.111
			27.520	28.274
			4.804 *	5.633
			29.503	31.225
			4.550 *	4.732
			4.444 *	5.911
			10.541	8.604
			13.585	12.596
			4.995 *	8.262
			16.032	9.149
			5.250 *	5.524
			5.228 *	7.774
			12.037	11.688
			16.745	16.131
			4.921 *	2.275
			5.122 *	5.195
			5.133 *	5.036
			15.271	13.446
			5.027 *	5.989
			4.963 *	5.323
			4.857 *	1.149
			4.751 *	1.001

## PBC21 F CALC

	H	K	L	F(OBS)	F(CALC)
	11			42.567	42.74
7	11	1		4.624 *	2.445
7	11	2		4.794 *	7.981
7	11	3		12.397	9.415
7	11	4		5.115 *	4.500
7	11	5		5.175 *	2.526
7	11	6		4.642	6.227
7	11	7		4.624 *	3.217
7	11	8		4.665 *	3.338
7	11	9		4.659 *	1.435
7	11	10		4.653 *	2.517
7	9			17.583	15.586
7	9	1		4.178 *	4.204
7	9	2		4.295 *	4.647
7	9	3		52.777	53.698
7	9	4		4.634 *	5.422
7	9	5		11.687	13.841
7	9	6		18.368	15.691
7	8	0		5.637 *	6.33
7	8	5		4.719 *	3.447
7	8	4		4.565 *	5.687
7	8	3		4.306 *	5.655
7	8	2		4.695	6.297
7	8	1		3.61 *	1.926
7	8	0		3.839 *	3.658
7	7			4.264	41.171
7	7	1		5.786 *	6.707
7	7	2		12.228	10.153
7	7	3		33.215	33.672
7	7	4		7.943	7.639
7	7	5		4.539 *	4.384
7	7	6		16.958	15.956
7	7	7		5.318 *	1.72
7	6	7		5.101 *	2.251
7	6	6		4.814 *	4.346
7	6	5		4.380 *	1.570
7	6	4		9.301	8.185
7	6	3		3.775 *	4.319
7	6	2		3.648 *	3.740
7	6	1		5.918	6.908
7	6	0		3.415 *	7.154
7	5	0		90.027	92.808
7	5	1		19.938	21.515
7	5	2		9.736	8.045
7	5	3		1.255	8.233
7	5	4		16.934	16.826
7	5	5		8.845	8.605
7	5	6		39.345	38.840
7	5	7		5.69 *	5.922
7	4	7		4.974 *	2.266
7	4	6		8.346	5.438
7	4	5		4.104 *	1.631
7	4	4		7.233	6.504
7	4	3		3.468 *	3.168
7	4	2		11.167	12.198
7	4	1		3.182 *	4.467

PROTO	PBC21	F CALC	(29)		
H	K	L	F(OBS)	F(CALC)	
	7	4	8	3.12 *	6.678
	7	3	9	3.384	30.204
	7	3	1	3.001 *	3.358
	7	3	2	12.302	12.271
	7	3	3	84.979	89.724
	7	3	4	6.204	4.512
	7	3	5	11.220	11.142
	7	3	6	4.412 *	3.685
	7	3	7	16.226	14.356
	7	2	8	5.186 *	1.923
	7	2	7	4.847 *	2.15
	7	2	6	4.274 *	0.193
	7	2	5	3.956 *	1.839
	7	2	4	15.006	15.204
	7	2	3	6.702	6.973
	7	2	2	2.906 *	2.999
	7	2	1	2.853 *	0.959
	7	1	0	52.835	55.610
	7	1	1	11.241	11.387
	7	1	2	24.689	24.682
	7	1	3	16.692	16.486
	7	1	4	3.542 *	3.291
	7	1	5	1.340	7.074
	7	1	6	45.241	42.261
	7	1	7	4.804 *	2.67
	7	1	8	5.143 *	2.091
	7	0	8	5.228 *	5.998
	7	0	7	4.656 *	5.000
	7	0	6	4.433 *	8.121
	7	0	5	3.892 *	0.609
	7	0	4	3.648 *	1.835
	7	0	3	3.213 *	0.000
	7	0	2	15.240	14.163
	7	0	1	2.779 *	7.674
	7	0	0	52.538	52.721
	8	0	0	3.086 *	0.700
	8	0	1	38.316	37.135
	8	0	2	3.447 *	0.000
	8	0	3	28.220	27.374
	8	0	4	4.072 *	0.000
	8	0	5	23.246	20.777
	8	0	6	4.783 *	0.000
	8	0	7	9.684	7.717
	8	1	7	15.780	14.067
	8	1	6	9.375	10.703
	8	1	5	11.644	10.253
	8	1	4	3.574 *	3.563
	8	1	3	32.802	33.900
	8	1	2	16.300	16.135
	8	1	1	2.991 *	4.011
	8	2	1	22.631	23.137
	8	2	1	29.302	30.044
	8	2	2	11.655	12.021
	8	2	3	14.688	12.912
	8	2	4	3.733 *	2.774
	8	2	5	22.610	21.713

H	K	L	F(OBS)	F(CALC)
8	2	6	15.897	13.742
8	2	7	14.860	13.336
8	3	7	14.731	13.346
8	3	6	4.719 *	8.113
8	3	5	18.835	19.181
8	3	4	15.611	14.299
8	3	3	1.170	8.914
8	3	2	7.296	5.916
8	3	1	27.976	3.696
8	3	0	3.129 *	3.825
8	4	1	21.263	19.964
8	4	1	14.115	14.568
8	4	2	15.971	15.766
8	4	3	3.691 *	2.452
8	4	4	7.540	7.892
8	4	5	13.76	11.212
8	4	6	8.686	4.618
8	4	7	5.122 *	4.030
8	5	7	5.143 *	2.249
8	5	6	4.847 *	3.379
8	5	5	9.969	10.281
8	5	4	28.443	30.280
8	5	3	8.134	8.150
8	5	2	13.967	15.082
8	5	1	6.808	6.058
8	5	0	3.457 *	2.256
8	6	0	25.166	24.787
8	6	1	3.733 *	4.923
8	6	2	20.129	18.725
8	6	3	3.988 *	2.659
8	6	4	17.753	16.386
8	6	5	4.687 *	4.953
8	6	6	19.057	16.703
8	7	6	5.016 *	1.293
8	7	5	4.698 *	4.490
8	7	4	21.910	25.924
8	7	3	4.147 *	7.203
8	7	2	8.389	9.578
8	7	1	19.842	10.850
8	7	0	3.744 *	3.403
8	8	0	27.404	25.178
8	8	1	19.683	20.626
8	8	2	4.178 *	6.255
8	8	3	10.637	9.864
8	8	4	4.666 *	7.893
8	8	5	19.959	17.529
8	8	6	14.476	12.780
8	9	5	5.122 *	4.114
8	9	4	4.857 *	1.660
8	9	3	4.475 *	3.786
8	9	2	11.443	9.197
8	9	1	19.980	21.423
8	9	0	4.263 *	10.302
8	10	0	4.571 *	2.798
8	10	1	4.603 *	6.017
8	10	2	19.609	17.102

H	K	L	F(OBS)	F(CALC)
8	11	3	11.485	8.565
8	10	4	10.032	10.185
8	11	5	5.228	* 4.544
8	11	4	11.294	10.595
8	11	3	5.154	* 5.685
8	11	2	15.165	15.083
8	11	1	4.921	* 6.651
8	11	0	4.762	* 4.842
8	12		10.064	9.046
8	12	1	10.085	8.899
8	12	2	5.141	* 3.726
8	12	3	5.313	* 7.022
9	12	1	5.165	* 6.098
9	12	0	5.218	* 5.206
9	11		10.869	8.934
9	11	1	10.902	10.812
9	11	2	20.071	16.385
9	11	3	15.823	16.537
9	10	4	12.928	11.849
9	10	3	4.942	* 4.945
9	10	2	17.276	15.156
9	10	1	10.529	11.080
9	10	0	4.687	* .100
9	9	0	4.603	* 7.515
9	9	1	11.623	9.306
9	9	2	10.287	9.487
9	9	3	9.382	7.056
9	9	4	5.037	* 8.080
9	9	5	12.175	9.137
9	8	5	5.083	* 3.191
9	8	4	12.928	12.931
9	8	3	4.613	* 1.158
9	8	2	4.444	* 5.020
9	8	1	20.998	18.532
9	8	0	4.231	* 6.993
9	7	0	12.498	12.405
9	7	1	11.931	10.508
9	7	2	4.253	* 2.296
9	7	3	9.046	6.041
9	7	4	4.677	* 3.772
9	7	5	15.134	13.863
9	7	6	5.239	* 1.445
9	6	5	5.037	* 2.563
9	6	4	4.804	* 2.654
9	6	3	18.029	15.523
9	6	2	4.189	* 3.831
9	6	1	7.614	5.618
9	6	0	7.434	6.265
9	5	0	3.850	* 6.365
9	5	1	7.116	3.818
9	5	2	3.733	* 5.699
9	5	3	22.419	22.783
9	5	4	15.791	15.510
9	5	5	17.965	17.778
9	5	6	4.518	* 3.233
9	5		11.740	10.227

O	PBC21	F CALC		
H	K	L	F(OBS)	F(CALC)
9	4	7	5.419 *	6.895
9	4	6	4.825 *	3.619
9	4	5	15.271	12.665
9	4	4	27.138	26.835
9	4	3	7.477	11.289
9	4	2	14.285	13.841
9	4	1	17.414	15.719
9	4	0	5.542 *	3.892
9	3	6	6.192	6.955
9	3	1	34.148	34.441
9	3	2	5.681 *	3.450
9	3	3	24.090	22.565
9	3	4	4.83 *	1.862
9	3	5	24.286	21.705
9	3	6	4.936 *	4.036
9	3	7	15.991	12.848
9	2	7	13.573	11.176
9	2	6	13.447	13.565
9	2	5	14.037	12.706
9	2	4	9.226	7.773
9	2	3	5.868 *	8.683
9	2	2	24.816	23.905
9	2	1	23.596	21.182
9	2	0	5.362 *	6.895
9	1	0	10.183	14.336
9	1	1	10.095	9.359
9	1	2	28.480	29.886
9	1	3	14.200	12.751
9	1	4	13.172	16.318
9	1	5	11.867	10.506
9	1	6	4.656 *	2.884
9	1	5	5.048 *	2.526
9	1	7	5.437 *	3.000
9	0	7	11.219	11.001
9	0	6	4.359 *	0.000
9	0	5	7.540	3.763
9	0	4	3.659 *	1.000
9	0	3	21.963	19.884
9	0	2	5.341 *	0.000
9	0	1	3.298 *	7.950
10	0	0	61.534	56.005
10	0	1	3.616 *	4.000
10	0	2	3.864 *	10.487
10	0	3	3.998 *	0.000
10	0	4	12.228	13.285
10	0	5	4.433 *	0.000
10	0	6	49.43	42.889
10	0	7	5.197 *	0.000
10	1	7	5.345 *	6.546
10	1	6	4.836 *	2.213
10	1	5	4.581 *	6.272
10	1	4	4.200 *	1.672
10	1	3	3.934 *	6.365
10	1	2	3.754 *	2.675
10	1	1	14.370	12.972
10	1	0	3.585 *	2.517

PROTO	PBC21	F CALC	(3)	
H	K	L	F(OBS)	F(CALC)
10	2	1	3.711 *	6.741
10	2	2	3.669 *	6.733
10	2	2	24.264	23.833
10	3	3	48.656	46.931
10	4	4	11.393	8.593
10	5	5	3.421	6.216
10	6	6	15.812	13.582
10	3	6	4.942 *	4.274
10	3	5	0.493	6.295
10	3	4	4.221 *	1.486
10	3	2	3.871 *	2.744
10	3	1	4.364	8.768
10	3	0	3.638 *	1.78
10	4	0	42.071	42.704
10	4	1	11.369	12.511
10	4	2	3.966 *	0.425
10	4	3	28.835	24.523
10	4	4	4.316 *	2.193
10	4	5	10.467	2.282
10	5	6	10.120	15.769
10	5	5	5.141 *	1.174
10	5	4	4.794 *	4.962
10	5	3	4.424 *	1.882
10	5	2	4.263 *	6.124
10	5	1	4.083 *	4.449
10	5	0	11.697	12.854
10	6	0	3.861 *	1.121
10	6	0	30.140	59.721
10	6	1	8.664	27.692
10	6	2	4.359 *	9.284
10	6	3	14.508	15.975
10	6	4	9.513	12.545
10	6	5	4.911 *	3.835
10	6	6	28.284	28.112
10	7	5	5.112 *	5.702
10	7	4	4.857 *	1.457
10	7	3	4.634 *	4.311
10	7	2	4.391 *	4.945
10	7	1	11.231	9.711
10	7	0	4.337 *	5.774
10	8	0	4.592 *	3.113
10	8	1	9.269	10.908
10	8	2	8.484	6.862
10	8	3	44.478	43.953
10	8	4	9.990	7.573
10	8	5	5.271 *	9.151
10	9	4	5.197 *	2.813
10	9	3	4.942 *	1.475
10	9	2	4.794 *	3.294
10	9	1	8.823	6.585
10	9	0	4.730 *	1.117
10	10	0	26.502	25.358
10	10	1	4.984 *	5.182
10	10	2	5.133 *	7.446
10	10	3	12.069	13.742
10	11	2	5.197 *	2.546

	PBC21	F CALC	H	K	L	F (NS)	F (CALC)
11	11	1	9.197	*	7.924		
11	11	0	9.165	*	2.285		
11	11	2	10.856		18.122		
11	10	1	10.936		16.645		
11	10	0	9.165	*	2.74		
11	9	0	8.185		7.271		
11	9	1	1.013		9.123		
11	9	2	9.143	*	7.287		
11	9	3	9.122	*	1.749		
11	8	4	9.159	*	3.799		
11	8	3	4.068	*	4.943		
11	8	2	4.719	*	2.769		
11	8	1	31.243		32.278		
11	8	0	9.693	*	1.762		
11	7		9.561	*	3.261		
11	7	1	4.465	*	1.612		
11	7	2	6.534	*	3.311		
11	7	3	11.649		1.306		
11	7	4	9.160	*	2.135		
11	7	5	9.228	*	2.255		
11	6	0	9.197	*	2.173		
11	6	4	37.649		39.662		
11	6	3	4.634	*	4.129		
11	6	2	29.663		30.232		
11	6	1	9.916		11.631		
11	6	0	4.316	*	11.875		
11	5		10.42		12.11		
11	5	1	4.380	*	5.571		
11	5	2	13.193		13.595		
11	5	3	4.433	*	3.154		
11	5	4	10.390		13.724		
11	5	5	1.143		8.846		
11	4	6	9.197	*	2.447		
11	4	5	21.553		23.818		
11	4	4	21.295		23.381		
11	4	3	8.268		9.553		
11	4	2	12.396		12.342		
11	4	1	25.728		29.030		
11	4	0	4.019	*	3.01		
11	3	5	4.141	*	3.873		
11	3	4	20.772		28.859		
11	3	3	4.189	*	2.034		
11	3	2	10.759		13.520		
11	3	1	4.624	*	1.551		
11	3	0	2.133		2.034		
11	3	6	5.133	*	3.844		
11	2	6	11.181		8.000		
11	2	5	20.014		24.207		
11	2	4	4.475	*	1.377		
11	2	3	8.860		9.007		
11	2	2	17.117		15.771		
11	2	1	38.147		36.751		
11	2	0	3.903	*	2.809		
11	1		29.468		19.457		
11	1	1	3.839	*	1.041		
11	1	2	17.742		17.881		

	PROTO	PBC21	F CALC	H	K	L	F (NS)	F (CALC)
				11	1	3	1.308	9.46
				11	1	4	13.469	12.635
				11	1	5	4.878	3.753
				11	1	6	5.197	5.963
				11	1	7	17.944	21.291
				11	1	8	4.719	9.094
				11	1	9	34.435	33.187
				11	1	0	4.178	9.000
				11	1	1	44.314	48.829
				11	1	2	3.956	9.000
				11	1	3	3.839	10.789
				12	0	0	25.601	26.593
				12	0	1	4.178	9.000
				12	0	2	54.966	53.915
				12	0	3	4.454	9.000
				12	0	4	33.120	31.599
				12	0	5	5.027	9.000
				12	1	5	4.963	2.693
				12	1	4	9.598	1.186
				12	1	3	4.380	3.987
				12	1	2	4.359	9.381
				12	1	1	4.178	4.736
				12	1	0	4.147	0.671
				12	2	0	4.576	6.314
				12	2	1	31.709	32.904
				12	2	2	4.401	4.786
				12	2	3	19.577	19.261
				12	2	4	4.804	2.366
				12	2	5	31.497	29.715
				12	3	5	5.048	6.113
				12	3	4	10.648	7.662
				12	3	3	4.560	4.657
				12	3	2	4.465	5.836
				12	3	1	4.284	6.389
				12	3	0	4.242	0.833
				12	4	0	15.886	13.842
				12	4	1	21.465	21.119
				12	4	2	11.613	10.986
				12	4	3	2.956	10.973
				12	4	4	10.764	9.285
				12	4	5	21.256	19.963
				12	4	6	5.271	4.444
				12	5	5	5.101	5.803
				12	5	4	4.815	6.228
				12	5	3	8.495	6.349
				12	5	2	4.497	4.363
				12	5	1	4.465	2.14
				12	5	0	27.340	30.144
				12	6	1	8.527	6.883
				12	6	2	36.810	36.226
				12	6	3	4.953	4.572
				12	6	4	23.374	24.131
				12	7	4	5.271	5.189
				12	7	3	5.080	4.938
				12	7	2	4.868	4.433
				12	7	1	4.698	1.590

H	K	L	F(MSI)	F(VALU)
12	7	0	4.740 *	4.821
12	8	0	8.919	6.477
12	8	1	28.188	26.035
12	8	2	16.096	8.951
12	8	3	17.074	16.436
12	9	2	5.271 *	2.994
12	9	1	5.101 *	2.209
12	9	0	5.080 *	2.577
13	8	1	18.273	17.608
13	8	0	5.133 *	2.412
13	7	0	5.218 *	7.982
13	7	1	16.685	9.982
13	7	2	5.112 *	4.515
13	7	3	13.066	12.847
13	6	3	5.101 *	2.742
13	6	2	23.002	23.537
13	6	1	4.963 *	6.354
13	6	0	4.783 *	3.856
13	5	0	22.101	21.802
13	5	1	11.422	11.960
13	5	2	18.951	18.624
13	5	3	5.006 *	2.297
13	5	4	13.755	13.848
13	4	4	5.250 *	7.445
13	4	3	4.974 *	3.571
13	4	2	12.164	10.549
13	4	1	18.803	18.972
13	4	0	4.613 *	5.455
13	3	0	11.740	11.350
13	3	1	18.517	17.167
13	3	2	16.595	9.292
13	3	3	11.538	9.666
13	3	4	5.027 *	4.325
13	2	5	13.818	12.815
13	2	4	5.037 *	6.699
13	2	3	4.762 *	4.602
13	2	1	22.748	23.008
13	2	0	4.391 *	3.012
13	1	0	4.359 *	1.863
13	1	1	4.475 *	2.250
13	1	2	4.581 *	2.031
13	1	3	6.686	6.982
13	1	4	5.165 *	6.807
13	1	5	5.260 *	1.427
13	0	5	5.250 *	0.000
13	0	4	32.590	32.174
13	0	3	4.719 *	0.000
13	0	2	25.739	25.968
13	0	1	4.391 *	0.000
13	0	0	4.433 *	0.872
14	0	0	40.851	39.624
14	0	1	4.751 *	0.000
14	0	2	15.080	12.987
14	0	3	4.984 *	0.000
14	0	4	12.143	13.069
14	1	4	5.186 *	1.974

PBC21	F CALC	(37)		
H	K	L	F(OBS)	F(CALC)
14	1	3	5.610 *	5.794
14	1	2	6.645	6.116
14	1	1	11.452	11.253
14	1	0	4.915 *	4.814
14	2	0	11.452	12.061
14	2	1	4.757	7.739
14	2	2	4.015 *	3.683
14	2	3	26.792	22.374
14	2	4	5.181 *	4.669
14	3	2	5.630 *	2.993
14	3	1	4.947 *	2.879
14	3	0	4.947 *	1.322
14	4	1	4.751 *	1.852
14	4	0	4.974 *	5.891
14	4	-1	4.942 *	3.309
14	4	-2	5.165 *	4.177
14	4	-3	15.791	15.923
14	5	3	5.228 *	5.557
14	5	2	5.165 *	1.383
14	5	1	15.796	7.998
14	5	0	5.169 *	2.559
14	5	-1	15.876	18.863
14	6	1	5.227 *	1.913
14	6	2	5.292 *	1.722
14	6	7	5.228 *	2.456
14	7	1	5.354 *	5.795
15	4	0	5.155 *	1.822
15	4	-1	5.165 *	0.669
15	3	0	5.166 *	17.952
15	3	1	5.203	2.943
15	3	2	5.197 *	2.943
15	2	2	5.154 *	5.367
15	2	1	5.154 *	4.288
15	2	0	4.963 *	0.500
15	1	0	5.165 *	4.983
15	1	1	5.122 *	3.2.2
15	1	2	17.010	16.041
15	2	1	5.181 *	0.223
15	0	1	5.27 *	0.000
15	0	0	5.165 *	4.552
13	2	2	4.613 *	3.206
13	3	3	4.651 *	1.862
13	1	1	4.632 *	0.000
7	2	1	5.298 *	6.364
7	2	3	5.298 *	18.510
6	2	5	19.492	18.510
5	4	2	2.074 *	2.496
5	3	3	4.407 *	6.052
4	4	1	2.651 *	7.119
3	1	3	32.483	34.316
3	5	1	16.258	17.116
3	14	4	5.483 *	6.782
2	11	2	21.886	23.752
2	7	3	13.076	13.224
2	4	1	26.812	29.888
2	2	1	62.666	67.347
1	2	0	1.517 *	1.368
1	5	1	15.473	18.292

PROTO	PBC21	F CALC	H	K	L	F(OBS)	F(CALC)
PROTO	PBC21	F CALC	1	16	0	5.520 *	2.517
			1	11	7	5.366 *	0.465
			0	3	16	2.672 *	0.000
			0	10	1	12.312	11.497
			0	7	3	29.175	32.0954
			0	6	1	15.653	14.797
			0	4	2	5.197	2.7179
PROTO	PBC21	F CALC	ALL REFLECTIONS	NUMERATOR			