

The crystal structure and extent of solid solution of geocronite

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Abstract

Geocronite ($\text{Pb}_{28}\text{As}_{4+x}\text{Sb}_{8-x}\text{S}_{48}$, $0 \leq x \leq 8$), an isostructural Sb-bearing analog of jordanite, is monoclinic, space group $P2_1/m$ with $a = 8.963(2)\text{\AA}$, $b = 31.93(2)\text{\AA}$, $c = 8.500(2)\text{\AA}$ and $\beta = 118.02(1)^\circ$. The asymmetric unit of geocronite contains three metal layers of four atoms each at approximately $y = 0.05$, $y = 0.15$, and $y = 0.25$. Each of the three layers contains three Pb and one semimetal (As or Sb) site. One of the Pb sites in the first layer is half occupied by semimetals. Of the four As sites in the asymmetric unit of jordanite, only three can expand to accommodate Sb in geocronite. These three expandable sites in the asymmetric unit account for eight Sb atoms in the unit cell. One semimetal site in the asymmetric unit is unable to expand, and this site accounts for four As atoms in the unit cell. The extent of Sb substitution for As in geocronite is thus limited to an $\text{As}/(\text{As}+\text{Sb})$ value of 0.33.

Introduction

Geocronite is one of 24 sulfosalt phases in the $\text{PbS}-\text{As}_2\text{S}_3-\text{Sb}_2\text{S}_3$ system. It is the most PbS-rich of the ternary phases and occurs in many hydrothermal deposits where Pb, As, and Sb mineralization is present.

Geocronite is the Sb-bearing analog of jordanite, $\text{Pb}_{28}\text{As}_{12}\text{S}_{48}$. Reported geocronite formulas vary within the range of $\text{Pb}_{28-30}(\text{As}, \text{Sb})_{12-14}\text{S}_{48-48}$ (Douglass *et al.*, 1954; Roland, 1968; Palache *et al.*, 1944, p. 395-396). Complete Sb substitution for As in geocronite has been reported as the mineral phase schulzite (Palache *et al.*, 1944, p. 396). However, the existence of this mineral has not been confirmed, and synthetic studies (250°-650°C) (Roland, 1968; Salanci and Moh, 1970; Walia and Chang, 1973; Garvin, 1973; Craig *et al.*, 1973; Birnie, 1975) have shown that the stable assemblage for the bulk composition corresponding to pure Sb geocronite is galena (PbS) plus boulangerite ($\text{Pb}_5\text{Sb}_4\text{S}_{11}$). Furthermore, electron microprobe analysis of 120 geocronite samples from 14 localities has shown a range of Sb substitution for As in 116 samples from an $\text{As}/(\text{As}+\text{Sb})$ value of 1.00 (jordanite) to 0.31 (± 0.02) (Birnie, 1975). There is a concentration of analyses at 0.33, and several equilib-

rium pairs of geocronite (0.33) plus boulangerite (0.00) were observed, indicating that this is the most Sb-rich geocronite that can exist stably within the pressure and temperature range represented by natural samples. Four analyses with $\text{As}/(\text{As}+\text{Sb})$ values between 0.20 and 0.30 apparently result from Sb contamination when probing a very fine-grained intimately intergrown aggregate of geocronite, boulangerite, and galena. Based on the ideal formula of jordanite, $\text{Pb}_{28}\text{As}_{12}\text{S}_{48}$ (Ito and Nowacki, 1974), geocronite may be assigned a formula of $\text{Pb}_{28}\text{As}_{4-x}\text{Sb}_{8-x}\text{S}_{48}$ with $0 \leq x \leq 8$. This compositional range plots in $\text{PbS}-\text{As}_2\text{S}_3-\text{Sb}_2\text{S}_3$ composition space along the line with $\text{PbS}/(\text{As}, \text{Sb})_2\text{S}_3 = 4.67$.

Jordanite is monoclinic with space group $P2_1/m$ (Douglass *et al.*, 1954). Reflections with h and l even are strong, indicative of a substructure with $a_{\text{sub}} = 1/2 a$, $b_{\text{sub}} = b$, and $c_{\text{sub}} = 1/2 c$. The cell parameters of jordanite are related to those of galena by $a = [1\bar{1}0]_{\text{gn}}$, $b = (10/3)[111]_{\text{gn}}$, and $c = [\bar{1}01]_{\text{gn}}$. On these grounds, Wuensch and Nowacki (1966) proposed that the substructure of jordanite is based on a $2 \times 2 \times 10$ array of PbS_6 octahedra stacked along the b axis. The close-packed array of sulfur atoms is interrupted at $y = 0.25$ and $y = 0.75$, where two sulfur layers directly overlie one another, creating metal sites at $y = 0.25$ and $y = 0.75$ having mirror symmetry and trigonal prismatic coordination with sulfur. This substructure model was based on an analysis

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Geocronite Observed and Calculated Structure Factors

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-9	0	2	283.959	-221.212	-9	4	8	212.584	-156.453
-9	2	2	250.679	-273.285	-9	6	8	140.961	136.035
-9	3	2	449.494	393.333	-9	7	8	177.575	127.454
-9	4	2	215.424	-181.074	-9	9	8	134.293	-76.991
-9	5	2	183.626	-165.931	-8	0	1	183.070	163.109
-9	6	2	211.843	212.989	-8	1	1	130.403	-113.465
-9	7	2	280.749	292.216	-8	5	1	164.115	-141.420
-9	8	2	123.240	77.839	-8	1	2	195.234	164.315
-9	9	2	136.762	-2.831	-8	3	2	139.479	-89.657
-9	10	2	206.409	110.980	-8	4	2	263.954	-240.529
-9	12	2	218.017	207.023	-8	5	2	887.442	-843.312
-9	13	2	374.661	-387.655	-8	9	2	186.713	179.353
-9	14	2	169.363	217.846	-8	11	2	156.706	-168.869
-9	15	2	141.707	229.274	-8	14	2	229.254	251.738
-9	16	2	142.998	-169.793	-8	15	2	611.440	718.700
-9	0	3	198.568	189.256	-8	17	2	143.739	161.488
-9	2	3	135.342	15.195	-8	19	2	171.647	-151.263
-9	4	3	156.150	151.595	-8	0	3	176.278	113.004
-9	6	3	158.311	-157.735	-8	4	3	179.057	-148.214
-9	9	3	142.258	74.275	-8	6	3	179.304	202.865
-9	10	3	160.101	-135.654	-8	7	3	139.479	71.716
-9	1	4	254.322	172.392	-8	15	3	126.081	31.528
-9	3	4	331.934	-238.352	-8	0	4	712.337	612.937
-9	4	4	283.959	-221.970	-8	1	4	632.009	529.201
-9	5	4	397.444	-370.159	-8	2	4	253.396	183.961
-9	6	4	195.913	133.546	-8	3	4	204.310	188.586
-9	7	4	386.145	-334.130	-8	5	4	156.397	-146.766
-9	9	4	213.078	188.468	-8	7	4	120.442	120.171
-9	11	4	200.544	-167.984	-8	8	4	147.012	-127.114
-9	13	4	178.131	222.998	-8	9	4	482.959	451.611
-9	15	4	235.614	233.404	-8	10	4	611.263	-602.952
-9	16	4	455.113	-451.711	-8	11	4	478.823	-455.694
-9	17	4	269.141	288.350	-8	12	4	288.405	-263.600
-9	19	4	191.776	-187.221	-8	13	4	280.810	-294.741
-9	0	5	226.044	-185.966	-8	15	4	147.938	198.402
-9	3	5	152.260	160.537	-8	19	4	214.806	-275.092
-9	10	5	153.001	150.739	-8	20	4	304.211	305.757
-9	13	5	173.376	-173.183	-8	21	4	457.583	458.436
-9	14	5	121.499	40.758	-8	22	4	219.314	228.458
-9	0	6	563.905	461.175	-8	23	4	214.251	195.788
-9	4	6	145.283	93.455	-8	25	4	167.881	-75.526
-9	7	6	131.761	121.057	-8	1	5	148.185	85.705
-9	9	6	300.939	301.143	-8	2	5	124.352	-91.296
-9	10	6	557.978	-551.833	-8	3	5	121.326	-87.773
-9	12	6	137.935	112.766	-8	4	5	149.729	-123.270
-9	13	6	223.389	-141.167	-8	5	5	194.369	-96.655
-9	14	6	163.621	-191.717	-8	6	5	230.958	-58.145
-9	3	7	186.157	-150.141	-8	7	5	117.622	-40.590
-9	13	7	140.343	-18.998	-8	16	5	128.983	4.050
-9	14	7	127.192	-89.003	-8	1	6	270.931	219.962
-9	0	8	145.653	-75.155	-8	2	6	429.613	-381.102
-9	2	8	162.263	-185.114	-8	3	6	573.599	501.956
-9	3	8	310.756	273.149	-8	4	6	262.534	-289.036

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-8	5	6	294.085	-276.563	-7	15	2	157.817	-99.179
-8	6	6	230.551	227.051	-7	17	2	128.797	132.797
-8	7	6	449.371	434.438	-7	19	2	169.672	211.145
-8	8	6	440.233	419.865	-7	20	2	425.044	-335.393
-8	9	6	372.438	363.799	-7	21	2	142.566	111.467
-8	10	6	159.669	102.370	-7	22	2	170.289	260.785
-8	11	6	199.189	-196.412	-7	0	3	117.560	156.725
-8	12	6	269.697	278.879	-7	1	3	112.312	-83.972
-8	13	6	360.769	-345.785	-7	3	3	163.374	178.251
-8	14	6	245.493	198.314	-7	5	3	162.324	145.119
-8	15	6	196.407	-209.001	-7	7	3	192.208	178.132
-8	16	6	335.948	-353.615	-7	10	3	120.647	-74.158
-8	17	6	336.009	-340.136	-7	20	3	134.848	59.345
-8	18	6	295.567	-321.368	-7	22	3	126.636	-127.864
-8	19	6	128.365	-87.799	-7	26	3	158.434	-167.661
-8	0	7	168.437	149.557	-7	27	3	183.255	197.423
-8	1	7	173.562	-152.863	-7	2	4	303.223	289.783
-8	2	7	127.809	22.022	-7	3	4	571.932	-520.477
-8	3	7	141.455	109.861	-7	4	4	406.397	329.052
-8	4	7	161.151	-103.958	-7	6	4	325.636	-290.387
-8	5	7	158.928	105.871	-7	7	4	248.148	-244.639
-8	10	7	273.524	-239.808	-7	8	4	124.969	74.107
-8	13	7	147.382	-180.669	-7	13	4	387.133	379.537
-8	15	7	128.365	68.455	-7	14	4	253.335	-304.765
-8	18	7	151.890	-114.011	-7	16	4	169.239	226.248
-8	19	7	161.583	43.130	-7	22	4	212.398	224.891
-8	20	7	140.405	149.864	-7	23	4	421.524	-462.115
-8	0	8	155.224	21.296	-7	24	4	376.698	376.253
-8	1	8	217.338	190.134	-7	26	4	193.320	-109.703
-8	3	8	304.396	-292.486	-7	5	5	115.584	-123.072
-8	4	8	433.317	-391.573	-7	6	5	129.600	-147.682
-8	5	8	760.559	-679.805	-7	7	5	141.393	-9.943
-8	6	8	406.098	413.915	-7	9	5	119.536	-139.475
-8	7	8	186.034	-202.877	-7	12	5	137.071	142.400
-8	9	8	229.254	186.921	-7	19	5	216.696	227.057
-8	11	8	165.041	-186.206	-7	21	5	130.588	173.714
-8	13	8	217.338	186.543	-7	1	6	137.688	-71.570
-8	14	8	349.963	325.979	-7	2	6	125.463	58.215
-8	15	8	507.904	505.319	-7	3	6	301.435	215.205
-7	0	1	270.252	263.894	-7	4	6	252.717	216.103
-7	3	1	157.879	-222.337	-7	6	6	230.983	-185.421
-7	7	1	158.249	-117.165	-7	7	6	291.739	232.445
-7	13	1	156.953	218.754	-7	16	6	467.647	462.564
-7	23	1	164.485	-213.637	-7	17	6	404.730	-404.293
-7	0	2	728.699	-622.322	-7	19	6	125.278	73.092
-7	2	2	135.836	102.027	-7	0	7	173.315	93.889
-7	4	2	154.853	-145.062	-7	13	7	122.800	175.574
-7	5	2	118.486	83.638	-7	0	8	242.653	-187.960
-7	6	2	133.119	113.362	-7	10	8	379.477	373.616
-7	9	2	336.688	-372.492	-7	11	8	265.607	-223.928
-7	10	2	701.409	809.635	-7	14	8	119.351	16.039
-7	13	2	204.495	251.537	-6	2	1	139.602	150.274
-7	14	2	176.587	239.932	-6	11	1	147.259	-107.721

H	K	L	F(OBS)	F(CALC)
-6	14	1	147.259	-279.685
-6	16	1	143.616	-106.002
-6	1	2	388.244	-221.443
-6	2	2	624.105	516.697
-6	3	2	742.159	-654.659
-6	4	2	392.073	300.728
-6	5	2	363.362	377.612
-6	6	2	336.688	-357.635
-6	7	2	609.472	-639.198
-6	8	2	525.748	-603.665
-6	9	2	403.372	-440.104
-6	11	2	209.064	263.507
-6	12	2	237.590	-324.614
-6	13	2	350.643	394.815
-6	14	2	197.024	-253.527
-6	15	2	243.147	-212.088
-6	16	2	253.149	269.661
-6	17	2	410.472	461.907
-6	18	2	413.498	440.891
-6	19	2	282.045	373.063
-6	23	2	270.993	-295.998
-6	24	2	197.889	222.721
-6	27	2	231.601	-312.752
-6	28	2	287.417	-380.765
-6	29	2	254.014	-278.538
-6	0	3	210.546	-216.282
-6	1	3	254.878	189.252
-6	3	3	160.348	-164.760
-6	5	3	179.921	152.202
-6	8	3	103.606	-139.024
-6	10	3	282.169	273.658
-6	12	3	144.912	113.966
-6	13	3	147.197	211.995
-6	19	3	128.859	-84.316
-6	20	3	170.845	-165.942
-6	29	3	148.185	142.503
-6	1	4	342.431	-239.521
-6	3	4	470.734	417.259
-6	4	4	672.945	591.177
-6	5	4	987.776	910.645
-6	6	4	575.204	-574.263
-6	7	4	412.818	419.042
-6	9	4	276.241	-283.739
-6	11	4	261.361	-292.601
-6	13	4	324.093	-307.819
-6	14	4	534.515	-575.558
-6	15	4	754.199	-782.483
-6	16	4	147.320	161.473
-6	17	4	324.155	-368.450
-6	19	4	206.594	183.119
-6	21	4	144.665	-163.900
-6	23	4	209.311	211.628
-6	24	4	370.833	429.614

H	K	L	F(OBS)	F(CALC)
-6	25	4	417.079	463.266
-6	3	5	212.275	-204.336
-6	4	5	253.273	216.591
-6	6	5	272.784	-256.776
-6	7	5	166.893	-76.313
-6	8	5	127.562	-0.764
-6	11	5	138.553	-109.302
-6	14	5	118.177	-107.820
-6	17	5	169.178	58.174
-6	24	5	134.540	16.145
-6	27	5	132.996	53.381
-6	0	6	1427.577	-1269.478
-6	1	6	638.615	-551.936
-6	2	6	221.783	-146.554
-6	3	6	151.581	-139.698
-6	5	6	167.511	-101.475
-6	9	6	335.515	-317.163
-6	10	6	1019.698	995.470
-6	11	6	388.430	363.230
-6	12	6	195.357	177.388
-6	15	6	119.536	-110.890
-6	19	6	206.162	302.097
-6	20	6	733.392	-749.535
-6	21	6	280.316	-287.114
-6	23	6	221.228	-179.421
-6	1	7	147.074	-86.587
-6	3	7	157.199	122.101
-6	4	7	203.446	140.744
-6	15	7	133.428	35.693
-6	17	7	152.013	-168.870
-6	22	7	125.216	-149.960
-6	0	8	136.392	-97.318
-6	1	8	123.055	-72.497
-6	2	8	344.653	287.844
-6	3	8	585.269	-492.114
-6	4	8	487.096	485.269
-6	6	8	436.466	-395.830
-6	7	8	533.577	-410.931
-6	8	8	450.297	-406.598
-6	9	8	208.447	-233.386
-6	12	8	312.979	-292.145
-6	13	8	487.652	472.411
-6	14	8	408.249	-435.103
-6	16	8	332.675	341.548
-6	17	8	371.388	328.330
-6	18	8	254.075	281.433
-5	0	1	277.044	241.786
-5	3	1	95.394	96.116
-5	4	1	165.782	194.759
-5	6	1	147.135	-217.945
-5	9	1	212.275	268.608
-5	12	1	123.179	-87.425
-5	19	1	226.291	-308.208

(4)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-5	1	2	209.682	144.888	-5	13	6	232.712	-231.523
-5	3	2	424.179	-388.724	-5	14	6	229.254	283.645
-5	4	2	394.110	-361.034	-5	16	6	169.363	-165.892
-5	5	2	195.357	-201.641	-5	18	6	218.264	242.988
-5	6	2	203.260	207.895	-5	19	6	165.782	126.977
-5	7	2	306.681	-329.869	-5	23	6	268.029	253.511
-5	12	2	103.050	63.674	-5	24	6	302.174	-356.289
-5	13	2	178.007	207.699	-5	25	6	175.476	146.041
-5	16	2	568.104	-651.844	-5	27	6	208.015	-177.570
-5	17	2	508.707	594.522	-5	28	6	218.573	-185.437
-5	18	2	165.844	-241.707	-5	29	6	179.674	-180.644
-5	26	2	318.536	431.547	-5	0	7	310.139	-311.192
-5	27	2	288.775	-407.870	-5	9	7	159.855	178.006
-5	29	2	152.939	68.426	-5	12	7	191.344	-189.825
-5	0	3	163.250	-148.796	-5	19	7	182.823	-241.663
-5	3	3	242.591	223.083	-5	5	8	145.530	126.086
-5	7	3	96.814	34.601	-5	6	8	187.763	175.822
-5	8	3	106.446	-70.961	-5	7	8	126.945	-127.327
-5	13	3	33.021	-304.432	-5	11	8	108.545	-33.015
-5	15	3	127.192	126.812	-5	14	8	207.335	-215.339
-5	16	3	148.061	188.971	-5	15	8	152.198	-178.628
-5	23	3	137.565	124.565	-5	16	8	121.820	-109.107
-5	26	3	181.527	-144.690	-5	17	8	269.017	290.519
-5	33	3	175.290	-97.339	-5	18	8	170.660	-143.845
-5	0	4	401.581	345.644	-5	19	8	130.773	40.757
-5	1	4	201.655	-147.214	-4	3	1	122.067	138.311
-5	2	4	136.577	-97.646	-4	4	1	257.407	-253.354
-5	9	4	122.500	128.950	-4	5	1	114.720	142.945
-5	10	4	653.434	-673.605	-4	6	1	234.132	276.178
-5	11	4	377.810	420.823	-4	14	1	120.709	197.633
-5	13	4	108.175	-171.061	-4	16	1	128.983	-125.392
-5	14	4	111.139	-79.854	-4	17	1	181.773	-61.371
-5	16	4	110.274	56.767	-4	27	1	141.023	-97.070
-5	20	4	330.637	377.787	-4	31	1	135.651	179.546
-5	21	4	393.925	-410.319	-4	0	2	2245.681	2039.013
-5	22	4	307.731	-296.239	-4	1	2	791.369	684.783
-5	28	4	244.592	-298.738	-4	2	2	164.362	126.251
-5	31	4	456.224	448.577	-4	3	2	207.397	164.173
-5	2	5	116.696	77.874	-4	5	2	153.989	-153.294
-5	5	5	212.151	-233.258	-4	7	2	119.598	105.391
-5	11	5	100.766	40.539	-4	9	2	375.710	389.284
-5	12	5	132.008	-174.936	-4	10	2	1218.636	-1426.482
-5	13	5	112.682	-97.783	-4	11	2	404.174	-442.119
-5	16	5	127.686	-190.961	-4	18	2	149.111	-88.733
-5	18	5	107.434	-17.707	-4	19	2	218.511	-318.381
-5	20	5	182.329	-136.530	-4	20	2	809.337	1016.769
-5	23	5	177.698	179.265	-4	21	2	312.238	414.469
-5	28	5	138.553	111.176	-4	22	2	218.449	281.201
-5	1	6	148.061	-105.996	-4	23	2	227.340	221.136
-5	3	6	255.989	218.772	-4	27	2	129.662	-17.671
-5	4	6	324.833	-282.144	-4	30	2	542.295	-645.580
-5	5	6	208.262	114.059	-4	31	2	223.883	-294.299
-5	8	6	164.547	-153.825	-4	1	3	166.523	123.640

H	K	L	F(OBS)	F(CALC)
-4	2	3	141.825	- 118.480
-4	3	3	241.727	- 210.158
-4	4	3	214.065	- 210.929
-4	5	3	93.048	- 37.664
-4	7	3	165.782	- 213.240
-4	8	3	127.377	220.661
-4	11	3	107.558	34.970
-4	13	3	172.327	152.573
-4	14	3	116.078	270.857
-4	17	3	169.980	213.673
-4	19	3	120.585	- 257.009
-4	27	3	124.352	- 84.354
-4	0	4	154.421	137.049
-4	1	4	132.749	91.770
-4	2	4	505.681	- 429.755
-4	3	4	872.439	773.269
-4	4	4	775.501	- 737.798
-4	5	4	93.603	- 103.843
-4	6	4	729.193	709.392
-4	7	4	951.594	934.358
-4	8	4	728.020	713.943
-4	9	4	288.405	279.555
-4	10	4	139.417	- 148.369
-4	12	4	348.481	405.611
-4	13	4	622.688	- 703.873
-4	14	4	618.795	696.293
-4	16	4	429.551	- 498.142
-4	17	4	452.273	- 545.064
-4	18	4	360.336	- 396.271
-4	20	4	126.451	186.940
-4	22	4	141.640	- 212.199
-4	23	4	372.870	384.195
-4	24	4	347.988	- 407.742
-4	26	4	276.920	279.938
-4	27	4	389.850	404.445
-4	28	4	307.792	290.482
-4	29	4	153.927	116.649
-4	33	4	281.281	- 255.555
-4	0	5	344.036	331.531
-4	1	5	168.066	- 123.637
-4	5	5	105.396	- 77.277
-4	8	5	129.909	123.270
-4	10	5	347.494	- 359.951
-4	20	5	131.885	131.622
-4	25	5	116.078	- 66.776
-4	28	5	188.071	225.020
-4	0	6	196.592	131.005
-4	1	6	213.139	195.952
-4	2	6	200.605	- 174.943
-4	3	6	609.534	- 566.812
-4	4	6	752.471	- 704.511
-4	5	6	560.262	- 503.697
-4	6	6	812.239	807.350

H	K	L	F(OBS)	F(CALC)
-4	7	6	692.456	- 692.482
-4	8	6	288.652	294.249
-4	9	6	154.112	159.812
-4	10	6	179.180	- 219.709
-4	11	6	185.046	- 183.427
-4	12	6	119.165	148.707
-4	13	6	457.830	472.599
-4	14	6	643.616	673.119
-4	15	6	457.644	519.009
-4	16	6	314.584	- 373.661
-4	17	6	358.916	418.836
-4	18	6	151.519	- 196.833
-4	19	6	128.427	- 90.762
-4	23	6	233.638	- 282.806
-4	24	6	426.587	- 457.987
-4	25	6	207.397	- 219.997
-4	26	6	334.527	353.144
-4	27	6	287.726	- 296.013
-4	28	6	193.567	156.486
-4	3	7	145.406	151.757
-4	4	7	141.208	- 108.126
-4	6	7	170.413	139.934
-4	7	7	123.497	112.236
-4	12	7	113.508	- 178.635
-4	14	7	156.459	139.100
-4	19	7	127.809	138.762
-4	21	7	143.986	- 103.484
-4	23	7	148.247	720.193
-4	24	7	182.206	- 136.583
-4	0	8	1487.159	1314.921
-4	1	8	170.166	125.116
-4	10	8	965.425	- 967.614
-4	20	8	742.715	789.754
-4	22	8	138.368	171.659
-3	0	1	153.927	178.948
-3	1	1	169.116	- 173.486
-3	2	1	182.823	- 166.318
-3	5	1	239.010	253.438
-3	6	1	138.368	- 211.850
-3	10	1	127.254	- 140.567
-3	12	1	120.771	247.144
-3	14	1	115.769	104.733
-3	15	1	126.513	- 97.526
-3	16	1	211.534	285.094
-3	20	1	190.973	125.504
-3	22	1	173.129	- 310.858
-3	26	1	166.152	- 252.395
-3	29	1	128.180	43.836
-3	36	1	438.380	181.464
-3	1	2	205.298	172.080
-3	3	2	479.440	- 448.404
-3	4	2	493.518	474.498
-3	5	2	197.889	- 173.589

H	K	L	F(OBS)	F(CALC)
12	6	2	231.168	- 249.038
13	8	2	278.094	281.232
14	9	2	196.468	225.080
15	12	2	96.999	- 55.530
16	13	2	267.412	330.912
17	14	2	268.215	- 365.821
18	16	2	138.615	188.140
19	17	2	122.006	- 132.533
20	18	2	237.960	- 336.753
21	19	2	173.129	- 201.355
22	21	2	154.421	163.872
23	23	2	348.667	- 393.947
24	24	2	388.862	522.196
25	25	2	226.723	- 219.448
26	27	2	178.748	186.684
27	28	2	166.523	196.163
28	33	2	262.472	269.973
29	34	2	280.502	- 265.444
30	0	3	250.679	216.174
31	1	3	188.442	- 152.574
32	2	3	97.864	- 87.292
33	4	3	90.022	- 27.371
34	9	3	305.199	- 368.630
35	12	3	150.284	189.130
36	15	3	97.740	121.840
37	19	3	295.999	405.201
38	21	3	145.283	254.379
39	23	3	157.693	113.956
40	29	3	240.801	- 245.039
41	34	3	157.447	37.127
42	35	3	148.185	92.679
43	2	4	165.473	118.481
44	3	4	157.447	96.161
45	5	4	225.920	- 168.695
46	6	4	171.771	- 153.026
47	7	4	235.491	209.114
48	14	4	174.426	225.131
49	15	4	242.097	262.515
50	16	4	162.263	225.073
51	17	4	389.541	- 464.321
52	18	4	264.448	309.494
53	24	4	233.700	- 285.353
54	25	4	252.470	- 224.829
55	26	4	294.888	- 301.493
56	27	4	371.018	312.214
57	34	4	206.039	207.296
58	1	5	138.800	- 88.529
59	5	5	104.100	58.358
60	6	5	173.129	196.289
61	7	5	176.340	206.219
62	8	5	129.230	109.782
63	11	5	125.031	116.777
64	12	5	124.846	- 174.952

H	K	L	F(OBS)	F(CALC)
13	15	5	137.133	134.391
14	15	5	157.076	- 188.467
15	16	5	228.699	- 229.741
16	17	5	109.348	- 138.819
17	21	5	134.354	- 115.062
18	23	5	128.242	- 14.502
19	26	5	199.247	220.913
20	27	5	122.500	88.648
21	28	5	161.830	147.832
22	30	5	170.536	12.066
23	33	5	164.856	16.831
24	3	6	106.755	- 8.757
25	9	6	122.993	84.349
26	11	6	475.118	- 500.203
27	18	6	115.769	11.254
28	21	6	503.396	562.853
29	0	7	118.054	- 56.314
30	2	7	114.041	- 20.169
31	5	7	133.552	150.212
32	7	7	183.502	- 135.764
33	8	7	122.253	112.326
34	13	7	228.946	218.553
35	14	7	166.461	212.691
36	16	7	132.088	160.215
37	19	7	117.869	- 160.304
38	20	7	146.456	80.932
39	23	7	195.357	- 189.563
40	24	7	145.530	- 135.927
41	2	8	180.662	- 121.776
42	3	8	205.792	188.498
43	5	8	139.356	- 109.421
44	6	8	174.241	175.712
45	7	8	233.391	231.593
46	15	8	161.398	182.155
47	17	8	314.893	- 367.280
48	18	8	252.100	- 226.277
49	0	8	491.890	- 449.143
50	1	1	105.482	73.313
51	8	1	119.844	- 178.802
52	10	1	289.393	460.362
53	18	1	159.546	348.172
54	20	1	185.355	- 149.187
55	24	1	167.943	126.613
56	0	2	299.333	- 222.861
57	2	2	260.990	- 241.789
58	2	2	356.817	287.551
59	3	2	864.659	822.890
60	4	2	966.289	981.991
61	5	2	559.460	549.608
62	6	2	1061.436	- 1170.190
63	7	2	1013.708	1184.497
64	8	2	487.590	- 566.572
65	9	2	177.451	- 222.639

H	K	L	F(OBS)	F(CALC)
12	6	2	231.168	- 249.038
12	6	2	278.094	281.232
12	6	2	196.468	225.080
12	6	2	96.999	- 55.530
13	6	2	267.412	330.912
14	6	2	268.215	- 365.921
16	6	2	138.615	188.140
17	6	2	122.006	- 132.533
18	6	2	237.960	- 336.753
19	6	2	173.129	- 201.355
21	6	2	154.421	163.872
23	6	2	348.667	- 393.947
24	6	2	388.862	522.196
25	6	2	226.723	- 219.448
27	6	2	178.748	186.684
28	6	2	166.523	196.163
33	6	2	262.472	269.973
34	6	2	280.502	- 265.444
34	0	2	250.679	216.174
34	2	2	188.442	- 152.574
34	4	2	97.864	- 87.292
34	9	2	90.022	- 27.371
12	3	3	305.199	- 368.630
15	3	3	150.284	189.130
19	3	3	97.740	121.840
21	3	3	295.999	405.201
23	3	3	145.283	254.979
29	3	3	157.693	113.956
34	3	3	240.801	- 245.039
35	3	3	157.447	37.127
35	2	4	148.185	92.679
35	3	4	165.473	118.481
35	4	4	157.447	96.161
35	6	4	225.920	- 168.695
35	7	4	171.771	- 153.026
14	4	4	235.491	209.114
15	4	4	174.426	225.131
16	4	4	242.097	253.515
16	4	4	162.263	225.073
17	4	4	389.541	- 464.321
18	4	4	264.448	309.494
24	4	4	233.700	- 285.353
25	4	4	252.470	- 224.829
26	4	4	294.888	- 301.493
27	4	4	371.018	312.214
34	4	4	206.039	207.296
34	5	4	138.800	- 88.529
34	5	4	104.100	58.358
34	6	4	173.129	196.289
34	7	4	176.340	206.219
34	8	4	129.230	109.782
11	5	5	125.031	116.777
12	5	5	124.846	- 176.952

H	K	L	F(OBS)	F(CALC)
13	5	5	137.133	134.391
15	5	5	157.076	- 188.467
16	5	5	228.699	- 229.761
17	5	5	109.348	- 138.819
21	5	5	134.354	- 115.062
23	5	5	128.242	- 14.502
26	5	5	199.247	220.913
27	5	5	122.500	88.648
28	5	5	161.830	147.832
30	5	5	170.536	12.066
33	5	5	164.856	16.831
3	6	6	106.755	- 8.757
9	6	6	122.993	84.349
11	6	6	475.118	- 500.203
18	6	6	115.769	11.254
21	6	6	503.396	562.853
2	7	7	118.054	- 56.314
2	7	7	114.041	- 20.169
7	7	7	133.552	150.212
7	7	7	183.502	- 135.764
8	7	7	122.253	112.326
13	7	7	228.946	218.553
14	7	7	166.461	212.691
16	7	7	132.088	160.215
19	7	7	117.869	- 160.304
20	7	7	146.456	80.932
23	7	7	195.357	- 183.563
24	7	7	145.530	- 135.927
2	8	8	180.442	- 121.776
3	8	8	205.792	188.488
5	8	8	139.356	- 109.421
6	8	8	174.241	175.712
6	8	8	233.391	231.593
15	8	8	161.398	182.155
17	8	8	314.893	- 367.280
18	8	8	252.100	- 226.277
0	1	1	491.850	- 449.143
1	1	1	103.482	73.313
1	1	1	119.844	- 178.802
10	1	1	289.393	460.362
18	1	1	159.546	348.172
20	1	1	185.355	- 149.187
24	1	1	167.943	126.613
0	2	2	299.333	- 222.861
1	2	2	260.990	- 241.789
2	2	2	356.817	287.551
3	2	2	864.659	822.890
4	2	2	966.289	981.991
5	2	2	359.460	549.608
6	2	2	1061.436	- 1170.190
7	2	2	1013.708	1184.497
8	2	2	487.590	- 566.572
9	2	2	177.451	- 222.639

H	K	L	F(OBS)	F(CALC)
-2	10	2	227.649	329.670
-2	11	2	192.702	276.278
-2	12	2	173.191	-254.892
-2	13	2	604.347	-731.998
-2	14	2	845.148	-1018.770
-2	15	2	592.925	710.151
-2	16	2	417.573	495.445
-2	17	2	518.956	-598.894
-2	18	2	244.011	284.574
-2	19	2	237.158	179.096
-2	20	2	200.544	-249.598
-2	21	2	146.086	-186.671
-2	22	2	130.403	145.629
-2	23	2	400.161	450.776
-2	24	2	540.813	605.718
-2	25	2	221.289	229.550
-2	26	2	404.668	-441.509
-2	27	2	336.874	341.303
-2	28	2	260.003	-206.717
-2	29	2	136.639	-32.256
-2	30	2	158.928	49.357
-2	33	2	273.833	-245.550
-2	34	2	419.054	-390.552
-2	36	2	181.835	168.833
-2	37	2	189.800	-302.257
-2	2	3	122.314	93.761
-2	3	3	229.748	-256.678
-2	4	3	201.285	212.779
-2	6	3	238.084	-207.358
-2	7	3	193.073	-190.113
-2	11	3	98.049	-44.702
-2	13	3	96.320	203.553
-2	14	3	181.094	-240.320
-2	17	3	193.381	125.011
-2	19	3	126.142	-196.460
-2	21	3	140.467	121.104
-2	23	3	170.536	-246.172
-2	24	3	168.684	175.237
-2	0	4	2406.831	-2435.354
-2	1	4	137.441	-117.631
-2	2	4	95.147	-9.198
-2	9	4	104.162	-120.641
-2	10	4	1420.106	1570.106
-2	15	4	106.693	11.796
-2	18	4	136.577	129.423
-2	20	4	1158.127	-1227.962
-2	22	4	280.316	-273.259
-2	30	4	733.762	728.658
-2	2	5	98.111	1.080
-2	7	5	139.170	134.932
-2	8	5	165.411	-277.396
-2	14	5	161.213	-241.183
-2	16	5	136.701	74.577

H	K	L	F(OBS)	F(CALC)
-2	17	5	165.782	-152.662
-2	18	5	112.991	281.313
-2	21	5	122.685	28.486
-2	0	6	250.741	-246.995
-2	1	6	146.641	106.917
-2	2	6	336.195	319.896
-2	3	6	636.763	-603.386
-2	4	6	715.116	675.132
-2	5	6	335.207	-311.520
-2	6	6	757.225	-713.352
-2	7	6	705.545	-704.502
-2	8	6	366.819	-382.499
-2	10	6	225.858	248.309
-2	11	6	136.948	-89.343
-2	12	6	195.789	-279.188
-2	13	6	545.073	545.140
-2	14	6	622.068	-692.308
-2	15	6	350.272	375.047
-2	16	6	328.477	324.108
-2	17	6	346.814	370.801
-2	18	6	215.980	268.264
-2	20	6	145.962	-183.109
-2	21	6	124.969	73.359
-2	22	6	136.392	172.955
-2	23	6	358.114	-327.611
-2	24	6	418.375	455.743
-2	26	6	284.700	-278.428
-2	27	6	254.508	-269.285
-2	28	6	190.356	-151.112
-2	30	6	150.099	67.641
-2	0	7	245.061	-254.768
-2	10	7	120.647	176.166
-2	11	7	157.447	-125.193
-2	22	7	135.834	-149.706
-2	25	7	129.291	49.237
-2	0	8	146.147	-144.139
-2	2	8	207.644	219.240
-2	3	8	482.527	434.050
-2	4	8	560.756	518.400
-2	5	8	161.398	143.021
-2	6	8	496.728	-485.515
-2	7	8	473.821	463.676
-2	8	8	384.787	-361.258
-2	9	8	194.987	162.762
-2	10	8	122.253	132.511
-2	12	8	187.269	-212.392
-2	13	8	389.788	-364.695
-2	14	8	437.763	-446.888
-2	15	8	133.675	-112.441
-2	16	8	391.579	405.114
-2	17	8	335.207	-334.508
-2	18	8	244.752	274.267
-2	20	8	149.296	-122.472

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	21	8	132.502	22.199	-1	24	4	192.455	-254.179
-1	1	1	115.090	117.601	-1	25	4	262.349	211.377
-1	2	1	143.554	-122.397	-1	26	4	263.707	-268.374
-1	3	1	103.112	115.015	-1	27	4	367.190	-372.787
-1	5	1	125.093	-172.773	-1	28	4	184.614	-195.993
-1	6	1	132.378	-216.176	-1	31	4	144.604	100.488
-1	12	1	159.299	274.271	-1	33	4	186.898	-150.088
-1	13	1	176.402	-261.640	-1	34	4	178.131	156.703
-1	15	1	129.538	204.843	-1	0	5	431.156	-421.990
-1	16	1	202.025	306.225	-1	1	5	126.636	119.688
-1	22	1	165.350	-280.888	-1	4	5	128.242	-119.526
-1	23	1	194.307	114.065	-1	9	5	301.494	339.036
-1	26	1	231.662	-261.025	-1	10	5	133.552	161.386
-1	29	1	142.690	-239.057	-1	11	5	106.137	-18.759
-1	36	1	161.398	203.624	-1	16	5	118.301	-120.774
-1	1	2	303.347	-268.790	-1	19	5	247.592	-331.016
-1	9	2	96.135	-53.789	-1	20	5	160.040	-167.279
-1	11	2	626.637	808.948	-1	24	5	123.981	-93.159
-1	19	2	131.699	-110.668	-1	29	5	251.914	193.480
-1	21	2	625.464	-681.953	-1	1	6	127.130	-114.398
-1	23	2	171.524	138.040	-1	3	6	276.365	267.155
-1	31	2	679.675	660.053	-1	4	6	402.446	362.954
-1	32	2	143.369	20.715	-1	5	6	260.558	220.374
-1	35	2	143.431	-69.169	-1	9	6	104.162	63.488
-1	1	3	123.117	111.952	-1	10	6	215.671	-166.685
-1	2	3	122.500	80.273	-1	13	6	245.617	-266.903
-1	3	3	132.626	132.487	-1	14	6	331.317	-386.169
-1	5	3	240.677	-249.360	-1	16	6	146.880	178.925
-1	7	3	161.275	128.154	-1	17	6	115.584	97.280
-1	12	3	116.757	-242.007	-1	18	6	183.688	-192.639
-1	13	3	200.420	-286.308	-1	23	6	220.981	255.174
-1	16	3	211.164	-271.424	-1	24	6	370.586	385.012
-1	19	3	153.680	197.734	-1	25	6	226.599	211.561
-1	20	3	165.411	-103.476	-1	27	6	164.547	-141.286
-1	22	3	203.754	272.973	-1	28	6	179.921	178.122
-1	23	3	265.004	201.266	-1	29	6	152.692	-171.427
-1	26	3	179.674	208.147	-1	1	7	253.619	249.525
-1	33	3	208.694	-51.207	-1	5	7	167.572	-126.436
-1	36	3	192.887	-197.639	-1	6	7	156.767	-142.156
-1	2	4	172.759	133.023	-1	7	7	159.978	-215.641
-1	3	4	199.124	-218.721	-1	11	7	119.042	-79.154
-1	5	4	153.927	157.498	-1	15	7	152.137	148.079
-1	6	4	187.824	-165.850	-1	17	7	153.618	148.104
-1	7	4	270.499	-286.912	-1	0	8	378.057	-287.814
-1	8	4	127.377	-147.934	-1	10	8	449.494	442.025
-1	14	4	151.951	170.102	-1	11	8	258.089	267.372
-1	15	4	221.166	-279.276	-1	20	8	252.285	-259.835
-1	16	4	171.895	170.286	0	3	1	146.394	-197.642
-1	17	4	447.950	534.815	0	4	1	172.821	-231.411
-1	18	4	306.434	367.863	0	5	1	82.613	-82.674
-1	19	4	144.542	93.336	0	6	1	88.355	77.496
-1	21	4	108.792	-38.039	0	7	1	143.307	-193.312
-1	23	4	148.432	79.680	0	8	1	113.176	297.719

H	K	L	F(OBS)	F(CALC)
0	13	1	108.298	227.079
0	14	1	216.350	327.799
C	16	1	150.963	-66.210
0	17	1	236.664	172.567
0	24	1	172.203	-113.629
0	0	2	295.320	293.448
0	1	2	206.286	-193.957
0	2	2	379.600	-372.381
0	3	2	801.557	840.986
0	4	2	855.891	-960.850
0	5	2	621.401	455.630
0	6	2	938.505	1113.000
0	7	2	995.803	1187.952
0	8	2	513.214	614.460
0	9	2	164.856	-171.722
0	10	2	253.273	-348.960
0	11	2	189.862	230.301
0	12	2	231.662	321.368
0	13	2	667.079	-767.343
0	14	2	909.362	1024.246
0	15	2	583.663	-640.877
0	16	2	447.333	-469.848
0	17	2	546.679	-578.089
0	18	2	287.664	-324.592
0	19	2	180.292	158.021
0	20	2	250.679	278.454
0	21	2	139.417	-155.953
0	22	2	132.502	-201.612
0	23	2	453.816	469.223
0	24	2	596.321	-596.507
0	25	2	175.167	204.603
0	26	2	421.771	404.063
0	27	2	338.973	327.100
0	28	2	255.002	204.880
0	30	2	152.198	-56.658
0	31	2	185.478	191.681
0	33	2	214.992	-261.577
0	34	2	389.171	410.204
0	37	2	267.659	-279.072
0	0	3	408.249	412.306
0	1	3	141.393	-83.921
0	10	3	273.031	-345.148
0	11	3	117.128	116.554
0	18	3	136.824	-320.986
0	19	3	115.893	-52.528
0	28	3	169.980	251.571
0	31	3	146.580	122.915
0	0	4	193.937	157.390
0	2	4	377.192	-360.758
0	3	4	747.963	-733.470
0	4	4	770.562	-790.893
0	6	4	752.903	800.101
0	7	4	840.641	-891.439

H	K	L	F(OBS)	F(CALC)
0	8	4	602.804	651.192
0	9	4	198.876	-221.957
0	10	4	140.158	-194.305
0	12	4	254.816	323.462
0	13	4	574.217	612.336
0	14	4	646.765	712.201
0	16	4	514.634	-559.604
0	17	4	482.959	551.682
0	18	4	329.526	-380.933
0	20	4	157.817	197.321
0	23	4	358.484	-330.115
0	24	4	388.491	-419.300
0	26	4	393.493	361.666
0	27	4	462.893	-449.382
0	28	4	357.002	284.082
0	33	4	259.632	255.893
0	34	4	241.727	214.940
0	2	5	141.084	-161.487
0	3	5	136.886	142.319
0	4	5	115.831	-93.165
0	6	5	111.756	137.913
0	10	5	130.403	4.763
0	11	5	117.745	-40.857
0	12	5	105.396	-70.410
0	14	5	116.881	151.403
0	18	5	124.908	-54.784
0	19	5	148.432	218.261
0	24	5	165.905	-283.829
0	0	6	1437.703	1278.944
0	1	6	438.998	-370.664
0	5	6	166.523	108.968
0	9	6	176.649	-124.839
0	10	6	1000.866	-1045.061
0	11	6	267.906	265.594
0	12	6	142.381	-163.693
0	14	6	139.726	130.909
0	19	6	154.359	114.647
0	20	6	715.918	776.065
0	21	6	242.838	-270.507
0	23	6	193.814	-171.910
0	2	7	125.093	78.308
0	3	7	169.301	64.783
0	4	7	127.007	-21.128
0	9	7	122.870	-129.980
0	1	8	179.365	-159.269
0	3	8	352.803	330.744
0	4	8	498.025	430.900
0	5	8	552.236	527.408
0	6	8	471.290	429.776
C	7	8	206.409	175.015
0	9	8	151.643	-133.439
0	13	8	209.620	-206.547
0	14	8	386.330	412.043

H	K	L	F(OBS)	F(CALC)
0	15	8	391.887	- 382.905
1	0	1	250.803	237.254
1	1	1	232.836	-200.145
1	9	1	385.898	-469.807
1	11	1	102.618	60.644
1	13	1	159.175	-174.119
1	19	1	364.164	450.516
1	23	1	186.713	132.251
1	27	1	138.985	-116.064
1	29	1	247.839	-273.029
1	31	1	160.410	-236.793
1	33	1	169.487	97.021
1	1	2	182.082	180.165
1	3	2	468.079	-474.112
1	4	2	522.475	-525.875
1	5	2	227.093	-224.686
1	6	2	228.760	278.630
1	8	2	267.906	-295.611
1	9	2	144.912	204.169
1	11	2	103.297	-97.894
1	13	2	346.629	349.033
1	14	2	357.373	422.486
1	16	2	159.916	-202.068
1	17	2	147.197	-124.035
1	18	2	271.672	316.144
1	19	2	142.998	-190.133
1	20	2	155.038	-130.235
1	23	2	392.073	-390.427
1	24	2	525.933	-540.565
1	25	2	322.055	-249.931
1	26	2	132.132	-77.769
1	27	2	217.091	171.701
1	28	2	270.005	-199.339
1	29	2	264.757	222.144
1	33	2	265.004	287.774
1	34	2	297.419	293.202
1	0	3	138.923	-134.155
1	1	3	152.445	-177.799
1	2	3	170.968	160.593
1	5	3	190.665	197.842
1	6	3	182.947	204.197
1	7	3	184.490	250.534
1	11	3	108.792	87.825
1	12	3	149.358	-218.241
1	14	3	104.656	12.637
1	15	3	193.381	-183.908
1	16	3	275.562	-289.421
1	20	3	141.084	-50.232
1	21	3	120.215	-15.375
1	23	3	124.661	-77.316
1	26	3	238.084	250.217
1	30	3	142.875	-37.519
1	31	3	144.727	41.047

H	K	L	F(OBS)	F(CALC)
1	0	4	459.497	415.796
1	1	4	197.086	198.427
1	9	4	128.118	-62.537
1	10	4	678.934	-732.296
1	11	4	407.694	-459.197
1	13	4	118.918	177.909
1	19	4	127.624	95.323
1	20	4	364.658	398.631
1	21	4	473.266	477.072
1	22	4	233.329	-216.397
1	29	4	151.087	-116.801
1	30	4	340.455	-246.668
1	31	4	559.398	-465.914
1	2	5	157.261	-68.849
1	3	5	248.395	-273.804
1	5	5	211.657	178.687
1	7	5	273.648	-252.882
1	9	5	106.631	79.991
1	13	5	243.270	288.452
1	14	5	127.995	102.339
1	16	5	149.420	200.126
1	21	5	145.839	38.891
1	23	5	279.699	-237.081
1	26	5	161.336	-114.468
1	27	5	162.695	59.326
1	2	6	136.330	-84.933
1	3	6	370.154	339.439
1	4	6	304.520	-237.308
1	5	6	149.605	120.443
1	6	6	225.179	227.432
1	7	6	347.617	314.894
1	9	6	130.835	-108.524
1	16	6	363.236	-373.990
1	17	6	450.791	-513.281
1	18	6	199.494	-178.285
1	20	6	134.786	84.688
1	26	6	279.637	272.263
1	3	7	342.729	345.799
1	6	7	175.784	-146.279
1	9	7	245.246	-228.628
1	12	7	120.894	5.594
1	19	7	179.365	174.274
1	20	7	130.588	139.165
1	2	8	160.966	-118.095
1	3	8	327.365	-298.044
1	4	8	318.721	-264.957
1	6	8	200.173	208.734
1	7	8	161.954	-154.840
2	0	1	156.273	-144.180
2	2	1	167.325	186.313
2	3	1	209.558	-234.097
2	4	1	161.522	185.605
2	6	1	120.709	-125.281

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	7	1	170.042	-244.501	2	17	4	309.830	309.654
2	8	1	101.754	-261.805	2	18	4	153.186	159.770
2	13	1	135.157	132.588	2	19	4	195.357	-147.000
2	14	1	199.124	-244.381	2	20	4	128.180	-151.725
2	15	1	132.749	-76.311	2	23	4	208.570	-218.568
2	17	1	156.150	180.151	2	24	4	485.800	436.135
2	19	1	149.729	-289.424	2	25	4	449.741	-461.215
2	21	1	150.222	-21.463	2	26	4	162.509	-125.894
2	24	1	164.053	313.208	2	27	4	152.569	-115.891
2	0	2	2086.135	-2032.271	2	29	4	264.880	152.459
2	1	2	639.727	585.233	2	31	4	186.219	-160.999
2	2	2	156.644	-117.299	2	0	5	209.867	-160.496
2	3	2	158.187	165.239	2	2	5	120.700	-150.236
2	5	2	151.828	-167.214	2	4	5	113.979	120.314
2	9	2	260.990	289.255	2	9	5	123.055	-145.093
2	10	2	1210.239	1454.268	2	14	5	204.063	-173.721
2	11	2	343.789	-386.807	2	2	6	374.784	332.675
2	13	2	148.247	-161.456	2	3	6	540.628	462.156
2	15	2	140.961	158.468	2	4	6	334.527	356.116
2	19	2	239.380	-225.695	2	5	6	199.309	-179.708
2	20	2	1051.742	-1025.277	2	6	6	269.511	-308.733
2	21	2	407.879	402.202	2	7	6	406.335	400.800
2	22	2	287.911	-277.049	2	8	6	369.474	-380.939
2	23	2	288.219	221.293	2	9	6	275.315	318.351
2	25	2	183.132	-101.312	2	11	6	173.376	-194.019
2	30	2	643.370	636.986	2	12	6	185.416	-237.947
2	31	2	229.316	-275.629	2	13	6	304.273	-270.954
2	35	2	156.520	104.616	2	14	6	203.878	-220.779
2	4	3	145.468	145.369	2	15	6	190.603	167.033
2	5	3	118.177	194.363	2	16	6	244.690	276.368
2	6	3	115.893	-136.171	2	17	6	343.480	-354.749
2	9	3	131.639	166.485	2	18	6	352.495	359.246
2	12	3	103.668	246.768	2	19	6	261.483	-316.727
2	14	3	190.912	-202.125	2	21	6	157.199	100.896
2	16	3	125.587	109.564	2	23	6	157.879	144.744
2	17	3	178.439	-47.259	2	8	7	155.718	-136.501
2	18	3	122.067	267.611	2	11	7	122.561	114.244
2	21	3	140.094	21.558	3	0	1	212.325	210.665
2	0	4	190.603	-183.878	3	3	1	262.843	294.206
2	1	4	282.663	256.595	3	5	1	186.343	-182.840
2	2	4	170.104	114.234	3	7	1	235.614	204.348
2	3	4	468.141	-445.515	3	12	1	169.301	-206.231
2	4	4	634.787	619.747	3	13	1	267.227	-353.259
2	5	4	801.557	-809.620	3	15	1	141.764	105.845
2	6	4	562.917	-569.776	3	16	1	162.571	-233.239
2	7	4	377.192	-374.095	3	23	1	262.719	221.558
2	9	4	252.902	226.265	3	26	1	249.939	152.863
2	10	4	118.424	194.829	3	33	1	172.080	-121.511
2	11	4	222.957	-221.331	3	1	2	198.568	147.300
2	13	4	331.996	310.935	3	2	2	100.272	69.937
2	14	4	523.463	-533.229	3	3	2	432.268	-449.707
2	15	4	607.002	690.510	3	4	2	371.512	369.292
2	16	4	178.007	156.584	3	5	2	195.851	-188.282

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	6	2	197.024	- 229.328	4	0	1	232.033	241.606
3	7	2	321.005	- 370.845	4	3	1	125.401	- 148.771
3	8	2	105.396	- 132.614	4	5	1	130.897	147.204
3	11	2	111.694	- 108.612	4	9	1	128.612	141.829
3	13	2	187.392	225.759	4	10	1	201.285	- 175.736
3	15	2	122.993	- 120.027	4	14	1	127.748	164.779
3	16	2	636.578	609.350	4	20	1	175.043	120.516
3	17	2	652.014	646.980	4	28	1	184.181	167.113
3	18	2	283.774	257.947	4	31	1	140.652	55.347
3	23	2	154.236	- 82.730	4	1	2	333.910	- 299.338
3	26	2	460.917	- 408.463	4	2	2	546.370	- 497.582
3	27	2	505.743	- 444.201	4	3	2	666.400	- 640.994
3	33	2	147.197	- 38.564	4	4	2	362.929	- 413.999
3	0	3	447.704	- 429.427	4	5	2	281.983	334.626
3	4	3	163.436	- 178.592	4	6	2	356.632	394.522
3	9	3	268.029	307.978	4	7	2	589.282	- 624.358
3	10	3	135.157	190.986	4	8	2	526.617	580.227
3	14	3	149.111	96.504	4	9	2	392.196	- 416.338
3	16	3	144.480	- 154.976	4	11	2	204.495	260.657
3	19	3	293.468	- 278.059	4	12	2	306.311	304.751
3	23	3	139.479	- 55.097	4	13	2	441.653	362.220
3	26	3	183.749	148.313	4	14	2	278.217	269.936
3	29	3	193.134	131.328	4	15	2	296.246	- 200.919
3	2	4	253.520	217.191	4	16	2	361.818	- 299.765
3	3	4	566.313	525.062	4	17	2	539.640	465.162
3	4	4	447.518	426.730	4	18	2	518.833	- 452.464
3	6	4	330.761	- 362.114	4	19	2	355.211	370.220
3	7	4	238.763	255.654	4	23	2	258.397	- 267.273
3	9	4	129.477	- 155.113	4	24	2	359.163	- 223.288
3	12	4	114.473	- 110.406	4	25	2	248.148	173.757
3	13	4	344.653	- 407.439	4	27	2	344.159	- 351.673
3	14	4	331.255	- 402.368	4	28	2	457.953	385.241
3	16	4	255.928	293.035	4	29	2	365.214	- 274.992
3	19	4	136.392	70.549	4	0	3	139.726	129.840
3	20	4	158.373	132.283	4	2	3	177.945	- 168.686
3	22	4	167.449	124.727	4	4	3	126.945	- 57.464
3	23	4	463.325	454.676	4	8	3	154.112	200.059
3	24	4	499.210	404.922	4	11	3	169.904	- 118.244
3	26	4	192.826	- 144.493	4	14	3	182.947	224.463
3	28	4	234.626	118.395	4	15	3	126.019	66.626
3	5	5	203.692	- 157.468	4	16	3	136.701	184.551
3	7	5	211.596	- 254.802	4	24	3	224.685	- 239.071
3	15	5	241.974	229.393	4	26	3	211.349	- 241.503
3	0	6	653.125	- 555.403	4	0	4	670.043	597.978
3	4	6	139.788	- 78.642	4	1	4	529.823	- 460.600
3	9	6	216.412	191.461	4	2	4	208.200	174.216
3	10	6	624.538	603.014	4	3	4	162.077	- 196.050
3	13	6	168.499	- 176.134	4	5	4	198.012	163.840
3	0	7	173.068	166.994	4	6	4	202.705	80.626
3	1	7	163.497	56.506	4	7	4	131.885	- 97.139
3	2	7	177.637	104.810	4	9	4	364.967	- 373.956
3	7	7	151.334	187.348	4	10	4	623.920	- 625.571
3	8	7	142.134	- 124.918	4	11	4	390.838	439.369

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	12	4	265.560	- 276.557	5	9	4	174.117	- 200.868
4	13	4	233.885	- 266.490	5	10	4	126.266	- 26.915
4	15	4	135.589	- 225.706	5	11	4	209.435	155.393
4	17	4	226.291	146.300	5	15	4	172.882	- 212.189
4	19	4	183.996	194.716	5	16	4	402.692	- 403.867
4	20	4	387.565	331.378	5	17	4	348.543	- 349.951
4	21	4	533.342	- 461.800	5	19	4	233.206	183.852
4	23	4	287.232	- 192.887	5	0	5	255.002	304.555
4	2	5	128.983	92.045	5	8	5	167.696	- 113.973
4	3	5	181.959	87.225	5	10	5	156.520	- 175.761
4	4	5	128.736	- 17.406	6	1	1	166.831	89.826
4	9	5	127.871	- 141.970	6	2	1	126.513	- 105.444
4	10	5	133.860	- 108.874	6	4	1	123.364	105.774
4	4	6	279.946	- 237.001	6	6	1	137.935	- 177.508
4	5	6	685.541	658.410	6	7	1	155.038	15.625
5	0	1	172.759	- 165.119	6	9	1	152.075	144.223
5	1	1	114.596	- 105.243	6	1	2	244.073	143.350
5	2	1	103.606	62.172	6	3	2	144.727	- 85.779
5	5	1	207.706	165.746	6	4	2	298.222	269.113
5	7	1	264.386	278.817	6	5	2	861.634	- 840.074
5	9	1	142.072	- 97.548	6	9	2	145.221	164.183
5	15	1	267.659	- 196.628	6	14	2	269.697	- 291.215
5	16	1	171.771	- 194.664	6	15	2	801.433	696.071
5	17	1	290.875	- 191.666	6	17	2	200.605	122.380
5	26	1	158.434	178.719	6	18	2	178.254	71.639
5	30	1	146.024	- 22.965	6	19	2	224.315	- 123.182
5	0	2	765.313	665.230	6	21	2	188.689	122.459
5	3	2	126.760	- 118.962	6	24	2	238.825	203.726
5	4	2	131.638	135.779	6	0	3	147.506	- 159.754
5	9	2	348.111	- 319.493	6	5	3	132.811	- 122.924
5	10	2	803.596	- 827.775	6	9	3	145.098	- 110.095
5	13	2	288.590	266.849	6	19	3	184.861	103.024
5	14	2	208.817	- 205.206	6	0	4	165.720	3.961
5	17	2	188.997	121.331	6	1	4	346.629	330.402
5	19	2	271.116	182.692	6	2	4	386.207	335.731
5	20	2	643.864	547.377	6	3	4	229.501	264.045
5	21	2	227.402	153.881	6	5	4	270.376	- 270.561
5	22	2	330.032	- 229.970	6	7	4	192.209	213.973
5	25	2	182.823	69.852	6	8	4	328.415	- 323.271
5	27	2	181.156	- 94.303	6	9	4	289.825	260.419
5	0	3	282.910	- 256.895	6	11	4	166.893	- 180.215
5	2	3	145.221	- 97.082	7	0	1	290.319	- 295.167
5	3	3	202.149	- 238.273	7	1	1	170.660	83.528
5	7	3	229.193	- 194.726	7	8	1	135.280	125.468
5	8	3	129.724	128.410	7	9	1	180.168	150.731
5	13	3	172.697	188.419	7	14	1	215.609	88.542
5	23	3	239.874	- 240.523	7	22	1	169.897	- 45.357
5	1	4	175.661	- 150.044	7	0	2	238.392	214.313
5	3	4	276.179	270.563	7	2	2	257.718	257.084
5	4	4	292.850	- 237.898	7	3	2	426.711	383.915
5	5	4	383.861	361.104	7	4	2	272.043	216.565
5	6	4	160.534	176.083	7	5	2	176.402	- 141.126
5	7	4	369.474	373.311	7	6	2	223.883	- 240.131

H	K	L	F(OBS)	F(CALC)
7	7	2	328.662	291.049
7	10	2	203.940	- 114.619
7	12	2	257.039	- 195.389
7	13	2	486.232	- 396.911
7	14	2	317.424	- 255.832
7	15	2	221.166	192.682
7	16	2	219.809	206.158
7	17	2	271.981	- 214.841
7	7	3	218.079	- 241.631
8	2	1	143.739	- 163.510
8	9	1	150.408	- 101.991
8	1	2	291.801	- 324.262
8	5	2	151.025	96.649
8	8	2	223.327	- 145.448