

AM-88-373

cd. 1001

Crystal chemistry of double-ring silicates: Structural, chemical, and optical
variation in osumilites

Thomas Armbruster, Roland Oberhänsli

For deposit: Table 3, 4, 5

American Mineralogist, 73, 5-6, 585-594.

pp 1) 1-25 (2)

for deposit

Table 3 (25 pages)

Observed and calculated structure factors of 8 natural osumilites. Structure factors flagged "LR" are smaller than 6 sigma ($F_{obs.}$) and were rejected.

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	7	28.39	29.60	4	4	6	40.87	40.26	2	2	7	9.84	9.98
2	2	8	91.40	91.73	4	4	6	40.10	39.26	2	2	7	31.39	31.20
2	2	9	43.26	44.01	4	4	6	2.87	3.43	2	2	7	2.58	1.06
2	2	10	49.00	49.14	4	4	6	7.65	7.46	2	2	7	4.62	2.04
2	2	11	20.73	20.79	4	4	6	4.68	1.66	2	2	7	17.70	17.83
2	2	12	15.80	16.75	4	4	6	8.90	7.41	2	2	7	38.57	38.33
2	2	13	28.13	28.44	4	4	6	24.24	24.48	2	2	7	3.72	3.50
2	2	14	76.68	74.77	5	5	6	4.52	5.61	3	3	7	20.81	21.12
2	2	15	13.47	12.40	5	5	6	4.02	5.21	3	3	7	39.28	39.62
2	2	16	6.39	5.44	5	5	6	14.64	15.36	3	3	7	13.27	13.30
2	2	17	24.89	25.21	5	5	6	12.71	12.50	3	3	7	28.23	28.70
3	3	0	10.79	10.45	5	5	6	4.95	3.90	3	3	7	25.12	24.93
3	3	1	34.56	35.57	5	5	6	8.87	9.77	3	3	7	11.61	11.98
3	3	2	19.93	20.66	5	5	6	17.35	17.49	3	3	7	7.61	7.95
3	3	3	60.78	61.63	5	5	6	1.46	3.80	3	3	7	5.64	3.86
3	3	4	15.03	15.39	5	5	6	4.93	2.54	3	3	7	6.87	6.43
3	3	5	53.62	52.96	5	5	6	10.26	8.79	3	3	7	18.02	17.99
3	3	6	13.30	12.97	5	5	6	5.16	6.25	3	3	7	30.55	30.84
3	3	7	0.00	3.43	5	5	6	60.91	62.56	3	3	7	40.13	38.99
3	3	8	2.06	6.06	5	5	6	41.57	40.91	3	3	7	3.54	23.70
3	3	9	19.54	19.03	5	5	6	62.80	63.40	3	3	7	24.05	21.30
3	3	10	2.71	3.99	6	6	6	30.62	30.38	4	4	7	20.51	23.45
3	3	11	4.19	3.00	6	6	6	11.22	10.52	4	4	7	22.96	24.57
3	3	12	17.67	16.68	6	6	6	36.65	35.68	4	4	7	1.41	2.55
3	3	13	36.05	36.15	6	6	6	3.71	2.03	4	4	7	6.52	6.83
3	3	14	22.37	21.93	6	6	6	4.90	0.34	4	4	7	53.68	55.39
3	3	15	20.40	20.74	6	6	6	23.13	22.71	4	4	7	17.84	18.66
3	3	16	0.00	3.69	6	6	6	52.43	53.62	4	4	7	3.29	3.18
4	4	0	7.58	8.18	6	6	6	18.74	19.29	4	4	7	46.76	45.66
4	4	1	53.82	53.33	6	6	6	9.22	12.40	4	4	7	5.02	5.09
4	4	2	8.76	8.23	6	6	6	30.55	30.38	4	4	7	6.29	7.97
4	4	3	14.40	14.26	6	6	6	19.19	11.29	4	4	7	8.47	10.73
4	4	4	0.00	2.15	6	6	6	9.55	19.55	5	5	7	33.23	33.21
4	4	5	48.12	48.03	6	6	6	33.17	32.75	5	5	7	6.93	10.66
4	4	6	12.33	12.03	6	6	6	24.95	23.65	5	5	7	5.37	3.66
4	4	7	1.87	6.05	6	6	6	56.71	37.22	5	5	7	21.39	21.54
4	4	8	23.25	23.31	6	6	6	7.31	9.76	5	5	7	12.41	12.79
4	4	9	53.50	54.78	6	6	6	41.79	42.87	5	5	7	5.39	2.64
4	4	10	18.08	18.43	6	6	6	23.85	24.07	5	5	7	31.19	31.20
4	4	11	25.97	25.25	6	6	6	39.40	39.40	5	5	7	4.89	7.20
4	4	12	5.45	5.97	6	6	6	11.55	11.22	5	5	7	30.06	30.77
4	4	13	25.89	25.74	6	6	6	5.32	1.08	5	5	7	5.03	6.27
4	4	14	3.56	5.71	6	6	6	31.38	31.29	5	5	7	15.23	15.02
4	4	15	23.98	24.14	6	6	6	24.28	24.54	5	5	7	42.63	42.53
5	5	0	42.13	42.28	6	6	6	16.16	16.90	6	6	7	8.49	7.95
5	5	1	33.33	32.68	6	6	6	13.44	12.91	6	6	7	17.45	16.78
5	5	2	6.62	4.54	6	6	6	6.55	9.05	6	6	7	0.00	2.33
5	5	3	17.99	17.55	6	6	6	32.77	33.20	6	6	7	63.24	61.79
5	5	4	3.49	5.22	6	6	6	5.39	8.06	6	6	7	11.98	12.12
5	5	5	6.89	5.98	6	6	6	21.70	21.32	6	6	7	33.63	32.53
5	5	6	9.76	10.50	6	6	6	36.26	36.49	6	6	7	1.78	2.12
5	5	7	41.55	40.75	6	6	6	50.70	50.75	6	6	7	28.58	27.80
0	0	6	36.11	34.67	6	6	6	14.03	14.82	6	6	7	40.31	40.03
0	0	7	140.18	138.58	6	6	6	30.72	31.81	6	6	7	4.68	7.39
0	0	8	130.69	129.70	6	6	6	0.00	1.04	6	6	7	147.63	146.24
0	0	9	19.90	20.06	6	6	6	68.17	68.59	6	6	7	27.37	27.51
0	0	10	89.77	88.02	6	6	6	67.26	66.98	6	6	7	35.55	35.11
0	0	11	80.30	81.49	6	6	6	4.43	0.34	6	6	7	53.46	52.97
0	0	12	46.63	48.36	6	6	6			6	6	7		

0	8	8	41.47	42.17	5	8	5	5.93	3.95	0	10	6	6.17	5.03
0	8	10	53.63	54.52	5	5	4	45.39	47.25	0	10	8	17.65	18.05
0	8	12	30.12	30.25	5	5	8	0.00	0.16	0	10	10	38.78	37.94
0	8	14	95.97	97.14	5	5	6	4.31	0.22	1	10	0	11.69	11.63
1	8	0	0.00	0.78	5	5	7	0.00	1.52	1	10	1	45.47	44.17
1	8	1	37.54	37.09	6	6	8	17.19	17.50	1	10	2	24.25	25.44
1	8	2	13.62	13.73	6	6	8	5.23	8.43	1	10	3	35.23	34.76
1	8	3	11.48	11.42	6	6	2	29.69	29.54	1	10	4	20.69	20.66
1	8	4	37.88	38.96	0	0	0	59.38	58.54	1	10	5	15.15	15.34
1	8	5	58.40	57.52	0	0	0	3.76	4.70	1	10	6	8.97	9.67
1	8	6	21.26	21.50	0	0	0	28.88	28.59	1	10	7	17.22	16.82
1	8	7	4.90	5.06	0	0	0	58.76	59.38	1	10	8	9.60	9.01
1	8	8	0.00	2.77	0	0	0	44.08	44.68	1	10	9	20.56	20.17
1	8	9	50.14	50.19	0	0	0	29.15	28.25	1	10	10	18.51	19.48
1	8	10	23.54	23.56	0	0	12	2.76	7.03	2	10	0	13.27	13.36
1	8	11	4.30	3.56	1	1	0	6.16	0.59	2	10	1	19.61	18.61
1	8	12	20.89	20.41	1	1	0	3.11	11.37	2	10	2	14.83	15.61
1	8	13	21.69	22.45	1	1	1	11.97	19.81	2	10	3	8.51	7.02
1	8	14	13.96	14.56	1	1	2	20.28	11.37	2	10	4	9.66	10.07
2	8	0	23.37	22.91	1	1	3	2.13	19.81	2	10	5	30.82	31.42
2	8	1	12.21	13.13	1	1	4	2.13	4.57	2	10	6	4.60	2.30
2	8	1	50.53	51.65	1	1	5	36.78	36.29	2	10	7	29.82	29.84
2	8	2	19.52	20.26	1	1	6	15.93	15.89	2	10	8	13.05	11.88
2	8	3	76.26	76.55	1	1	7	28.86	27.87	3	10	0	32.70	31.90
2	8	4	27.58	27.49	1	1	8	3.64	3.55	3	10	1	2.80	1.31
2	8	5	36.53	38.38	1	1	9	16.39	16.34	3	10	2	30.83	31.08
2	8	6	5.95	7.51	1	1	10	18.09	17.12	3	10	3	21.97	21.38
2	8	7	35.74	35.74	1	1	11	0.00	2.58	3	10	4	15.00	15.09
2	8	8	14.20	13.18	2	2	0	9.80	12.11	0	11	0	17.66	16.77
2	8	9	55.69	55.53	2	2	1	13.38	12.91	0	11	1	38.58	37.46
2	8	10	6.65	4.92	2	2	2	0.00	0.48	0	11	2	27.53	27.15
2	8	11	38.90	39.02	2	2	3	8.34	7.72	0	11	3	18.81	17.04
2	8	12	20.29	20.79	2	2	4	5.11	0.24	0	11	4	10.32	10.81
2	8	13	13.56	13.53	2	2	5	3.40	2.40	0	11	5	39.86	38.75
3	8	0	32.91	32.82	2	2	6	17.77	18.61	1	11	0	22.11	22.39
3	8	1	21.07	21.09	2	2	7	6.51	6.26	1	11	1	65.57	63.90
3	8	2	30.21	30.80	2	2	8	5.02	5.20	1	11	2	10.52	9.94
3	8	3	26.87	27.25	2	2	9	1.20	4.08	2	11	3	0.00	3.57
3	8	4	49.08	48.66	2	2	10	39.76	39.37	2	11	4	8.57	11.15
3	8	5	14.25	14.72	2	2	11	44.43	44.97	2	11	5	56.41	56.43
3	8	6	7.05	7.04	3	3	0	0.00	22.41	1	11	6	32.01	32.93
3	8	7	8.95	9.23	3	3	1	0.00	44.97	2	11	7	9.33	10.98
3	8	8	33.79	34.11	3	3	2	0.00	3.15	2	11	8	1.00	3.57
3	8	9	34.86	34.39	3	3	3	30.01	31.15	2	11	9	8.31	9.95
3	8	10	14.94	13.68	3	3	4	16.52	16.46	2	11	10	56.41	56.43
3	8	11	8.64	9.74	3	3	5	68.66	68.79	0	12	0	32.01	32.93
4	8	0	4.47	3.14	3	3	6	27.01	27.13	0	12	2	9.33	10.98
4	8	1	4.22	7.80	3	3	7	0.96	4.28	0	12	4	1.00	3.57
4	8	2	20.65	20.72	3	3	8	28.76	29.29	2	11	0	0.00	3.57
4	8	3	3.01	7.21	4	4	0	51.77	51.47	2	11	1	8.57	11.15
4	8	4	3.79	3.96	4	4	1	5.02	4.93	2	11	2	56.41	56.43
4	8	5	18.55	18.85	4	4	2	5.29	4.81	2	11	3	32.01	32.93
4	8	6	8.87	9.17	4	4	3	5.55	0.42	0	12	0	9.33	10.98
4	8	7	9.17	7.47	4	4	4	6.04	0.65	0	12	2	1.00	3.57
4	8	8	8.65	12.04	4	4	5	17.00	17.81	0	12	4	8.57	11.15
4	8	9	8.65	23.41	4	4	6	17.99	18.10	0	12	6	56.41	56.43
5	8	0	36.49	37.10	0	0	0	8.72	10.79	0	12	8	32.01	32.93
5	8	1	5.21	6.08	0	0	10	17.49	16.90	0	12	10	9.33	10.98
5	8	2	13.30	13.55	0	0	10	59.54	59.34	0	12	12	1.00	3.57

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	0	147.68	150.14	0	0	2	7.81	0.00	1	1	1	109.34	113.59
0	0	0	179.14	187.43	0	1	2	22.29	21.84	1	1	1	37.09	35.86
0	0	0	51.82	57.46	1	1	1	141.49	139.08	1	1	1	38.73	39.50
0	0	0	280.81	281.46	1	1	2	72.94	72.19	1	1	1	33.53	33.03
0	0	0	78.88	80.66	1	1	3	49.93	50.16	1	1	1	43.29	43.08
0	0	0	63.19	65.47	1	1	4	33.23	35.67	1	1	1	3.90	1.08
0	0	0	196.73	192.79	1	1	5	11.99	5.90	1	1	1	53.08	52.54
0	0	0	100.18	100.18	1	1	6	34.80	33.43	1	1	1	9.28	11.24
0	0	0	45.30	45.26	1	1	7	8.75	10.13	1	1	1	15.71	15.90
0	0	0	65.81	62.65	1	1	8	12.16	13.34	1	1	1	19.53	19.57
0	0	0	50.05	47.53	1	1	9	73.72	59.90	1	1	1	65.90	63.85
0	0	0	75.09	73.39	1	1	10	80.96	84.26	1	1	1	89.13	88.63
0	0	0	5.52	0.00	1	1	11	7.95	12.13	1	1	1	16.30	16.71
0	0	0	98.08	97.56	1	1	12	41.32	41.60	1	1	1	7.65	6.42
0	0	0	5.63	0.00	1	1	13	5.72	3.69	1	1	1	5.19	3.22
0	0	0	9.34	4.11	1	1	14	38.22	37.97	1	1	1	5.56	3.46
0	0	0	2.29	0.00	1	1	15	14.89	14.58	1	1	1	11.74	13.20
0	0	0	21.08	19.79	1	1	16	43.91	45.08	1	1	1	54.35	54.21
0	0	0	8.92	0.00	1	1	17	40.08	39.02	1	1	1	24.97	25.89
0	0	0	23.76	21.42	1	1	18	33.76	33.36	1	1	1	64.40	66.04
0	0	0	53.80	53.47	1	1	19	160.47	159.93	1	1	1	8.48	13.37
0	0	0	5.16	0.00	1	1	20	83.85	85.23	1	1	1	12.32	12.61
0	0	0	29.55	30.11	1	1	21	55.57	54.20	1	1	1	17.68	15.15
0	0	0	8.86	0.00	1	1	22	188.81	186.09	1	1	1	11.36	15.03
0	0	0	23.53	23.03	1	1	23	172.02	170.23	1	1	1	9.56	9.27
0	0	0	6.51	0.00	1	1	24	48.99	50.07	1	1	1	39.38	37.47
0	0	0	14.30	13.16	1	1	25	38.31	38.40	1	1	1	15.03	17.75
0	0	0	8.84	0.00	1	1	26	38.00	80.87	1	1	1	13.01	11.85
0	0	0	8.53	7.38	1	1	27	16.87	38.46	1	1	1	8.01	5.48
0	0	0	111.41	111.82	1	1	28	74.54	19.57	1	1	1	10.06	8.02
0	0	0	112.02	109.95	1	1	29	7.57	73.30	1	1	1	55.02	54.46
0	0	0	165.80	167.92	1	1	30	30.29	29.42	1	1	1	123.54	126.60
0	0	0	24.05	24.43	1	1	31	22.92	0.00	1	1	1	16.22	18.12
0	0	0	43.41	43.28	1	1	32	2.13	21.55	1	1	1	84.59	83.54
0	0	0	90.73	91.45	1	1	33	3.46	0.00	1	1	1	35.60	34.71
0	0	0	53.01	52.59	1	1	34	88.10	88.45	1	1	1	25.25	22.22
0	0	0	6.91	5.74	1	1	35	4.33	0.00	1	1	1	9.80	8.95
0	0	0	13.54	17.58	1	1	36	88.91	89.23	1	1	1	46.98	45.76
0	0	0	49.03	47.31	1	1	37	5.89	0.00	1	1	1	26.52	25.74
0	0	0	96.75	95.98	1	1	38	6.29	25.68	1	1	1	0.00	0.00
0	0	0	0.00	0.00	1	1	39	9.80	13.41	1	1	1	48.83	47.65
0	0	0	92.96	89.27	1	1	40	6.11	0.00	1	1	1	27.73	28.84
0	0	0	6.54	0.00	1	1	41	26.66	25.83	1	1	1	3.29	0.00
0	0	0	147.63	146.88	1	1	42	10.44	0.00	1	1	1	27.02	24.85
0	0	0	7.46	0.00	1	1	43	10.36	13.18	1	1	1	24.36	24.36
0	0	0	4.36	5.49	1	1	44	0.00	0.00	1	1	1	6.85	6.50
0	0	0	0.00	0.00	1	1	45	11.77	11.50	1	1	1	74.79	76.50
0	0	0	60.15	60.99	1	1	46	7.07	0.00	1	1	1	5.52	0.00
0	0	0	5.10	0.00	1	1	47	50.32	47.06	1	1	1	6.32	1.44
0	0	0	68.75	68.51	1	1	48	32.79	37.29	1	1	1	8.50	0.00
0	0	0	4.00	0.00	1	1	49	13.07	15.43	1	1	1	22.71	23.10
0	0	0	51.24	50.36	1	1	50	71.86	64.70	1	1	1	6.61	0.00
0	0	0	4.77	0.00	1	1	51	105.48	102.30	1	1	1	6.28	9.77
0	0	0	10.16	6.10	1	1	52	111.31	113.39	1	1	1	2.73	0.00
0	0	0	1.98	0.00	1	1	53	42.12	42.97	1	1	1	37.81	39.01
0	0	0	13.51	13.66	1	1	54	29.80	30.76	1	1	1	4.88	0.00
0	0	0	6.79	0.00	1	1	55	19.72	20.76	1	1	1	0.00	0.00
0	0	0	38.77	36.62	1	1	56	0.00	0.00	1	1	1	0.00	0.00

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	4	8	38.37	38.05	1	1	1	25.91	25.36	1	1	1	2.48	2.02
4	4	10	97.58	97.38	1	1	1	36.09	36.36	1	1	1	24.11	23.99
4	4	12	60.85	61.95	1	1	1	39.39	38.00	1	1	1	9.09	4.12
4	4	14	6.18	2.41	1	1	1	58.89	60.86	1	1	1	23.61	22.90
4	4	16	33.56	33.92	1	1	1	33.61	32.49	1	1	1	17.67	19.04
0	0	0	141.36	137.61	1	1	1	52.87	52.09	1	1	1	18.01	20.38
0	0	1	5.96	0.00	1	1	1	25.88	26.94	1	1	1	5.80	27.73
0	0	2	34.28	34.28	1	1	1	5.31	6.85	1	1	1	27.93	9.67
0	0	3	5.19	0.00	1	1	1	7.70	19.41	1	1	1	11.04	4.81
0	0	4	26.54	25.52	1	1	1	18.45	17.90	1	1	1	6.49	6.66
0	0	5	4.86	0.00	1	1	1	14.66	1.40	1	1	1	5.60	6.66
0	0	6	16.66	19.16	1	1	1	9.19	1.40	1	1	1	22.98	25.03
0	0	7	3.14	0.00	1	1	1	25.36	34.98	1	1	1	9.19	2.60
0	0	8	42.29	43.70	1	1	1	35.24	35.83	1	1	1	24.63	25.85
0	0	9	0.00	0.00	1	1	1	26.87	27.89	1	1	1	3.18	2.56
0	0	10	9.75	14.46	1	1	1	21.16	20.03	1	1	1	13.95	17.30
0	0	11	14.64	18.10	1	1	1	7.34	24.67	1	1	1	40.16	41.85
0	0	12	5.82	0.00	1	1	1	24.09	24.67	1	1	1	36.05	35.08
0	0	13	8.61	0.00	1	1	1	49.60	50.10	1	1	1	22.79	43.50
0	0	14	47.51	47.63	1	1	1	10.69	15.17	1	1	1	0.00	22.80
0	0	15	3.68	0.00	1	1	1	8.97	8.31	1	1	1	34.05	33.98
0	0	16	19.34	22.47	1	1	1	42.17	42.11	1	1	1	8.39	11.57
0	0	17	7.24	0.00	1	1	1	21.70	21.99	1	1	1	6.30	3.26
0	0	18	10.33	6.19	1	1	1	7.62	4.76	1	1	1	8.79	7.27
1	1	0	4.39	2.40	1	1	1	34.31	34.32	1	1	1	31.54	31.60
1	1	1	63.67	62.71	1	1	1	46.62	48.58	1	1	1	35.36	37.41
1	1	2	49.74	49.53	1	1	1	21.66	22.64	1	1	1	14.73	19.30
1	1	3	63.72	63.95	1	1	1	22.10	24.66	1	1	1	5.96	2.02
1	1	4	59.71	59.52	1	1	1	7.09	1.68	1	1	1	24.88	26.23
1	1	5	10.96	15.15	1	1	1	22.09	24.04	1	1	1	4.09	1.03
1	1	6	1.54	0.98	1	1	1	5.94	2.76	1	1	1	14.41	19.83
1	1	7	8.62	10.83	1	1	1	18.84	21.23	1	1	1	18.36	19.20
1	1	8	51.89	52.89	1	1	1	44.75	45.01	1	1	1	37.86	37.35
1	1	9	65.16	65.93	1	1	1	40.71	40.23	1	1	1	36.40	37.09
1	1	10	31.77	32.49	1	1	1	10.63	8.27	1	1	1	19.99	20.55
1	1	11	29.08	29.75	1	1	1	23.48	23.01	1	1	1	39.47	40.22
1	1	12	44.64	45.29	1	1	1	8.23	4.33	1	1	1	35.08	35.97
1	1	13	7.29	9.12	1	1	1	9.63	10.35	1	1	1	40.63	40.44
1	1	14	36.21	35.62	1	1	1	17.48	20.55	1	1	1	23.95	26.32
1	1	15	25.80	24.85	1	1	1	39.85	37.78	1	1	1	8.15	0.44
1	1	16	20.54	24.79	1	1	1	53.72	52.01	1	1	1	43.17	43.69
1	1	17	169.99	169.78	1	1	1	6.65	0.00	1	1	1	25.96	25.76
2	2	0	81.56	80.71	1	1	1	150.41	148.43	1	1	1	23.17	22.55
2	2	1	27.45	26.96	1	1	1	4.31	0.00	1	1	1	11.51	11.00
2	2	2	54.74	55.98	1	1	1	136.91	137.70	1	1	1	11.96	19.10
2	2	3	69.47	71.47	1	1	1	3.56	0.00	1	1	1	29.49	30.61
2	2	4	36.77	35.50	1	1	1	4.78	33.88	1	1	1	7.41	7.19
2	2	5	91.50	89.74	1	1	1	7.37	0.00	1	1	1	17.96	19.75
2	2	6	26.85	28.24	1	1	1	3.59	15.45	1	1	1	23.59	23.05
2	2	7	98.99	100.06	1	1	1	93.90	92.26	1	1	1	45.10	45.28
2	2	8	42.12	41.29	1	1	1	7.43	0.00	1	1	1	4.66	1.65
2	2	9	31.90	30.77	1	1	1	83.86	84.60	1	1	1	25.88	28.21
2	2	10	16.96	19.24	1	1	1	8.23	0.00	1	1	1	12.20	14.91
2	2	11	5.91	1.86	1	1	1	53.17	55.61	1	1	1	62.45	62.88
2	2	12	26.80	26.62	1	1	1	0.00	0.00	1	1	1	9.47	1.97
2	2	13	79.68	78.87	1	1	1	48.69	47.25	1	1	1	32.65	32.47
2	2	14	10.77	11.13	1	1	1	10.55	0.00	1	1	1	48.23	49.43
2	2	15	12.07	14.81	1	1	1	57.64	56.96	1	1	1	10.22	13.75
2	2	16	19.99	22.61	1	1	1			1	1	1		

H K L F(OBS) F(CALC) H K L F(OBS) F(CALC) H K L F(OBS) F(CALC)

0	11	7	6.99	LR	0.00
0	11	8	0.00	LR	3.92
1	11	0	3.42	LR	0.75
1	11	1	35.99		35.66
1	11	2	20.58		22.40
1	11	3	18.03	LR	20.68
1	11	4	30.47		30.08
1	11	5	58.08		57.45
1	11	6	11.65	LR	3.44
2	11	0	9.81	LR	7.45
2	11	1	8.23	LR	4.48
2	11	2	22.42		24.41
0	12	0	53.56		53.87
0	12	1	0.00	LR	0.00
0	12	2	36.30		36.52
0	12	3	8.35	LR	0.00
0	12	4	14.08	LR	19.58

OSUMILITE NICKENICH (EIFEL) FROM NAT.HIST. MUSEUM BERN

STRUCTURE FACTORS

PAGE 1

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	0	122.27	120.28	1	2	19	36.55	36.14	3	3	3	122.01	120.75	3	3	3	9.60	7.96
0	0	0	212.85	217.49	1	2	0	134.22	135.52	1	2	4	36.32	34.96	1	2	4	16.40	16.68
0	0	0	27.65	34.13	2	2	2	62.24	63.92	3	3	3	109.16	107.80	3	3	3	5.37	4.10
0	0	0	270.22	267.36	2	2	4	35.86	34.67	3	3	6	7.70	9.03	3	3	6	71.13	71.52
0	0	0	98.85	99.58	2	2	6	169.01	167.32	3	3	8	35.66	35.71	3	3	8	31.08	31.59
0	0	0	44.72	48.33	2	2	8	153.95	154.64	3	3	10	72.89	71.87	3	3	10	18.49	19.25
0	0	0	187.77	186.71	2	2	10	35.81	37.43	3	3	12	23.59	23.58	3	3	12	48.47	49.39
0	0	0	92.55	95.52	2	2	12	25.97	25.34	3	3	14	37.33	36.67	3	3	14	59.74	61.88
0	0	0	61.04	60.23	2	2	14	71.15	69.90	3	3	16	0.00	3.29	3	3	16	4.66	4.11
0	0	0	58.42	54.17	2	2	16	29.59	29.68	3	3	18	40.54	39.01	3	3	18	22.07	23.02
0	0	0	19.96	18.26	2	2	18	12.59	12.59	3	3	20	0.94	4.74	3	3	20	0.00	1.27
0	0	0	49.07	48.08	2	2	20	46.74	46.11	3	3	22	67.69	67.91	3	3	22	9.32	7.98
0	0	0	79.48	77.06	0	0	2	2.56	0.20	0	0	4	44.91	47.10	0	0	4	0.00	2.17
0	0	0	25.58	22.52	0	0	4	0.00	1.03	0	0	6	44.23	43.70	0	0	6	0.00	2.15
0	0	0	38.75	37.51	0	0	6	70.54	69.91	0	0	8	39.90	41.10	0	0	8	0.00	6.87
0	0	0	10.24	8.89	0	0	8	72.55	71.83	0	0	10	87.59	90.25	0	0	10	5.34	6.87
0	0	0	45.96	45.80	0	0	10	0.00	3.06	0	0	12	11.61	10.83	0	0	12	0.00	5.55
0	0	0	21.75	22.78	0	0	12	4.03	3.87	0	0	14	14.96	13.86	0	0	14	27.99	29.01
0	0	0	14.52	15.17	0	0	14	16.21	15.26	0	0	16	20.50	20.06	0	0	16	64.70	66.71
0	0	0	7.64	6.91	0	0	16	3.93	2.86	0	0	18	47.73	48.60	0	0	18	141.57	142.13
0	0	0	0.00	141.10	0	0	18	0.00	1.87	0	0	20	69.24	66.30	0	0	20	44.51	46.75
1	1	1	139.19	141.10	1	1	0	69.68	67.25	1	1	4	87.77	87.39	1	1	4	28.41	26.92
1	1	1	85.74	82.73	1	1	1	34.64	39.33	1	1	2	41.50	40.28	1	1	2	91.62	89.89
1	1	1	141.86	141.94	1	1	2	4.03	3.06	1	1	4	7.03	8.44	1	1	4	54.96	55.02
1	1	1	3.97	0.65	1	1	4	71.15	64.65	1	1	6	44.93	45.42	1	1	6	10.92	9.11
1	1	1	64.74	65.08	1	1	6	87.57	85.82	1	1	8	27.19	27.98	1	1	8	27.15	26.58
1	1	1	77.84	77.04	1	1	8	114.61	114.02	1	1	10	47.52	48.65	1	1	10	130.58	128.89
1	1	1	41.23	39.62	1	1	10	27.11	26.46	1	1	12	0.00	0.07	0	0	12	20.48	20.50
1	1	1	21.32	21.09	1	1	12	30.70	29.96	1	1	14	0.00	0.00	0	0	14	40.08	40.50
1	1	1	6.52	3.59	1	1	14	1.64	5.32	1	1	16	72.95	74.23	1	1	16	9.41	8.47
1	1	1	39.15	39.13	1	1	16	114.89	117.24	1	1	18	18.87	18.31	1	1	18	36.57	35.58
1	1	1	115.78	113.74	1	1	18	26.71	25.10	1	1	20	2.18	3.44	1	1	20	27.86	27.56
0	0	0	169.80	169.68	1	1	20	39.73	40.51	1	1	22	30.53	31.33	1	1	22	10.41	9.94
0	0	0	17.53	13.71	1	1	22	25.21	25.07	1	1	24	11.73	10.89	1	1	24	46.56	47.12
0	0	0	48.09	46.64	1	1	24	46.03	45.60	1	1	26	0.00	0.00	1	1	26	19.21	20.22
0	0	0	82.96	83.39	1	1	26	5.85	9.62	1	1	28	4.28	6.39	1	1	28	16.09	14.43
0	0	0	64.44	64.61	1	1	28	54.56	54.66	1	1	30	23.95	24.04	1	1	30	13.37	13.47
0	0	0	2.50	3.87	1	1	30	0.00	4.01	1	1	32	12.43	12.04	1	1	32	67.04	66.96
0	0	0	22.58	21.63	1	1	32	15.90	17.51	1	1	34	12.88	11.57	1	1	34	49.84	49.44
0	0	0	46.22	45.83	1	1	34	16.73	15.98	1	1	36	92.05	91.79	1	1	36	50.03	51.29
0	0	0	41.38	41.45	1	1	36	68.71	69.81	1	1	38	26.21	26.91	1	1	38	50.25	50.10
0	0	0	142.65	141.41	1	1	38	69.73	69.41	1	1	40	4.33	3.78	1	1	40	58.55	59.30
0	0	0	50.87	50.10	1	1	40	20.79	19.27	1	1	42	27.83	28.98	1	1	42	27.35	28.47
0	0	0	51.68	53.05	1	1	42	11.76	10.75	1	1	44	33.66	33.09	1	1	44	0.00	0.55
0	0	0	12.37	13.72	1	1	44	3.46	1.53	1	1	46	33.66	33.64	1	1	46	21.59	23.17
0	0	0	11.81	16.11	1	1	46	12.86	13.63	1	1	48	61.40	63.64	1	1	48	52.15	51.93
0	0	0	18.85	16.88	1	1	48	43.29	43.24	1	1	50	58.40	58.76	1	1	50	59.72	58.95
0	0	0	3.83	11.85	1	1	50	26.56	26.91	1	1	52	74.55	76.12	1	1	52	32.32	32.57
0	0	0	3.04	11.75	1	1	52	51.96	54.63	1	1	54	36.01	36.28	1	1	54	22.03	22.03
0	0	0	58.79	60.35	1	1	54	15.90	15.34	1	1	56	14.26	15.01	1	1	56	46.39	46.36
0	0	0	63.71	65.05	1	1	56	24.27	24.61	1	1	58	4.07	5.06	1	1	58	17.06	17.05
0	0	0	82.89	86.36	1	1	58	21.24	21.88	1	1	60	29.35	30.57	1	1	60	37.22	37.28
0	0	0	0.00	1.07	1	1	60	0.00	2.72	1	1	62	31.11	31.00	1	1	62	20.39	19.90
0	0	0	41.86	43.09	1	1	62	7.75	7.22	1	1	64	36.98	37.77	1	1	64	25.19	25.96
0	0	0	40.10	40.29	1	1	64	19.99	20.19	1	1	66	17.22	17.47	1	1	66	82.86	83.54
0	0	0	9.96	8.84	1	1	66	4.78	3.16	1	1	68	9.94	6.82	1	1	68	0.00	4.80
0	0	0	46.88	48.20	1	1	68	0.00	5.85	1	1	70	26.32	26.66	1	1	70	54.41	56.24
0	0	0	34.73	35.30	1	1	70	16.35	14.95	1	1	72	28.59	28.20	1	1	72	37.41	37.20
0	0	0			1	1	72			1	1	74			1	1	74	75.75	74.91

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	2	28.73	29.89	2	2	2	45.03	44.66	2	7	9	9.31	9.68
2	2	2	86.40	88.44	4	4	6	55.17	55.10	2	7	10	29.70	29.87
2	2	2	42.20	43.55	4	4	6	0.00 LR	3.04	2	7	11	0.00	1.75
2	2	2	50.88	50.35	4	4	6	16.94 LR	16.31	2	7	12	1.72	3.16
2	2	2	19.22	20.00	4	4	6	0.00 LR	3.66	2	7	13	18.63	17.40
2	2	2	17.11	17.27	4	4	6	12.19	40.03	2	7	14	38.00	37.99
2	2	2	27.82	27.44	4	4	6	21.41	34.77	3	3	7	16.94	17.10
2	2	2	72.01	72.05	4	4	6	10.41	39.73	3	3	7	37.81	37.99
2	2	2	12.05	12.05	5	5	6	0.00 LR	9.44	3	3	7	16.74	17.01
2	2	2	6.43	4.68	5	5	6	17.98	13.91	3	3	7	26.49	26.59
2	2	2	24.66	24.63	5	5	6	11.16	15.92	3	3	7	28.59	28.66
2	2	2	13.86	13.14	5	5	6	0.00 LR	16.32	3	3	7	9.03	9.04
2	2	2	36.98	37.96	5	5	6	6.91	13.94	3	3	7	10.61	11.12
2	2	2	24.75	25.22	5	5	6	20.17	27.77	3	3	7	6.38	2.94
2	2	2	62.11	63.11	5	5	6	0.00 LR	1.99	3	3	7	6.10	9.92
2	2	2	51.48	54.28	5	5	6	0.00 LR	6.17	3	3	7	16.03	16.07
2	2	2	17.12	17.12	5	5	6	18.83	18.72	3	3	7	33.25	33.92
2	2	2	4.09	4.09	5	5	6	17.44	17.51	3	3	7	37.74	37.90
2	2	2	2.39	2.72	5	5	6	6.97 LR	7.13	3	3	7	0.94	3.68
2	2	2	21.72	20.72	5	5	6	6.42 LR	7.91	3	3	7	20.84	20.87
2	2	2	9.85	8.66	6	6	6	75.01	76.50	4	4	7	20.66	21.43
2	2	2	2.77	2.13	6	6	6	41.59	41.91	4	4	7	23.79	23.76
2	2	2	20.59	19.61	6	6	6	28.58	29.11	4	4	7	21.54	22.59
2	2	2	36.05	37.36	6	6	6	13.95	14.19	4	4	7	0.00	2.90
2	2	2	22.86	22.79	6	6	6	43.96	43.57	4	4	7	0.00	4.28
2	2	2	20.29	21.11	6	6	6	30.09	31.70	4	4	7	54.93	54.26
2	2	2	0.00	5.36	6	6	6	89.34	91.85	4	4	7	18.42	18.95
2	2	2	12.85	13.09	6	6	6	32.84	33.85	4	4	7	0.00	3.07
2	2	2	53.52	52.65	6	6	6	76.69	79.14	4	4	7	2.02	1.87
2	2	2	10.13	10.51	6	6	6	42.55	40.83	4	4	7	45.95	45.17
2	2	2	15.30	15.11	6	6	6	30.37	29.78	4	4	7	0.00	3.21
2	2	2	0.00	45.05	6	6	6	13.50	12.37	4	4	7	6.35	7.06
2	2	2	16.08	15.09	6	6	6	16.10	16.94	4	4	7	9.59	9.77
2	2	2	44.71	45.05	6	6	6	57.84	58.16	5	5	7	34.60	36.25
2	2	2	5.00	5.92	6	6	6	6.45 LR	4.89	5	5	7	8.69	9.65
2	2	2	26.33	26.06	6	6	6	17.31	17.90	5	5	7	0.00	0.85
2	2	2	52.94	52.94	6	6	6	32.07	31.95	5	5	7	21.67	20.61
2	2	2	18.44	18.53	6	6	6	10.40	10.35	5	5	7	9.77	8.98
2	2	2	25.69	25.84	6	6	6	8.10	8.39	5	5	7	0.00	2.23
2	2	2	6.63	5.14	6	6	6	38.78	38.90	5	5	7	32.30	32.76
2	2	2	25.50	24.93	6	6	6	25.19	25.53	5	5	7	6.91	6.67
2	2	2	1.81	3.02	6	6	6	7.84	7.62	5	5	7	31.09	31.48
2	2	2	23.95	23.63	6	6	6	14.32	14.89	5	5	7	0.00	6.37
2	2	2	34.83	35.32	6	6	6	10.69	11.11	5	5	7	12.24	11.88
2	2	2	28.55	28.82	6	6	6	29.49	30.12	6	6	7	39.59	39.33
2	2	2	0.00	6.61	6	6	6	30.13	29.99	6	6	7	9.05	9.19
2	2	2	11.71	12.02	6	6	6	3.19 LR	1.10	6	6	7	17.25	17.52
2	2	2	10.36	9.71	6	6	6	11.04	10.77	6	6	7	5.51	2.66
2	2	2	6.45	6.13	6	6	6	15.59 LR	17.40	6	6	7	60.58	59.76
2	2	2	8.47	9.02	6	6	6	17.77 LR	17.89	6	6	7	13.85	14.04
2	2	2	36.50	35.35	6	6	6	45.92 LR	44.87	6	6	7	30.45	30.90
2	2	2	135.95	136.80	6	6	6	20.50	20.97	6	6	7	4.62	1.64
2	2	2	124.67	125.88	6	6	6	6.51	5.59	7	7	7	37.87	36.46
2	2	2	17.72	18.00	6	6	6	46.63	47.74	7	7	7	2.46	9.82
2	2	2	30.10	32.11	6	6	6	18.73	18.42	7	7	7	141.14	141.71
2	2	2	86.28	86.01	6	6	6	3.98 LR	3.78	7	7	7	36.43	35.99
2	2	2	79.05	80.08	6	6	6	43.82 LR	42.90	7	7	7	51.16	50.52
2	2	2	46.96	48.00	6	6	6	33.17	33.29	7	7	7	56.57	55.46

H K L F(OBS) F(CALC) H K L F(OBS) F(CALC) H K L F(OBS) F(CALC)

0	8	12	27.88	28.04	5	8	5	6.12	LR	0.58	0	10	10	36.08	35.64
0	8	14	92.49	92.23	5	8	6	3.44	LR	0.72	1	10	10	9.99	9.33
1	8	0	3.15	3.46	5	8	7	0.00	LR	1.74	1	10	1	45.28	43.38
1	8	1	35.26	34.77	6	8	0	14.86		14.54	1	10	2	22.11	22.24
1	8	2	16.75	16.84	6	8	1	9.41		9.64	1	10	3	33.48	33.25
1	8	3	9.11	9.32	6	8	2	27.36		26.42	1	10	4	16.25	18.25
1	8	4	41.43	41.47	0	9	0	57.76		58.43	1	10	5	15.33	15.17
1	8	5	55.86	55.13	0	9	2	0.00	LR	3.80	1	10	6	12.02	11.94
1	8	6	17.57	17.30	0	9	4	31.54		31.24	1	10	7	17.26	16.91
1	8	7	6.34	4.69	0	9	6	60.61		59.44	1	10	8	11.23	10.27
1	8	8	0.00	0.29	0	9	8	44.92		44.17	1	10	9	20.15	20.21
1	8	9	48.81	48.47	0	9	10	30.40		29.21	1	10	10	16.13	17.32
1	8	10	26.96	25.89	0	9	12	7.60		7.70	2	10	0	13.88	13.87
1	8	11	5.51	2.87	1	9	0	38.51		38.62	2	10	1	18.43	18.84
1	8	12	21.63	21.85	1	9	1	0.00	LR	0.18	2	10	2	12.36	12.82
1	8	13	20.39	20.91	1	9	2	0.00	LR	4.61	2	10	3	3.44	8.07
1	8	14	11.89	12.52	1	9	3	10.84		11.15	2	10	4	1.73	4.38
2	8	0	19.21	17.63	1	9	4	14.81		15.19	2	10	5	19.81	19.93
2	8	1	12.98	12.59	1	9	5	2.69	LR	3.71	2	10	6	29.55	29.39
2	8	2	48.18	48.16	1	9	6	38.15		38.86	0	10	7	0.00	2.69
2	8	3	19.62	19.88	1	9	7	15.05		16.12	2	10	8	28.73	28.40
2	8	4	74.07	74.93	1	9	8	30.29		30.26	3	10	0	9.57	9.92
2	8	5	25.34	26.09	1	9	9	0.00	LR	4.18	3	10	1	34.29	33.01
2	8	6	34.21	35.68	1	9	10	13.61		13.18	3	10	2	0.00	0.40
2	8	7	6.43	6.59	1	9	11	17.99		17.44	3	10	3	32.59	32.39
2	8	8	32.69	33.29	1	9	12	0.00	LR	0.45	3	10	4	23.40	22.86
2	8	9	11.14	11.91	2	9	0	11.70		11.42	3	10	5	21.66	21.95
2	8	10	54.05	54.09	2	9	1	12.93		12.60	0	11	0	11.54	11.35
2	8	11	0.00	4.10	2	9	2	3.90	LR	1.14	0	11	2	16.05	16.10
2	8	12	36.91	36.65	2	9	3	6.30	LR	6.03	0	11	4	33.49	32.87
2	8	13	18.12	19.10	2	9	4	1.60	LR	0.74	0	11	6	24.38	24.45
2	8	14	10.65	9.90	2	9	5	0.00	LR	1.35	0	11	8	16.15	14.26
3	8	0	32.50	32.54	2	9	6	19.11		19.55	1	11	0	1.79	7.26
3	8	1	22.27	22.41	2	9	7	0.00	LR	5.78	1	11	1	40.90	38.67
3	8	2	30.07	30.14	2	9	8	14.32		14.61	1	11	2	16.20	16.25
3	8	3	28.00	27.99	2	9	9	0.00	LR	6.35	1	11	3	23.29	22.66
3	8	4	48.70	48.70	2	9	10	0.00	LR	3.96	1	11	4	26.08	26.41
3	8	5	11.17	11.45	2	9	11	21.25		20.95	1	11	5	62.51	63.00
3	8	6	6.56	6.58	3	9	0	35.71		34.24	1	11	6	4.16	3.23
3	8	7	4.55	5.84	3	9	1	43.27	LR	44.34	2	11	0	5.17	7.53
3	8	8	32.44	34.15	3	9	2	5.43	LR	0.19	2	11	1	2.92	3.81
3	8	9	34.80	34.52	3	9	3	30.43		30.45	2	11	2	10.13	11.22
3	8	10	14.22	12.86	3	9	4	17.90		18.37	2	11	3	9.59	9.77
3	8	11	11.97	10.53	3	9	5	65.51		65.36	2	11	0	54.09	52.28
3	8	12	6.19	5.76	3	9	6	24.58		24.15	0	12	0	29.94	31.20
4	8	0	8.84	9.64	3	9	7	4.53	LR	4.86	0	12	2	8.46	9.70
4	8	1	18.29	18.13	3	9	8	26.16		26.33	0	12	4		
4	8	2	0.00	5.60	3	9	9	50.48		49.45					
4	8	3	37.15	37.23	4	9	0	3.77	LR	3.12					
4	8	4	5.83	5.99	4	9	1	4.66	LR	3.58					
4	8	5	14.83	15.55	4	9	2	3.39	LR	5.01					
4	8	6	7.40	7.16	4	9	3	0.00	LR	0.76					
4	8	7	0.00	6.02	4	9	4	0.00	LR	0.58					
4	8	8	13.05	13.65	4	9	5	17.68		17.98					
4	8	9	21.87	20.74	4	9	6	18.63		18.48					
4	5	10	36.99	36.88	0	10	0	15.56		15.06					
5	8	0	7.68	6.27	0	10	2	14.28		14.23					
5	8	1	11.31	12.65	0	10	4	55.35		56.06					
5	8	2	3.30	5.05	0	10	6	0.00	LR	3.69					
5	8	3	45.94	44.75	0	10	8	15.87		14.95					

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	2	146.58	145.96	1	2	19	36.02	36.08	3	3	0	105.01	102.99
0	0	4	185.16	192.31	2	2	0	154.96	156.84	3	3	2	56.32	53.95
0	0	6	50.61	59.10	2	2	2	87.13	87.51	3	3	4	123.86	123.58
0	0	8	279.85	285.83	2	2	4	56.41	53.34	3	3	6	24.53	25.71
0	0	10	85.72	88.84	2	2	6	185.77	182.90	3	3	8	22.26	21.76
0	0	12	56.39	58.62	2	2	8	170.37	168.89	3	3	10	35.25	35.41
0	0	14	199.84	200.21	2	2	10	53.99	54.64	3	3	12	83.76	84.47
0	0	16	104.18	107.41	2	2	12	38.38	38.14	3	3	14	27.45	26.73
0	0	18	51.63	51.38	2	2	14	81.08	79.48	3	3	16	5.95	4.48
0	0	20	65.73	62.60	2	2	16	38.84	38.71	3	3	18	47.01	46.34
0	1	0	30.31	28.83	2	2	18	21.61	21.83	3	3	0	18.13	17.52
0	1	2	63.97	62.10	3	3	0	74.95	76.54	4	4	2	55.75	55.02
0	1	4	94.42	91.65	3	3	2	20.24	20.78	4	4	4	34.35	34.26
0	1	6	14.15	12.56	3	3	4	20.15	19.78	4	4	6	42.09	40.12
0	1	8	30.01	29.51	3	3	6	89.43	89.40	4	4	8	35.69	34.92
0	1	10	19.33	17.72	3	3	8	90.76	90.39	4	4	10	79.80	80.65
0	1	12	51.96	52.27	3	3	10	13.25	13.05	4	4	12	3.13	3.94
0	1	14	26.38	26.98	3	3	12	10.73	9.88	4	4	14	15.95	15.80
0	1	16	19.69	20.12	3	3	14	29.27	28.74	4	4	16	15.30	14.93
0	1	18	12.59	12.49	3	3	16	11.60	11.73	4	4	18	42.60	43.37
0	1	20	8.35	6.95	3	3	18	2.35	2.94	4	4	0	89.10	87.99
1	1	0	118.09	119.08	1	1	0	59.53	57.34	1	1	0	83.23	82.20
1	1	2	111.52	108.68	1	1	2	37.46	41.73	1	1	2	63.93	62.13
1	1	4	165.32	167.37	1	1	4	9.70	9.56	1	1	4	2.00	6.03
1	1	6	24.97	23.61	1	1	6	71.12	63.12	1	1	6	64.77	64.54
1	1	8	47.12	46.17	1	1	8	99.61	96.55	1	1	8	57.08	55.97
1	1	10	93.93	94.37	1	1	10	113.50	114.65	1	1	10	14.25	14.33
1	1	12	52.68	51.77	1	1	12	32.11	32.01	1	1	12	48.42	48.04
1	1	14	14.21	12.13	1	1	14	29.46	29.19	1	1	14	12.14	12.08
1	1	16	49.37	48.83	1	1	16	10.77	10.72	1	1	16	69.87	71.38
1	1	18	79.50	81.60	1	1	18	116.05	117.17	1	1	18	32.13	31.40
0	2	0	104.50	100.45	1	1	0	42.06	42.38	1	1	0	5.47	6.44
0	2	2	159.72	157.51	1	1	2	32.57	31.94	1	1	2	41.71	43.01
0	2	4	0.00	0.78	1	1	4	46.59	45.22	1	1	4	9.54	9.71
0	2	6	57.98	57.16	1	1	6	4.57	5.68	1	1	6	12.21	13.10
0	2	8	77.09	75.10	1	1	8	56.97	57.41	1	1	8	8.18	8.52
0	2	10	59.76	59.43	1	1	10	18.45	17.78	1	1	10	34.09	33.84
0	2	12	3.23	1.69	1	1	12	8.26	8.63	1	1	12	11.24	11.17
0	2	14	17.74	17.37	1	1	14	21.24	20.77	1	1	14	20.49	19.66
0	2	16	43.04	42.04	1	1	16	71.21	72.13	1	1	16	81.07	80.70
0	2	18	23.53	24.80	1	1	18	76.32	76.04	1	1	18	31.61	32.35
1	1	0	142.34	141.56	2	2	0	23.87	23.38	2	2	0	6.47	6.12
1	1	2	61.08	59.78	2	2	2	0.00	0.68	2	2	2	26.88	28.16
1	1	4	20.08	22.36	2	2	4	4.34	2.45	2	2	4	69.24	69.59
1	1	6	14.46	8.59	2	2	6	10.06	2.93	2	2	6	50.85	50.70
1	1	8	30.25	28.33	2	2	8	51.98	51.73	2	2	8	6.47	5.20
1	1	10	13.67	11.18	2	2	10	28.28	29.15	2	2	10	69.37	69.87
1	1	12	59.23	12.82	2	2	12	59.44	60.03	2	2	12	44.22	43.25
1	1	14	67.91	59.98	2	2	14	13.42	13.46	2	2	14	19.17	20.13
1	1	16	85.31	87.07	2	2	16	16.72	16.94	2	2	16	4.17	6.07
1	1	18	7.55	7.17	2	2	18	19.76	19.50	2	2	18	24.96	25.20
1	1	20	43.99	43.45	2	2	20	13.99	13.85	2	2	20	33.22	32.89
1	1	22	5.17	5.50	2	2	22	8.20	8.26	2	2	22	32.58	28.39
1	1	24	40.12	39.74	2	2	24	39.43	38.51	2	2	24	27.93	28.39
1	1	26	14.41	13.69	2	2	26	20.02	20.12	2	2	26	13.76	13.92
1	1	28	45.94	48.01	2	2	28	10.34	10.43	2	2	28	7.62	7.93
1	1	30	37.61	37.79	2	2	30	5.07	5.15	2	2	30	14.57	13.92
1	1	32	17.14	17.14	2	2	32	11.03	10.87	2	2	32	36.60	37.15
1	1	34	82.87	82.87	2	2	34	1.03	1.03	2	2	34	21.51	20.85
1	1	36	92.17	92.17	2	2	36	1.03	1.03	2	2	36	2.85	2.85

F(CALC)		F(CALC)		F(CALC)		F(CALC)		F(CALC)					
H	K	L	F(OBS)	H	K	L	F(OBS)	H	K				
2	2	7	29.68	4	4	6	58.09	2	2	7	10	22.83	
		8	102.55			10	3.71 LR			11	0.00 LR		
		9	41.19			11	17.05 LR			12	17.76 LR		
		10	43.35			12	0.00 LR			13	18.54 LR		
		11	18.41			13	41.41 LR			14	42.93 LR		
		12	25.33			14	30.74 LR			15	3.06 LR		
		13	81.85			15	42.27 LR			16	5.03 LR		
		14	9.28			16	10.08 LR			17	34.57 LR		
		15	11.16			17	20.57 LR			18	20.98 LR		
		16	23.78			18	9.30 LR			19	23.73 LR		
		17	21.79			19	16.07 LR			20	27.80 LR		
		18	34.40			20	3.38 LR			21	9.20 LR		
		19	30.88			21	8.66 LR			22	18.16 LR		
		20	37.35			22	29.29 LR			23	4.93 LR		
		21	28.54			23	3.83 LR			24	15.52 LR		
		22	55.14			24	9.41 LR			25	16.40 LR		
		23	21.56			25	18.94 LR			26	34.11 LR		
		24	2.15			26	10.22 LR			27	36.13 LR		
		25	3.20			27	8.32 LR			28	8.07 LR		
		26	22.64			28	12.15 LR			29	20.74 LR		
		27	12.30			29	77.47 LR			30	27.55 LR		
		28	1.46			30	49.37 LR			31	20.45 LR		
		29	36.91			31	44.10 LR			32	31.79 LR		
		30	27.24			32	24.03 LR			33	4.15 LR		
		31	21.11			33	52.87 LR			34	15.54 LR		
		32	9.38			34	41.79 LR			35	49.11 LR		
		33	20.98			35	104.53 LR			36	26.28 LR		
		34	49.94			36	39.10 LR			37	3.76 LR		
		35	18.73			37	73.93 LR			38	9.47 LR		
		36	10.56			38	39.74 LR			39	41.27 LR		
		37	8.12			39	10.24 LR			40	12.02 LR		
		38	44.29			40	11.52 LR			41	8.50 LR		
		39	20.30			41	64.18 LR			42	16.75 LR		
		40	6.59			42	9.90 LR			43	40.45 LR		
		41	29.81			43	7.03 LR			44	13.44 LR		
		42	52.81			44	31.95 LR			45	4.39 LR		
		43	23.86			45	21.77 LR			46	6.65 LR		
		44	0.82			46	6.51 LR			47	0.00 LR		
		45	2.70			47	52.85 LR			48	40.35 LR		
		46	20.40			48	22.77 LR			49	8.15 LR		
		47	58.36			49	20.94 LR			50	37.95 LR		
		48	39.47			50	14.34 LR			51	2.44 LR		
		49	3.10			51	23.54 LR			52	10.95 LR		
		50	26.40			52	30.14 LR			53	33.22 LR		
		51	4.56			53	40.93 LR			54	4.32 LR		
		52	2.81			54	19.19 LR			55	22.02 LR		
		53	17.79			55	6.82 LR			56	4.45 LR		
		54	51.82			56	11.67 LR			57	63.32 LR		
		55	47.61			57	0.00 LR			58	8.02 LR		
		56	149.19			58	49.17 LR			59	25.30 LR		
		57	141.34			59	19.25 LR			60	2.16 LR		
		58	34.56			60	3.97 LR			61	21.51 LR		
		59	17.03			61	46.81 LR			62	52.76 LR		
		60	98.96			62	11.34 LR			63	125.32 LR		
		61	87.21			63	5.26 LR			64	19.33 LR		
		62	53.32			64	47.70 LR			65	32.79 LR		
		63	47.37			65	2.30 LR			66	60.34 LR		
		64	46.65			66	7.61 LR			67	30.33 LR		
		65	46.65			67				68			
		66	46.65			68				69			

H K L F(OBS) F(CALC) H K L F(OBS) F(CALC) H K L F(OBS) F(CALC)

0	8	10	54.42	52.72	5	8	5	51.89	52.59	0	10	0	13.91	14.13
0	8	12	26.57	26.34	5	8	5	0.00 LR	0.80	0	10	2	8.56	9.11
0	8	14	83.92	83.88	5	8	6	6.91 LR	7.25	0	10	4	50.58	50.08
1	8	0	9.80	8.75	5	8	7	4.70 LR	1.42	0	10	6	0.00 LR	2.42
1	8	1	40.19	40.38	6	8	0	12.26	12.43	0	10	8	14.02	14.13
1	8	2	22.86	22.68	6	8	1	8.18	6.45	0	10	10	31.90	31.59
1	8	3	12.75	13.31	6	8	2	12.17	11.65	1	10	0	14.26	14.31
1	8	4	48.89	47.01	6	8	3	21.99	21.65	1	10	1	40.62	40.85
1	8	5	60.49	60.24	0	9	0	71.55	72.98	1	10	2	32.37	32.54
1	8	6	13.36	13.44	0	9	2	14.70	14.32	1	10	3	33.16	32.86
1	8	7	3.18 LR	4.80	0	9	4	22.97	23.16	1	10	4	31.06	30.46
1	8	8	5.25	4.70	0	9	6	65.46	65.14	1	10	5	12.79	12.58
1	8	9	52.83	52.77	0	9	8	51.39	51.01	1	10	6	7.78	6.19
1	8	10	31.53	31.11	0	9	10	23.41	22.59	1	10	7	16.53	17.03
1	8	11	6.82	6.11	0	9	12	4.37 LR	2.16	1	10	8	4.26 LR	4.57
1	8	12	26.36	25.65	1	9	0	43.01 LR	43.18	1	10	9	18.83	17.54
1	8	13	23.83	24.84	1	9	1	3.80 LR	2.54	1	10	10	27.76	28.15
1	8	14	9.75	9.42	1	9	2	11.03	10.98	2	10	0	3.66 LR	2.97
2	8	0	33.26	33.78	1	9	3	10.80	10.87	2	10	1	17.60	17.66
2	8	1	13.31	13.11	1	9	4	9.09	7.63	2	10	2	9.92	10.01
2	8	2	57.77	59.47	1	9	5	9.00	7.48	2	10	3	4.71 LR	6.63
2	8	3	19.36	19.72	1	9	6	36.83	37.43	2	10	4	8.76	7.96
2	8	4	80.47	80.85	1	9	7	16.07	16.05	2	10	5	18.54	18.41
2	8	5	23.43	24.03	1	9	8	31.33	30.65	2	10	6	22.26	22.52
2	8	6	47.35	47.05	1	9	9	1.00 LR	0.17	2	10	7	4.17 LR	1.95
2	8	7	6.81	6.54	1	9	10	7.69	7.64					
2	8	8	43.66	42.87	1	9	11	18.31	17.87					
2	8	9	11.52	11.28	1	9	12	4.98 LR	6.01					
2	8	10	60.71	60.05	2	9	0	19.68	19.86					
2	8	11	4.77 LR	5.96	2	9	1	9.27	8.75					
2	8	12	45.06	45.46	2	9	2	4.96 LR	5.65					
2	8	13	18.46	18.68	2	9	3	6.77 LR	6.53					
3	8	0	7.28	7.29	2	9	4	4.92 LR	5.08					
3	8	1	35.39	36.15	2	9	5	10.03	9.76					
3	8	2	27.84	27.99	2	9	6	24.46	24.70					
3	8	3	34.49	33.88	2	9	7	0.00 LR	5.19					
3	8	4	32.87	33.02	2	9	8	22.12	22.16					
3	8	5	50.12	50.93	2	9	9	4.39 LR	1.62					
3	8	6	7.54	6.64	2	9	10	0.00 LR	0.51					
3	8	7	7.87	7.72	2	9	11	20.78	20.58					
3	8	8	0.00 LR	2.50	3	9	0	45.81	45.57					
3	8	9	36.13	35.45	3	9	1	40.44	40.65					
3	8	10	41.15	40.15	3	9	2	7.54	8.12					
3	8	11	17.18	16.76	3	9	3	29.29	29.08					
3	8	12	13.22	13.69	3	9	4	10.59	10.45					
4	8	0	7.56	6.40	3	9	5	63.05	62.66					
4	8	1	0.00 LR	7.28	3	9	6	33.43	33.42					
4	8	2	13.80	13.75	3	9	7	4.07 LR	4.55					
4	8	3	6.74	7.20	3	9	8	36.87	36.18					
4	8	4	30.82	29.58	3	9	9	48.01	46.36					
4	8	5	6.23	6.60	4	9	0	1.99 LR	1.06					
4	8	6	13.65	14.20	4	9	1	10.19	10.19					
4	8	7	5.63 LR	5.89	4	9	2	9.16	9.85					
4	8	8	2.73 LR	4.95	4	9	3	6.51	5.16					
4	8	9	12.44	13.07	4	9	4	10.72	7.77					
4	8	10	15.81	16.06	4	9	5	24.35	24.03					
5	8	0	32.03	30.25	4	9	6	22.02	21.47					
5	8	1	0.00 LR	4.74	4	9	7	4.60 LR	5.18					
5	8	2	19.67	19.95	4	9	8	39.38	38.37					
5	8	3	4.13 LR	1.60	5	9	9	11.84	11.13					

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	2	30.01	30.82	4	6	16	47.26	47.71	2	7	9	8.72	9.16
2	2	2	104.61	103.80	4	6	0	44.31	43.04	2	7	10	23.77	23.07
2	2	2	40.93	41.34	4	6	0	6.77	5.92	2	7	11	2.24	1.35
2	2	2	44.60	43.65	4	6	2	18.15	18.84	2	7	12	9.96	9.27
2	2	2	17.69	17.84	4	6	3	0.00	2.17	2	7	13	18.95	18.94
2	2	2	9.93	9.69	4	6	4	25.77	24.03	2	7	14	46.02	45.24
2	2	2	24.49	24.90	4	6	5	15.55	15.42	2	7	15	3.71	4.34
2	2	2	84.30	83.51	5	6	6	2.85	4.03	2	7	0	7.83	7.09
2	2	2	9.09	9.20	5	6	1	25.29	24.64	3	7	1	35.25	34.88
2	2	2	11.89	12.31	5	6	2	15.77	15.73	3	7	2	21.98	21.98
2	2	2	23.93	24.36	5	6	3	9.84	9.22	3	7	3	22.18	22.74
2	2	2	22.88	22.24	5	6	4	20.61	11.10	3	7	4	28.73	28.80
3	3	3	37.19	37.98	5	6	5	23.99	24.57	3	7	5	7.88	8.15
3	3	3	30.53	30.54	5	6	6	4.57	4.50	3	7	6	19.09	18.96
3	3	3	58.64	59.50	5	6	7	18.21	18.88	3	7	7	2.56	3.04
3	3	3	28.39	27.87	5	6	8	0.00	2.03	3	7	8	15.35	14.62
3	3	3	55.43	55.74	5	6	9	15.08	15.39	3	7	9	16.13	16.05
3	3	3	21.67	21.37	5	6	10	4.46	3.93	3	7	10	33.24	33.79
3	3	3	4.28	3.94	5	6	11	60.24	60.80	3	7	11	36.74	36.25
3	3	3	5.30	3.90	5	6	12	48.62	47.38	3	7	12	7.89	8.03
3	3	3	23.77	23.97	5	6	13	53.10	53.54	3	7	13	20.11	19.65
3	3	3	12.89	12.48	5	6	14	37.78	37.85	4	7	0	28.97	28.88
3	3	3	25.12	25.61	5	6	15	0.00	0.86	4	7	1	20.13	20.52
3	3	3	37.06	37.46	5	6	16	38.44	38.51	4	7	2	31.46	31.60
3	3	3	28.07	27.51	5	6	17	3.08	0.86	4	7	3	2.14	2.26
3	3	3	10.04	10.11	5	6	18	20.02	20.07	4	7	4	15.81	14.95
3	3	3	22.16	21.99	5	6	19	36.61	36.21	4	7	5	48.64	49.56
3	3	3	50.57	49.92	5	6	20	42.82	43.02	4	7	6	27.38	27.32
4	4	4	20.43	20.70	5	6	21	21.94	22.15	4	7	7	3.45	3.30
4	4	4	11.36	10.48	5	6	22	5.93	5.58	4	7	8	10.53	10.66
4	4	4	8.59	8.53	5	6	23	35.10	34.82	4	7	9	40.87	41.18
4	4	4	43.83	44.24	5	6	24	10.68	10.83	4	7	10	12.46	12.66
4	4	4	22.00	22.14	5	6	25	22.58	22.35	4	7	11	8.16	8.51
4	4	4	7.72	7.03	5	6	26	27.71	27.94	4	7	12	17.20	17.22
4	4	4	30.83	30.22	5	6	27	32.33	31.34	5	7	0	13.19	13.28
4	4	4	51.93	53.17	5	6	28	34.97	35.11	5	7	1	22.41	2.07
4	4	4	24.82	24.91	5	6	29	22.82	23.08	5	7	2	22.42	7.26
4	4	4	22.91	22.91	5	6	30	40.71	40.93	5	7	3	7.71	0.61
4	4	4	2.36	1.79	5	6	31	36.12	35.18	5	7	4	41.14	41.67
4	4	4	4.40	4.62	5	6	32	16.49	17.20	5	7	5	8.61	8.75
4	4	4	21.31	20.94	5	6	33	36.91	36.80	5	7	6	39.22	39.69
4	4	4	61.25	60.16	5	6	34	19.97	20.59	5	7	7	3.52	3.12
4	4	4	41.16	41.76	5	6	35	28.85	29.58	5	7	8	11.65	10.82
4	4	4	2.13	2.15	5	6	36	13.07	12.66	5	7	9	34.72	34.19
4	4	4	28.88	29.46	5	6	37	16.28	16.28	6	7	0	3.58	3.26
4	4	4	5.48	4.79	5	6	38	29.69	29.82	6	7	1	23.06	23.03
4	4	4	5.08	4.67	5	6	39	2.68	3.17	6	7	2	0.00	1.73
4	4	4	18.39	18.76	5	6	40	19.36	19.10	6	7	3	65.32	65.79
4	4	4	53.96	54.26	5	6	41	29.04	29.36	6	7	4	8.65	8.44
4	4	4	49.93	48.39	5	6	42	54.02	53.84	6	7	5	23.93	23.73
0	0	0	147.11	144.15	4	6	1	8.66	8.77	6	7	6	3.63	2.35
0	0	0	140.37	137.12	4	6	2	5.30	5.11	6	7	7	21.51	21.15
0	0	0	38.49	37.95	4	6	3	32.28	32.45	6	7	8	56.20	54.96
0	0	0	15.01	15.97	4	6	4	72.16	72.43	7	7	0	0.00	1.29
0	0	0	101.35	99.41	4	6	5	58.71	58.75	7	7	1	124.35	122.37
0	0	0	91.30	90.56	4	6	6	0.00	0.49	7	7	2	32.04	20.57
0	0	0	56.90	56.32	4	6	7	0.00	0.49	7	7	3	32.04	31.95
0	0	0			4	6	8			7	7	4	40.33	39.37

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0	8	8	32.61	32.44	5	8	3	1.40	LR	1.56	5	9	1	11.17	11.22
0	8	10	53.70	52.27	5	8	4	53.42	LR	53.77	0	10	0	14.68	14.16
0	8	12	27.72	27.28	5	8	5	0.00	LR	0.07	0	10	2	10.08	10.00
0	8	14	85.05	84.25	5	8	6	7.00	LR	7.64	0	10	4	51.58	52.16
1	8	0	8.74	8.13	5	8	7	3.04	LR	13.69	0	10	6	0.00	1.95
1	8	1	41.85	42.00	6	8	0	13.59		13.69	0	10	8	13.91	14.28
1	8	2	23.42	23.29	6	8	1	7.32		6.83	0	10	10	33.61	32.81
1	8	3	13.98	14.65	6	8	2	22.03		22.33	1	10	0	15.04	14.86
1	8	4	48.81	48.15	6	8	3	11.52		11.27	1	10	2	41.15	41.30
1	8	5	62.24	61.16	0	9	0	75.56		74.07	1	10	2	33.78	33.96
1	8	6	13.48	13.11	0	9	2	15.18		15.47	1	10	3	33.75	33.12
1	8	7	6.36	5.92	0	9	4	24.35		25.09	1	10	5	33.67	33.19
1	8	8	4.85	4.74	0	9	6	67.62		67.05	1	10	5	13.01	12.43
1	8	8	55.88	54.38	0	9	8	53.18		51.65	1	10	6	6.89	6.48
1	8	9	33.08	32.79	0	9	10	24.76		24.59	1	10	7	18.81	18.00
1	8	10	5.73	5.67	0	9	12	3.29	LR	1.26	1	10	8	3.79	4.40
1	8	11	26.96	26.84	1	9	0	44.76		44.81	1	10	8	18.22	17.55
1	8	12	26.95	26.30	1	9	1	4.94		4.48	1	10	9	18.22	17.55
1	8	13	9.86	9.71	1	9	1	11.66		11.74	1	10	10	30.52	30.32
1	8	14	37.24	36.34	1	9	2	12.05		11.93	2	10	0	2.11	3.68
2	8	0	12.87	13.38	1	9	3	8.11		7.66	2	10	1	17.46	17.43
2	8	1	61.39	62.18	1	9	4	8.74		8.30	2	10	2	11.57	11.46
2	8	2	19.05	18.84	1	9	5	37.44		36.99	2	10	3	7.30	6.75
2	8	3	84.64	82.84	1	9	6	15.23		14.57	2	10	4	8.71	8.79
2	8	4	23.00	23.16	1	9	7	31.71		31.36	2	10	5	19.33	19.49
2	8	5	49.69	49.75	1	9	8	0.00	LR	1.17	2	10	6	23.63	23.57
2	8	6	7.61	6.94	1	9	9	7.75		7.46	2	10	7	0.00	1.01
2	8	7	45.44	45.05	1	9	10	18.90		18.00	2	10	8	9.80	9.10
2	8	8	11.50	11.98	1	9	11	5.99		6.29	3	10	0	34.73	34.23
2	8	9	62.93	62.59	1	9	12	22.15		22.26	3	10	1	5.89	6.08
2	8	10	8.14	7.57	2	9	0	8.60		8.42	3	10	2	31.34	31.13
2	8	11	48.38	47.89	2	9	1	7.58		7.40	3	10	3	30.12	29.61
2	8	12	18.75	19.22	2	9	2	6.32		6.10	3	10	4	28.36	28.32
2	8	13	17.32	17.36	2	9	3	3.70	LR	5.23	3	10	5	9.60	9.61
3	8	0	36.92	37.50	2	9	4	10.70		10.71	0	11	0	23.41	23.23
3	8	1	29.02	28.79	2	9	5	27.17		27.08	0	11	2	42.90	42.90
3	8	2	35.24	35.75	2	9	6	5.56		5.36	0	11	4	17.19	16.59
3	8	3	34.73	34.58	2	9	7	25.32		24.71	0	11	6	11.61	10.47
3	8	4	52.40	53.52	2	9	8	0.00	LR	2.04	0	11	8	3.39	3.44
3	8	5	6.33	6.17	2	9	9	3.68	LR	1.67	1	11	0	38.55	38.16
3	8	6	8.08	7.78	2	9	10	21.47		21.09	1	11	1	18.79	19.38
3	8	7	0.00	1.96	3	9	0	47.70		46.99	1	11	2	23.70	22.98
3	8	8	37.72	37.63	3	9	1	42.16		41.02	1	11	3	32.26	32.05
3	8	9	42.30	42.01	3	9	2	9.15		9.16	1	11	4	61.60	58.82
3	8	10	17.28	16.82	3	9	3	27.52		28.93	1	11	5	0.66	0.61
3	8	11	14.71	15.12	3	9	4	8.96		9.32	1	11	6	1.29	4.76
3	8	12	6.27	5.72	3	9	5	63.05		62.66	2	11	7	5.65	5.01
4	8	0	8.68	7.96	3	9	6	36.08	LR	36.10	2	11	0	0.00	LR
4	8	1	14.78	14.98	3	9	7	0.00	LR	4.40	2	11	1	17.68	17.51
4	8	2	6.10	6.35	3	9	8	38.71		38.38	2	11	2	9.25	8.89
4	8	3	29.72	30.24	3	9	9	48.23		47.54	2	11	3	72.15	70.54
4	8	4	8.38	8.05	4	9	0	0.00	LR	1.35	0	12	0	37.14	37.85
4	8	5	15.40	15.78	4	9	1	10.82		10.97	0	12	2	9.98	10.91
4	8	6	6.75	6.31	4	9	2	11.11		11.51	1	11	4	0.00	LR
4	8	7	5.59	5.57	4	9	3	6.13		6.57	1	11	6	17.51	17.51
4	8	8	13.89	13.92	4	9	4	9.67		9.08	2	11	7	8.89	8.89
4	8	9	16.25	16.89	4	9	5	25.60		26.10	2	11	8	70.54	70.54
5	8	0	31.15	30.67	4	9	6	22.84		23.05	0	12	0	37.14	37.85
5	8	1	1.85	4.22	4	9	7	4.95		5.07	0	12	2	9.98	10.91
5	8	2	20.31	21.14	5	9	0	41.10		39.73	0	12	4	0.00	LR

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	2	148.33	142.57	3	3	3	105.68	105.41	3	4	2	4.04	LR
0	0	4	196.38	198.30	3	3	2	49.13	51.14	3	4	3	19.66	20.21
0	0	6	44.75	52.82	3	3	6	123.97	122.09	3	4	4	9.59	8.32
0	0	8	291.88	287.16	3	3	4	21.77	23.23	3	4	5	64.62	65.60
0	0	10	85.97	87.43	3	3	6	24.67	24.63	3	4	6	38.02	37.36
0	0	12	54.35	56.60	3	3	8	82.47	83.58	3	4	7	17.42	18.04
0	0	14	201.39	199.41	3	3	10	33.54	33.53	3	4	8	57.03	57.08
0	0	16	104.94	108.24	3	3	12	30.68	29.38	3	4	9	56.54	57.66
0	0	18	54.95	55.37	3	3	14	6.87	2.63	3	4	10	9.35	8.98
0	0	20	65.66	62.60	3	3	16	46.94	46.64	3	4	11	23.28	23.41
0	1	0	24.34	22.35	0	4	18	12.18	12.56	3	4	12	0.00	LR
0	1	2	57.51	56.95	0	4	0	61.35	59.23	3	4	13	4.10	LR
0	1	4	90.89	87.52	0	4	4	35.10	36.85	3	4	14	0.00	LR
0	1	6	17.26	15.03	0	4	6	42.69	41.60	3	4	15	0.00	LR
0	1	8	32.98	32.52	0	4	8	37.44	36.94	3	4	16	13.15	11.70
0	1	10	17.33	15.96	0	4	10	82.41	83.85	3	4	17	7.82	LR
0	1	12	51.22	52.02	0	4	12	6.90	5.84	4	4	0	13.96	16.25
0	1	14	26.25	26.76	0	4	14	15.11	14.85	4	4	2	79.17	79.14
0	1	16	17.74	18.81	0	4	16	17.30	17.13	4	4	4	155.66	157.58
0	1	18	10.06	11.49	0	4	18	46.46	46.78	4	4	6	53.33	55.04
0	0	0	0.00	6.92	0	4	0	88.95	85.44	4	4	8	35.60	35.38
0	1	0	115.50	120.75	1	4	1	85.62	83.58	4	4	10	100.90	100.09
1	1	1	101.77	105.60	1	4	2	60.41	59.68	4	4	12	66.68	67.04
1	1	4	163.35	162.95	1	4	3	4.32	7.57	4	4	14	0.00	LR
1	1	6	21.63	20.85	1	4	4	60.68	60.02	4	4	16	34.90	35.49
1	1	8	49.92	49.55	1	4	5	55.45	55.59	4	5	0	144.80	140.60
1	1	10	92.37	92.31	1	4	6	18.02	16.41	0	5	2	26.62	27.04
1	1	12	52.12	50.81	1	4	7	49.44	49.12	0	5	4	36.28	35.66
1	1	14	14.30	13.97	1	4	8	10.62	10.44	0	5	6	17.26	16.10
1	1	16	10.65	9.89	1	4	9	68.77	71.79	0	5	8	44.21	42.96
1	1	18	50.18	48.11	1	4	10	30.14	30.46	0	5	10	25.97	25.94
0	0	2	77.97	79.02	1	4	11	6.62	6.40	0	5	12	14.47	14.78
0	0	4	107.38	104.38	1	4	12	41.90	40.92	0	5	14	55.70	55.59
0	0	6	163.14	161.04	1	4	13	4.90	9.97	0	5	16	23.82	25.13
0	0	8	3.81	3.96	1	4	14	9.20	10.59	0	5	18	13.51	13.65
0	0	10	56.58	55.08	1	4	15	8.40	9.19	0	5	0	8.86	8.79
0	0	12	80.38	78.11	1	4	16	31.92	31.72	1	5	1	65.95	65.71
0	0	14	62.69	62.26	1	4	17	3.30	11.64	1	5	2	56.27	55.07
0	0	16	6.15	0.35	1	4	18	19.97	18.89	1	5	3	50.30	52.41
0	0	18	18.46	18.01	1	4	0	84.29	83.25	1	5	4	53.73	53.37
0	0	2	43.99	44.70	2	2	4	32.29	32.86	1	5	5	57.19	59.03
0	0	4	28.55	28.59	2	2	2	4.85	2.77	1	5	6	19.12	20.14
1	1	2	139.23	141.67	2	2	4	28.05	29.31	1	5	7	0.00	LR
1	1	4	55.02	56.28	2	2	3	29.84	29.02	1	5	8	16.91	18.29
1	1	6	53.12	54.42	2	2	4	29.84	29.02	1	5	9	52.87	50.62
1	1	8	16.04	18.29	2	2	6	52.80	52.68	1	5	10	63.94	63.10
1	1	10	26.65	24.92	2	2	8	0.00	2.91	1	5	11	31.63	31.36
1	1	12	13.30	12.96	2	2	9	71.84	71.84	1	5	12	25.37	25.34
1	1	14	12.86	10.56	2	2	10	42.26	42.37	1	5	13	47.10	46.56
1	1	16	60.71	60.13	2	2	11	16.73	18.07	1	5	14	12.72	12.37
1	1	18	69.56	69.13	2	2	12	4.78	4.39	1	5	15	37.81	37.73
1	1	2	84.07	86.12	2	2	13	27.29	27.13	1	5	16	22.37	22.60
1	1	4	43.61	43.58	2	2	14	32.34	32.40	1	5	17	26.30	26.14
1	1	6	6.10	7.24	2	2	15	34.82	34.29	2	2	5	165.21	165.25
1	1	8	41.13	40.30	2	2	16	27.09	27.31	2	2	5	80.19	79.52
1	1	10	13.08	13.17	2	2	17	16.86	16.13	2	2	5	13.20	14.44
1	1	12	47.95	49.49	2	2	18	12.01	8.18	2	2	5	50.40	51.78
1	1	14	37.90	39.20	2	2	0	34.33	34.80	2	2	5	83.51	84.04
1	1	16			3	3	1	23.61	22.97	2	2	5	33.58	33.34
1	1	18			3	3	1			3	3	4	89.05	88.87

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	7	29.28	30.74	0	6	16	44.82	44.98	4	6	8	41.99	41.36
2	2	8	100.32	101.73	1	6	0	44.31	44.04	2	7	10	59.46	58.22
2	2	9	41.47	41.97	1	6	1	0.00	3.88	2	7	11	5.73	4.61
2	2	10	45.66	45.15	1	6	2	16.48	16.81	2	7	12	15.84	16.91
2	2	11	18.79	18.38	1	6	3	0.00	1.38	2	7	13	0.00	1.66
2	2	12	12.40	11.75	1	6	4	21.03	20.18	2	7	14	41.63	42.11
2	2	13	24.86	25.05	1	6	5	25.19	25.47	2	7	15	33.43	33.29
2	2	14	81.13	81.51	1	6	6	13.39	13.37	2	7	16	45.96	43.86
2	2	15	9.55	9.68	1	6	7	0.00	3.11	3	7	0	10.06	9.55
2	2	16	9.49	10.68	1	6	8	23.42	23.43	3	7	1	19.14	19.55
2	2	17	23.84	24.66	1	6	9	12.44	13.40	3	7	2	0.00	2.76
3	3	5	36.88	38.14	1	6	10	5.24	6.60	3	7	3	12.57	10.18
3	3	6	27.49	28.83	1	6	11	23.48	23.70	3	7	4	15.50	16.67
3	3	7	59.06	60.97	1	6	12	5.60	3.68	3	7	5	27.80	27.98
3	3	8	27.26	26.57	1	6	13	19.08	18.95	3	7	6	0.00	3.32
3	3	9	55.93	55.94	1	6	14	6.07	1.92	3	7	7	7.73	10.36
3	3	10	19.41	19.94	1	6	15	7.58	14.50	3	7	8	11.84	19.36
3	3	11	6.08	4.42	1	6	16	2.02	4.28	3	7	9	3.36	10.32
3	3	12	0.00	2.36	1	6	17	57.86	60.86	3	7	10	12.12	8.16
3	3	13	22.68	23.39	2	6	0	45.93	45.37	3	7	11	47.99	78.33
3	3	14	13.04	12.01	2	6	1	55.22	55.44	3	7	12	79.99	49.10
3	3	15	0.00	2.60	2	6	2	34.89	35.55	4	7	0	42.27	43.45
3	3	16	24.09	24.33	2	6	3	0.00	1.11	4	7	1	21.39	22.20
3	3	17	37.46	37.81	2	6	4	38.69	37.51	4	7	2	51.82	52.22
3	3	18	25.47	25.99	2	6	5	0.00	0.72	4	7	3	42.86	42.04
3	3	19	21.58	21.24	2	6	6	6.51	0.28	4	7	4	101.99	103.69
3	3	20	7.43	8.97	2	6	7	19.46	20.68	4	7	5	37.20	37.58
4	4	5	19.11	20.02	2	6	8	36.15	35.56	4	7	6	72.23	75.05
4	4	6	51.32	50.13	2	6	9	45.03	45.15	4	7	7	48.86	47.39
4	4	7	17.34	17.60	2	6	10	21.29	20.93	4	7	8	39.81	40.13
4	4	8	11.55	10.93	2	6	11	6.38	6.77	4	7	9	11.39	10.24
4	4	9	0.00	6.73	2	6	12	32.41	33.61	4	7	10	6.79	10.28
4	4	10	43.53	43.66	2	6	13	7.29	10.96	4	7	11	64.10	64.05
4	4	11	20.90	20.66	2	6	14	20.86	21.10	4	7	12	8.19	9.98
4	4	12	6.62	6.70	2	6	15	29.84	28.52	5	7	0	4.96	9.49
4	4	13	29.16	29.35	2	6	16	35.27	35.11	5	7	1	30.87	31.46
4	4	14	21.69	22.38	3	6	0	17.12	18.19	5	7	2	20.78	19.85
4	4	15	23.64	23.85	3	6	1	39.67	39.87	5	7	3	6.89	6.18
4	4	16	0.00	0.80	3	6	2	31.54	30.97	5	7	4	51.48	52.20
4	4	17	23.56	23.45	3	6	3	33.21	33.80	5	7	5	22.98	22.98
4	4	18	3.52	3.33	3	6	4	15.05	15.43	5	7	6	17.91	18.17
4	4	19	21.98	21.47	3	6	5	2.28	0.22	5	7	7	13.71	14.53
5	5	0	52.72	52.63	3	6	6	34.38	35.28	5	7	8	21.25	20.27
5	5	1	37.83	38.46	3	6	7	21.99	21.61	5	7	9	39.03	38.85
5	5	2	0.00	2.44	3	6	8	24.41	24.68	6	7	0	6.66	6.66
5	5	3	24.82	24.34	3	6	9	13.62	12.90	6	7	1	18.86	18.39
5	5	4	0.00	1.30	3	6	10	14.03	13.87	6	7	2	5.86	5.86
5	5	5	7.40	4.34	3	6	11	28.52	29.89	6	7	3	12.29	13.48
5	5	6	15.51	15.84	3	6	12	0.00	4.23	6	7	4	0.00	0.16
5	5	7	49.70	49.06	3	6	13	19.71	19.61	6	7	5	49.74	48.68
5	5	8	47.07	45.45	3	6	14	30.37	30.96	6	7	6	19.05	20.33
0	0	6	150.10	149.29	4	6	0	52.28	52.28	6	7	7	1.52	1.09
0	0	7	141.34	139.47	4	6	1	6.34	9.59	6	7	8	48.47	48.26
0	0	8	32.29	33.00	4	6	2	31.49	32.09	6	7	9	13.06	11.90
0	0	9	17.23	19.92	4	6	3	0.00	3.78	6	7	10	0.00	5.31
0	0	10	98.20	98.38	4	6	4	71.93	70.78	6	7	11	48.39	49.07
0	0	11	88.52	89.71	4	6	5	58.68	59.99	6	7	12	0.00	6.05
0	0	12	53.12	54.93	4	6	6	0.00	0.05	6	7	13	38.12	37.37

F(CALC)

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F(CALC)

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H K L

0	8	8	0	0	0	35.51	35.51	0.00	LR	2.51	5	9	1	12.80	12.06
0	8	10	0	5	3	52.89	52.89	50.36	LR	51.29	5	10	0	14.42	14.17
0	8	12	0	5	4	27.85	27.85	0.00	LR	0.35	0	10	2	9.74	11.16
0	8	14	0	5	5	86.71	86.71	0.00	LR	5.36	0	10	4	52.18	53.29
1	8	0	1	5	6	6.94	6.94	0.00	LR	1.65	0	10	6	0.00	0.37
1	8	1	1	6	7	39.51	39.51	14.72	LR	14.08	0	10	8	13.57	14.05
1	8	2	1	6	8	21.18	21.18	4.90	LR	7.48	0	10	10	33.41	33.04
1	8	3	1	6	8	13.17	13.17	22.85	LR	23.06	1	10	0	14.93	13.26
1	8	4	1	6	8	46.45	46.45	6.38	LR	11.59	1	10	1	42.02	41.62
1	8	5	0	6	9	59.30	59.30	71.79	LR	70.62	1	10	2	30.45	30.47
1	8	6	0	6	9	13.80	13.80	10.87	LR	12.04	1	10	3	32.51	32.51
1	8	7	1	6	9	5.88	5.88	26.17	LR	26.60	1	10	4	29.15	29.15
1	8	8	0	6	9	3.89	3.89	66.56	LR	65.22	1	10	5	14.45	13.09
1	8	9	0	6	9	52.49	52.49	49.09	LR	50.06	1	10	6	3.75	7.75
1	8	10	0	6	9	30.36	30.36	25.33	LR	26.06	1	10	7	18.14	17.80
1	8	11	0	6	9	4.13	4.13	5.47	LR	2.30	1	10	8	0.00	6.01
1	8	12	1	6	9	25.98	25.98	42.84	LR	42.85	1	10	9	19.59	18.46
1	8	13	1	6	9	24.78	24.78	6.05	LR	3.72	1	10	10	25.68	26.40
1	8	14	1	6	9	4.88	4.88	6.80	LR	9.94	2	10	0	1.87	7.30
2	8	0	1	6	9	30.99	30.99	10.92	LR	11.79	2	10	1	17.31	17.31
2	8	1	1	6	9	12.18	12.18	8.91	LR	8.89	2	10	2	12.45	11.56
2	8	2	1	6	9	58.57	58.57	6.49	LR	7.16	2	10	3	0.00	6.43
2	8	3	1	6	9	18.22	18.22	38.09	LR	37.07	2	10	4	0.00	7.19
2	8	4	1	6	9	81.59	81.59	14.66	LR	14.27	2	10	5	20.30	19.18
2	8	5	1	6	9	22.80	22.80	31.87	LR	30.87	2	10	6	25.30	25.12
2	8	6	1	6	9	46.37	46.37	5.58	LR	0.20	2	10	7	4.83	1.26
2	8	7	1	6	9	5.36	5.36	9.84	LR	8.64	2	10	8	23.60	23.54
2	8	8	1	6	9	41.12	41.12	16.81	LR	17.35	3	10	0	8.74	8.73
2	8	9	1	6	9	11.46	11.46	0.00	LR	4.71	3	10	1	34.07	33.80
2	8	10	1	6	9	61.21	61.21	19.92	LR	18.92	3	10	2	5.19	4.59
2	8	11	1	6	9	6.44	6.44	7.22	LR	9.69	3	10	3	31.03	31.05
2	8	12	1	6	9	44.86	44.86	6.10	LR	6.22	3	10	4	28.28	27.90
2	8	13	1	6	9	18.97	18.97	0.00	LR	6.05	3	10	5	25.15	26.39
3	8	0	1	6	9	8.05	8.05	6.91	LR	4.15	0	11	0	6.94	7.73
3	8	1	1	6	9	35.41	35.41	6.51	LR	7.96	0	11	2	20.89	20.93
3	8	2	1	6	9	27.25	27.25	24.77	LR	24.82	0	11	4	39.79	38.74
3	8	3	1	6	9	32.67	32.67	3.71	LR	5.42	0	11	6	17.66	18.02
3	8	4	1	6	9	32.24	32.24	20.96	LR	21.47	0	11	8	13.54	10.24
3	8	5	1	6	9	51.57	51.57	7.94	LR	0.51	0	11	0	5.76	3.97
3	8	6	0	6	9	6.98	6.98	4.80	LR	0.88	1	11	1	38.87	38.19
3	8	7	0	6	9	7.50	7.50	20.50	LR	21.03	1	11	2	17.96	18.34
3	8	8	0	6	9	2.62	2.62	43.41	LR	43.12	1	11	3	22.55	22.51
3	8	9	0	6	9	36.40	36.40	41.18	LR	40.65	1	11	4	29.75	30.32
3	8	10	0	6	9	39.41	39.41	0.00	LR	6.68	1	11	5	60.93	59.29
3	8	11	1	6	9	15.45	15.45	28.17	LR	28.47	1	11	6	3.98	0.64
3	8	12	1	6	9	14.09	14.09	7.70	LR	11.48	1	11	7	9.02	4.54
4	8	0	1	6	9	6.02	6.02	61.96	LR	62.38	2	11	0	4.39	4.97
4	8	1	1	6	9	8.65	8.65	32.99	LR	32.35	2	11	1	3.46	2.29
4	8	2	1	6	9	16.04	16.04	5.93	LR	4.14	2	11	2	14.81	15.69
4	8	3	1	6	9	5.96	5.96	35.19	LR	34.91	2	11	3	9.49	9.07
4	8	4	1	6	9	32.00	32.00	48.14	LR	47.07	0	12	0	66.99	65.26
4	8	5	0	6	9	8.24	8.24	0.00	LR	0.76	0	12	2	35.35	36.03
4	8	6	0	6	9	15.73	15.73	8.16	LR	8.18	0	12	4	12.95	11.10
4	8	7	0	6	9	6.42	6.42	9.67	LR	9.69	0	12	2	12.95	11.10
4	8	8	0	6	9	5.22	5.22	4.75	LR	4.65	0	12	4	12.95	11.10
4	8	9	0	6	9	14.29	14.29	5.86	LR	6.34	0	12	2	12.95	11.10
4	8	10	0	6	9	18.10	18.10	23.01	LR	23.27	0	12	2	12.95	11.10
5	8	0	1	6	9	31.85	31.85	20.35	LR	21.80	0	12	2	12.95	11.10
5	8	1	1	6	9	4.88	4.88	0.00	LR	4.57	0	12	2	12.95	11.10
5	8	2	1	6	9	18.35	18.35	37.03	LR	36.96	0	12	2	12.95	11.10

OSUMILITE HAYASAKI (JAPAN) SAMPLE FROM D.WONES

STRUCTURE FACTORS

PAGE 1

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	0	2	153.24	154.01	1	1	2	37.61	36.74	3	3	0	100.56	99.55
0	0	2	180.23	188.26	2	2	2	161.10	163.51	3	3	2	55.96	57.24
0	0	6	50.25	59.30	2	2	4	91.57	92.07	3	3	4	128.30	128.24
0	0	8	285.10	291.84	2	2	4	61.57	59.72	3	3	5	28.23	28.96
0	0	10	77.90	80.94	2	2	6	184.83	186.75	3	3	6	20.26	19.69
0	0	12	59.77	60.99	2	2	8	172.41	173.72	3	3	8	88.07	87.59
0	0	14	200.83	202.37	2	2	10	56.63	56.53	3	3	10	37.20	37.16
0	0	16	109.01	109.87	2	2	12	41.65	40.60	3	3	12	27.14	26.22
0	0	18	51.96	51.63	2	2	14	83.17	82.80	3	3	14	2.59	5.67
0	0	20	67.03	64.58	2	2	16	43.03	42.59	3	3	16	49.61	48.89
0	1	0	27.05	25.24	2	2	18	23.00	23.30	3	3	18	16.16	15.61
0	1	2	61.36	61.14	3	3	0	82.88	80.29	0	0	0	59.83	56.43
0	1	4	92.35	92.08	0	0	2	24.53	25.02	0	0	2	32.81	33.91
0	1	6	13.77	11.15	0	0	4	27.93	26.31	0	0	4	40.92	40.40
0	1	8	31.30	30.06	0	0	6	92.45	93.28	0	0	6	35.33	35.25
0	1	10	19.49	17.93	0	0	8	93.40	92.97	0	0	8	78.71	81.77
0	1	12	54.09	53.21	0	0	10	15.04	14.11	0	0	10	16.18	15.98
0	1	14	27.83	28.18	0	0	12	12.98	11.77	0	0	12	13.90	14.82
0	1	16	18.97	20.39	0	0	14	31.71	31.05	0	0	14	43.73	44.79
0	1	18	14.35	12.83	0	0	16	13.96	13.75	0	0	16	96.55	92.68
0	1	20	6.43	7.29	0	0	18	0.00	3.47	0	0	18	85.52	82.27
1	1	0	109.58	113.41	1	1	0	60.66	57.32	1	1	0	68.09	67.61
1	1	2	114.33	114.07	1	1	2	39.81	44.38	1	1	2	6.26	6.73
1	1	4	169.20	171.24	1	1	4	9.57	9.85	1	1	4	68.23	66.45
1	1	6	29.37	29.25	1	1	6	70.65	63.33	1	1	6	54.69	54.54
1	1	8	43.90	42.87	1	1	8	100.58	96.95	1	1	8	12.45	11.91
1	1	10	99.23	97.26	1	1	10	115.43	115.57	0	0	10	51.22	49.75
1	1	12	55.93	54.44	1	1	12	31.24	32.28	0	0	12	14.27	14.19
1	1	14	12.06	10.67	1	1	14	28.41	27.96	0	0	14	68.56	70.06
1	1	16	14.44	13.39	1	1	16	10.49	10.37	0	0	16	35.48	35.51
1	1	18	50.32	50.86	1	1	18	117.79	121.20	0	0	18	8.58	7.79
1	1	20	81.91	81.39	1	1	20	35.29	34.64	0	0	20	44.89	44.99
0	2	0	105.44	101.41	1	1	0	42.26	42.48	0	0	0	9.80	8.40
0	2	2	155.46	157.91	1	1	2	32.91	32.60	0	0	2	14.43	14.02
0	2	4	0.00	1.27	1	1	4	48.78	48.63	0	0	4	14.43	14.02
0	2	6	56.87	57.68	1	1	6	0.00	5.15	1	1	6	8.39	9.51
0	2	8	75.59	75.08	1	1	8	57.38	56.65	1	1	8	34.68	34.51
0	2	10	61.96	60.25	1	1	10	8.20	9.68	1	1	10	10.33	10.32
0	2	12	0.00	1.27	1	1	12	21.52	21.06	1	1	12	22.55	21.88
0	2	14	17.23	17.15	1	1	14	22.85	22.37	1	1	14	83.59	80.79
0	2	16	42.94	43.05	1	1	16	73.72	73.09	1	1	16	36.18	35.60
0	2	18	22.63	22.85	1	1	18	78.43	75.47	1	1	18	5.58	5.54
1	1	0	140.49	141.87	2	2	0	25.58	23.40	2	2	0	5.58	5.54
1	1	2	60.43	59.90	2	2	2	0.00	0.74	2	2	2	28.49	29.80
1	1	4	55.03	54.66	2	2	4	5.69	3.10	2	2	4	28.40	27.49
1	1	6	18.35	20.73	2	2	6	5.11	0.53	2	2	6	68.52	70.90
1	1	8	29.39	7.60	2	2	8	6.76	7.36	2	2	8	0.00	51.60
1	1	10	13.80	12.60	2	2	10	52.96	52.27	2	2	10	70.90	70.81
1	1	12	14.77	13.74	2	2	12	28.85	29.38	2	2	12	43.67	45.31
1	1	14	57.91	60.20	2	2	14	59.85	60.84	2	2	14	17.61	19.42
1	1	16	68.16	70.45	2	2	16	16.78	17.00	2	2	16	4.75	4.81
1	1	18	83.89	85.90	2	2	18	19.68	19.65	2	2	18	25.70	25.43
1	1	20	9.38	7.81	2	2	20	14.49	14.58	2	2	20	34.37	33.39
1	1	22	45.60	44.37	2	2	22	11.01	9.17	2	2	22	27.41	27.49
1	1	24	0.00	5.48	2	2	24	40.06	39.79	2	2	24	15.04	14.82
1	1	26	39.46	40.09	2	2	26	21.47	21.13	2	2	26	14.70	13.89
1	1	28	15.04	14.13	2	2	28	9.84	11.93	2	2	28	15.96	18.89
1	1	30	49.13	49.46	2	2	30	6.19	4.25	2	2	30	14.70	13.82
1	1	32	39.39	39.43	2	2	32	10.81	10.85	2	2	32	40.42	38.65
1	1	34			2	2	34			2	2	34	21.15	20.88

STRUCTURE FACTORS		STRUCTURE FACTORS		STRUCTURE FACTORS		STRUCTURE FACTORS								
H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	2	29.37	30.97	4	4	6	49.92	48.01	2	2	2	40.93	40.48
2	2	2	108.07	107.76	4	4	6	44.01	43.71	2	2	2	60.01	60.59
2	2	2	42.49	40.88	4	4	6	4.86	5.51	2	2	2	7.51	7.51
2	2	2	17.61	18.09	4	4	6	19.27	19.00	2	2	2	18.53	17.24
2	2	2	6.99	9.10	4	4	6	0.00	24.54	2	2	2	5.27	0.63
2	2	2	23.68	24.03	4	4	6	25.84	27.52	2	2	2	43.73	32.36
2	2	2	85.36	85.22	4	4	6	14.90	15.36	2	2	2	32.52	45.96
2	2	2	8.93	8.87	5	5	6	2.85	3.80	2	2	2	46.54	11.30
2	2	2	12.69	13.00	5	5	6	14.75	15.05	2	2	2	11.93	11.78
2	2	2	22.86	23.90	5	5	6	4.95	5.57	2	2	2	0.00	1.86
2	2	2	23.87	22.76	5	5	6	10.15	10.97	2	2	2	8.17	17.88
2	2	2	38.65	38.63	5	5	6	24.89	24.95	2	2	2	28.72	29.22
2	2	2	31.22	31.05	5	5	6	6.74	6.36	2	2	2	0.00	3.76
2	2	2	60.34	60.76	5	5	6	18.94	18.58	2	2	2	4.35	11.95
2	2	2	29.75	28.76	5	5	6	0.00	22.10	2	2	2	9.08	19.99
2	2	2	56.61	56.67	5	5	6	15.46	15.54	2	2	2	20.57	19.99
2	2	2	22.29	21.72	5	5	6	0.00	4.03	2	2	2	9.08	8.59
2	2	2	6.84	4.38	5	5	6	61.04	62.26	2	2	2	5.72	8.81
2	2	2	0.00	4.25	5	5	6	0.00	4.03	2	2	2	12.07	13.35
2	2	2	24.23	24.04	5	5	6	47.80	47.76	2	2	2	80.18	80.73
2	2	2	11.57	12.63	5	5	6	54.53	54.44	2	2	2	52.17	53.03
2	2	2	7.76	2.29	5	5	6	38.49	38.41	2	2	2	49.97	50.17
2	2	2	26.26	25.84	5	5	6	4.42	4.61	2	2	2	25.31	25.42
2	2	2	36.79	37.58	5	5	6	39.89	39.18	2	2	2	45.67	46.08
2	2	2	26.50	27.66	5	5	6	0.00	0.85	2	2	2	65.67	66.96
2	2	2	22.37	21.33	5	5	6	5.18	5.56	2	2	2	108.05	109.69
2	2	2	10.69	10.59	5	5	6	20.79	20.71	2	2	2	39.85	39.76
2	2	2	21.96	22.13	5	5	6	37.13	36.43	2	2	2	71.96	74.66
2	2	2	50.91	49.76	5	5	6	42.66	43.34	2	2	2	51.19	49.88
2	2	2	20.42	20.70	5	5	6	20.93	21.73	2	2	2	42.68	43.53
2	2	2	9.70	9.51	5	5	6	4.30	4.14	2	2	2	11.41	11.40
2	2	2	44.68	44.17	5	5	6	0.00	35.08	2	2	2	7.24	10.10
2	2	2	22.96	22.35	5	5	6	27.15	27.29	2	2	2	66.93	66.08
2	2	2	8.06	6.95	5	5	6	33.18	32.41	2	2	2	13.06	11.45
2	2	2	30.47	30.56	5	5	6	27.85	27.29	2	2	2	6.66	6.21
2	2	2	53.92	53.41	5	5	6	34.47	34.93	2	2	2	23.67	22.72
2	2	2	24.89	24.98	5	5	6	22.80	23.79	2	2	2	0.00	0.00
2	2	2	0.00	1.26	5	5	6	41.10	40.50	2	2	2	57.96	58.04
2	2	2	22.78	23.17	5	5	6	38.34	36.20	2	2	2	22.31	22.65
2	2	2	7.56	4.63	5	5	6	17.10	17.50	2	2	2	0.00	0.00
2	2	2	21.23	20.76	5	5	6	7.69	0.54	2	2	2	41.88	41.78
2	2	2	63.41	60.59	5	5	6	36.91	37.59	2	2	2	6.51	6.95
2	2	2	43.77	42.50	5	5	6	20.16	20.11	2	2	2	21.60	21.68
2	2	2	5.41	4.21	5	5	6	12.49	13.16	2	2	2	8.09	6.95
2	2	2	30.10	30.32	5	5	6	16.44	17.17	2	2	2	11.19	11.54
2	2	2	3.36	5.16	5	5	6	0.00	2.97	2	2	2	0.00	0.54
2	2	2	0.00	18.48	5	5	6	18.43	18.90	2	2	2	0.00	0.54
2	2	2	17.84	55.38	5	5	6	30.39	29.50	2	2	2	52.02	50.51
2	2	2	55.38	49.85	5	5	6	55.35	54.07	2	2	2	20.43	20.28
2	2	2	153.59	155.69	5	5	6	7.84	8.72	2	2	2	0.00	3.42
2	2	2	145.25	146.35	5	5	6	31.88	32.86	2	2	2	48.93	49.10
2	2	2	40.37	39.97	5	5	6	5.25	4.82	2	2	2	8.30	9.60
2	2	2	13.89	14.93	5	5	6	71.79	73.76	2	2	2	2.16	5.91
2	2	2	102.11	102.61	5	5	6	59.08	59.28	2	2	2	52.23	51.53
2	2	2	89.51	92.51	5	5	6	4.45	0.14	2	2	2	6.33	5.86
2	2	2	54.95	57.58	5	5	6			2	2	2	38.77	38.87

0	8	0	32.63	32.16	7.45	1.52	11.52	5	9	1	11.52
0	8	10	53.62	52.91	55.70	55.43	17.99	5	9	2	17.99
0	8	12	27.40	27.53	0.00	0.11	14.94	0	10	0	14.94
0	8	14	82.66	84.93	8.14	8.32	5.84	0	10	2	5.84
1	8	0	10.12	8.65	7.27	2.07	51.31	0	10	4	51.31
1	8	1	43.10	42.32	13.13	14.13	4.30	0	10	6	4.30
1	8	1	24.05	23.55	0.00	6.98	13.64	0	10	8	13.64
1	8	3	14.64	15.01	23.15	22.32	32.03	0	10	10	32.03
1	8	4	49.77	49.26	11.76	11.48	14.41	1	10	0	14.41
1	8	5	61.98	61.88	77.97	76.33	41.55	1	10	1	41.55
1	8	6	13.02	12.96	17.02	16.24	34.48	1	10	2	34.48
1	8	7	7.60	6.06	24.24	24.91	33.45	1	10	3	33.45
1	8	8	7.05	5.00	69.66	69.40	35.13	1	10	4	35.13
1	8	9	54.25	54.76	52.97	53.59	9.47	1	10	5	9.47
1	8	10	33.13	32.82	24.62	23.96	0.00	1	10	6	0.00
1	8	11	4.76	5.40	7.51	1.31	18.02	1	10	7	18.02
1	8	12	26.81	27.47	45.25	45.30	4.58	1	10	8	4.58
1	8	13	25.48	26.51	8.27	4.88	17.11	1	10	9	17.11
1	8	14	7.77	9.59	11.17	12.40	31.13	1	10	10	31.13
2	8	0	37.63	37.74	12.05	11.81	8.48	2	10	0	8.48
2	8	1	13.52	12.96	8.44	6.82	17.43	2	10	1	17.43
2	8	1	62.74	64.31	7.87	8.50	0.00	2	10	2	0.00
2	8	2	17.53	18.52	36.75	37.38	4.48	2	10	3	4.48
2	8	3	82.96	84.87	14.20	14.27	9.38	2	10	4	9.38
2	8	4	23.41	22.99	31.72	31.54	18.65	2	10	5	18.65
2	8	5	49.18	50.88	0.00	1.73	23.05	2	10	6	23.05
2	8	6	9.86	7.34	5.64	6.85	0.00	2	10	7	0.00
2	8	7	46.18	45.78	19.30	17.95	22.03	2	10	8	22.03
2	8	8	11.02	11.79	8.63	6.80	8.85	2	10	9	8.85
2	8	9	64.29	63.96	21.96	22.20	34.40	2	10	10	34.40
2	8	10	8.29	7.62	0.00	8.44	5.36	3	10	2	5.36
2	8	11	49.80	48.43	3.40	7.67	31.00	3	10	3	31.00
2	8	12	19.71	19.20	5.32	6.10	30.80	3	10	4	30.80
2	8	13	7.75	6.93	6.91	4.66	28.68	3	10	5	28.68
3	8	0	36.99	37.32	10.69	11.05	17.47	3	10	6	17.47
3	8	1	27.80	29.26	27.24	27.54	9.49	3	10	7	9.49
3	8	2	35.18	35.81	0.00	5.48	23.65	3	10	8	23.65
3	8	3	34.35	35.17	23.70	24.51	43.82	3	10	9	43.82
3	8	4	52.15	54.26	5.29	2.08	17.82	3	10	10	17.82
3	8	5	6.03	6.11	2.69	1.65	0.00	3	10	0	0.00
3	8	6	5.60	8.09	21.65	21.26	0.00	3	10	1	0.00
3	8	7	0.00	1.94	49.24	47.84	38.57	3	10	2	38.57
3	8	8	37.84	37.80	40.20	40.64	18.72	3	10	3	18.72
3	8	9	42.14	42.35	8.56	9.56	22.22	3	10	4	22.22
3	8	10	16.63	16.56	27.95	28.77	32.92	3	10	5	32.92
3	8	11	16.01	15.55	8.85	9.24	60.02	3	10	6	60.02
3	8	12	5.51	6.14	64.39	63.15	0.00	3	10	7	0.00
4	8	0	7.81	8.25	37.27	36.35	0.00	3	10	8	0.00
4	8	1	14.81	15.08	7.97	4.31	3.08	3	10	9	3.08
4	8	2	7.90	6.30	38.64	38.74	7.22	3	10	10	7.22
4	8	3	29.80	30.12	48.04	47.21	18.75	3	10	0	18.75
4	8	4	6.25	8.39	6.43	1.37	2.76	3	10	1	2.76
4	8	5	16.04	16.41	9.84	10.85	73.64	3	10	2	73.64
4	8	6	8.30	6.28	11.02	11.43	38.25	3	10	3	38.25
4	8	7	0.00	5.46	0.00	7.13	6.74	3	10	4	6.74
4	8	8	14.50	14.41	8.47	8.91	0.00	3	10	5	0.00
4	8	9	16.25	16.75	26.13	26.18	9.01	3	10	6	9.01
4	8	10	30.28	30.74	22.73	23.25	72.73	3	10	7	72.73
5	8	0	0.00	4.02	0.00	4.80	38.60	0	12	0	38.60
5	8	1	21.39	21.46	39.96	40.97	11.50	0	12	1	11.50

STRUCTURE FACTORS F(CALC) F(OBS) LR

Table with 14 columns: H, K, L, F(OBS), F(CALC), LR, H, K, L, F(OBS), F(CALC), LR, H, K, L, F(OBS), F(CALC), LR. It contains numerical data for multiple rows, including observations and calculated values, with 'LR' indicating load ratios.

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	2	2	26.96	29.05	4	6	8	45.59	46.57	2	2	9	0.00	9.60
2	2	2	98.99	96.26	4	6	9	56.84	50.80	2	2	10	24.03	27.09
2	2	2	41.43	45.77	4	6	10	8.03	1.03	2	2	11	0.00	0.67
2	2	2	45.92	43.67	4	6	11	13.00	17.28	2	2	12	0.00	3.18
2	2	2	24.11	22.28	4	6	12	7.19	3.94	2	2	13	13.50	16.52
2	2	2	8.03	17.15	4	6	13	37.34	38.29	2	2	14	35.95	39.36
2	2	2	30.49	31.15	4	6	14	34.27	34.67	2	2	15	9.64	3.48
2	2	2	76.88	75.37	5	6	0	36.34	40.94	3	3	0	16.63	17.91
2	2	2	0.00	15.38	5	6	1	7.50	5.58	3	3	1	48.26	43.43
2	2	2	10.44	7.62	5	6	2	9.71	14.45	3	3	2	9.24	15.74
2	2	2	28.46	26.43	5	6	3	6.17	8.23	3	3	3	33.34	32.51
2	2	2	0.00	18.42	5	6	4	20.62	18.54	3	3	4	21.40	25.75
2	2	2	27.60	23.42	5	6	5	9.47	12.17	3	3	5	22.28	19.43
2	2	2	52.60	53.57	5	6	6	29.00	30.51	3	3	6	13.29	8.85
2	2	2	23.85	14.25	5	6	7	5.70	5.70	3	3	7	0.00	3.46
2	2	2	51.37	46.75	5	6	8	0.00	16.70	3	3	8	12.68	8.31
2	2	2	22.31	15.84	5	6	9	19.08	18.40	3	3	9	28.69	23.38
2	2	2	0.00	1.39	5	6	10	17.87	18.40	3	3	10	30.37	33.35
2	2	2	0.00	2.36	5	6	11	11.09	8.99	3	3	11	40.25	38.45
2	2	2	17.21	15.00	5	6	12	0.00	7.63	3	3	12	0.00	2.50
2	2	2	0.00	13.68	6	6	0	78.68	80.11	3	3	13	29.95	29.02
2	2	2	0.00	33.68	6	6	2	45.13	43.88	4	4	0	21.32	18.74
2	2	2	0.00	1.12	6	6	4	34.86	30.33	4	4	2	24.28	24.74
2	2	2	19.69	17.98	6	6	6	24.47	27.32	4	4	4	24.13	26.89
2	2	2	34.56	33.24	6	6	8	51.05	51.27	4	4	6	10.77	3.91
2	2	2	25.87	26.59	6	6	10	35.81	31.15	4	4	8	0.00	11.62
2	2	2	22.48	20.89	6	6	12	94.38	91.98	4	4	10	56.26	56.55
2	2	2	7.86	6.22	6	6	0	33.38	36.81	4	4	12	21.57	16.99
2	2	2	8.89	7.90	6	6	2	36.45	38.77	4	4	4	5.65	5.05
2	2	2	59.37	54.57	6	6	4	31.96	29.56	4	4	6	0.00	0.65
2	2	2	6.59	10.75	6	6	6	11.86	8.66	4	4	8	6.33	46.61
2	2	2	20.09	15.06	6	6	8	18.02	15.72	4	4	10	0.00	10.56
2	2	2	9.89	9.58	6	6	10	18.02	15.72	4	4	12	0.00	9.45
2	2	2	54.93	52.15	6	6	12	57.75	57.44	4	4	14	13.00	13.25
2	2	2	12.00	11.27	6	6	14	10.73	6.86	4	4	16	40.01	33.97
2	2	2	0.00	6.64	6	6	16	0.00	10.19	5	5	0	12.59	9.02
2	2	2	10.24	24.22	6	6	0	0.00	10.19	5	5	2	0.00	2.74
2	2	2	22.22	24.22	6	6	2	36.54	33.10	5	5	4	18.17	11.96
2	2	2	60.78	57.75	6	6	4	15.97	15.36	5	5	6	0.00	11.96
2	2	2	16.32	23.63	6	6	6	12.98	9.41	5	5	8	0.00	3.28
2	2	2	24.17	24.04	6	6	8	42.96	44.88	5	5	10	32.93	32.88
2	2	2	0.00	1.82	6	6	10	26.46	17.56	5	5	12	9.05	7.44
2	2	2	29.74	27.76	6	6	12	14.90	12.62	5	5	14	36.14	34.01
2	2	2	0.00	8.09	6	6	14	14.20	18.79	5	5	16	0.00	9.56
2	2	2	27.08	25.69	6	6	16	18.64	18.79	5	5	18	12.98	12.77
2	2	2	46.21	48.57	6	6	18	31.80	33.81	6	6	20	32.38	39.52
2	2	2	34.43	33.90	6	6	20	30.06	31.99	6	6	22	3.40	7.52
2	2	2	12.05	7.16	6	6	22	0.00	2.91	6	6	24	6.91	19.19
2	2	2	21.38	21.07	6	6	24	18.92	14.83	6	6	26	3.47	2.57
2	2	2	0.00	3.83	6	6	26	16.10	12.00	6	6	28	53.46	63.40
2	2	2	0.00	2.43	6	6	28	13.78	11.96	6	6	30	13.62	10.28
2	2	2	0.00	3.83	6	6	30	10.04	5.59	6	6	32	33.02	32.69
2	2	2	45.04	41.97	6	6	32	45.29	47.31	6	6	34	11.37	1.81
2	2	2	38.37	35.58	6	6	34	16.29	18.09	6	6	36	24.16	25.87
2	2	2	143.42	142.22	6	6	36	0.00	2.87	6	6	38	42.30	38.61
2	2	2	137.09	136.71	6	6	38	40.59	44.91	6	6	40	0.00	3.65
2	2	2	23.09	24.85	6	6	40	13.06	18.45	6	6	42	0.00	148.63
2	2	2	23.02	26.31	6	6	42	0.00	4.47	6	6	44	145.76	3.65
2	2	2	100.10	94.55	6	6	44	45.12	42.56	6	6	46	23.94	25.98
2	2	2	87.03	85.29	6	6	46	8.39	8.12	6	6	48	40.02	40.25
2	2	2	46.06	47.70	6	6	48	35.88	34.91	6	6	50	53.04	52.91
2	2	2	0.00	0.00	6	6	50	0.00	0.00	6	6	52	0.00	0.00

STRUCTURE FACTORS
H K L F(OBS) F(CALC)

H K L F(OBS) F(CALC)

0	0	0	37.05	42.30	0.00	LR	3.59
0	0	8	62.04	59.64	47.51	LR	49.15
0	0	12	28.61	27.55	0.00	LR	0.38
0	0	14	100.02	101.73	0.00	LR	1.11
1	1	8	0.00	4.75	0.00	LR	1.26
1	1	8	35.49	34.72	0.00	LR	13.24
1	1	8	18.04	15.89	13.64	LR	6.25
1	1	8	9.80	9.96	30.07	LR	27.80
1	1	8	37.67	41.20	61.73	LR	55.87
1	1	8	56.76	55.71	11.71	LR	7.34
1	1	8	23.96	20.33	23.80	LR	22.31
1	1	8	0.00	0.71	48.39	LR	54.02
1	1	8	0.00	1.16	41.66	LR	44.46
1	1	8	50.53	49.29	10.53	LR	20.42
1	1	8	21.97	25.24	43.70	LR	4.41
1	1	8	0.00	8.13	0.00	LR	39.96
1	1	8	9.03	23.25	0.00	LR	1.94
1	1	8	20.21	24.68	11.85	LR	3.27
1	1	8	3.60	12.91	12.30	LR	7.51
1	1	8	28.27	28.34	10.74	LR	19.60
2	2	8	0.00	14.92	0.00	LR	2.53
2	2	8	53.95	54.53	41.99	LR	40.10
2	2	8	22.51	23.32	15.50	LR	17.77
2	2	8	78.67	75.62	31.48	LR	29.63
2	2	8	33.71	29.96	0.00	LR	3.80
2	2	8	39.79	42.13	0.00	LR	17.59
2	2	8	0.00	6.85	0.00	LR	18.80
2	2	8	38.86	37.59	20.94	LR	1.35
2	2	8	14.62	14.50	10.77	LR	10.96
2	2	8	56.36	55.19	5.52	LR	15.64
2	2	8	10.32	4.59	13.17	LR	4.59
2	2	8	40.28	40.54	11.07	LR	11.78
2	2	8	20.48	22.93	10.65	LR	3.62
2	2	8	0.00	12.13	7.24	LR	0.15
2	2	8	26.84	27.96	0.00	LR	19.65
2	2	8	22.83	23.07	18.56	LR	4.22
2	2	8	27.47	25.36	12.12	LR	4.87
2	2	8	30.86	31.07	16.39	LR	6.08
2	2	8	43.34	43.02	9.20	LR	1.59
2	2	8	0.00	13.93	11.76	LR	20.73
2	2	8	13.60	9.42	41.26	LR	43.03
2	2	8	5.81	9.00	45.23	LR	47.52
2	2	8	29.68	31.01	11.59	LR	5.90
2	2	8	17.77	16.17	29.34	LR	34.67
2	2	8	16.06	13.15	5.86	LR	16.22
2	2	8	7.35	5.73	29.16	LR	72.32
2	2	8	0.00	2.60	0.00	LR	27.76
2	2	8	15.46	19.45	0.00	LR	6.50
2	2	8	36.47	38.05	32.62	LR	53.70
2	2	8	12.13	3.25	14.44	LR	5.93
2	2	8	20.32	16.43	8.64	LR	3.06
2	2	8	0.00	5.15	13.59	LR	6.42
2	2	8	11.69	8.10	0.00	LR	0.27
2	2	8	0.00	6.09	11.20	LR	6.12
2	2	8	21.71	24.62	7.98	LR	12.74
2	2	8	35.41	33.97	21.29	LR	19.82
2	2	8	0.00	5.36	29.34	LR	29.55
2	2	8	13.45	13.13	6.31	LR	10.94
2	2	8			21.65	LR	17.22

Table 4. Fractional atomic coordinates, displacement parameters, and site occupancies (F).

	Antarctica	Norway	Eifel B93	Eifel Nick.	Japan Shimizu	Japan Hayasaki	Sardinia	Oregon	
C	P(K)	0.91(1)	0.90(1)	0.48(1)	0.69(1)	0.74(1)	0.76(1)	0.75(1)	0.69(1)
	x	0	0	0	0	0	0	0	
	y	0	0	0	0	0	0	0	
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	
	B _{eq.}	2.37(3)	2.59(9)	2.50(9)	2.69(4)	2.78(2)	2.80(3)	2.89(4)	2.68(3)
	U ₁₁	0.0255(7)	0.029(3)	0.029(3)	0.030(1)	0.0307(8)	0.031(1)	0.032(1)	0.030(1)
	U ₂₂	0.0255	0.029	0.029	0.030	0.0307	0.031	0.032	0.030
	U ₃₃	0.031(1)	0.031(4)	0.028(4)	0.033(2)	0.034(1)	0.034(1)	0.035(2)	0.032(1)
	U ₁₂	0.0127	0.014	0.014	0.015	0.015	0.016	0.016	0.016
A	P(Fe)	0.01(1)	0.16(2)	0.67(1)	0.01(1)	0.56(1)	0.58(1)	0.41(1)	0.51(1)
	x	1/3	1/3	1/3	1/3	1/3	1/3	1/3	
	y	2/3	2/3	2/3	2/3	2/3	2/3	2/3	
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	
	B _{eq.}	0.61(2)	0.67(5)	0.69(2)	0.58(2)	0.699(7)	0.66(1)	0.66(1)	0.734(8)
	U ₁₁	0.0054(6)	0.007(1)	0.0068(5)	0.0053(6)	0.0072(2)	0.0066(3)	0.0068(3)	0.0073(3)
	U ₂₂	0.0054	0.007	0.0068	0.0053	0.0072	0.0066	0.0068	0.0073
	U ₃₃	0.0107(8)	0.009(2)	0.0105(7)	0.0098(8)	0.0099(3)	0.0097(4)	0.0090(5)	0.0100(3)
	U ₁₂	0.0027	0.0035	0.0034	0.0027	0.0036	0.0033	0.0034	0.0038
Γ1	Si, Al								
	x	0.24821(6)	0.2501(2)	0.2466(1)	0.24734(6)	0.24750(4)	0.24738(6)	0.24725(7)	0.24775(6)
	y	0.35359(6)	0.3554(2)	0.3538(1)	0.35333(7)	0.35074(5)	0.35055(6)	0.35136(7)	0.35119(6)
	z	0.39206(4)	0.3921(1)	0.39217(5)	0.39204(4)	0.39191(3)	0.39187(4)	0.39189(4)	0.39208(3)
	B _{eq.}	0.756(9)	0.72(2)	1.03(1)	0.813(9)	0.769(8)	0.758(9)	0.80(1)	0.859(9)
	U ₁₁	0.0086(3)	0.0084(8)	0.0113(5)	0.0094(3)	0.0088(2)	0.088(3)	0.0093(3)	0.0099(3)
	U ₂₂	0.0099(3)	0.0100(8)	0.0137(5)	0.0107(3)	0.0105(2)	0.0105(3)	0.0115(3)	0.0118(3)
	U ₃₃	0.0077(3)	0.0058(6)	0.0100(3)	0.0080(3)	0.0068(2)	0.0069(2)	0.0068(3)	0.0077(2)
	U ₁₂	0.0055(2)	0.0046(6)	0.0063(4)	0.0060(2)	0.0055(2)	0.0056(2)	0.0060(2)	0.0062(2)
	U ₁₃	0.0015(2)	0.0010(6)	0.0018(4)	0.0016(2)	0.0013(1)	0.0014(2)	0.0014(2)	0.0012(2)
	U ₂₃	0.0017(2)	0.0010(6)	0.0006(5)	0.0017(2)	0.0013(1)	0.0014(2)	0.0015(2)	0.0011(2)
Γ2	P(Fe)	0.01(1)	0.03(1)	0.08(1)	0.08(1)	0.06(1)	0.07(1)	0.06(1)	0.06(1)
	x	1/2	1/2	1/2	1/2	1/2	1/2	1/2	
	y	1/2	1/2	1/2	1/2	1/2	1/2	1/2	
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	
	B _{eq.}	0.70(1)	0.75(4)	1.91(3)	1.15(1)	0.753(8)	0.77(1)	0.82(1)	0.99(1)
	U ₁₁	0.0091(5)	0.010(1)	0.029(1)	0.0163(5)	0.0102(3)	0.0105(5)	0.0116(4)	0.0139(4)
	U ₂₂	0.0091	0.010	0.029	0.0163	0.0102	0.0105	0.0116	0.0139
	U ₃₃	0.0068(5)	0.006(1)	0.0117(8)	0.0091(5)	0.0063(3)	0.0069(5)	0.0061(5)	0.0079(4)
	U ₁₂	0.0072(5)	0.007(1)	0.026(1)	0.0137(5)	0.0073(5)	0.0080(4)	0.0089(5)	0.0107(4)
Γ1	Al								
	x	0.1229(3)	0.1238(8)	0.1252(4)	0.1237(3)	0.1198(2)	0.1198(3)	0.1207(3)	0.1204(3)
	y	0.4079(3)	0.4090(7)	0.4085(4)	0.4071(3)	0.4044(2)	0.4041(3)	0.4049(3)	0.4061(3)
	z	0	0	0	0	0	0	0	
	B _{eq.}	1.63(4)	1.6(1)	1.86(6)	1.71(4)	1.75(3)	1.66(4)	1.69(5)	1.74(4)
	U ₁₁	0.026(1)	0.025(4)	0.026(2)	0.027(1)	0.0278(9)	0.027(1)	0.027(1)	0.026(1)
	U ₂₂	0.020(1)	0.017(3)	0.024(2)	0.022(1)	0.0214(9)	0.019(1)	0.021(1)	0.023(1)
	U ₃₃	0.0072(9)	0.009(2)	0.010(1)	0.0079(9)	0.0086(6)	0.0080(9)	0.007(1)	0.0081(8)
	U ₁₂	0.011(1)	0.004(3)	0.010(2)	0.012(1)	0.0118(7)	0.010(1)	0.010(1)	0.012(1)
2									
	x	0.2166(2)	0.2196(6)	0.2208(4)	0.2176(2)	0.2145(2)	0.2144(2)	0.2152(2)	0.2159(2)
	y	0.2847(2)	0.2911(6)	0.2878(3)	0.2851(2)	0.2833(2)	0.2830(2)	0.2833(2)	0.2851(2)
	z	0.1320(1)	0.1327(3)	0.1323(2)	0.1318(1)	0.13159(9)	0.1319(1)	0.1316(1)	0.1313(1)
	B _{eq.}	2.35(3)	2.5(1)	2.69(5)	2.34(3)	2.28(2)	2.30(3)	2.33(4)	2.31(3)
	U ₁₁	0.028(1)	0.029(3)	0.032(2)	0.027(1)	0.0261(7)	0.025(1)	0.027(1)	0.0260(9)
	U ₂₂	0.035(1)	0.043(3)	0.036(2)	0.033(1)	0.0336(7)	0.035(1)	0.035(2)	0.034(1)
	U ₃₃	0.0228(9)	0.021(2)	0.029(1)	0.0245(9)	0.0228(6)	0.0233(9)	0.0223(9)	0.0236(8)
	U ₁₂	0.0244(9)	0.030(3)	0.027(1)	0.0238(9)	0.0233(6)	0.0239(9)	0.024(1)	0.0232(8)
	U ₁₃	-0.0017(8)	-0.005(2)	0.006(1)	-0.0001(8)	-0.0011(5)	-0.0011(7)	-0.0015(8)	-0.0004(7)
	U ₂₃	-0.0048(8)	-0.004(2)	0.001(1)	-0.0025(8)	-0.0036(6)	-0.0036(7)	-0.0035(8)	-0.0018(7)
3									
	x	0.1398(2)	0.1383(5)	0.1416(3)	0.1410(2)	0.1373(1)	0.1371(2)	0.1383(2)	0.1375(2)
	y	0.4934(2)	0.4936(5)	0.4949(3)	0.4937(2)	0.4904(1)	0.4905(2)	0.4913(2)	0.4909(2)
	z	0.1790(1)	0.1789(3)	0.1790(1)	0.1787(1)	0.17887(8)	0.1789(1)	0.1787(1)	0.17918(9)
	B _{eq.}	1.18(2)	1.25(6)	1.68(4)	1.27(2)	1.32(2)	1.30(2)	1.34(3)	1.34(2)
	U ₁₁	0.0138(7)	0.016(2)	0.022(1)	0.0153(7)	0.0164(5)	0.0159(7)	0.0163(8)	0.0160(7)
	U ₂₂	0.0155(7)	0.016(2)	0.023(1)	0.0169(7)	0.0176(5)	0.0167(7)	0.0177(8)	0.0184(7)
	U ₃₃	0.0117(7)	0.012(2)	0.0140(8)	0.0120(7)	0.0120(5)	0.0123(7)	0.0124(7)	0.0122(6)
	U ₁₂	0.0087(6)	0.010(2)	0.015(1)	0.0102(6)	0.0106(4)	0.0098(6)	0.0102(7)	0.0105(6)
	U ₁₃	-0.0037(6)	-0.003(2)	-0.002(1)	-0.0036(6)	-0.0028(4)	-0.0030(6)	-0.0034(7)	-0.0020(5)
	U ₂₃	-0.0049(6)	-0.005(2)	-0.002(1)	-0.0048(6)	-0.0049(4)	-0.0048(6)	-0.0054(8)	-0.0041(5)

Note: Standard deviations are in parentheses. The displacement parameters are of the form:

$$\langle r^2 \rangle = \frac{1}{3} (U_{11} + U_{22} + U_{33})$$

Table 5. Selected interatomic distances and angles

	Antarctica	Norway	Eifel B93	Eifel Nk.	Japan Shi.	Japan Hay.	Sardinia	Oregon
C-01 (12x)	3.099(2)	3.141(8)	3.120(4)	3.100(3)	3.099(2)	3.096(2)	3.097(3)	3.115(2)
A (Mg,Fe,Al) octahedron								
A-03 (6x)	2.118(2)	2.128(5)	2.100(3)	2.110(2)	2.151(2)	2.154(2)	2.142(2)	2.145(2)
03-03(3x)	2.553(3)	2.544(8)	2.542(5)	2.560(3)	2.579(2)	2.577(3)	2.577(3)	2.568(3)
03-03(3x)	2.964(3)	2.991(9)	2.945(5)	2.951(3)	2.987(2)	2.992(3)	2.980(4)	2.982(3)
03-03(6x)	3.219(2)	3.238(7)	3.185(4)	3.200(2)	3.285(2)	3.288(2)	3.262(4)	3.277(3)
T1 (Si,Al) tetrahedron								
T1-01	1.6197(7)	1.616(2)	1.617(1)	1.6171(9)	1.6185(7)	1.6182(9)	1.618(1)	1.6208(8)
T1-02	1.625(4)	1.622(12)	1.622(7)	1.620(4)	1.621(3)	1.624(4)	1.622(4)	1.620(4)
T1-02	1.635(3)	1.658(8)	1.626(4)	1.628(3)	1.630(2)	1.629(3)	1.628(3)	1.630(3)
T1-03	1.630(2)	1.621(4)	1.638(4)	1.627(2)	1.632(1)	1.635(2)	1.629(2)	1.636(2)
O1-T1-02	111.4(2)	110.9(6)	111.3(3)	111.1(2)	111.3(1)	111.3(2)	111.2(2)	111.3(2)
O1-T1-03	111.3(1)	111.7(3)	111.0(2)	111.3(2)	110.9(1)	110.9(1)	111.0(1)	110.9(1)
O1-T1-02	112.1(2)	112.2(5)	112.2(3)	111.9(2)	111.6(2)	111.9(1)	111.6(3)	111.7(2)
O2-T1-03	110.1(1)	109.1(4)	109.5(2)	110.1(1)	110.4(1)	110.4(1)	110.5(1)	110.0(1)
O2-T1-02	105.6(1)	108.1(3)	107.9(2)	106.3(1)	106.0(1)	105.9(1)	105.9(1)	106.9(1)
O3-T1-02	105.9(1)	104.6(4)	104.7(2)	106.0(1)	106.3(1)	106.2(4)	106.3(2)	105.8(1)
T2 (Al,Mg,Fe) tetrahedron								
T2-03 (4x)	1.767(3)	1.756(9)	1.772(5)	1.775(3)	1.766(2)	1.764(3)	1.769(3)	1.762(3)
03-03 (2x)	2.553(3)	2.544(8)	2.542(5)	2.560(3)	2.579(2)	2.577(3)	2.577(3)	2.568(3)
03-03 (2x)	2.889(3)	2.862(8)	2.905(5)	2.906(3)	2.888(2)	2.885(3)	2.893(3)	2.884(3)
03-03 (2x)	3.178(2)	3.162(6)	3.198(3)	3.195(2)	3.155(2)	3.153(2)	3.168(2)	3.152(2)
03-T2-03(2x)	92.5(1)	92.8(3)	91.6(2)	92.3(1)	93.81(7)	93.8(1)	93.5(1)	93.5(1)
03-T2-03(2x)	109.7(1)	109.2(3)	110.1(2)	109.9(1)	109.75(8)	109.7(1)	109.7(1)	109.8(1)
03-T2-03(2x)	128.2(1)	128.5(2)	128.9(1)	128.33(7)	126.56(4)	126.63(7)	127.08(7)	126.80(6)
T1-01-T1	145.2(2)	145.7(5)	145.0(3)	145.6(2)	145.3(1)	145.3(2)	145.5(2)	144.5(1)
T1-02-T1	153.3(1)	153.8(3)	153.8(2)	153.8(1)	154.0(1)	153.7(1)	153.9(1)	154.4(1)
T1-03-T2	124.3(1)	124.8(2)	123.9(1)	124.0(1)	125.05(6)	125.07(8)	124.8(1)	125.0(2)

Note: standard deviations are in parentheses.