

## Roebingite, $\text{Pb}_2\text{Ca}_6(\text{SO}_4)_2(\text{OH})_2(\text{H}_2\text{O})_4[\text{Mn}(\text{Si}_3\text{O}_9)_2]$ : its crystal structure and comments on the lone pair effect

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### Abstract

Roebingite,  $\text{Pb}_2\text{Ca}_6(\text{SO}_4)_2(\text{OH})_2(\text{H}_2\text{O})_4[\text{Mn}(\text{Si}_3\text{O}_9)_2]$ , monoclinic holosymmetric,  $a = 13.208(4)$ ,  $b = 8.287(2)$ ,  $c = 13.089(9)\text{\AA}$ ,  $\beta = 106.65(6)^\circ$ , space group  $C2/m$ , possesses a  $2[\text{Mn}(\text{Si}_3\text{O}_9)_2]^{10-}$  corner-linked sheet oriented parallel to  $c\{001\}$ , the plane of perfect micaceous cleavage.  $R = 0.066$  for 2479 nonequivalent reflections.

The large cations are tucked between the  $[\text{Mn}(\text{Si}_3\text{O}_9)_2]$  sheets. All vertices of the  $\text{MnO}_6$  octahedron link to the  $(\text{Si}_3\text{O}_9)$  radicals which are oligosilicate three-membered rings and are geometrically similar to the rings in paragenetically related margarosanite,  $\text{PbCa}_2[\text{Si}_3\text{O}_9]$ . Coordination polyhedra include  $\text{Pb}\phi_7$  (maximal point symmetry  $mm2$ );  $\text{Ca}(1)\phi_8$  distorted square antiprisms;  $\text{Ca}(2)\phi_7$  polyhedra similar to  $\text{Pb}\phi_7$ ;  $\text{MnO}_6$  octahedra;  $\text{SiO}_4$ ,  $\text{SO}_4$  tetrahedra. Mean bond distances are:  $\text{Pb}-\text{O}$  2.82 (2.22 to 3.42),  $\text{Ca}(1)-\text{O}$  2.53,  $\text{Ca}(2)-\text{O}$  2.43,  $\text{Mn}-\text{O}$  2.22,  $\text{Si}(1)-\text{O}$  1.64,  $\text{Si}(2)-\text{O}$  1.62 and  $\text{S}-\text{O}$  1.47\AA.

The packing efficiency, defined as the volume of the unit cell divided by the total number of anions in that cell, is usually close to the values of hcp or ccp oxysalt structures for most minerals which don't have channels. This value,  $V_E$ , is unusually large for  $\text{Pb}(\text{II})$  oxysalts. By including the number of lone pair cations for that cell, the value,  $V_{E+L}$ , is more reasonable and approximates the packing efficiencies for oxysalts with those cations of similar size but stripped of all valence electrons.

### Introduction

Roebingite is an exotic phase, presently known from two localities. It was described from the type locality at Franklin, New Jersey (Penfield and Foote, 1897) as a sulfite-bearing silicate; Blix (1931) showed that it is a sulfate-bearing silicate, based on the Franklin material and a more recent find from Långban, Sweden where it occurred as fracture fillings. Foit (1966) examined its crystallographic character on coarse platy Långban material. We agree with his findings, except that the space group appears to be  $C2/m$ , not  $C2/c$ . Finally, Dunn et al. (1982) reported several new chemical analyses on roebingite, but the differences from the Blix analysis are small. We include their chemical analysis for a Långban roebingite in Table 1.

The senior author has long been interested in roebingite; over fifteen years ago, crystals were secured from the Swedish Natural History Museum with plans of eventual-

ly unravelling its structure, and especially determining the role of the sulfur cation. More recently, increased interest in  $\text{Pb}(\text{II})$  from oxysalt and sulfosalt environments and the micaceous nature of the material prompted a more detailed structure investigation.

### Experimental procedure

At least ten chemical analyses have been reported in the literature, and three are selected for Table 1. One of the motivations for the present study concerns the formal charge on sulfur: is it  $\text{S}^{4+}$  or  $\text{S}^{6+}$ ? Penfield and Foote (1897) were cautious in their study and reported  $\text{SO}_2$  as the oxide. However, Blix (1931) re-investigated the problem, analyzing Franklin material and the recent find of Långban material. He concluded that sulfur occurred as  $\text{SO}_3$ , a conclusion we similarly make on the basis of structure study, for Långban material at least.

A small vial of palest pink flakes from Långban,

Moore, P.B. and Shen, J.

Table 3. Roebbingite. Structure factors.  $R=0.066$

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR										ROEBLINGITE DATA RED 2/19/82										PAGE 1					
H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC						
4	0	0	43	-31	0	4	0	545	495	13	7	0	39	-46	8	12	0	50	25	15	1	1	1	56	-64
6	0	0	164	-151	2	4	0	61	-45	15	7	0	89	-88	1	13	0	55	37	17	1	1	1	55	53
8	0	0	30	-16	4	4	0	35	-27	17	7	0	46	-35	5	13	0	86	-87	-18	2	1	1	85	-95
10	0	0	169	164	6	4	0	179	-173	0	8	0	252	249	-20	0	1	87	80	-16	2	1	1	76	-64
14	0	0	56	-65	8	4	0	88	86	2	8	0	61	-55	-18	0	1	55	-58	-14	2	1	1	65	-72
18	0	0	71	75	10	4	0	193	191	4	8	0	53	-31	-16	0	1	55	-191	-12	2	1	1	141	134
20	0	0	119	123	12	4	0	40	28	6	8	0	100	-91	-14	0	1	77	-69	-10	2	1	1	75	69
3	1	1	163	153	14	4	0	104	-91	8	8	0	54	58	-10	0	1	65	61	-8	2	1	1	148	-145
5	1	1	173	-178	16	4	0	40	-26	10	8	0	133	129	-8	0	1	65	-63	-6	2	1	1	112	-115
7	1	1	280	-279	18	4	0	50	32	12	8	0	56	40	-6	0	1	446	-461	-4	2	1	1	111	-116
9	1	1	98	190	1	5	0	129	110	14	8	0	76	-77	-4	0	1	178	179	-2	2	1	1	260	230
11	1	1	194	95	3	5	0	100	-78	16	8	0	42	-36	0	0	1	235	226	0	2	1	1	282	240
15	1	1	154	-151	5	5	0	306	-285	1	9	0	50	33	2	0	1	44	-14	0	2	2	1	281	-300
19	1	1	46	32	7	5	0	169	157	3	9	0	52	-9	2	0	1	231	-231	2	2	2	1	238	-237
2	2	2	411	334	9	5	0	62	51	5	9	0	151	-143	4	0	1	145	144	6	2	2	1	121	-125
4	2	2	57	-49	11	5	0	142	-142	7	9	0	52	16	8	0	1	145	144	8	2	2	1	121	-125
6	2	2	244	-242	15	5	0	43	31	9	9	0	155	152	4	0	1	145	144	8	2	2	1	122	113
8	2	2	94	93	19	5	0	485	471	11	9	0	135	60	12	0	1	36	-35	12	2	2	1	165	-170
10	2	2	215	211	19	5	0	137	-130	15	9	0	175	185	14	0	1	111	-124	14	2	2	1	165	-170
12	2	2	105	106	4	6	0	190	-183	15	9	0	51	45	18	0	1	58	-73	16	2	2	1	81	-31
14	2	2	87	-94	6	6	0	67	-48	2	10	0	125	-122	-15	1	1	71	-57	20	2	2	1	46	51
16	2	2	101	-97	6	6	0	96	88	8	10	0	97	89	-13	1	1	70	64	-17	3	3	1	73	-61
18	2	2	93	93	8	6	0	38	31	10	10	0	78	69	-11	1	1	245	238	-13	3	3	1	149	149
20	2	2	45	51	10	6	0	50	-40	12	10	0	48	33	-9	1	1	64	63	-11	3	3	1	164	161
5	3	3	92	82	14	6	0	46	-27	1	11	0	73	77	-7	1	1	206	-201	-9	3	3	1	68	-60
7	3	3	164	-150	16	6	0	113	113	5	11	0	81	-84	-5	1	1	95	-96	-7	3	3	1	257	-245
9	3	3	61	-53	18	6	0	120	121	5	11	0	79	-83	-3	1	1	180	183	-5	3	3	1	288	-285
11	3	3	258	259	3	7	0	157	-139	7	11	0	90	-77	-1	1	1	224	226	-1	3	3	1	276	222
13	3	3	132	129	5	7	0	101	-84	9	11	0	88	80	1	1	1	31	48	3	3	3	1	239	210
15	3	3	62	-51	7	7	0	89	-85	11	11	0	54	49	3	1	1	279	-281	5	3	3	1	107	-109
17	3	3	160	-153	9	7	0	127	123	12	12	0	183	208	9	1	1	263	253	7	7	7	1	122	121
17	3	3	51	-51	11	7	0	97	91	6	12	0	76	-75	13	1	1	136	-139	9	3	3	1	140	127

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ROEBLINGITE DATA RED 2/19/82

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC						
11	3	3	56	-56	-10	6	6	1	58	59	8	8	1	95	84	12	12	1	85	74	7	9	1	138	135
13	3	3	141	-145	-8	6	6	1	135	-111	8	8	1	50	-38	2	12	1	86	-89	9	1	1	42	41
15	3	3	79	-76	-6	6	6	1	142	-139	8	8	1	222	-207	4	12	1	135	-130	11	1	1	231	-234
17	3	3	87	98	-2	6	6	1	210	177	8	8	1	59	62	6	12	1	51	-37	13	1	1	96	-85
19	3	3	105	112	0	6	6	1	52	52	8	8	1	47	-58	8	12	1	52	52	17	1	1	125	115
-15	4	4	146	-149	2	6	6	1	279	-257	14	8	1	81	-84	-1	13	1	99	87	-18	1	1	117	-112
-12	4	4	95	96	4	6	6	1	239	-224	16	8	1	53	-3	3	13	1	56	-50	-14	1	1	61	65
-8	4	4	38	-41	6	6	6	1	71	-69	-13	9	1	73	58	0	0	2	51	-43	-12	2	2	92	93
-6	4	4	277	-273	8	6	6	1	81	98	-11	9	1	170	156	-20	0	93	-100	-8	2	2	57	-68	
-2	4	4	238	220	10	6	6	1	126	133	-9	9	1	77	-62	-18	0	102	98	-6	2	2	118	-121	
0	4	4	105	85	12	6	6	1	110	-104	-7	9	1	133	-127	-14	0	338	355	-4	2	2	385	389	
2	4	4	124	-118	14	6	6	1	63	-44	-5	9	1	127	-124	-12	0	68	-71	-2	2	2	155	137	
4	4	4	358	-359	-17	7	7	1	68	-68	-1	9	1	176	176	-8	0	79	-72	0	2	2	51	58	
8	4	4	115	120	-15	7	7	1	51	-30	3	9	1	61	49	-6	0	77	-80	2	2	2	379	-388	
10	4	4	35	18	-13	7	7	1	129	75	9	9	1	73	-76	-4	0	105	108	4	2	2	187	-188	
12	4	4	63	-65	-11	7	7	1	70	110	9	9	1	121	117	-2	0	172	192	6	2	2	284	280	
14	4	4	101	-101	-9	7	7	1	145	-142	11	9	1	84	-94	0	0	243	-249	8	2	2	74	75	
18	4	4	83	90	-7	7	7	1	111	-111	13	9	1	85	-94	2	2	250	247	10	2	2	134	136	
-18	5	5	60	-61	-5	7	7	1	154	138	-6	10	1	89	68	4	4	97	93	12	2	2	70	-63	
-13	5	5	55	44	-3	7	7	1	65	67	-2	10	1	113	116	0	0	230	233	16	2	2	84	80	
-11	5	5	250	227	-1	7	7	1	90	84	0	10	1	56	66	8	8	92	94	-13	3	3	172	-176	
-9	5	5	54	25	1	7	7	1	146	-140	2	10	1	135	-117	10	0	171	-171	-7	3	3	242	-250	
-7	5	5	114	-108	3	7	7	1	51	-57	4	10	1	145	-136	18	0	81	91	-5	3	3	298	267	
-5	5	5	78	-70	5	7	7	1	128	125	8	10	1	65	62	-19	1	59	-59	-3	3	3	224	184	
-3	5	5	122	124	7	7	7	1	141	123	12	10	1	89	73	-13	1	108	-103	1	3	3	236	-222	
-1	5	5	288	239	9	7	7	1	41	35	-9	11	1	85	-55	1	1	163	-164	-1	3	3	211	-221	
3	5	5	238	-216	11	7	7	1	113	-101	-7	11	1	63	-51	-5	1	67	57	3	3	3	40	22	
7	5	5	92	96	13	7	7	1	81	-73	3	11	1	113	112	-3	1	325	-338	7	3	3	21	22	
13	5	5	240	241	15	7	7	1	80	77	-7	11	1	113	112	5	1	219	226	9	3	3	103	104	
-13	6	6	114	-113	-17	8	8	1	94	-84	3	11	1	104	-104	-3	1	219	226	11	3	3	224	-223	
-14	6	6	87	-80	-16	8	8	1	68	63	9	11	1	107	107	3	1	241	-248	13	3	3	58	-79	
-12	6	6	131	-122	-12	8	8	1	183	-172	7	11	1	86	85	1	1	70	69	15	3	3	41	4	

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ROEBLINGITE DATA RED 2/19/82 PAGE 3

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
17	3	2	107	99	-4	6	2	190	178	-3	9	2	171	163	-4	0	3	194	189	-2	2	3	66	66
-18	4	2	82	-85	0	6	2	43	15	1	9	2	55	-54	0	0	3	200	-211	0	2	3	497	-480
-12	4	2	216	211	2	6	2	174	-162	3	9	2	187	-179	0	0	3	69	-81	2	2	3	106	-109
-10	4	2	83	-79	4	6	2	44	-31	5	9	2	42	23	4	0	3	224	211	4	2	3	74	69
-8	4	2	65	-65	6	6	2	257	263	11	9	2	97	-86	6	0	3	243	243	6	2	3	268	267
-4	4	2	185	168	8	6	2	105	105	13	9	2	85	-76	8	0	3	94	-93	8	2	3	37	39
-2	4	2	319	275	10	6	2	40	-37	-14	10	2	56	43	10	0	3	51	-37	10	2	3	212	-209
0	4	2	100	-82	12	6	2	97	-106	-12	10	2	109	93	12	0	3	140	-147	12	2	3	119	-121
2	4	2	351	-345	14	6	2	72	-72	-8	10	2	69	-49	14	0	3	90	82	14	2	3	58	54
4	4	2	35	25	16	6	2	58	62	-4	10	2	147	142	16	0	3	104	90	18	2	3	45	29
6	4	2	92	98	-13	7	2	110	111	-2	10	2	74	69	18	0	3	41	-10	-19	3	3	73	-66
8	4	2	198	196	-9	7	2	134	-146	2	10	2	141	-140	-15	1	3	128	127	-17	3	3	70	-64
12	4	2	98	107	-7	7	2	140	-146	6	10	2	105	98	-13	1	3	63	67	-15	3	3	109	109
16	4	2	68	51	-3	7	2	167	137	8	10	2	79	73	-11	1	3	66	-68	-13	3	3	76	81
18	4	2	69	69	-1	7	2	86	72	-9	11	2	119	-115	-9	1	3	66	-68	-11	3	3	75	75
-19	5	2	50	-54	1	7	2	124	-118	-7	11	2	88	-85	-9	1	3	118	122	-9	3	3	182	-160
-17	5	2	113	-114	3	7	2	116	-123	-3	11	2	61	65	-5	1	3	250	245	-7	3	3	79	81
-13	5	2	136	128	7	7	2	101	91	1	11	2	81	-99	-3	1	3	438	446	-5	3	3	311	284
-9	5	2	123	-123	9	7	2	49	60	3	11	2	55	-37	-1	1	3	107	-114	-3	3	3	175	170
-7	5	2	282	-280	11	7	2	205	-206	9	11	2	60	49	1	1	3	132	-138	-1	3	3	127	-122
-5	5	2	53	53	13	7	2	74	-41	11	11	2	148	-138	1	1	3	52	-54	1	3	3	88	-83
-3	5	2	194	147	15	7	2	43	-19	-4	12	2	48	53	5	1	3	170	162	3	3	3	95	-91
1	5	2	103	-82	-12	8	2	123	113	2	12	2	85	-90	7	1	3	83	-78	5	3	3	387	430
3	5	2	103	-82	-12	8	2	77	-55	6	12	2	96	96	9	1	3	90	-93	7	3	3	195	202
5	5	2	113	116	-6	8	2	49	-30	8	12	2	79	81	11	1	3	174	173	9	3	3	41	-33
7	5	2	98	98	-4	8	2	177	153	3	13	2	61	62	15	1	3	90	-93	11	3	3	78	78
11	5	2	165	-165	-2	8	2	180	159	3	13	2	111	-117	17	1	3	63	70	15	3	3	165	162
13	5	2	88	-94	2	8	2	210	-204	-18	0	3	110	-117	-20	2	3	87	-88	-20	4	3	52	-39
17	5	2	110	108	4	8	2	66	-57	-16	0	3	111	-128	-18	2	3	64	-65	-18	4	3	126	-117
-18	6	2	98	-101	6	8	2	73	78	-14	0	3	146	159	-14	2	3	127	143	-16	4	3	61	71
-14	6	2	131	127	8	8	2	150	-57	-12	0	3	66	-73	-12	2	3	72	69	-14	4	3	129	123
-12	6	2	197	184	12	8	2	52	53	-10	0	3	107	-102	-10	2	3	142	-145	-10	4	3	145	-37
-8	6	2	65	-69	-7	9	2	202	-183	-8	0	3	249	-261	-8	2	3	104	-104	-8	4	3	223	-229
-6	6	2	124	-115	-5	9	2	55	64	-6	0	3	63	68	-4	2	3	139	131	-6	4	3	139	135

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

ROEBLINGITE DATA RED 2/19/82

PAGE 4

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-4	4	3	134	123	12	6	3	69	-72	5	9	3	118	130	2	0	4	41	48	-6	2	4	298	299
-2	4	3	140	-119	14	6	3	66	69	7	9	3	146	144	0	0	4	165	157	-4	2	4	85	86
0	4	3	169	-164	16	6	3	49	40	11	9	3	72	-70	6	0	4	158	161	0	2	4	60	-60
2	4	3	187	-192	-15	7	3	120	118	-14	10	3	59	84	8	0	4	65	-55	2	2	4	53	67
4	4	3	98	91	-9	7	3	159	-150	-10	10	3	81	-80	10	0	4	160	-158	4	2	4	410	434
6	4	3	284	293	-7	7	3	58	24	-8	10	3	89	-79	12	0	4	76	69	8	2	4	211	-204
8	4	3	68	-78	-5	7	3	207	181	-4	10	3	61	50	14	0	4	62	55	4	2	4	112	-111
10	4	3	74	-71	-3	7	3	250	212	0	10	3	134	-136	18	0	4	65	-56	10	2	4	160	151
12	4	3	154	-154	-1	7	3	62	-47	6	10	3	132	131	-21	1	4	89	-70	16	2	4	52	60
-15	5	3	98	101	3	7	3	112	-101	10	10	3	59	-74	-19	1	4	54	-77	-19	3	4	75	-68
-13	5	3	66	67	3	7	3	60	-57	12	10	3	63	-68	-15	1	4	50	42	-15	3	4	114	115
-11	5	3	69	-75	5	7	3	188	185	-9	11	3	125	-116	-13	1	4	51	-44	-11	3	4	221	-221
-9	5	3	225	-217	7	7	3	40	31	-5	11	3	157	148	-11	1	4	157	-166	-9	3	4	89	-86
-7	5	3	124	107	9	7	3	48	-45	-3	11	3	98	100	-9	1	4	78	-74	-5	3	4	137	126
-5	5	3	202	175	11	7	3	53	-56	3	11	3	81	-77	-7	1	4	201	197	-3	3	4	477	-82
-3	5	3	347	312	13	7	3	41	-9	-8	12	3	104	98	-5	1	4	239	237	-1	3	4	159	-175
-1	5	3	91	-83	15	7	3	159	158	-6	12	3	87	-87	-3	1	4	120	-124	1	3	4	81	83
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9	5	3	76	-85	4	8	3	110	-113	6	12	3	80	94	7	1	4	31	-33	11	3	4	55	-50
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17	5	3	72	74	10	8	3	79	-79	-20	0	4	55	-62	13	1	4	97	97	-20	4	4	62	-46
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-14	6	3	164	-166	-15	9	3	66	41	-14	0	4	91	-115	17	1	4	80	-77	-16	4	4	92	97
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6	6	3	132	140	-1	9	3	104	-103	-2	0	4	248	-236	-10	2	4	162	-167	-4	4	4	93	-91
10	6	3	113	-117	1	9	3	85	-83	0	0	4	312	-314	-8	2	4	107	-107	-2	4	4	93	-91

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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6	4	4	96	94	14	6	4	98	101	5	9	4	103	91	-12	0	5	96	-91	17	1	5	94	38
8	4	4	153	-153	-11	7	4	169	-156	7	9	4	98	-108	-10	0	5	38	-28	-18	2	5	64	60
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12	4	4	65	69	-5	7	4	141	128	11	9	4	60	-60	-6	0	5	168	168	-12	2	5	320	-318
14	4	4	62	63	-3	7	4	45	-37	13	9	4	69	-36	-4	0	5	168	-181	-8	2	5	110	100
16	4	4	82	81	-1	7	4	279	-275	-12	10	4	84	-64	-2	0	5	81	-71	-6	2	5	156	150
18	4	4	89	-82	1	7	4	83	-85	-10	10	4	84	-68	0	0	5	164	-173	-4	2	5	43	30
19	5	4	53	37	3	7	4	44	45	-6	10	4	89	89	0	0	5	205	206	-2	2	5	331	-344
15	5	4	86	-73	5	7	4	77	75	-4	10	4	58	39	2	4	0	234	225	2	2	5	213	225
13	5	4	86	-73	5	7	4	44	45	-6	10	4	89	89	0	0	5	158	-146	4	2	5	84	-89
11	5	4	102	-107	9	7	4	136	-138	-2	10	4	49	-45	8	0	5	252	-242	6	2	5	70	-77
9	5	4	53	-47	11	7	4	41	-25	0	10	4	42	-57	8	0	5	34	-29	8	2	5	292	-291
7	5	4	171	162	13	7	4	85	83	4	10	4	135	140	10	0	5	44	30	10	2	5	47	47
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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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-14	4	5	115	-108	-8	6	62	65	65	-9	5	5	84	87	-8	0	6	124	115
-12	4	5	176	-161	-6	6	73	69	69	-7	9	5	157	151	-6	0	6	239	234
-10	4	5	97	-92	-2	6	183	-174	-34	-5	9	5	106	85	-4	0	6	57	-45
-8	4	5	127	114	0	6	37	-34	195	-3	9	5	109	-100	-2	0	6	248	-242
-6	4	5	188	184	2	6	189	195	66	-1	9	5	91	88	0	0	6	302	308
-4	4	5	115	-105	4	6	70	66	66	1	9	5	86	76	2	0	6	61	52
-2	4	5	124	-117	8	6	245	-250	52	3	9	5	72	76	0	0	6	200	-195
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2	4	5	190	190	-17	7	94	92	92	11	9	5	125	117	10	0	6	242	234
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8	4	5	169	-171	-7	7	226	217	47	-8	10	5	71	116	18	0	6	91	-81
12	4	5	85	74	-3	7	156	-157	36	-6	10	5	88	84	-19	1	6	85	86
14	4	5	127	129	5	7	244	251	36	-4	10	5	47	-23	-19	1	6	85	86
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-15	5	5	122	115	9	7	53	-43	43	8	10	5	145	-136	-11	1	6	75	-74
-13	5	5	76	-79	9	7	43	53	53	-7	11	5	100	-107	-9	1	6	141	141
-11	5	5	50	-33	13	7	64	64	64	-3	11	5	93	-90	-5	1	6	83	-75
-9	5	5	69	56	-14	8	114	-94	94	3	11	5	174	179	-3	1	6	294	-302
-7	5	5	115	-109	-12	8	187	-155	55	7	11	5	49	-41	-1	1	6	103	108
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5	5	5	72	-69	0	8	88	-87	87	2	12	5	64	-55	9	1	6	111	105
7	5	5	145	-143	2	8	107	99	99	6	12	5	48	-43	11	1	6	44	36
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11	5	5	44	47	8	8	131	-135	135	1	13	5	73	73	15	1	6	67	-67
13	5	5	62	-61	8	8	64	59	59	-18	0	6	66	75	17	1	6	146	151
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-18	6	5			14	8					0	6				2	6		

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
-14	4	6	67	-63	-14	6	6	100	-89	-9	9	6	126	119	8	0	7	73	71	8	2	7	48	41
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-10	4	6	220	210	-10	6	6	61	59	-3	9	6	136	-133	14	0	7	220	-210	12	2	7	40	-43
-8	4	6	179	169	-8	6	6	200	189	1	9	6	86	84	16	0	7	76	-78	14	2	7	63	-67
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-2	4	6	117	-124	-2	6	6	36	-39	11	9	6	66	49	-13	1	7	61	-45	-15	3	7	111	-121
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2	4	6	99	107	2	6	6	125	131	-8	10	6	142	135	-9	1	7	222	215	-9	3	7	96	38
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6	4	6	151	-150	6	6	6	182	-183	-4	10	6	91	97	-5	1	7	168	-169	-5	3	7	114	-111
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10	4	6	162	160	12	6	6	191	183	10	10	6	77	72	-1	1	7	259	267	-1	3	7	254	201
12	4	6	112	101	14	6	6	46	27	-9	11	6	63	60	3	3	7	149	165	3	3	7	121	152
14	4	6	85	84	16	6	6	62	50	-3	11	6	119	-121	1	1	7	67	-141	1	3	7	247	-248
16	4	6	97	85	18	6	6	137	-127	-1	11	6	58	62	3	3	7	148	-147	3	3	7	90	-89
18	4	6	91	-74	-13	7	7	120	109	1	11	6	101	83	5	1	7	36	-37	5	3	7	77	63
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42	4	6	63	-52	2	8	6	78	84	-8	0	7	131	129	-6	2	7	292	-292	-4	4	7	101	117
44	4	6	89	84	6	8	6	80	-78	-4	0	7	226	-225	-4	2	7	68	74	-4	4	7	235	-240
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52	4	6	84	-66	15	9	6	73	-68	4	0	7	51	-46	4	2	7	141	-137	10	4	7	131	-129

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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-15	5	7	97	-102	1	7	7	120	126	-5	11	7	77	-78	1	1	8	63	-56	3	3	186	-197	
-13	5	7	57	-53	3	7	7	60	-62	-1	11	7	61	63	3	1	8	230	-228	5	3	97	-101	
-11	5	7	137	109	5	7	7	124	-127	1	11	7	85	94	5	1	8	129	-126	7	3	89	85	
-9	5	7	146	145	5	7	7	46	2	5	11	7	75	78	7	1	8	106	100	9	3	172	168	
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8	6	7	63	51	7	9	7	87	-88	-19	1	8	43	-28	-17	2	8	144	-135	-9	5	72	74	
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12	6	7	61	-49	11	9	7	98	33	-15	1	8	98	97	-15	3	8	149	-152	-7	5	271	-272	
-14	6	7	116	-118	-10	10	7	58	81	-13	1	8	90	87	-13	3	8	51	57	-5	5	56	-50	
-17	7	7	88	-49	-4	10	7	142	-148	-11	1	8	90	87	-11	3	8	102	93	-5	5	153	150	
-15	7	7	80	-79	0	10	7	60	79	-9	1	8	75	56	-9	3	8	96	93	3	5	214	-216	
-9	7	7	173	167	4	10	7	93	-98	-7	1	8	275	-282	-7	3	8	95	-85	7	5	92	-92	
-7	7	7	79	-77	6	10	7	63	-70	-5	1	8	80	-76	-5	3	8	77	83	7	5	79	76	
-5	7	7	116	-115	-11	11	7	65	26	-3	1	8	56	55	-3	3	8	184	191	9	5	64	51	

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ROEBLINGITE DATA RED 2/19/82 PAGE 9

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
13	5	8	99	-98	-2	8	8	100	102	-18	0	9	139	-135	-2	2	9	134	136	4	4	9	56	-42
-18	6	8	57	22	0	8	8	77	74	-14	0	9	43	3	0	2	9	47	-41	6	4	9	110	109
-16	6	8	58	-59	2	8	8	76	-88	-10	0	9	95	-98	2	2	9	133	-128	10	4	9	110	109
-14	6	8	104	90	6	8	8	41	-28	-8	0	5	255	-249	4	2	9	76	-78	10	4	9	137	-134
-12	6	8	109	99	8	8	8	155	162	-4	0	9	255	257	6	2	9	78	74	-17	5	9	57	-54
-10	6	8	87	91	12	8	8	52	-40	-2	0	9	137	-140	8	2	9	122	113	-13	5	9	175	164
-8	6	8	101	-109	-15	9	9	67	-67	0	0	9	27	-10	10	2	9	126	-125	-11	5	9	49	52
-6	6	8	195	-195	-11	9	9	59	-47	2	0	9	362	-362	12	2	9	107	-107	-9	5	9	47	-59
-4	6	8	111	112	-9	9	9	106	105	4	0	9	68	-71	-19	3	9	86	-80	-7	5	9	48	-48
-2	6	8	135	133	-7	9	9	110	-116	6	0	9	68	67	-17	3	9	76	-57	-3	5	9	253	259
0	6	8	244	258	-1	9	9	79	79	8	0	9	33	13	-15	3	9	78	71	-1	5	9	34	-27
4	6	8	79	-75	1	9	9	44	-51	12	0	9	104	-99	-13	3	9	140	143	1	5	9	135	-131
6	6	8	37	22	3	9	9	159	-166	16	0	9	93	79	-11	3	9	122	113	3	5	9	102	-102
8	6	8	113	114	5	9	9	48	-44	-19	1	9	55	-59	-9	3	9	112	-105	5	5	9	86	86
10	6	8	39	-6	7	9	9	67	70	-17	1	9	78	-58	-7	3	9	167	-169	7	5	9	163	161
12	6	8	51	-39	9	9	9	87	83	-13	1	9	173	173	-5	3	9	31	5	9	5	67	54	
14	6	8	84	-73	-12	10	8	51	66	-11	1	9	76	74	-3	3	9	131	128	11	5	9	57	-55
-15	7	8	112	-118	-10	10	8	73	75	-9	1	9	71	-63	1	3	9	32	-21	-18	6	9	64	-54
-13	7	8	82	86	-6	10	8	116	-112	-7	1	9	293	-296	3	3	9	116	-120	-16	6	9	39	-81
-11	7	8	78	66	-2	10	8	89	96	-3	1	9	116	-123	5	3	9	148	146	-14	6	9	41	14
-7	7	8	127	-121	0	10	8	101	116	1	1	9	158	-159	7	3	9	143	139	-10	6	9	137	-142
-5	7	8	69	-55	2	10	8	78	-71	3	1	9	116	-123	9	3	9	159	59	-8	6	9	97	-92
-3	7	8	54	45	4	10	8	44	47	5	1	9	127	126	11	3	9	105	-107	-6	6	9	76	-62
-1	7	8	130	131	6	10	8	47	11	7	1	9	166	164	13	3	9	101	-89	-4	6	9	165	173
1	7	8	78	-77	8	10	8	95	93	9	1	9	88	87	15	3	9	62	57	-2	6	9	157	-96
3	7	8	103	-102	-11	11	8	68	52	11	1	9	75	-67	-18	4	9	118	-113	0	6	9	177	-184
5	7	8	121	-119	-7	11	8	91	-93	13	1	9	40	-56	-14	4	9	56	46	2	6	9	82	-89
7	7	8	69	70	-5	11	8	69	-72	-16	2	9	63	-56	-12	4	9	78	76	4	6	9	69	73
7	7	8	101	97	-1	11	8	111	114	-14	2	9	78	82	-8	4	9	43	-32	8	6	9	47	-60
9	7	8	55	-42	3	11	8	62	-64	-12	2	9	137	131	-6	4	9	161	167	10	6	9	52	-43
11	7	8	49	-39	5	11	8	55	-72	-10	2	9	129	-121	-4	4	9	42	34	-17	7	9	71	-58
13	7	8	72	-71	-6	12	8	70	-74	-8	2	9	139	-125	-2	4	9	67	66	-15	7	9	45	57
-16	8	8	95	106	0	12	8	88	84	-6	2	9	128	-124	0	4	9	67	66	-15	7	9	45	57
-12	8	8	96	-106	0	12	8	108	116	-4	2	9	141	-136	2	4	9	223	-228	-13	7	9	100	88

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-11	7	9	78	72	-4	10	9	97	99	-5	1	10	142	139	1	3	10	149	-149	-18	6	10	66	-69
-9	7	9	62	-46	-2	10	9	57	60	-3	1	10	31	-14	3	3	10	48	-53	-16	6	10	77	59
-7	7	9	75	-68	2	10	9	83	-100	-1	1	10	112	-122	5	3	10	108	101	-14	6	10	87	62
-5	7	9	54	36	4	10	9	50	-37	1	1	10	169	-177	7	3	10	38	7	-12	6	10	85	85
-3	7	9	145	135	6	10	9	41	45	5	1	10	175	170	9	3	10	133	-134	-10	6	10	93	-90
-1	7	9	40	33	8	10	9	49	47	7	1	10	46	45	11	3	10	128	-116	-8	6	10	93	-23
3	7	9	88	-87	-7	11	9	54	-48	9	1	10	67	-71	-18	4	10	61	-51	-6	6	10	109	111
5	7	9	106	-111	-5	11	9	82	82	11	1	10	161	-150	-14	4	10	133	130	-4	6	10	121	-53
7	7	9	103	118	-3	11	9	86	80	15	1	10	57	37	-10	4	10	146	-142	-2	6	10	60	-54
7	7	9	92	89	1	11	9	59	-54	-18	2	10	84	-75	-8	4	10	41	33	0	6	10	95	-94
7	7	9	75	78	3	11	9	105	-98	-16	2	10	81	71	-6	4	10	47	20	2	6	10	102	-113
9	7	9	70	54	5	11	9	86	90	-14	2	10	42	36	-4	4	10	282	291	4	6	10	142	103
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-12	8	9	134	-131	-2	12	9	67	-55	-8	2	10	147	-145	0	4	10	141	-142	10	6	10	82	-75
-8	8	9	43	-56	-18	0	10	179	166	-6	2	10	53	-54	2	4	10	84	-89	12	6	10	72	-75
-6	8	9	70	82	-14	0	10	65	57	-4	2	10	142	139	4	4	10	32	36	-15	7	10	56	41
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0	8	9	125	-130	-8	0	10	134	40	0	2	10	208	-220	14	4	10	44	44	-9	7	10	82	-86
2	8	9	71	65	-6	0	10	57	46	4	2	10	132	136	14	4	10	76	76	-5	7	10	84	83
6	8	9	58	-44	-4	0	10	262	258	6	2	10	95	86	-19	5	10	144	-125	-3	7	10	52	45
10	8	9	144	147	-4	0	10	164	-116	8	2	10	40	34	-15	5	10	82	75	-1	7	10	105	-110
-13	9	9	59	44	0	0	10	164	-166	8	2	10	40	34	-13	5	10	82	75	-1	7	10	99	-95
-11	9	9	59	44	0	0	10	164	-166	8	2	10	40	34	-11	5	10	82	75	-1	7	10	99	-95
-9	9	9	69	-68	2	0	10	44	44	10	2	10	67	42	-9	5	10	157	-155	3	7	10	106	95
-7	9	9	59	-70	4	0	10	83	77	14	2	10	117	115	-9	5	10	66	-63	5	7	10	106	95
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-1	9	9	36	-13	10	0	10	33	33	-15	3	10	80	81	-5	5	10	35	-36	11	7	10	91	-08
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7	9	9	123	129	-15	1	10	117	-114	-9	3	10	168	-171	-1	5	10	147	-152	-14	8	10	106	61
9	9	9	39	26	-13	1	10	98	99	-7	3	10	129	-135	3	5	10	38	42	-10	8	10	106	-109
-12	10	9	73	58	-11	1	10	73	-83	-5	3	10	148	153	5	5	10	160	159	-6	8	10	37	38
-10	10	9	57	-61	-11	1	10	180	-178	-3	3	10	139	144	9	5	10	53	-45	0	8	10	193	193
-8	10	9	108	-106	-7	1	10	93	-91	-1	3	10	68	-66	11	5	10	139	-134	0	8	10	87	-92

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR										ROEBLINGITE DATA RED 2/19/82										PAGE 11				
H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
2	8	10	97	-92	14	0	11	120	114	-11	3	11	80	-64	9	5	11	99	-96	-1	9	11	125	-133
6	8	10	09	88	-17	1	11	76	78	-9	3	11	71	-67	-16	6	11	117	114	1	9	11	57	53
8	8	10	43	28	-15	1	11	146	143	-7	3	11	187	193	-12	6	11	137	-90	3	9	11	56	45
10	8	10	59	-60	-13	1	11	54	-60	-5	3	11	145	142	-10	6	11	109	-110	5	9	11	104	1.5
-9	9	10	144	-140	-11	1	11	121	-117	-3	3	11	59	64	-6	6	11	66	61	-10	10	11	64	-58
-7	9	10	51	-41	-9	1	11	86	-86	-1	3	11	199	-204	-4	6	11	60	62	-4	10	11	47	32
-5	9	10	97	100	-7	1	11	153	153	-3	3	11	156	159	-2	6	11	116	-116	-2	10	11	102	-114
1	9	10	125	-130	-5	1	11	144	140	5	3	11	144	145	0	6	11	54	-48	0	10	11	84	-30
5	9	10	88	83	-3	1	11	74	68	9	3	11	65	-54	4	6	11	92	85	-7	11	11	105	93
7	9	10	42	-38	-1	1	11	139	-137	11	3	11	53	-45	6	6	11	68	84	-4	10	11	49	40
-10	10	10	68	-77	1	1	11	33	33	13	3	11	108	103	8	6	11	143	-148	-5	11	11	45	31
-8	10	10	41	-8	-16	4	11	95	91	-16	4	11	96	86	-15	7	11	73	78	-1	11	11	53	-45
-6	10	10	59	61	-12	4	11	129	129	-10	4	11	39	8	-9	7	11	57	-70	-16	0	12	42	34
-4	10	10	116	119	7	1	11	92	-92	-8	4	11	157	-151	-11	7	11	90	153	-14	0	12	60	-62
0	10	10	65	-65	9	1	11	103	-100	-2	4	11	128	127	-7	7	11	62	76	-12	0	12	140	-141
2	10	10	70	-85	-18	2	11	101	92	-6	4	11	134	-142	-5	7	11	62	58	-10	0	12	80	86
4	10	10	63	67	-14	2	11	63	-58	4	4	11	198	-201	-3	7	11	83	-80	-8	0	12	80	12
6	10	10	49	54	-16	2	11	44	49	4	4	11	118	120	-1	7	11	116	110	-6	0	12	143	141
-7	11	10	49	-62	-12	2	11	75	-68	8	4	11	73	-60	5	7	11	92	97	-4	0	12	81	-73
-5	11	10	55	38	-10	2	11	75	-68	8	4	11	61	-58	7	7	11	74	-67	-2	0	12	212	-284
-1	11	10	108	-103	-8	2	11	75	-77	10	4	11	61	-58	9	7	11	66	-61	2	0	12	95	92
1	11	10	55	-42	-10	2	11	54	63	-17	5	11	132	142	-14	8	11	37	-4	4	0	12	118	107
-16	0	11	158	158	-6	2	11	76	90	-15	5	11	53	-61	-10	8	11	92	-92	12	0	12	109	-101
-10	0	11	220	-223	-4	2	11	109	111	-13	5	11	117	-115	-8	8	11	67	-92	4	0	12	68	57
-8	0	11	54	58	0	2	11	167	-173	-9	5	11	101	101	-6	8	11	102	105	-17	1	12	68	57
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-2	0	11	52	-40	6	2	11	151	146	-3	5	11	123	-125	6	8	11	96	100	-9	1	12	76	81
0	0	11	100	-101	8	2	11	147	-149	-1	5	11	62	58	8	8	11	69	-65	-5	1	12	164	162
2	0	11	48	47	10	2	11	51	-32	1	3	11	58	50	-13	9	11	56	-33	-5	1	12	70	65
4	0	11	171	166	-17	3	11	61	47	3	5	11	102	99	-7	9	11	77	77	-3	1	12	136	-138
8	0	11	126	-115	-14	3	11	86	47	5	5	11	81	-78	-5	9	11	123	120	-1	1	12	157	-156
10	0	11	63	-65	-15	3	11	86	81	7	5	11	81	-78	-5	9	11	123	120	-1	1	12	157	-156

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

ROEBLINGITE DATA RED 2/19/82

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
1	1	1	50	46	-16	4	12	111	116	6	6	12	47	-35	-10	0	13	63	58	8	2	13	87	-82
3	1	1	60	56	-12	4	12	124	-113	8	6	12	45	-33	-8	0	13	114	112	10	2	13	100	103
7	1	1	121	-118	-8	4	12	67	68	-13	7	12	127	-127	-6	0	13	124	-132	-15	3	13	48	-109
9	1	1	56	64	-6	4	12	93	95	-11	7	12	67	-53	-4	0	13	148	-145	-13	3	13	113	-109
11	1	1	60	64	-4	4	12	94	95	-7	7	12	97	92	0	0	13	68	-67	-11	3	13	61	65
13	1	1	81	79	-2	4	12	108	-106	-5	7	12	78	76	0	0	13	67	70	-9	3	13	153	145
18	2	1	106	111	0	4	12	61	60	-3	7	12	148	-150	2	0	13	205	205	-7	3	13	125	124
14	2	1	78	82	2	4	12	135	133	-1	7	12	90	-94	4	0	13	72	-70	-5	3	13	81	-65
16	2	1	36	33	4	4	12	130	134	1	7	12	38	50	6	0	13	61	-55	-3	3	13	67	-63
12	2	1	95	-92	8	4	12	123	-119	5	7	12	39	7	8	0	13	48	31	-1	3	13	34	-23
10	2	1	49	169	12	4	12	53	56	7	7	12	123	-123	10	0	13	139	-131	1	3	13	163	164
8	2	1	170	169	-17	5	12	58	47	9	7	12	39	-27	10	0	13	46	51	5	3	13	93	-89
6	2	1	60	54	-15	5	12	77	78	-14	8	12	49	12	-15	1	13	34	46	7	3	13	49	-39
4	2	1	95	-98	-13	5	12	85	-84	-12	8	12	87	-80	-13	1	13	85	-87	9	3	13	71	87
2	2	1	71	71	-11	5	12	93	-92	-8	8	12	53	47	-11	1	13	85	79	11	3	13	110	100
2	2	1	252	254	-9	5	12	74	81	-6	8	12	77	73	-9	1	13	132	128	-16	4	13	57	-48
4	2	1	104	108	-7	5	12	165	165	-4	8	12	57	-56	-7	1	13	137	91	-14	4	13	108	-104
6	2	1	65	-65	-5	5	12	33	23	-2	8	12	91	-91	-5	1	13	118	-115	-12	4	13	103	-93
8	2	1	58	-48	-3	5	12	84	-77	0	8	12	46	61	-3	1	13	118	-115	-10	4	13	36	24
10	2	1	117	107	3	5	12	135	-135	2	8	12	134	134	3	1	13	175	170	-8	4	13	98	90
12	2	1	85	75	5	5	12	60	60	4	8	12	94	90	5	1	13	60	54	-6	4	13	46	-53
15	3	1	49	18	7	5	12	38	-34	8	8	12	91	-92	7	1	13	36	-42	-4	4	13	102	-101
13	3	1	102	-98	9	5	12	86	-79	-7	9	12	85	74	11	1	13	74	-69	-4	4	13	45	-32
11	3	1	130	-128	11	5	12	46	-38	-5	9	12	52	-60	-16	2	13	105	93	2	4	13	50	53
9	3	1	32	18	-16	6	12	42	51	-3	9	12	68	-64	-14	2	13	37	12	0	4	13	141	134
7	3	1	95	95	-12	6	12	79	-80	-1	9	12	78	79	-10	2	13	205	-200	6	4	13	117	-120
3	3	1	181	-183	-8	6	12	122	117	3	9	12	78	79	-8	2	13	54	35	8	4	13	95	-91
1	3	1	75	-95	-6	6	12	54	-62	-4	10	12	74	76	-4	2	13	68	53	10	4	13	59	-53
3	3	1	94	80	-2	6	12	114	-105	2	10	12	51	-58	0	2	13	99	-95	-11	5	13	87	-95
7	3	1	180	-180	0	6	12	42	-56	-3	11	12	75	-83	2	2	13	56	59	-9	5	13	77	71
9	3	1	81	-79	2	6	12	142	143	-14	0	13	41	-17	4	2	13	57	-67	-5	5	13	92	-7
18	4	1	46	46	4	6	12	59	62	-12	0	13	83	-76	6	2	13	164	-157	5	5	13	115	-116

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-3	5	13	120	-121	-5	9	13	51	-40	-10	2	14	239	234	-5	5	14	95	-88	-14	0	15	40	-27
1	5	13	125	122	-3	9	13	60	-64	-6	2	14	86	-86	-3	5	14	50	-53	-12	0	15	40	99
3	5	13	53	65	1	9	13	72	68	-2	2	14	50	38	-1	5	14	125	118	-10	0	15	126	126
7	5	13	88	-79	-8	10	13	38	-20	0	2	14	154	151	1	5	14	83	90	-8	0	15	98	-92
9	5	13	54	55	-4	10	13	85	-90	0	2	14	114	-111	3	5	14	56	-57	-6	0	15	98	-92
-14	6	13	83	-81	-16	10	13	49	42	10	2	14	108	99	5	5	14	131	-128	-4	0	15	74	-63
-12	6	13	36	-25	-16	10	13	90	-84	-15	3	14	85	-88	-16	6	14	84	-75	-2	0	15	55	-57
-10	6	13	61	51	-14	10	13	81	-73	-11	3	14	130	67	-14	6	14	39	-24	4	0	15	189	-101
-8	6	13	41	41	-10	10	13	110	100	-9	3	14	57	67	-12	6	14	58	-43	4	0	15	65	55
-6	6	13	44	-24	-8	10	13	50	43	-7	3	14	70	68	-10	6	14	141	141	6	0	15	88	73
-4	6	13	183	-186	-6	10	13	46	-36	-5	3	14	195	-192	-6	6	14	65	-51	8	0	15	88	73
0	6	13	91	86	-4	10	13	58	-63	-3	3	14	104	-98	-2	6	14	42	55	10	0	15	46	30
2	6	13	105	99	-2	10	13	148	150	-1	3	14	128	123	4	6	14	140	-124	-15	1	15	46	30
6	6	13	105	-99	0	10	13	120	115	5	3	14	51	26	6	6	14	123	-124	-13	1	15	73	63
8	6	13	105	-99	2	10	13	40	43	9	3	14	63	-70	6	6	14	53	-48	-11	1	15	83	79
-13	7	13	54	-57	4	10	13	121	-107	7	3	14	45	43	-11	7	14	79	71	-7	1	15	99	-97
-7	7	13	143	141	6	10	13	141	-135	-16	4	14	58	52	-7	7	14	41	-48	-5	1	15	46	-51
-5	7	13	62	56	8	10	13	125	115	-14	4	14	84	-81	-5	7	14	131	-132	-3	1	15	113	115
-3	7	13	108	-113	10	10	13	114	98	-12	4	14	47	51	-1	7	14	118	107	-1	1	15	140	141
-3	7	13	146	152	-15	11	14	71	-70	-12	4	14	65	-51	5	7	14	122	-124	3	1	15	57	-35
5	7	13	44	-46	-9	11	14	73	57	-8	4	14	48	47	-12	8	14	41	47	5	1	15	57	-35
-14	8	13	100	-97	-7	11	14	92	-90	-6	4	14	44	44	-10	8	14	119	122	7	1	15	92	66
-11	8	13	104	-100	-7	11	14	135	-134	-6	4	14	44	44	-6	8	14	61	-41	9	1	15	109	66
-8	8	13	83	73	-3	11	14	51	-46	-4	4	14	99	-31	-4	8	14	45	-41	-8	2	15	64	-64
-6	8	13	38	-38	-3	11	14	137	137	-2	4	14	105	98	-2	8	14	72	77	-6	2	15	150	-143
-4	8	13	80	-76	-1	11	14	90	-84	0	4	14	66	-60	4	8	14	56	61	-6	2	15	135	-132
2	8	13	49	41	3	11	14	44	-34	4	4	14	94	83	-7	9	14	89	-76	0	2	15	49	-35
4	8	13	104	-105	5	11	14	160	-155	8	4	14	81	81	-5	9	14	106	-79	2	2	15	129	-117
6	8	13	76	-79	7	11	14	36	1	10	4	14	88	81	-9	9	14	71	-71	8	2	15	102	69
-11	9	13	60	-79	9	11	14	41	38	-15	5	14	57	47	-1	9	14	58	-71	8	2	15	56	40
-9	9	13	47	53	-16	11	14	56	49	-11	5	14	56	56	-1	9	14	40	58	-13	3	15	81	30
-7	9	13	96	97	-14	12	14	39	-3	-7	5	14	89	-89	3	9	14	41	-25	-9	3	15	52	-50

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ROEBLINGITE DATA RED 2/19/82

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC					
-7	3	15	154	-161	-13	7	15	39	31	-8	2	16	127	-123	-12	6	16	98	109	-10	2	17	81	-72
-3	3	15	98	89	-11	7	15	72	74	-4	2	16	69	55	-7	6	16	141	-136	-8	2	17	79	-60
-1	3	15	137	138	-7	7	15	87	-86	-2	2	16	90	82	-2	6	16	63	57	-6	2	17	45	-3
1	3	15	36	38	-3	7	15	57	57	2	2	16	135	-117	2	6	16	85	82	-4	2	17	130	129
3	3	15	115	-101	-1	7	15	111	120	4	2	16	47	38	0	6	16	46	1	-2	2	17	60	-58
5	3	15	54	-49	3	7	15	88	-84	6	2	16	68	67	2	6	16	67	-55	0	2	17	37	-39
7	3	15	41	26	-8	8	15	80	-90	8	2	16	90	81	4	6	16	58	55	2	2	17	44	-47
-12	4	15	72	64	-6	8	15	61	-65	-13	3	16	80	72	-11	7	16	52	-41	4	2	17	53	55
-10	4	15	95	90	-2	8	15	73	-69	-11	3	16	57	-59	-9	7	16	39	-30	6	2	17	79	76
-8	4	15	127	-131	2	8	15	58	-63	-9	3	16	45	5	-7	7	16	100	-101	-13	3	17	94	-93
-6	4	15	95	-88	-7	9	15	82	-81	-7	3	16	80	-66	-5	7	16	63	61	-9	3	17	42	-48
-2	4	15	71	60	-5	9	15	50	-46	-5	3	16	109	106	-3	7	16	62	61	-5	3	17	62	63
0	4	15	52	57	-3	9	15	97	96	-3	3	16	84	80	1	7	16	93	-89	-3	3	17	59	55
2	4	15	116	-105	-1	9	15	74	77	-1	3	16	38	28	3	7	16	70	-56	-1	3	17	87	-73
4	4	15	97	48	-14	0	16	157	156	3	3	16	163	-152	-8	8	16	58	-56	1	3	17	70	-35
8	4	15	57	48	-8	0	16	104	100	7	3	16	106	99	-4	8	16	76	72	5	3	17	114	109
-15	5	15	55	-52	-8	0	16	126	-129	3	3	16	106	99	0	8	16	39	-31	-12	4	17	146	-139
-13	5	15	41	56	-6	0	16	88	-88	-14	4	16	138	130	-10	0	17	197	-194	-10	4	17	50	27
-11	5	15	63	66	-4	0	16	143	143	-12	4	16	41	41	-8	0	17	51	-48	-8	4	17	40	-46
-7	5	15	86	-79	-2	0	16	93	76	-6	4	16	80	-65	-6	0	17	90	88	-6	4	17	35	75
-5	5	15	57	-55	6	0	16	130	121	-4	4	16	63	-65	-4	4	17	106	98	-4	4	17	86	-98
-3	5	15	111	115	8	0	16	66	66	-2	4	16	130	126	0	0	17	117	-107	0	4	17	57	-33
-1	5	15	101	-78	-9	1	16	83	-84	2	4	16	59	54	4	4	17	94	-87	2	4	17	86	64
3	5	15	87	87	-9	1	16	103	93	-2	4	16	59	54	4	4	17	70	67	4	4	17	86	64
5	5	15	51	-44	-7	1	16	141	-135	6	4	16	124	114	-13	1	17	82	42	-13	5	17	53	60
7	5	15	90	96	-5	1	16	90	75	-13	5	16	89	78	-11	1	17	42	-45	-9	5	17	39	-32
-12	6	15	49	44	-3	1	16	59	63	-7	5	16	115	-124	-9	1	17	63	-48	-5	5	17	147	137
-10	6	15	118	-113	1	1	16	150	-153	-5	5	16	59	59	-5	1	17	143	134	-3	5	17	69	62
-6	6	15	57	-45	3	1	16	63	-61	-3	5	16	46	51	-3	1	17	74	66	-1	5	17	72	-54
-4	6	15	83	76	7	1	16	79	66	-1	5	16	71	68	-1	1	17	76	-74	-12	6	17	111	-53
-2	6	15	59	-62	-14	2	16	60	60	1	5	16	151	-145	1	1	17	84	-73	-10	6	17	72	-89
0	6	15	83	-89	-12	2	16	92	79	3	5	16	54	-48	5	1	17	137	121	-10	6	17	111	-105
2	6	15	113	-100	-10	2	16	37	-13	-14	6	16	76	79	7	1	17	50	44	-8	6	17	49	-86

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR										ROEBLINGITE DATA RED 2/19/82										PAGE 15				
H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-6	6	17	50	45	3	1	18	92	86	-2	4	18	72	-75	-1	1	19	37	-27	-8	0	20	80	85
-4	6	17	123	122	5	1	18	73	66	-11	5	18	111	-106	1	1	19	96	93	-6	0	20	34	-4
0	6	17	61	-46	-12	2	18	65	-58	-7	5	18	46	41	3	1	19	71	69	-4	0	20	99	-84
2	6	17	76	-75	-10	2	18	128	-111	-3	5	18	56	-62	-8	2	19	105	109	-7	1	20	46	34
-9	7	17	58	-50	-6	2	18	67	65	-1	5	18	118	-112	-6	2	19	63	57	-5	1	20	50	-48
-7	7	17	56	52	-8	2	18	104	89	-10	6	18	56	-42	-4	2	19	79	-68	-3	1	20	50	-39
-5	7	17	75	65	-4	2	18	81	78	-8	6	18	64	69	-2	2	19	150	-135	-8	2	20	65	60
-3	7	17	54	53	-2	2	18	40	-37	-6	6	18	92	79	0	2	19	37	-20	-6	2	20	38	-34
1	7	17	80	-77	0	2	18	79	-74	-4	6	18	38	43	-9	3	19	46	51	-4	2	20	86	-76
-12	0	18	74	-74	2	2	18	44	44	-2	6	18	81	-72	-7	3	19	122	108	-2	2	20	48	-53
-8	0	18	36	23	4	2	18	81	69	0	6	18	82	-71	-7	3	19	46	51	0	2	20	118	112
-6	0	18	156	144	-11	3	18	126	-125	-5	7	18	65	65	-3	3	19	58	-42	-5	3	20	103	112
-4	0	18	60	47	-5	3	18	70	69	-10	0	19	41	-40	-1	3	19	68	-67	-3	3	20	66	-65
-2	0	18	143	-136	-3	3	18	47	-44	-8	0	19	136	131	-1	3	19	91	89	-1	3	20	37	34
-4	0	18	107	95	-1	3	18	81	-68	-6	0	19	52	-43	-8	4	19	130	131	-8	4	20	73	68
4	0	18	99	-106	3	3	18	53	51	-2	0	19	111	-110	-2	4	19	143	-137	-4	4	20	114	-107
-11	1	18	49	43	-12	4	18	74	-75	0	0	19	36	22	0	4	19	43	-22	-6	0	21	86	-73
-5	1	18	77	-76	-10	4	18	54	-54	2	0	19	82	79	-9	5	19	39	-2	-4	0	21	102	-87
-3	1	18	130	-122	-6	4	18	133	132	-7	1	19	91	81	-3	5	19	83	72	-4	0	21	102	-87
-1	1	18	49	-27	-4	4	18	58	49	-3	1	19	56	-46	-3	5	19	65	-49	-5	1	21	99	-84

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