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Okenite, $Ca_{10}Si_{18}O_{46} \cdot 18H_2O$: the first example of a chain and sheet silicate

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Abstract

The crystal structure of okenite, $Ca_{10}Si_{18}O_{46} \cdot 18H_2O$, was solved with triclinic space group $P\bar{1}$ $a = 9.69$, $b = 7.28$, $c = 22.02$Å, $\alpha = 92.7°$, $\beta = 100.1°$, $\gamma = 110.9°$. The structure is composed of the following structural units: (a) tetrahedral sheets S, with composition $(Si_6O_{15})^{-6}$, characterized by five- and eight-membered rings of silicate tetrahedra, with five tetrahedra pointing in one direction and one tetrahedron pointing in the other direction; (b) three-repeat double chains C, with composition $(Si_6O_{16})^{-8}$ and characterized by four- and six-membered rings, made up by pairing two wollastonite chains, which point in opposite directions; (c) octahedral double chains O, formed by two strands of octahedra. These structural units are connected by corner sharing to give the complex layer SOCOS, with composition $[Ca_8(Si_6O_{16})(Si_6O_{15})_2(H_2O)_6]^{-4}$. Such complex layers alternate in the structure with sheets $[Ca_2(H_2O)_9 \cdot 3H_2O]^{+4}$. Weak supercell reflections revealed a larger unit cell with doubled a and b parameters in the unconventional space group $C\bar{1}$.

Introduction

Okenite, a hydrated calcium silicate, has long been of interest to a large number of mineralogists and crystal chemists: its consistent association with gyrolite and zeolites in basalts seemed indicative of some structural relations among them. Of particular interest is the role of water molecules in the structure of okenite, the definition of which could lead to an understanding of the dehydration mechanism which, according to Heller's X-ray studies (Gard and Taylor, 1956), leads topotactically to the formation of wollastonite.

Okenite was first described from Disko Island (Greenland) and was subsequently found in various other localities, such as Crestmore (California), Scawt Hill (Northern Ireland), Bordö (Faröer Islands), Bombay (India), usually in basalts. The most comprehensive account of its crystallographic properties was given by Gard and Taylor (1956) who studied a specimen from Bombay, India, consisting of fibrous aggregates. These authors studied okenite by electron diffraction, as single crystals of sufficient size for X-ray diffraction were not available. The results indicated that the crystals were triclinic with $a = 9.84$, $b = 7.20$, $c = 21.33$Å, $\alpha = 90.0°$, $\beta = 103.9°$, $\gamma = 111.5°$. The fiber direction was [010], with repeated lamellar twinning across the cleavage plane {001}. On the basis of the cell volume and a chemical analysis by Christie (1925), Gard and Taylor (1956) proposed that the cell contents are $Ca_9Si_{18}O_{63}H_{36}$, or $Ca_9(Si_6O_{15})_3 \cdot 18H_2O$.

Gard and Taylor (1956) also studied a mineral from Crestmore, California, which was previously characterized as okenite on the basis of its chemical composition and optical properties, and demonstrated that it was in fact a new species for which they proposed the name nekoite. Crystal structures for both minerals were hypothesized by Mamedov and Belov (1958) on the basis of the chemical composition and unit cell dimensions. The crystal structure of nekoite was recently solved by Alberti and Galli (1980) who showed that it was in many respects different from the structural model of Mamedov and Belov (1958).

The present work was undertaken to determine the crystal structure of okenite in order to further our understanding of the crystal chemistry of the hydrated calcium silicates.

Experimental

A specimen of okenite from Kolhapur District, Maharastra State, India, donated by Prof. E. Passaglia, was used in this study. Careful examination of a large number of crystals from this specimen and testing by preliminary Weissenberg photographs resulted in the selection of crystals of sufficient quality for intensity measurement. By means of Weissenberg and precession photographs the lattice parameters were determined on a small fragment cut from a long lath-shaped crystal. The same crystal fragment was used to collect intensity data with a Philips PW 1100 single crystal diffractometer, after obtaining refined lattice parameters by least squares fitting of 20 medium range θ values: $a = 9.69(1)$, $b = 7.28(1)$, $c = 22.02(4)$Å, $\alpha = 92.7(2)°$, $\beta = 100.1(3)°$, $\gamma = 110.9(1)°$.

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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR SUBCELL OF OKENITE

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
5	0	0	66	70	4	0	1	61	-83	1	-1	2	55	53	-3	-2	3	83	-91	-5	0	4	39	-46
-5	1	0	62	66	-4	0	1	74	94	4	-1	2	49	-38	3	-1	3	41	-38	-4	0	4	89	101
-3	1	0	43	-61	-3	0	1	41	52	-5	0	2	31	31	-2	-1	3	39	-55	-3	0	4	95	-98
1	1	0	46	51	-4	0	1	73	-87	-4	0	2	103	-127	4	0	3	78	-93	-2	0	4	48	-60
2	1	0	27	7	-5	0	1	31	45	-3	0	2	153	-174	1	0	3	29	27	0	0	4	75	82
3	1	0	48	-61	2	1	1	82	-91	-2	0	2	49	-49	-2	0	3	50	-52	2	0	4	124	-122
4	1	0	33	-47	1	1	1	46	-59	1	0	2	70	76	-3	0	3	206	-221	4	0	4	31	-33
-5	2	0	127	137	0	1	1	25	-33	3	0	2	49	53	4	1	3	43	-77	-3	1	4	154	-178
-3	2	0	30	-24	-3	1	1	103	-112	-4	1	2	45	-50	2	1	3	33	-32	-2	1	4	31	-40
-1	2	0	36	21	-5	1	1	56	-61	-1	1	2	58	82	1	1	3	63	56	-1	1	4	51	-56
0	2	0	59	81	3	2	1	56	62	0	1	2	37	26	0	1	3	38	-29	0	1	4	71	59
1	2	0	51	66	-1	2	1	31	-41	1	1	2	90	104	-1	1	3	39	-55	1	1	4	66	-54
2	2	0	73	76	-5	2	1	30	-16	2	1	2	36	-54	-2	1	3	62	82	-5	2	4	54	-63
3	2	0	145	163	1	3	1	80	-98	4	1	2	28	39	-4	1	3	29	31	-4	2	4	46	64
-5	3	0	87	86	0	3	1	37	-47	-5	2	2	48	-57	-5	1	3	33	41	-2	2	4	74	-92
2	3	0	103	101	-2	3	1	43	-63	-3	2	2	66	74	3	2	3	75	-99	0	2	4	85	-61
3	-4	1	45	50	-4	3	1	44	-47	-1	2	2	47	-45	2	2	3	50	-48	1	2	4	69	-65
2	-4	1	402	265	-5	3	1	60	60	0	2	2	180	-192	1	2	3	32	-25	2	2	4	56	53
5	-3	1	31	-35	-2	4	1	37	18	1	2	2	75	72	0	2	3	328	-292	-5	3	4	53	68
2	-3	1	41	28	-3	4	1	68	-77	2	2	2	72	-80	-1	2	3	52	-47	-3	3	4	58	70
-1	-3	1	34	39	1	-4	2	58	-55	-5	3	2	56	60	-5	2	3	117	-126	-1	3	4	45	-31
-2	-3	1	43	33	2	-4	2	62	5	-2	3	2	34	24	1	3	3	28	19	0	3	4	37	-35
5	-2	1	95	100	-1	-3	2	32	-48	-1	3	2	31	35	-2	4	3	45	-53	1	3	4	39	-49
3	-2	1	30	32	2	-3	2	77	-64	-3	4	2	31	-41	1	-4	4	80	-61	3	-3	5	40	-29
2	-2	1	76	80	3	-3	2	79	-93	-2	4	2	45	-46	2	-4	4	38	-28	2	-3	5	111	84
1	-2	1	115	-82	4	-3	2	31	-27	3	-4	3	47	54	-2	-3	4	73	71	1	-3	5	55	30
0	-2	1	55	-66	-3	-2	2	71	-79	1	-4	3	40	-25	2	-3	4	47	35	0	-3	5	62	47
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-2	-2	1	52	-50	0	-2	2	37	-46	-2	-3	3	102	108	-1	-2	4	64	-56	2	-2	5	37	24
-3	-2	1	68	83	1	-2	2	55	-30	5	-2	3	78	-77	1	-2	4	84	-77	1	-2	5	41	38
5	-1	1	41	-43	2	-2	2	139	-138	4	-2	3	35	-29	3	-2	4	117	-119	-1	-2	5	56	48
2	-1	1	96	109	3	-2	2	60	57	3	-2	3	73	74	-4	-1	4	36	-42	-2	-2	5	42	33
1	-1	1	33	-21	4	-2	2	39	-45	2	-2	3	243	-227	1	-1	4	45	-44	3	-1	5	50	51
0	-1	1	61	-74	5	-2	2	61	64	0	-2	3	51	35	2	-1	4	64	57	2	-1	5	122	110
-1	-1	1	34	36	-2	-1	2	84	-99	-1	-2	3	84	74	3	-1	4	74	-75	1	-1	5	60	55
5	0	1	54	63	-1	-1	2	67	66	-2	-2	3	45	55	4	-1	4	30	-27	0	-1	5	49	-47

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
-1	-1	5	65	55	0	-1	6	56	52	2	0	7	69	79	0	-3	9	91	64	4	2	0	87	81
-2	-1	5	53	-48	1	-1	6	77	73	1	0	7	78	-61	3	-2	9	39	-36	6	2	0	39	53
-4	-1	5	46	61	2	-1	6	66	-60	0	0	7	193	186	1	-2	9	74	-74	-8	3	0	35	40
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2	0	5	117	112	-5	0	6	86	93	-3	0	7	79	73	3	-1	9	31	-42	-7	4	0	44	49
1	0	5	106	88	-3	0	6	119	113	3	1	7	42	-48	-1	-1	9	39	39	-6	4	0	37	-22
0	0	5	37	-45	-2	0	6	83	-87	-1	1	7	116	-124	2	0	9	60	-50	3	4	0	60	77
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-4	0	5	172	180	1	0	6	101	91	0	2	7	126	96	-4	0	9	77	-78	-3	5	0	38	38
3	1	5	30	44	2	0	6	99	103	-2	2	7	33	41	2	1	9	78	-59	-2	5	0	66	48
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-3	1	5	45	51	1	1	6	71	62	-3	3	7	35	50	-4	2	9	46	-49	3	-6	1	64	43
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-4	-1	6	37	-43	0	-1	7	71	-68	-1	2	8	90	-79	-7	1	0	50	62	-5	-4	1	49	61
-3	-1	6	28	-6	-1	-1	7	80	-64	1	2	8	106	-91	-6	1	0	58	62	9	-3	1	49	-60
-2	-1	6	38	-75	-2	-1	7	44	-44	-1	3	8	71	-52	6	1	0	48	74	-3	-3	1	34	25
-1	-1	6	67	56	3	0	7	64	65	2	-3	9	60	-56	-6	2	0	37	29	-4	-3	1	35	43

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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7	-2	1	46	-54	7	-4	2	45	35	-1	-4	3	111	-126	3	-5	4	43	22	8	-4	5	63	-64
6	-2	1	75	82	-4	-3	2	37	-41	8	-3	3	43	42	5	-5	4	74	-73	5	-4	5	37	-30
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-7	-2	1	36	-41	-7	-2	2	62	-86	-4	-3	3	57	-61	7	-5	4	45	-38	-1	-4	5	36	12
6	-1	1	33	-35	-6	-2	2	102	-146	7	-2	3	47	-55	-4	-4	4	54	55	-2	-4	5	62	61
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-8	2	1	81	-75	7	0	2	38	45	7	0	3	58	69	7	-4	4	71	-76	7	0	5	35	41
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-5	4	1	55	-66	3	3	2	84	93	-9	2	3	66	68	7	-2	4	119	-127	5	2	5	37	51
-6	4	1	130	-147	-7	4	2	36	45	-6	3	3	51	58	-7	0	4	77	95	4	2	5	35	59
-8	4	1	38	-44	-5	4	2	72	-85	3	4	3	93	-102	-6	0	4	73	85	-9	2	5	59	64
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-2	6	1	51	-56	-4	5	2	34	41	-8	4	3	40	48	3	2	4	89	-104	4	4	5	54	-52
-4	6	1	45	-53	-1	5	2	56	77	-9	4	3	40	34	2	3	4	65	66	0	4	5	93	93
-5	6	1	48	-53	0	5	2	42	-60	2	5	3	48	-53	-7	4	4	50	-58	-1	4	5	104	80
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6	-6	2	46	-37	4	-6	3	107	-87	-5	5	3	64	-70	-3	6	4	54	49	-8	4	5	49	59
-1	-5	2	56	-67	2	-6	3	76	-56	-8	5	3	40	58	5	-6	5	60	-62	0	5	5	53	-54
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6	-5	2	47	-51	3	-5	3	74	64	-2	6	3	77	-113	6	-5	5	56	-46	-6	5	5	38	-30
-4	-4	2	37	-26	2	-5	3	72	37	-6	6	3	34	36	4	-5	5	88	75	-2	6	5	61	53
-3	-4	2	43	47	0	-5	3	59	-65	-7	6	3	36	-40	2	-5	5	89	-68	-3	6	5	114	103
-2	-4	2	88	-94	8	-4	3	59	58	-1	-6	4	65	-79	1	-5	5	38	-22	-5	6	5	35	50
-1	-4	2	35	-34	6	-4	3	77	-85	1	-6	4	39	-31	0	-5	5	57	-49	1	-6	6	49	47

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
2	-6	6	51	-54	1	3	6	31	20	3	2	7	37	38	-5	-2	8	64	-67	4	-2	9	92	-92
3	-6	6	90	65	-7	4	6	57	66	2	2	7	59	57	-4	-2	8	33	-25	-3	-2	9	77	-56
5	-5	6	44	-36	-5	4	6	40	49	-6	2	7	38	-38	5	-2	8	55	58	-4	-2	9	53	-54
6	-6	6	45	52	-4	4	6	55	-62	-7	2	7	111	-125	6	-2	8	50	53	-6	-2	9	40	-49
3	-5	6	43	46	-3	4	6	31	42	3	3	7	38	-39	7	-2	6	34	25	5	-1	9	71	-74
0	-5	6	121	-107	-2	4	6	57	63	1	3	7	33	-31	-7	-1	8	44	-49	-4	-1	9	42	46
1	-5	6	38	33	0	4	6	48	38	-7	3	7	49	-53	5	0	8	36	44	-5	-1	9	67	68
2	-5	6	36	21	2	4	6	74	-73	3	4	7	77	83	-5	1	8	35	-39	4	0	9	104	-106
3	-5	6	69	50	3	4	6	70	70	0	4	7	69	59	-9	2	8	68	-76	-5	0	9	61	59
4	-5	6	53	48	-6	5	6	39	-42	-1	4	7	37	-25	0	3	8	48	-43	-6	0	9	49	-52
6	-5	6	38	39	-4	5	6	34	-33	-2	4	7	86	72	1	3	8	69	-55	-7	0	9	39	-41
-4	-4	6	67	61	-3	5	6	74	-77	-4	4	7	63	-65	2	3	8	72	58	6	1	9	37	-51
-3	-4	6	82	78	-1	5	6	65	59	-6	4	7	57	-80	-6	4	8	75	-92	-7	1	9	37	40
-2	-4	6	92	93	-5	6	6	36	57	2	5	7	49	-53	-2	4	8	49	47	2	2	9	174	-154
-1	-4	6	126	122	-2	6	6	80	68	0	5	7	40	39	-5	5	8	47	-49	1	2	9	60	-38
3	-4	6	68	52	4	-6	7	101	85	-5	5	7	53	-74	-3	5	8	40	33	-5	2	9	97	-111
4	-4	6	84	80	3	-6	7	80	50	-3	6	7	63	-65	-2	5	8	41	26	-6	2	9	52	-68
6	-4	6	45	-43	1	-6	7	76	52	2	-6	8	50	39	-1	5	8	52	-45	-7	2	9	52	58
8	-4	6	64	-57	5	-5	7	47	-54	4	-6	8	78	65	0	5	8	93	-85	-1	3	9	75	64
-4	-3	6	49	-45	3	-5	7	55	53	-1	-5	8	68	-59	-5	6	8	76	-100	-2	3	9	50	44
-2	-3	6	42	25	2	-5	7	48	33	2	-5	8	88	-72	3	-6	9	45	-29	-4	3	9	35	-34
5	-3	6	106	106	-1	-5	7	44	34	3	-5	8	37	-26	1	-6	9	62	-47	3	4	9	75	-73
-7	-2	6	40	56	7	-4	7	77	75	4	-5	8	50	36	0	-6	9	42	-43	2	4	9	128	-115
6	-2	6	63	71	2	-4	7	111	79	5	-5	8	54	-43	4	-5	9	63	55	0	4	9	84	-63
7	-2	6	50	62	1	-4	7	46	35	-5	-4	8	76	-77	-1	-5	9	67	-58	-3	4	9	41	-46
8	-2	6	66	-70	0	-4	7	91	-79	-3	-4	8	44	-43	-2	-5	9	51	33	-6	4	9	44	-56
-7	-1	6	38	35	-3	-4	7	51	58	-2	-4	8	120	-101	-3	-5	9	41	33	-7	4	9	78	94
-5	-1	6	38	49	-4	-4	7	75	78	0	-4	8	70	-54	6	-4	9	56	-56	1	5	9	37	20
7	-1	6	44	46	4	-3	7	35	-28	2	-4	8	91	69	0	-4	9	42	25	-1	5	9	60	57
-7	0	6	37	-25	-4	-3	7	40	-35	4	-4	8	50	48	-2	-4	9	54	-47	-3	5	9	56	-58
-6	0	6	62	74	-5	-2	7	39	-43	5	-4	8	48	50	-3	-4	9	47	44	-4	5	9	47	-62
5	0	6	48	59	7	0	7	60	67	6	-4	8	58	46	-4	-4	9	42	-37	-2	6	9	104	-90
7	0	6	88	95	5	0	7	57	82	7	-4	8	60	65	3	-3	9	65	-55	1	-6	10	85	-62
4	2	6	34	35	-5	0	7	54	46	-3	-3	8	55	-44	-5	-3	9	43	49	3	-6	10	49	-26
5	2	6	47	56	-7	0	7	56	-59	3	-3	8	68	-68	6	-2	9	50	50	4	-6	10	89	-69
6	2	6	40	-49	6	2	7	35	31	-7	-2	8	64	-80	5	-2	9	38	32	0	-5	10	52	-38

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
1	-5	10	54	55	-5	4	10	46	-56	2	-5	12	54	-37	-5	2	12	71	-85	-1	-1	13	55	-51
-3	-4	10	104	86	0	4	10	59	-50	3	-5	12	59	53	-4	2	12	69	81	-2	-1	13	121	-121
-2	-4	10	82	-83	2	4	10	47	-35	4	-5	12	135	123	-1	2	12	55	61	-7	-1	13	55	-52
0	-4	10	61	-45	-2	5	10	66	65	-4	-4	12	42	38	1	2	12	73	-72	2	0	13	224	206
1	-4	10	55	-37	0	5	10	46	39	-2	-4	12	109	79	2	2	12	49	-39	1	0	13	120	109
4	-4	10	88	-92	1	-6	11	93	-72	-1	-4	12	82	75	3	2	12	48	-47	0	0	13	31	-35
6	-4	10	116	-109	3	-5	11	45	40	0	-4	12	85	62	4	2	12	69	76	-1	0	13	34	39
7	-4	10	63	-52	1	-5	11	66	-44	3	-4	12	46	41	-7	3	12	57	-67	-2	0	13	78	-77
-4	-3	10	72	-69	-1	-5	11	47	39	4	-4	12	87	76	-5	3	12	31	-35	-3	0	13	34	41
2	-3	10	54	-45	4	-4	11	70	-65	6	-4	12	69	61	2	3	12	40	45	-5	0	13	44	55
5	-3	10	60	57	-1	-4	11	55	-46	-5	-3	12	53	54	-5	4	12	45	55	-7	0	13	66	-68
6	-3	10	40	-57	4	-3	11	46	-38	-1	-3	12	70	46	-1	4	12	73	61	2	1	13	38	-26
-7	-2	10	36	38	2	-3	11	92	87	0	-3	12	71	55	0	4	12	108	85	1	1	13	35	30
-6	-2	10	44	-51	1	-3	11	119	100	3	-3	12	64	-54	1	4	12	65	-57	0	1	13	43	-37
-4	-2	10	50	-52	0	-3	11	44	33	6	-3	12	53	61	-6	5	12	35	-35	-1	1	13	78	-78
-3	-2	10	125	-109	-1	-3	11	43	31	-3	-2	12	37	-44	-5	5	12	45	-63	-2	1	13	38	-46
4	-2	10	100	-100	-2	-2	11	128	106	-1	-2	12	87	89	-4	5	12	58	-58	-4	1	13	34	-38
7	-2	10	40	-63	-4	-2	11	56	47	1	-2	12	77	69	-1	-5	13	63	-44	-5	1	13	52	53
-7	0	10	40	40	5	-1	11	38	51	3	-2	12	44	-41	-2	-5	13	42	18	-6	1	13	42	-32
-5	0	10	120	119	4	-1	11	41	52	6	-2	12	88	93	5	-4	13	88	-76	-8	1	13	36	-30
3	0	10	37	45	3	-1	11	41	42	-7	-1	12	36	-38	4	-4	13	85	78	4	2	13	84	76
4	0	10	116	-109	-6	-1	11	38	47	-6	-1	12	38	26	3	-4	13	71	60	2	2	13	32	-19
5	0	10	59	-72	5	0	11	76	-84	-3	-1	12	59	-50	0	-4	13	54	-40	-3	2	13	111	123
-5	1	10	67	63	3	0	11	65	60	2	-1	12	41	29	-3	-4	13	38	26	-5	2	13	103	-118
4	1	10	42	-41	2	2	11	44	26	3	-1	12	36	-26	0	-3	13	35	29	-7	2	13	52	-58
-6	2	10	64	-66	-1	2	11	75	72	5	-1	12	42	-41	-1	-3	13	90	-77	1	3	13	39	-23
-5	2	10	85	-98	-3	2	11	36	37	-7	0	12	64	76	-2	-3	13	100	-80	-1	3	13	48	44
1	2	10	74	59	-6	2	11	47	51	-4	0	12	55	52	-4	-3	13	86	-71	0	4	13	144	115
2	2	10	45	-40	-3	3	11	74	80	1	0	12	77	75	6	-2	13	66	70	-1	4	13	42	28
3	2	10	59	63	-6	3	11	39	48	2	0	12	71	70	5	-2	13	46	-51	-2	4	13	35	-31
-6	3	10	41	37	2	4	11	70	68	3	0	12	59	-56	4	-2	13	42	-35	-4	4	13	46	-55
-4	3	10	33	45	0	4	11	55	58	4	0	12	73	70	-3	-2	13	129	-107	-7	4	13	52	52
-3	3	10	56	65	-6	4	11	39	54	5	0	12	51	-45	6	-1	13	39	40	-3	5	13	57	-65
0	3	10	34	-34	-2	5	11	40	26	-5	1	12	52	-58	5	-1	13	47	-40	-4	5	13	63	-68
3	3	10	66	58	-4	5	11	43	54	-4	1	12	31	-34	3	-1	13	34	-23	-1	-5	14	46	26
-7	4	10	54	59	-2	-5	12	46	37	-3	1	12	32	-34	0	-1	13	68	-66	0	-4	14	85	-65

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
1	-4	14	65	53	-1	4	14	94	-82	-2	4	15	44	50	1	-3	17	66	58	-4	-1	19	41	34
4	-4	14	97	92	2	-5	15	80	-82	-3	4	15	70	-79	0	-3	17	102	96	-4	0	19	85	89
-4	-3	14	55	-47	3	-4	15	89	-78	-4	4	15	40	-44	-3	-3	17	83	62	-5	1	19	39	-45
-3	-3	14	72	54	0	-4	15	63	-62	0	-4	16	58	-47	4	-2	17	96	-93	-1	2	19	81	83
0	-3	14	40	24	-1	-4	15	44	33	1	-4	16	126	-101	-5	-2	17	128	119	-2	-2	20	73	66
1	-3	14	88	70	4	-3	15	106	-96	-3	-3	16	56	-47	4	-1	17	46	45	-3	-1	20	49	-46
-5	-2	14	87	-77	3	-3	15	78	-82	0	-3	16	93	70	1	-1	17	45	40	-1	1	20	69	-79
-4	-2	14	41	35	-1	-3	15	36	-31	1	-3	16	49	-45	-1	-1	17	46	43	9	0	0	77	-65
-3	-2	14	57	-57	4	-2	15	41	-51	-3	-2	16	53	-50	-5	-1	17	37	32	-7	1	0	62	62
-1	-2	14	107	93	3	-2	15	65	-70	0	-2	16	76	70	2	0	17	53	47	-6	1	0	64	62
2	-2	14	59	-59	2	-2	15	35	-10	1	-2	16	49	49	-2	0	17	35	52	-5	1	0	75	66
-4	-1	14	31	-32	0	-2	15	50	-45	2	-2	16	42	40	-3	0	17	53	56	0	1	0	105	88
-2	-1	14	48	-38	-1	-2	15	61	-56	3	-2	16	86	-84	-5	0	17	118	122	1	1	0	60	51
-7	0	14	41	-37	-3	-2	15	53	-47	4	-2	16	82	-84	-5	1	17	62	68	3	1	0	79	-61
-6	0	14	42	36	4	-1	15	36	-33	-5	-1	16	43	53	1	2	17	60	60	4	1	0	52	-47
-5	0	14	81	76	3	-1	15	49	-47	-5	-1	16	62	56	-3	2	17	39	30	6	1	0	88	74
-2	0	14	105	-100	0	-1	15	37	-31	-1	0	16	92	-98	-1	3	17	47	42	-5	2	0	143	137
-1	0	14	99	96	2	0	15	36	-40	0	0	16	64	59	2	-2	18	63	-50	0	2	0	118	81
0	0	14	42	38	1	0	15	168	-156	2	0	16	49	50	3	-2	18	53	50	1	2	0	98	86
1	0	14	48	-55	-1	0	15	130	-117	-7	1	16	50	56	-5	-1	18	64	-60	2	2	0	99	76
2	0	14	121	119	-2	0	15	111	-112	-4	1	16	54	59	-1	-1	18	39	46	3	2	0	213	163
3	0	14	54	39	-4	0	15	51	55	-2	1	16	56	66	-5	0	18	54	61	4	2	0	109	81
4	0	14	40	-38	-6	0	15	38	-39	0	1	16	47	49	-4	0	18	37	27	5	2	0	50	-37
-5	1	14	39	39	-7	0	15	60	-62	1	1	16	37	41	-2	0	18	74	78	2	0	0	46	57
-3	1	14	48	-51	2	1	15	39	-33	-6	2	16	45	-59	1	0	18	61	-55	5	0	0	70	70
2	1	14	67	-62	1	1	15	38	-40	-2	2	16	53	54	3	0	18	69	62	7	0	0	77	89
4	1	14	48	-53	-3	1	15	42	-38	1	2	16	65	-65	-6	1	18	37	-36	-7	1	0	56	62
-7	2	14	82	-94	-5	1	15	38	-46	2	2	16	97	-90	-4	1	18	49	-47	-6	1	0	60	62
-4	2	14	71	-78	2	2	15	88	-85	-2	3	16	82	92	-3	1	18	51	-44	-5	1	0	60	66
-2	2	14	31	-33	1	2	15	122	-117	-1	3	16	52	58	-2	2	18	42	42	0	1	0	96	88
0	2	14	51	-46	-1	2	15	63	58	0	3	16	46	35	-1	2	18	61	66	1	1	0	52	51
-3	3	14	53	52	-3	2	15	72	-76	-5	4	16	53	60	1	2	18	78	87	3	1	0	61	-61
-1	3	14	41	-42	-5	2	15	36	-31	-2	4	16	45	49	1	-2	19	127	114	4	1	0	56	-47
0	3	14	89	-81	-7	2	15	66	-68	2	-4	17	62	57	0	-2	19	60	55	6	1	0	83	74
1	3	14	57	-49	-7	3	15	37	-42	3	-3	17	51	58	-3	-2	19	58	-49	-5	2	0	129	137
-4	4	14	83	-101	-1	4	15	81	-61	2	-3	17	46	44	0	-1	19	49	-47	0	2	0	110	81

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR SUBCELL OF OKENITE

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
1	2	0	92	66	5	-2	1	85	100	-4	3	1	54	-47	6	-2	2	154	165	0	5	2	78	-80
2	2	0	95	76	2	-2	1	78	80	-5	3	1	65	60	-5	-1	2	61	57	1	5	2	50	-45
3	2	0	196	163	1	-2	1	69	-82	6	4	1	77	64	-2	-1	2	105	-99	-3	6	2	67	67
4	2	0	101	81	0	-2	1	85	-85	-3	4	1	68	-77	-1	-1	2	62	66	-2	6	2	67	-66
-6	3	0	89	101	-1	-2	1	86	-57	-5	4	1	63	-66	1	-1	2	52	53	0	-7	3	72	81
-5	3	0	80	66	-2	-2	1	72	-50	-6	4	1	135	-147	-5	0	2	44	31	4	-6	3	83	-87
0	3	0	48	36	-3	-2	1	91	83	0	5	1	143	-108	-4	0	2	133	-127	-1	-6	3	54	-45
2	3	0	146	101	-4	-2	1	54	-44	4	6	1	71	51	-3	0	2	192	-174	-2	-6	3	93	-84
-2	4	0	245	254	2	-1	1	84	109	2	6	1	67	59	-2	0	2	63	-49	-4	-6	3	57	-49
3	4	0	94	77	0	-1	1	65	-74	-2	6	1	54	-58	1	0	2	62	76	3	-5	3	61	64
6	4	0	74	55	-1	-1	1	39	36	-4	6	1	53	-53	3	0	2	58	53	0	-5	3	75	-65
-5	5	0	82	-83	8	0	1	80	79	-8	6	1	68	-76	6	0	2	88	81	8	-4	3	58	58
1	5	0	49	-41	5	0	1	62	63	-2	-6	2	74	-45	9	0	2	96	98	6	-4	3	69	-85
2	5	0	92	-61	4	0	1	72	-83	-1	-5	2	98	-87	-4	1	2	53	-50	4	-4	3	45	-64
4	5	0	87	66	-2	0	1	93	94	0	-5	2	147	-130	-1	1	2	73	82	2	-4	3	38	-39
0	7	0	75	53	-3	0	1	56	52	-7	-4	2	71	-56	1	1	2	114	104	-1	-4	3	138	-126
4	-8	1	96	108	-4	0	1	85	-87	-3	-4	2	71	47	2	1	2	42	-54	5	-3	3	71	85
2	-8	1	71	57	-5	0	1	46	45	-2	-4	2	126	-94	4	1	2	45	39	2	-3	3	50	-50
4	-6	1	73	65	-7	0	1	118	112	-1	-4	2	64	-34	6	1	2	53	-44	-2	-3	3	133	108
2	-6	1	73	68	-9	0	1	66	-68	0	-4	2	48	47	-9	2	2	59	-59	-4	-3	3	67	-61
-1	-6	1	125	86	2	1	1	118	-91	1	-4	2	49	-55	-8	2	2	109	-112	5	-2	3	80	-77
6	-5	1	60	-63	1	1	1	63	-59	6	-4	2	55	-47	-5	2	2	51	-57	3	-2	3	63	74
4	-5	1	59	64	0	1	1	36	-33	-7	-3	2	55	38	-3	2	2	82	74	2	-2	3	206	-227
1	-5	1	47	47	-3	1	1	110	-112	-1	-3	2	70	-48	-1	2	2	41	-45	0	-2	3	50	35
-1	-5	1	54	-34	-5	1	1	58	-61	2	-3	2	61	-64	0	2	2	246	-192	-1	-2	3	90	74
7	-4	1	75	87	5	2	1	88	-81	3	-3	2	74	-93	1	2	2	107	72	-2	-2	3	54	55
2	-4	1	238	263	4	2	1	106	92	5	-3	2	54	54	2	2	2	105	-80	-3	-2	3	88	-91
0	-4	1	92	81	3	2	1	75	62	-7	-2	2	98	-86	4	2	2	149	123	-6	-2	3	72	-71
-1	-4	1	56	35	-2	2	1	53	-76	-6	-2	2	165	-146	9	2	2	73	71	-2	-1	3	50	-55
-2	-4	1	99	-59	-6	2	1	129	-131	-4	-2	2	140	-130	-5	3	2	59	60	-6	-1	3	81	75
-3	-4	1	58	43	-8	2	1	52	-75	-3	-2	2	89	-79	3	3	2	121	93	7	0	3	72	69
-5	-4	1	68	61	-9	2	1	71	-69	-1	-2	2	101	82	-5	4	2	81	-85	6	0	3	63	56
-1	-3	1	69	59	4	3	1	66	-51	0	-2	2	40	-46	-2	4	2	50	-46	5	0	3	118	-110
-4	-3	1	45	43	1	3	1	130	-98	2	-2	2	124	-136	2	4	2	73	-56	4	0	3	96	-93
-5	-3	1	56	56	0	3	1	65	-47	3	-2	2	43	57	4	4	2	73	58	-2	0	3	49	-52
6	-2	1	68	62	-2	3	1	57	-63	5	-2	2	55	54	-1	5	2	81	77	-3	0	3	247	-221

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	1	3	65	-77	-2	-3	4	81	71	0	2	4	71	-61	-4	-1	5	59	61	-5	4	5	113	119
2	1	3	40	-32	7	-2	4	117	-127	-2	2	4	96	-92	-2	-1	5	46	-48	-3	4	5	41	51
1	1	3	82	56	5	-2	4	94	-114	-4	2	4	59	64	-1	-1	5	59	55	-1	4	5	92	80
-1	1	3	53	-55	3	-2	4	101	-119	-5	2	4	64	-63	0	-1	5	42	-47	0	4	5	100	93
-2	1	3	79	82	2	-2	4	204	-209	-7	2	4	60	-69	1	-1	5	40	55	4	4	5	64	-52
-3	1	3	36	31	1	-2	4	58	-77	2	3	4	86	66	2	-1	5	97	110	0	5	5	66	-54
-8	1	3	55	41	0	-2	4	106	-91	1	3	4	60	-49	3	-1	5	45	51	-3	6	5	101	103
5	2	3	114	-95	-1	-2	4	56	-56	0	3	4	41	-35	-7	0	5	87	79	-2	6	5	66	53
3	2	3	116	-99	-3	-2	4	91	-84	-3	3	4	68	70	-6	0	5	86	80	3	-6	6	63	65
2	2	3	68	-48	-4	-2	4	61	56	-5	3	4	65	68	-4	0	5	203	180	3	-5	6	56	50
1	2	3	44	-25	-7	-2	4	76	80	2	4	4	49	41	-3	0	5	115	99	0	-5	6	101	-107
0	2	3	349	-252	3	-1	4	64	-75	-6	4	4	61	69	1	0	5	91	88	-3	-5	6	53	45
-1	2	3	43	-47	2	-1	4	58	57	-5	5	4	71	-78	2	0	5	104	112	4	-4	6	64	80
-5	2	3	128	-126	-4	-1	4	50	-42	1	6	4	60	-61	6	0	5	66	-67	3	-4	6	45	52
-7	2	3	65	-61	-7	-1	4	59	-60	0	6	4	66	52	-5	1	5	65	-57	1	-4	6	67	62
-9	2	3	81	68	6	0	4	68	-76	0	7	4	83	76	-3	1	5	63	51	-1	-4	6	158	122
2	3	3	74	-55	5	0	4	88	-100	-2	-6	5	95	89	-2	1	5	54	43	-2	-4	6	90	93
0	3	3	51	46	2	0	4	117	-122	4	-6	5	71	-72	-1	1	5	75	77	-3	-4	6	81	78
-3	3	3	64	-58	0	0	4	72	82	5	-6	5	58	-62	0	1	5	55	41	-4	-4	6	69	61
-5	3	3	55	-70	-2	0	4	56	-60	7	-6	5	74	-90	1	1	5	83	77	5	-3	6	90	106
3	5	3	89	-77	-3	0	4	111	-98	-1	-5	5	65	-37	3	1	5	42	44	2	-3	6	82	-97
1	6	3	96	-80	-4	0	4	93	101	0	-5	5	49	-49	4	1	5	74	78	0	-3	6	63	53
-1	6	3	76	-68	-5	0	4	53	-46	2	-5	5	61	-68	-9	2	5	63	64	-4	-3	6	47	-45
-2	6	3	110	-113	-6	0	4	99	85	4	-5	5	69	75	-4	2	5	94	92	6	-2	6	64	71
-1	-6	4	113	-79	-7	0	4	103	95	-2	-4	5	69	61	-3	2	5	131	133	2	-2	6	73	69
4	-6	4	66	-71	6	1	4	63	65	4	-4	5	48	42	-2	2	5	42	-42	1	-2	6	45	54
7	-5	4	57	-71	1	1	4	73	-54	6	-4	5	69	-64	-1	2	5	45	41	0	-2	6	80	76
-4	-5	4	75	72	0	1	4	55	59	2	-3	5	85	84	0	2	5	49	51	-1	-2	6	184	153
-2	-5	4	42	-26	-1	1	4	58	-56	3	-3	5	42	-29	1	2	5	85	-68	-2	-2	6	56	53
5	-5	4	73	-73	-2	1	4	45	-40	-7	-2	5	80	67	4	2	5	62	59	3	-1	6	48	-59
7	-4	4	61	-76	-3	1	4	194	-178	-2	-2	5	43	33	5	2	5	68	51	2	-1	6	57	-60
4	-4	4	53	-61	-6	1	4	54	51	-1	-2	5	56	48	-5	3	5	72	72	1	-1	6	64	73
1	-4	4	52	-61	5	2	4	97	-99	0	-2	5	140	-128	-2	3	5	55	48	0	-1	6	54	52
0	-4	4	57	-53	3	2	4	130	-104	3	-2	5	57	-56	2	3	5	90	73	-1	-1	6	62	56
-1	-4	4	248	-167	2	2	4	66	53	5	-2	5	59	-65	5	3	5	61	60	-2	-1	6	77	-75
-4	-4	4	63	55	1	2	4	79	-65	-5	-1	5	62	56	-7	4	5	54	59	-4	-1	6	46	-43

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
7	0	6	73	95	0	-1	7	65	-68	5	-4	8	44	50	-7	-3	9	64	57	3	4	9	80	-73
5	0	6	44	59	1	-1	7	52	-54	4	-4	8	50	48	0	-3	9	70	64	-4	5	9	65	-62
4	0	6	79	-86	-9	0	7	108	-108	2	-4	8	67	69	2	-3	9	56	-56	-1	5	9	56	57
3	0	6	46	-63	-7	0	7	64	-59	0	-4	8	59	-54	3	-3	9	45	-55	-2	6	9	87	-90
2	0	6	79	105	-5	0	7	56	48	-2	-4	8	104	-101	-4	-2	9	56	-54	4	-6	10	71	-69
1	0	6	85	91	-3	0	7	90	73	-5	-4	8	69	-77	-3	-2	9	68	-58	1	-6	10	65	-62
-1	0	6	160	164	-2	0	7	186	-155	-7	-4	8	79	-82	-1	-2	9	99	-82	-2	-6	10	63	-72
-2	0	6	92	-87	-1	0	7	41	42	3	-3	8	59	-68	1	-2	9	66	-74	6	-4	10	96	-109
-3	0	6	132	113	0	0	7	156	186	3	-2	8	65	-70	4	-2	9	74	-92	4	-4	10	77	-92
-5	0	6	102	93	1	0	7	60	-61	1	-2	8	97	-108	-5	-1	9	64	68	0	-4	10	56	-45
-6	0	6	67	74	2	0	7	72	79	-2	-2	8	75	-74	-4	-1	9	50	46	-1	-4	10	109	-89
1	1	6	59	62	3	0	7	60	65	-5	-2	8	64	-67	5	-1	9	51	-74	-2	-4	10	66	-63
-4	1	6	52	-39	5	0	7	64	82	-7	-2	8	88	-80	-6	0	9	66	-52	-3	-4	10	90	86
5	2	6	62	56	7	0	7	66	67	-3	-1	8	68	-65	-5	0	9	71	59	5	-3	10	51	57
0	2	6	152	123	-3	1	7	46	-47	8	0	8	88	94	-4	0	9	83	-78	2	-3	10	48	-45
-3	2	6	76	79	-2	1	7	48	-41	-1	0	8	85	-77	2	0	9	47	-50	-4	-3	10	64	-69
-4	2	6	64	-61	-1	1	7	127	-124	-2	0	8	70	-69	4	0	9	92	-106	4	-2	10	81	-100
-4	3	6	49	-36	-7	2	7	139	-125	-4	0	8	98	-96	-9	1	9	52	41	2	-2	10	164	-185
5	4	6	74	55	-6	2	7	46	-38	-9	0	8	98	-87	-3	1	9	49	42	1	-2	10	74	-69
3	4	6	85	70	-4	2	7	65	-55	-1	1	8	54	53	2	1	9	54	-59	0	-2	10	53	54
2	4	6	86	-73	-3	2	7	74	69	-3	1	8	111	-102	-7	2	9	62	58	-1	-2	10	56	-54
-4	4	6	53	-62	0	2	7	103	96	1	2	8	83	-91	-6	2	9	73	-68	-3	-2	10	105	-109
-7	4	6	75	66	2	2	7	66	57	-1	2	8	91	-79	-5	2	9	117	-111	-4	-2	10	49	-52
-3	5	6	75	-77	-7	3	7	49	-53	-3	2	8	79	-70	-4	2	9	54	-49	2	-1	10	51	-56
-2	5	6	61	68	-6	4	7	73	-80	-9	2	8	85	-76	-3	2	9	85	-82	5	0	10	62	-72
1	-8	7	66	69	-4	4	7	87	-85	2	3	8	75	58	-1	2	9	117	-111	4	0	10	89	-109
-1	-4	7	50	35	-2	4	7	85	72	1	3	8	51	-55	0	2	9	127	-120	2	0	10	67	-70
0	-4	7	79	-79	0	4	7	60	59	-1	3	8	56	-52	1	2	9	47	-38	-2	0	10	65	-60
2	-4	7	79	79	3	4	7	95	83	-6	4	8	91	-92	2	2	9	147	-154	-3	0	10	131	-118
7	-4	7	54	75	-5	5	7	68	-74	2	5	8	56	-36	-2	3	9	52	44	-4	0	10	42	-52
-1	-3	7	89	-70	2	5	7	57	-53	0	5	8	99	-85	-1	3	9	69	64	-5	0	10	115	119
1	-3	7	42	40	-3	6	7	62	-65	0	6	8	63	-55	-7	4	9	82	94	1	1	10	46	64
-1	-2	7	88	67	4	-6	8	62	65	-5	6	8	93	-100	-6	4	9	55	-56	-2	1	10	44	-39
1	-2	7	42	41	2	-5	8	64	-72	-1	-5	9	67	-58	-3	4	9	58	-46	-5	1	10	75	63
2	-2	7	143	161	1	-5	8	70	-69	0	-5	9	65	-46	0	4	9	72	-83	3	2	10	52	63
-1	-1	7	69	-64	-1	-5	8	70	-59	6	-4	9	56	-56	2	4	9	140	-115	1	2	10	68	59

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
0	2	10	152	-151	2	3	11	58	54	-1	4	12	64	61	-3	-3	14	60	54	-7	2	15	80	-68
-2	3	10	75	76	-9	4	11	77	84	-5	4	12	60	55	2	-2	14	60	-59	-4	2	15	75	-72
-3	2	10	45	-42	-1	4	11	70	84	-3	6	12	80	73	-1	-2	14	86	93	-3	2	15	69	-76
-5	2	10	106	-98	2	4	11	74	68	-5	-5	13	79	-73	-3	-2	14	61	-57	-1	2	15	63	58
-8	2	10	85	-86	-6	6	11	88	93	0	-5	13	57	-52	-5	-2	14	83	-77	1	2	15	108	-117
3	3	10	65	58	2	-7	12	65	54	4	-4	13	82	78	2	0	14	83	119	2	2	15	80	-85
-3	3	10	53	65	0	-6	12	100	93	5	-4	13	54	-76	-2	0	14	92	-100	-4	4	15	59	-44
-7	4	10	68	59	-2	-6	12	79	75	-4	-3	13	68	-71	-5	0	14	91	76	-3	4	15	83	-79
-1	5	10	99	93	4	-5	12	110	123	-2	-3	13	82	-80	-3	1	14	58	-51	1	-4	16	89	-101
-6	6	10	77	82	4	-4	12	74	76	-1	-3	13	69	-77	-4	2	14	60	-78	3	-2	16	66	-64
1	-5	11	85	-72	0	-4	12	53	62	-3	-2	13	111	-107	-5	2	14	50	-41	-4	-2	16	89	-75
4	-5	11	63	-56	-1	-4	12	76	75	-1	-2	13	76	92	-7	2	14	90	-94	-1	0	16	82	-98
4	-4	11	52	-65	-2	-4	12	95	79	1	-2	13	61	75	0	3	14	71	-81	-2	1	16	54	66
-2	-3	11	67	52	-5	-4	12	62	64	-2	-1	13	115	-121	-3	3	14	54	52	-4	1	16	75	59
1	-3	11	86	100	-1	-3	12	57	46	-1	-1	13	47	-51	-1	4	14	93	-82	2	2	16	75	-90
2	-3	11	76	67	-5	-3	12	53	54	0	-1	13	56	-66	-4	4	14	92	-101	-7	2	16	73	80
-7	-2	11	81	68	6	-2	12	70	93	-8	0	13	97	-97	-9	4	14	73	-74	-8	2	16	68	71
-2	-2	11	105	106	1	-2	12	52	69	-7	0	13	74	-68	2	5	14	66	-59	-2	3	16	86	92
-1	-2	11	56	-58	-1	-2	12	79	69	-2	0	13	63	-77	-6	6	14	70	-68	-3	4	16	69	-63
2	-2	11	51	-63	-2	-2	12	180	168	1	0	13	97	109	1	-5	15	64	-65	-5	4	16	57	60
1	-1	11	75	76	-1	-1	12	47	49	2	0	13	177	206	-5	-4	15	71	-65	-7	4	16	67	74
2	-1	11	114	126	-3	-1	12	57	-50	-5	1	13	55	53	0	-4	15	53	-62	-3	-4	17	77	66
-7	0	11	153	142	4	0	12	62	70	-1	1	13	72	-78	3	-4	15	78	-78	0	-3	17	80	96
-5	0	11	74	85	1	0	12	57	75	-7	2	13	63	-58	-6	-3	15	61	51	-5	-2	17	105	119
-4	0	11	126	116	-4	0	12	58	52	-5	2	13	131	-116	-5	-3	15	71	65	4	-2	17	81	-93
0	0	11	73	70	-7	0	12	82	76	-3	2	13	127	123	3	-3	15	71	-82	-5	0	17	130	122
3	0	11	56	60	-5	1	12	70	-56	4	2	13	74	76	4	-3	15	79	-98	-3	0	17	55	56
5	0	11	73	-64	4	2	12	66	76	-4	4	13	58	-55	-5	-2	15	114	-110	-5	1	17	70	68
0	1	11	75	73	1	2	12	57	-72	0	4	13	116	115	-2	-2	15	121	-121	-7	2	17	85	83
5	1	11	55	67	-1	2	12	59	61	-4	5	13	66	-68	-1	-2	15	52	-56	-3	-4	18	65	49
-9	2	11	89	87	-4	2	12	85	81	-3	5	13	70	-65	-7	0	15	77	-62	-5	-1	18	64	-60
-6	2	11	52	51	-5	2	12	79	-85	-5	6	13	81	86	-4	0	15	59	55	-2	0	18	68	78
-4	2	11	209	207	-4	3	12	72	-81	0	-5	14	64	-57	-2	0	15	113	-112	-5	0	18	76	61
-2	2	11	60	53	-7	3	12	71	-67	4	-4	14	70	92	-1	0	15	118	-117	1	2	18	54	67
-1	2	11	66	72	1	4	12	53	-57	0	-4	14	55	-65	1	0	15	138	-156	0	-4	19	62	67
-3	3	11	86	80	0	4	12	105	85	1	-3	14	63	70	6	0	15	55	-60	1	-2	19	102	114

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR SUBCELL OF OREMITE

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	0	19	89	89	-4	3	19	62	-63	-1	1	20	69	-79	9	4	0	141	27	-9	-4	3	168	-36
-1	2	19	73	83	-5	0	20	52	-54	-5	2	20	71	-62										

SUMMARY OF ERRORS FOR THIS JOB

ERROR NUMBER	NUMBER OF ERRORS
209	1