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Crystal structure of cappelenite, $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$: a silicoborate sheet structure

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Abstract

Cappelenite, $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$, is based on a $^2_\infty[Si_3B_6O_{24}]$ tetrahedral corner-sharing sheet consisting of $[B_6O_{18}]$ six-membered and $[Si_3B_6O_{27}]$ nine-membered rings. The nine-membered rings are isomorphic to the insular $[Si_3Si_6O_{27}]$ rings in eudialyte. It is trigonal, a = 10.67(2), c = 4.680(2)Å, Z = 1, space group $P3$ with pronounced $P6mm$ symmetry through the *Zellengleich* relation $P3 \rightarrow P3ml \rightarrow P6mm$. R = 0.063 for 1450 independent reflections. The structure also is based on the $\{(6 \cdot 4 \cdot 3 \cdot 4)^4\}$ semi-regular net when the Y atoms are joined together in a plane parallel to {001} and may occur in other structures such as melanocerite, caryocerite, tritomite, *etc.* $[BaO_{12}]$ defines an hexagonal antiprism; $[YO_7F]$, square antiprisms; $[SiO_4]$ and $[BO_4]$, tetrahedra. The (Y,RE):F = 3:1 ratio appears to be characteristic for these lanthanide silicate compounds. Mean distances are $^{[12]}$Ba–O = 2.96, $^{[8]}$Y(1)–O = 2.38, $^{[8]}$Y(2)–O = 2.43, $^{[4]}$B(1)–O = 1.48, $^{[4]}$B(2)–O = 1.47 and $^{[4]}$Si–O = 1.64Å. The fluoride distances are 3F(1)–Y(1) = 2.38 and 3F(2)–Y(2) = 2.34Å.

Introduction

Cappelenite was named by the famous mineralogist–petrologist W. C. Brøgger (1885) honoring its discoverer, Mr. D. Cappelen of Holden, Norway. Only two specimens were found by Mr. Cappelen on the eastern side of the island Lille-Arø, a part of the nepheline syenites and pegmatitic syenitic veins in the mineralogically complex and classic Langesundfjord of Southern Norway. Brøgger (1890), in a definitive study, described the mineralogy of this region, which included over seventy species. Of these, over half were exotic titano- and zirconosilicates, beryllosilicates, borosilicates of alkalies, lanthanides and actinides, the last-mentioned usually occurring in a metamict state and amorphous to X-radiation. To restore crystallinity, such phases are usually heated, but it is not clear in powder diffraction studies whether reconstituted material is in fact representative of the original species, or is a product of recrystallization and/or decomposition of the parent structure. Therefore, Brøgger and coworkers afford a valuable service to our science through careful goniometric study and detailed chemical analyses.

Brøgger reported two specimens of this curious mineral, one a free crystal 2 cm in length and 1.5 cm in width, and a hand specimen displaying a broken crystal. Our interest in crystal-chemical systematics of the lanthanide silicates and borosilicates such as cerite, törnebohmite, steenstrupine, *etc.*, led to cappelenite, which has an unusual composition. Brøgger (1890) suggested $R^{3+}BO_3 \cdot R^{2+}SiO_3$ where R^{3+} = Y, La, Nd and R^{2+} = Ba, Ca, Na_2, K_2. Strunz (1970) proposed (Ba, *etc.*) (Y, *etc.*)$_2$ $(B_2O_5)(SiO_4)$. Povarennykh (1972) offered $BaY_2(BSiO_5)(BO_4)$. More recently, Ramdohr and Strunz (1978) suggested $BaY_6B_6Si_3O_{25}$. Our crystal structure analysis admits the proposed composition $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$.

Experimental details

Fragments of the type material (collected by D. Cappelen, 1879) were kindly provided by Dr. Gunnar Raade of the Mineralogical-Geological Museum, University of Oslo. Small clear pale yellowish chips failed to provide any single crystal diffraction pattern and a metamict state was assumed. We were encouraged by Pabst (1961) who obtained excellent single crystal photographs of davidite through thermal reconstitution of previous metamict material. He reconstituted grains at temperatures between 1150°–1375°C. Lima de Faria (1956) noted that once reconstitution took place, the duration of heat treatment did not lead to further changes—a conclusion which Pabst also made.

For cappelenite, we were in essentially uncharted

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Table 2. Cappelenite. |Fo|, |Fc| tables. ~~[illegible]~~ Shen and Moore

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CAPPELENITE DATA RED 1Ø/25/82

H	K	L	FO	FC
-1	[illegible]	Ø	9	12
Ø	[illegible]	Ø	7	14
1	1	Ø	1Ø	5
-3	2	Ø	126	119
-2	[illegible]	Ø	27	16
-1	2	Ø	8	5
Ø	2	Ø	28	18
1	[illegible]	Ø	123	121
2	[illegible]	Ø	91	88
[illegible]	[illegible]	Ø	27	23
[illegible]	[illegible]	Ø	15	9
-3	3	Ø	47	36
-2	3	Ø	125	12Ø
-1	3	Ø	123	12Ø
Ø	3	Ø	43	39
1	[illegible]	Ø	12	14
2	3	Ø	27	25
3	3	Ø	241	232
-7	4	Ø	27	25
-5	4	Ø	38	36
-4	4	Ø	148	147
-3	4	Ø	15	8
-2	4	Ø	91	88
-1	4	Ø	12	14
Ø	[illegible]	Ø	149	144
1	[illegible]	Ø	37	37
2	4	Ø	7	1Ø
3	4	Ø	27	27
4	4	Ø	58	57
-9	5	Ø	84	82
-8	[illegible]	Ø	32	31
-7	[illegible]	Ø	1Ø	12
-6	[illegible]	Ø	56	56
-5	5	Ø	191	181

H	K	L	FO	FC
-4	5	Ø	38	37
-3	5	Ø	27	24
-2	5	Ø	26	26
-1	5	Ø	37	36
Ø	5	Ø	19Ø	179
1	5	Ø	59	52
2	5	Ø	9	7
3	5	Ø	33	32
4	5	Ø	85	81
5	5	Ø	72	68
-11	6	Ø	33	35
-9	6	Ø	58	51
-8	6	Ø	141	139
-7	6	Ø	57	53
-6	6	Ø	36	3Ø
-5	6	Ø	56	54
-3	6	Ø	24Ø	232
-2	6	Ø	8	9
-1	6	Ø	58	53
Ø	6	Ø	36	32
1	6	Ø	55	56
2	6	Ø	141	139
3	6	Ø	57	54
4	6	Ø	11	8
5	6	Ø	36	35
6	6	Ø	117	113
-13	7	Ø	29	28
-12	7	Ø	14	4
-11	7	Ø	3Ø	32
-1Ø	7	Ø	25	27
-9	7	Ø	39	36
-8	7	Ø	7Ø	65
-7	7	Ø	19	1Ø
-6	7	Ø	57	54

H	K	L	FO	FC
-5	7	Ø	11	1Ø
-4	7	Ø	27	26
-3	7	Ø	26	26
-2	7	Ø	11	8
-1	7	Ø	52	57
Ø	7	Ø	11	18
1	7	Ø	71	67
2	7	Ø	35	36
3	7	Ø	26	24
4	7	Ø	32	3Ø
6	7	Ø	29	24
-15	8	Ø	47	45
-14	8	Ø	24	23
-12	8	Ø	18	21
-11	8	Ø	136	131
-1Ø	8	Ø	2Ø	17
-9	8	Ø	18	2Ø
-8	8	Ø	19	27
-7	8	Ø	69	66
-6	8	Ø	14Ø	14Ø
-5	8	Ø	31	31
-4	8	Ø	57	57
-3	8	Ø	32	32
-2	8	Ø	138	139
-1	8	Ø	67	67
Ø	8	Ø	19	17
1	8	Ø	18	14
2	8	Ø	2Ø	21
3	8	Ø	132	133
4	8	Ø	18	16
5	8	Ø	15	1Ø
6	8	Ø	23	25
7	8	Ø	46	48
8	8	Ø	81	81

H	K	L	FO	FC
-17	9	Ø	29	29
-15	9	Ø	26	24
-14	9	Ø	74	74
-13	9	Ø	21	19
-12	9	Ø	22	25
-11	9	Ø	32	33
-1Ø	9	Ø	12	7
-9	9	Ø	131	128
-8	9	Ø	15	15
-7	9	Ø	37	33
-6	9	Ø	58	53
-5	9	Ø	83	82
-4	9	Ø	83	81
-3	9	Ø	56	53
-2	9	Ø	34	4Ø
-1	9	Ø	2Ø	16
Ø	9	Ø	131	126
2	9	Ø	33	34
3	9	Ø	24	26
4	9	Ø	23	21
5	9	Ø	77	72
6	9	Ø	24	3Ø
7	9	Ø	17	7
8	9	Ø	28	32
-17	1Ø	Ø	21	6
-16	1Ø	Ø	16	12
-14	1Ø	Ø	45	43
-13	1Ø	Ø	16	16
-12	1Ø	Ø	48	47
-1Ø	1Ø	Ø	53	5Ø
-8	1Ø	Ø	19	18
-7	1Ø	Ø	27	26
-5	1Ø	Ø	7Ø	69
-4	1Ø	Ø	14	9

H	K	L	FO	FC
-3	1Ø	Ø	26	24
-2	1Ø	Ø	2Ø	19
Ø	1Ø	Ø	51	51
1	1Ø	Ø	16	9
2	1Ø	Ø	47	44
3	1Ø	Ø	18	15
4	1Ø	Ø	45	45
-17	11	Ø	72	68
-14	11	Ø	3Ø	34
-13	11	Ø	55	52
-12	11	Ø	73	72
-11	11	Ø	36	31
-9	11	Ø	35	33
-8	11	Ø	133	13Ø
-7	11	Ø	34	31
-6	11	Ø	35	36
-5	11	Ø	36	33
-4	11	Ø	33	32
-3	11	Ø	131	133
-2	11	Ø	32	34
-1	11	Ø	18	1Ø
Ø	11	Ø	32	37
1	11	Ø	73	71
2	11	Ø	56	51
3	11	Ø	32	34
-16	12	Ø	42	37
-15	12	Ø	73	7Ø
-14	12	Ø	17	18
-13	12	Ø	17	7
-12	12	Ø	14	5
-11	12	Ø	71	72
-1Ø	12	Ø	46	44
-9	12	Ø	24	26
-8	12	Ø	13	23

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CAPPELENITE DATA RED 1Ø/25/82

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	12	Ø	115	113	Ø	14	Ø	94	97	-5	4	1	54	56	-2	6	1	14	14	-1Ø	8	1	11	5
-5	12	Ø	12	2	-12	15	Ø	68	7Ø	-4	4	1	1Ø8	1Ø4	-1	6	1	1Ø	3	-9	8	1	18	16
-4	12	Ø	2Ø	15	-9	15	Ø	29	26	-3	4	1	58	52	Ø	6	1	67	68	-8	8	1	76	73
-3	12	Ø	24	26	-8	15	Ø	47	45	-2	4	1	46	44	1	6	1	89	9Ø	-7	8	1	58	58
-2	12	Ø	44	46	-7	15	Ø	45	47	-1	4	1	65	54	2	6	1	112	11Ø	-6	8	1	112	112
-1	12	Ø	74	71	-6	15	Ø	26	26	Ø	4	1	96	1Ø4	3	6	1	23	23	-5	8	1	28	23
Ø	12	Ø	13	11	-3	15	Ø	66	69	1	[illegible]	1	42	42	4	6	1	33	31	-4	8	1	46	44
2	12	Ø	2Ø	18	-13	16	Ø	41	37	2	[illegible]	1	12	13	5	6	1	33	37	-3	8	1	46	43
3	12	Ø	75	71	-12	16	Ø	43	37	3	4	1	31	32	6	6	1	93	93	-2	8	1	111	11Ø
4	[illegible]	Ø	39	36	-9	16	Ø	14	1Ø	4	4	1	47	43	-13	7	1	44	37	-1	8	1	6Ø	61
-16	13	Ø	41	41	-8	16	Ø	79	81	-9	5	1	89	88	-12	7	1	19	12	Ø	8	1	49	5Ø
-11	13	Ø	52	51	-4	16	Ø	35	37	-8	5	1	28	24	-11	7	1	34	32	1	8	1	23	22
-9	13	Ø	21	22	-3	16	Ø	39	41	-7	5	1	1Ø	8	-1Ø	7	1	5Ø	51	2	8	1	12	13
-8	13	Ø	14	16	Ø	Ø	1	166	178	-6	5	1	33	28	-9	7	1	13	11	3	8	1	116	117
-7	13	Ø	27	25	-1	1	1	14	19	-5	5	1	168	164	-8	7	1	6Ø	57	4	8	1	24	23
-6	13	Ø	29	25	Ø	1	1	1Ø	6	-4	5	1	53	57	-7	7	1	35	28	6	8	1	37	4Ø
-5	13	Ø	13	15	1	1	1	55	61	-3	5	1	41	35	-6	7	1	9Ø	89	7	8	1	48	44
-4	13	Ø	22	19	-3	2	1	183	174	-2	5	1	5Ø	52	-4	7	1	5Ø	53	8	8	1	45	47
-3	13	Ø	18	17	-2	2	1	63	6Ø	-1	5	1	42	44	-3	7	1	31	32	-17	9	1	19	19
-2	13	Ø	53	51	-1	2	1	54	62	Ø	5	1	158	163	-2	7	1	26	27	-16	9	1	22	13
Ø	13	Ø	14	6	Ø	2	1	75	74	1	5	1	9	4	-1	7	1	91	91	-15	9	1	23	17
1	13	Ø	17	4	1	2	1	179	18Ø	2	5	1	27	29	Ø	7	1	42	36	-14	9	1	97	95
2	13	Ø	4Ø	4Ø	2	2	1	48	47	3	5	1	45	43	1	7	1	6Ø	59	-13	9	1	28	27
-1[illegible]	[illegible]	Ø	1ØØ	97	-5	3	1	41	37	4	5	1	99	98	2	7	1	26	17	-12	9	1	21	19
-12	14	Ø	17	18	-4	3	1	6Ø	53	5	5	1	73	69	3	7	1	46	47	-11	9	1	21	27
-11	14	Ø	29	37	-3	3	1	69	67	-11	6	1	16	13	4	7	1	36	34	-1Ø	9	1	19	2Ø
-1Ø	14	Ø	44	45	-2	3	1	173	172	-1Ø	6	1	33	31	5	7	1	16	11	-9	9	1	13Ø	123
-9	14	Ø	72	78	-1	3	1	179	179	-9	6	1	23	28	6	7	1	37	36	-8	9	1	16	15
-8	14	Ø	25	23	Ø	3	1	41	39	-8	6	1	114	114	7	7	1	18	13	-7	9	1	14	13
-7	14	Ø	13	1Ø	1	3	1	65	56	-7	6	1	92	9Ø	-15	8	1	49	45	-6	9	1	22	26
-6	14	Ø	23	25	2	3	1	51	53	-6	6	1	51	48	-14	8	1	25	26	-5	9	1	87	88
-5	14	Ø	77	74	3	3	1	19Ø	185	-5	6	1	34	28	-13	8	1	14	16	-4	9	1	98	97
-4	14	Ø	45	43	-7	4	1	51	52	-4	6	1	28	24	-12	8	1	39	36	-3	9	1	24	22
-3	[illegible]	Ø	31	34	-6	4	1	28	24	-3	6	1	19Ø	188	-11	8	1	117	117	-2	9	1	28	16

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	9	1	23	19	-6	11	1	14	15	-11	13	1	59	56	1	1	2	15	16	-3	5	2	42	47
Ø	9	1	123	126	-5	11	1	34	38	-9	13	1	28	27	-3	2	2	132	137	-2	5	2	54	51
1	9	1	29	28	-4	11	1	34	34	-8	13	1	17	17	-2	2	2	11	7	-1	5	2	26	29
3	9	1	28	29	-3	11	1	115	116	-7	13	1	43	39	-1	2	2	14	14	Ø	5	2	122	125
4	9	1	3Ø	28	-2	11	1	15	9	-6	13	1	38	37	Ø	2	2	42	44	1	5	2	19	19
5	9	1	81	85	-1	11	1	14	8	-4	13	1	3Ø	29	1	2	2	133	139	2	5	2	18	18
6	9	1	18	14	Ø	11	1	39	37	-2	13	1	65	64	2	2	2	75	76	3	5	2	57	57
8	9	1	26	26	1	11	1	71	71	Ø	13	1	14	16	-5	3	2	45	48	4	5	2	84	82
-17	10	1	3Ø	22	2	11	1	61	63	3	13	1	32	37	-4	3	2	4Ø	4Ø	5	5	2	56	57
-15	1Ø	1	19	16	3	11	1	21	2Ø	-14	14	1	8Ø	77	-3	3	2	1Ø5	1Ø2	-11	6	2	26	25
-14	[illegible]	1	34	31	4	11	1	25	19	-12	14	1	24	24	-2	3	2	131	138	-9	6	2	63	63
-13	1Ø	1	16	13	5	11	1	21	2Ø	-11	14	1	25	33	-1	3	2	134	139	-8	6	2	122	12Ø
-12	1Ø	1	34	34	-15	12	1	69	65	-1Ø	14	1	3Ø	29	Ø	3	2	46	47	-7	6	2	79	83
-11	1Ø	1	16	1Ø	-14	12	1	27	23	-9	14	1	91	91	1	3	2	54	54	-6	6	2	15	5
-1Ø	1Ø	1	37	34	-13	12	1	14	1Ø	-8	14	1	24	27	2	3	2	54	5Ø	-5	6	2	36	34
[illegible]	[illegible]	1	18	19	-12	12	1	36	31	-7	14	1	2Ø	14	3	3	2	133	139	-4	6	2	14	18
-7	1Ø	1	51	52	-11	12	1	75	78	-6	14	1	34	41	-7	4	2	32	36	-3	6	2	134	138
-6	1Ø	1	3Ø	29	-1Ø	12	1	34	34	-5	14	1	8Ø	82	-6	4	2	17	17	-2	6	2	33	35
-5	1Ø	1	72	67	-9	12	1	14	17	-4	14	1	34	35	-5	4	2	27	28	-1	6	2	19	2Ø
-4	1Ø	1	33	31	-8	12	1	37	33	-2	14	1	25	28	-4	4	2	98	98	Ø	6	2	46	47
-3	1Ø	1	45	48	-7	12	1	17	11	Ø	14	1	69	75	-3	4	2	4Ø	41	1	6	2	66	69
-1	1Ø	1	3Ø	3Ø	-6	12	1	91	95	-14	15	1	21	12	-2	4	2	73	78	2	6	2	122	124
Ø	1Ø	1	31	29	-5	12	1	13	11	-12	15	1	65	66	-1	4	2	53	55	3	6	2	2Ø	19
2	1Ø	1	31	34	-4	12	1	19	21	-11	15	1	2Ø	16	Ø	4	2	124	132	4	6	2	13	9
4	1Ø	1	37	34	-3	12	1	25	3Ø	-8	15	1	44	47	1	4	2	28	29	5	6	2	44	41
-15	11	1	19	14	-2	12	1	32	32	-7	15	1	45	42	2	4	2	33	34	6	6	2	99	97
-14	11	1	33	36	-1	12	1	7Ø	71	-4	15	1	25	18	3	4	2	35	35	-13	7	2	41	41
-13	11	1	61	56	Ø	12	1	42	43	-3	15	1	55	62	4	4	2	13	12	-12	7	2	19	16
-12	11	1	77	76	2	12	1	29	27	-13	16	1	4Ø	4Ø	-9	5	2	88	89	-11	7	2	33	36
-11	11	1	2Ø	19	3	12	1	64	62	-8	16	1	41	45	-8	5	2	29	28	-1Ø	7	2	24	25
-1Ø	[illegible]	1	19	13	-16	13	1	42	38	-3	16	1	32	35	-7	5	2	16	1Ø	-9	7	2	15	17
-9	11	1	2Ø	27	-15	13	1	26	1Ø	Ø	Ø	2	166	177	-6	5	2	34	33	-8	7	2	46	48
-8	11	1	114	119	-13	13	1	23	21	-1	1	2	41	47	-5	5	2	127	128	-7	7	2	51	5Ø
-7	11	1	32	32	-12	13	1	15	8	Ø	1	2	38	37	-4	5	2	26	28	-6	7	2	77	81

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CAPPELENITE DATA RED 1Ø/25/82

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	7	2	1Ø	12	-14	9	2	71	7Ø	1	1Ø	2	23	24	-3	12	2	32	32	-9	15	2	32	34
-4	7	2	33	33	-13	9	2	3Ø	32	2	1Ø	2	45	44	-2	12	2	47	46	-8	15	2	36	38
-3	7	2	35	33	-12	9	2	13	16	3	1Ø	2	28	27	-1	12	2	65	71	-7	15	2	39	41
-2		2	18	16	-11	9	2	3Ø	3Ø	4	1Ø	2	46	45	Ø	12	2	17	4	-4	15	2	24	29
-1		2	67	68	-1Ø	9	2	2Ø	17	-16	11	2	18	14	2	12	2	17	26	-3	15	2	5Ø	57
Ø		2	46	44	-9	9	2	1Ø7	1Ø5	-15	11	2	19	2Ø	3	12	2	52	58	-8	16	2	47	53
1	7	2	48	51	-8	9	2	14	18	-14	11	2	39	38	-15	13	2	2Ø	12	-6	16	2	2Ø	15
2		2	14	14	-7	9	2	11	16	-13	11	2	53	51	-14	13	2	18	11	Ø	Ø	3	161	169
3	7	2	49	51	-6	9	2	62	63	-12	11	2	65	62	-11	13	2	5Ø	5Ø	-1	1	3	24	28
4	7	2	17	11	-5	9	2	87	89	-11	11	2	27	28	-1Ø	13	2	21	2Ø	Ø	1	3	2Ø	18
6	7	2	3Ø	29	-4	9	2	82	83	-1Ø	11	2	3Ø	29	-9	13	2	3Ø	32	1	1	3	23	23
7		2	28	26	-3	9	2	21	16	-9	11	2	34	29	-8	13	2	25	26	-3	2	3	1Ø3	1Ø4
-15		2	4Ø	41	-2	9	2	11	13	-8	11	2	88	93	-7	13	2	38	4Ø	-2	2	3	37	44
-13		2	25	27	-1	9	2	34	32	-7	11	2	34	35	-6	13	2	26	28	-1	2	3	23	25
-12		2	16	5	Ø	9	2	98	1ØØ	-6	11	2	25	24	-5	13	2	21	2Ø	Ø	2	3	59	63
-11		2	91	94	1	9	2	23	24	-5	11	2	43	41	-4	13	2	17	17	1	2	3	1Ø8	113
-1Ø	8	2	22	19	2	9	2	17	17	-4	11	2	15	11	-3	13	2	25	24	2	2	3	53	57
-9	8	2	18	15	3	9	2	32	32	-3	11	2	88	91	-2	13	2	42	43	-5	3	3	3Ø	35
-8	8	2	42	36	4	9	2	19	18	-2	11	2	19	17	-1	13	2	19	9	-4	3	3	19	16
-7	8	2	45	47	5	9	2	82	81	-1	11	2	26	25	Ø	13	2	17	21	-3	3	3	82	84
-6	8	2	119	119	6	9	2	18	17	Ø	11	2	46	45	1	13	2	22	6	-2	3	3	1Ø1	1Ø3
-5		2	3Ø	3Ø	-14	1Ø	2	4Ø	38	1	11	2	67	7Ø	-14	14	2	76	76	-1	3	3	1Ø6	112
-4		2	12	1Ø	-13	1Ø	2	26	22	2	11	2	36	4Ø	-11	14	2	36	38	Ø	3	3	28	31
-3		2	57	55	-12	1Ø	2	51	48	3	11	2	2Ø	23	-1Ø	14	2	37	39	1	3	3	45	44
-2	8	2	124	126	-11	1Ø	2	31	3Ø	4	11	2	23	29	-9	14	2	69	68	2	3	3	17	15
-1	8	2	47	5Ø	-1Ø	1Ø	2	53	52	5	11	2	29	21	-8	14	2	19	9	3	3	3	142	145
Ø	8	2	26	26	-9	1Ø	2	17	18	-16	12	2	3Ø	26	-7	14	2	27	25	-7	4	3	26	29
1	8	2	33	31	-8	1Ø	2	22	19	-15	12	2	52	54	-6	14	2	25	29	-6	4	3	4Ø	41
3	8	2	9Ø	93	-7	1Ø	2	24	25	-12	12	2	36	38	-5	14	2	81	8Ø	-5	4	3	26	31
5	8	2	19	17	-5	1Ø	2	56	59	-11	12	2	61	63	-4	14	2	42	42	-4	4	3	46	47
6	8	2	28	29	-4	1Ø	2	15	16	-1Ø	12	2	49	5Ø	-3	14	2	23	2Ø	-3	4	3	21	15
7	8	2	45	41	-3	1Ø	2	47	51	-9	12	2	18	15	-2	14	2	21	26	-2	4	3	51	56
8	8	2	53	52	-1	1Ø	2	25	21	-7	12	2	15	14	Ø	14	2	64	74	-1	4	3	46	44
-15	9	2	28	33	Ø	1Ø	2	46	45	-6	12	2	97	96	-12	15	2	51	54	Ø	4	3	37	42

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CAPPELENITE DATA RED 1Ø/25/82

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	[illegible]	3	15	16	5	6	3	34	35	Ø	8	3	24	29	-8	1Ø	3	28	31	-1Ø	12	3	36	35
2	[illegible]	[illegible]	34	37	6	6	3	78	78	1	8	3	31	3Ø	-7	1Ø	3	3Ø	26	-9	12	3	17	21
4	[illegible]	3	31	32	-13	7	3	39	36	2	8	3	28	23	-6	1Ø	3	16	21	-8	12	3	36	37
-9	5	3	62	63	-12	7	3	17	17	3	8	3	8Ø	83	-5	1Ø	3	6Ø	62	-7	12	3	2Ø	15
-8	[illegible]	3	18	19	-11	7	3	15	16	4	8	3	22	24	-4	1Ø	3	25	26	-6	12	3	72	78
-7	5	3	16	13	-1Ø	7	3	32	25	6	8	3	43	42	-3	1Ø	3	37	36	-4	12	3	23	23
-6	5	3	36	36	-9	7	3	14	16	7	8	3	3Ø	27	-2	1Ø	3	31	26	-3	12	3	41	41
-5	5	3	115	121	-8	7	3	35	37	-15	9	3	33	29	-1	1Ø	3	25	25	-2	12	3	34	34
-4	5	3	27	31	-7	7	3	29	25	-14	9	3	69	7Ø	Ø	1Ø	3	34	35	-1	12	3	41	46
-3	5	3	28	36	-6	7	3	58	64	-13	9	3	25	21	1	1Ø	3	12	1Ø	Ø	12	3	29	29
-2	5	3	2Ø	16	-5	7	3	15	13	-12	9	3	18	2Ø	2	1Ø	3	33	38	2	12	3	28	29
-1	[illegible]	3	12	12	-4	7	3	26	3Ø	-11	9	3	36	33	3	1Ø	3	19	12	-14	13	3	21	19
Ø	[illegible]	3	111	116	-2	7	3	24	25	-1Ø	9	3	21	18	4	1Ø	3	32	31	-11	13	3	41	43
1	[illegible]	3	22	26	-1	7	3	52	54	-9	9	3	84	86	-15	11	3	2Ø	17	-1Ø	13	3	17	13
2	5	3	24	29	Ø	7	3	19	19	-8	9	3	13	8	-14	11	3	41	4Ø	-9	13	3	21	22
3	[illegible]	3	46	46	1	7	3	37	42	-7	9	3	14	16	-13	11	3	42	43	-8	13	3	21	19
4	[illegible]	3	66	7Ø	2	7	3	22	18	-6	9	3	53	53	-12	11	3	54	56	-7	13	3	33	35
5	5	3	61	62	3	7	3	36	34	-5	9	3	57	62	-11	11	3	18	19	-6	13	3	36	35
[illegible]	[illegible]	3	17	2Ø	4	7	3	19	17	-4	9	3	66	69	-1Ø	11	3	15	18	-4	13	3	22	17
-1Ø	5	3	22	23	6	7	3	38	35	-3	9	3	22	21	-9	11	3	31	32	-2	13	3	53	55
-9	[illegible]	3	52	51	-15	8	3	37	33	-2	9	3	19	2Ø	-8	11	3	85	87	Ø	13	3	22	22
-8	6	3	93	92	-14	8	3	26	25	-1	9	3	28	3Ø	-6	11	3	2Ø	2Ø	1	13	3	18	13
-7	[illegible]	3	62	61	-13	8	3	17	19	Ø	9	3	91	95	-5	11	3	34	35	-11	14	3	34	4Ø
[illegible]	6	3	43	5Ø	-12	8	3	39	38	1	9	3	24	28	-4	11	3	13	12	-1Ø	14	3	26	28
[illegible]	6	3	34	35	-11	8	3	88	89	2	9	3	19	19	-3	11	3	82	84	-9	14	3	67	7Ø
-4	[illegible]	3	4Ø	38	-1Ø	8	3	31	35	3	9	3	4Ø	42	-2	11	3	21	2Ø	-8	14	3	27	26
-3	[illegible]	3	14Ø	145	-8	8	3	56	53	4	9	3	22	18	Ø	11	3	45	48	-7	14	3	2Ø	16
-2	5	3	33	38	-7	8	3	33	34	5	9	3	63	64	1	11	3	45	49	-6	14	3	4Ø	4Ø
-1	[illegible]	3	21	23	-6	8	3	89	94	-15	1Ø	3	21	18	2	11	3	55	55	-5	14	3	57	64
Ø	[illegible]	3	74	76	-5	8	3	19	2Ø	-14	1Ø	3	31	31	3	11	3	18	19	-4	14	3	33	32
[illegible]	[illegible]	[illegible]	53	52	-4	8	3	32	32	-12	1Ø	3	35	34	4	11	3	21	21	-3	14	3	19	21
2	[illegible]	3	89	95	-3	8	3	46	46	-11	1Ø	3	15	2Ø	-14	12	3	22	19	-2	14	3	24	27
3	5	3	2Ø	19	-2	8	3	89	93	-1Ø	1Ø	3	44	43	-12	12	3	53	49	-9	15	3	34	29
4	[illegible]	3	25	26	-1	8	3	39	4Ø	-9	1Ø	3	18	16	-11	12	3	53	55	-8	15	3	37	34

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CAPPELENITE DATA RED 1Ø/25/82

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	[illegible]	3	26	25	-7	5	4	25	23	-1Ø	7	4	16	8	4	8	4	2Ø	16	3	1Ø	4	23	21
-5	5	3	2Ø	7	-6	5	4	53	53	-9	7	4	21	19	5	8	4	19	18	4	1Ø	4	32	28
Ø	[illegible]	4	128	137	-5	5	4	91	9Ø	-8	7	4	26	26	6	8	4	37	41	-13	11	4	27	3Ø
-1		4	28	35	-4	5	4	37	39	-7	7	4	16	21	-14	9	4	55	55	-12	11	4	49	49
Ø	1	4	4Ø	41	-3	5	4	26	23	-6	7	4	41	43	-13	9	4	29	24	-11	11	4	18	16
1	[illegible]	4	32	37	-2	5	4	63	64	-5	7	4	25	23	-12	9	4	23	24	-1Ø	11	4	21	23
-3	2	4	65	66	-1	5	4	28	25	-4	7	4	34	37	-11	9	4	4Ø	42	-9	11	4	4Ø	42
-2	[illegible]	4	12	9	Ø	5	4	82	85	-3	7	4	16	17	-1Ø	9	4	22	18	-8	11	4	7Ø	72
-1		4	33	36	1	5	4	21	24	-2	7	4	2Ø	22	-9	9	4	82	8Ø	-7	11	4	33	37
Ø		4	48	48	2	5	4	2Ø	23	-1	7	4	36	36	-8	9	4	19	2Ø	-6	11	4	24	21
1	[illegible]	[illegible]	76	75	3	5	4	47	51	Ø	7	4	17	15	-7	9	4	17	2Ø	-5	11	4	46	48
2	[illegible]	4	23	25	4	5	4	49	47	1	7	4	39	42	-6	9	4	5Ø	54	-3	11	4	76	81
-5		4	25	24	5	5	4	31	32	2	7	4	37	36	-5	9	4	52	52	-2	11	4	18	22
-4		4	19	25	-11	6	4	2Ø	21	3	7	4	32	33	-4	9	4	49	46	-1	11	4	17	16
-3		4	64	55	-1Ø	6	4	15	13	4	7	4	17	13	-3	9	4	31	35	Ø	11	4	43	45
-2		4	62	64	-9	6	4	52	54	5	7	4	15	14	-2	9	4	34	36	1	11	4	45	45
-1		4	75	74	-8	6	4	67	7Ø	6	7	4	2Ø	1Ø	-1	9	4	29	3Ø	2	11	4	31	33
Ø		[illegible]	23	27	-7	6	4	43	42	7	7	4	18	12	Ø	9	4	72	72	-12	12	4	17	16
1	[illegible]	4	31	34	-6	6	4	14	18	-13	8	4	22	23	1	9	4	24	21	-11	12	4	47	5Ø
2		4	64	54	-5	6	4	5Ø	53	-11	8	4	69	73	2	9	4	2Ø	2Ø	-1Ø	12	4	15	18
3		4	95	97	-4	6	4	27	29	-1Ø	8	4	16	13	3	9	4	39	41	-9	12	4	22	22
-7		4	34	39	-3	6	4	95	97	-9	8	4	21	18	5	9	4	5Ø	48	-8	12	4	22	17
-6		4	3Ø	28	-2	6	4	15	16	-8	8	4	46	49	-14	1Ø	4	21	16	-7	12	4	2Ø	15
-5		4	32	37	-1	6	4	22	25	-7	8	4	26	26	-13	1Ø	4	2Ø	22	-6	12	4	55	61
-4		4	6Ø	61	Ø	6	4	61	64	-6	8	4	67	7Ø	-12	1Ø	4	22	21	-5	12	4	18	15
-3		4	23	25	1	6	4	36	34	-5	8	4	14	19	-11	1Ø	4	25	21	-4	12	4	2Ø	18
-2		4	2Ø	25	2	6	4	68	65	-4	8	4	15	12	-1Ø	1Ø	4	29	3Ø	-3	12	4	38	38
-1		4	3Ø	34	3	6	4	29	37	-3	8	4	49	49	-9	1Ø	4	2Ø	22	-2	12	4	23	2Ø
Ø		4	71	74	4	6	4	17	14	-2	8	4	65	67	-7	1Ø	4	18	9	-1	12	4	45	42
1	[illegible]	4	26	3Ø	5	6	4	47	49	-1	8	4	4Ø	43	-5	1Ø	4	3Ø	33	Ø	12	4	21	18
2		4	17	17	6	6	4	61	61	Ø	8	4	17	4	-3	1Ø	4	33	32	1	12	4	18	13
3	4	4	16	17	-13	7	4	26	26	1	8	4	31	3Ø	-2	1Ø	4	15	15	-11	13	4	3Ø	31
-9	5	4	52	56	-12	7	4	17	17	2	8	4	18	16	-1	1Ø	4	14	19	-1Ø	13	4	16	18
[illegible]	[illegible]	4	2Ø	18	-11	7	4	33	35	3	8	4	78	79	2	1Ø	4	17	2Ø	-9	13	4	2Ø	24

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
[illegible]	[illegible]	[illegible]	25	24	-2	4	5	34	33	4	6	5	24	27	-12	9	5	17	14	-5	11	5	42	44
[illegible]	[illegible]	[illegible]	22	23	-1	4	5	3Ø	35	5	6	5	47	45	-11	9	5	38	35	-3	11	5	48	48
-8	[illegible]	4	18	9	Ø	4	5	53	52	6	6	5	52	51	-1Ø	9	5	16	8	-2	11	5	2Ø	16
-5	[illegible]	4	18	18	2	4	5	32	28	-12	7	5	22	19	-9	9	5	5Ø	49	Ø	11	5	36	38
-4	[illegible]	4	16	1Ø	3	4	5	15	9	-11	7	5	2Ø	22	-8	9	5	15	16	-1Ø	12	5	21	21
-3	[illegible]	[illegible]	25	19	4	4	5	27	24	-9	7	5	2Ø	15	-7	9	5	17	15	-9	12	5	18	13
-2	[illegible]	4	28	29	-9	5	5	36	34	-8	7	5	23	22	-6	9	5	49	5Ø	-8	12	5	16	21
[illegible]	[illegible]	4	56	56	-8	5	5	17	21	-7	7	5	27	3Ø	-5	9	5	34	36	-7	12	5	22	2Ø
[illegible]	[illegible]	4	36	41	-7	5	5	18	14	-6	7	5	36	37	-4	9	5	37	37	-6	12	5	48	48
[illegible]	[illegible]	[illegible]	47	48	-6	5	5	37	37	-5	7	5	19	14	-3	9	5	18	14	-3	12	5	34	34
[illegible]	[illegible]	4	29	28	-5	5	5	52	51	-4	7	5	25	24	-2	9	5	18	14	-2	12	5	17	18
Ø	[illegible]	5	1Ø6	96	-4	5	5	16	22	-2	7	5	15	14	-1	9	5	37	37	Ø	Ø	6	65	62
-1	[illegible]	5	27	26	-3	5	5	22	23	-1	7	5	22	22	Ø	9	5	57	59	-1	1	6	27	24
[illegible]	[illegible]	5	27	31	-2	5	5	46	48	Ø	7	5	22	23	1	9	5	15	14	Ø	1	6	25	27
[illegible]	[illegible]	5	14	9	Ø	5	5	55	56	1	7	5	28	28	2	9	5	15	15	-3	2	6	34	33
[illegible]	[illegible]	5	48	48	1	5	5	19	18	2	7	5	17	17	3	9	5	33	31	Ø	2	6	47	44
[illegible]	[illegible]	5	31	34	3	5	5	5Ø	51	3	7	5	26	26	-12	1Ø	5	22	2Ø	1	2	6	41	38
[illegible]	[illegible]	5	53	57	4	5	5	38	36	5	7	5	18	11	-11	1Ø	5	17	15	-5	3	6	27	22
1	[illegible]	5	51	49	5	5	5	27	28	-11	8	5	53	53	-1Ø	1Ø	5	3Ø	28	-4	3	6	22	24
2	[illegible]	5	34	31	-11	6	5	21	13	-1Ø	8	5	24	27	-9	1Ø	5	17	9	-3	3	6	56	55
-5	[illegible]	5	22	24	-1Ø	6	5	23	24	-9	8	5	2Ø	15	-8	1Ø	5	26	25	-2	3	6	33	32
[illegible]	3	5	15	21	-9	6	5	51	5Ø	-8	8	5	52	54	-7	1Ø	5	19	8	-1	3	6	43	38
-3	[illegible]	5	71	71	-8	6	5	55	54	-7	8	5	23	19	-6	1Ø	5	25	23	Ø	3	6	33	31
-2	[illegible]	5	46	49	-7	6	5	39	39	-6	8	5	52	53	-5	1Ø	5	28	28	1	3	6	36	37
-1	[illegible]	5	51	5Ø	-6	6	5	27	26	-5	8	5	21	19	-4	1Ø	5	25	26	2	3	6	36	32
[illegible]	[illegible]	[illegible]	26	22	-5	6	5	35	36	-4	8	5	23	26	-3	1Ø	5	25	25	3	3	6	53	51
1	[illegible]	[illegible]	34	35	-4	6	5	29	27	-3	8	5	49	53	-2	1Ø	5	19	18	-7	4	6	22	23
2	[illegible]	[illegible]	46	48	-3	6	5	75	74	-2	8	5	54	51	Ø	1Ø	5	22	14	-6	4	6	29	28
[illegible]	3	[illegible]	77	75	-2	6	5	3Ø	31	-1	8	5	23	27	1	1Ø	5	17	14	-5	4	6	18	17
-7	4	5	24	25	-1	6	5	18	17	Ø	8	5	29	31	2	1Ø	5	16	22	-4	4	6	29	19
-6	[illegible]	5	3Ø	31	Ø	6	5	54	55	1	8	5	39	39	-9	11	5	35	34	-3	4	6	23	24
[illegible]	[illegible]	5	19	22	1	6	5	25	24	2	8	5	19	16	-8	11	5	52	54	-1	4	6	35	36
[illegible]	[illegible]	5	3Ø	26	2	6	5	53	54	3	8	5	49	49	-7	11	5	21	23	Ø	4	6	26	21
[illegible]	4	5	13	22	3	6	5	15	14	4	8	5	21	21	-6	11	5	21	15	1	4	6	17	12

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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
2	4	6	15	7	-6	6	6	18	13	1	7	6	26	21	0	9	6	41	36	0	3	7	16	14
3	[illegible]	6	16	17	-5	6	6	37	36	2	7	6	27	26	-7	10	6	18	7	1	3	7	30	28
4	4	6	14	16	-4	6	6	29	27	3	7	6	20	17	-6	10	6	19	16	2	3	7	33	33
-9	[illegible]	6	33	27	-3	6	6	51	51	-8	8	6	43	38	-5	10	6	20	23	3	3	7	33	29
-8	[illegible]	6	26	26	-1	6	6	24	22	-7	8	6	15	14	-4	10	6	18	20	-6	4	7	22	22
-7	5	6	17	17	0	6	6	53	52	-6	8	6	28	31	-3	10	6	17	18	-4	4	7	17	9
-6	5	6	39	36	1	6	6	20	16	-5	8	6	25	27	0	0	7	29	29	-2	4	7	30	18
-5	[illegible]	6	54	49	2	6	6	34	33	-4	8	6	19	16	-1	1	7	18	12	-1	4	7	33	27
-3	5	6	25	22	3	6	6	17	13	-3	8	6	34	37	0	1	7	35	29	0	4	7	23	21
-2	[illegible]	6	36	34	4	6	6	23	20	-2	8	6	31	33	1	1	7	15	11	1	4	7	19	13
0	[illegible]	6	48	42	-10	7	6	15	6	-1	8	6	27	23	-3	2	7	25	21	2	4	7	27	17
1	[illegible]	6	20	21	-9	7	6	24	17	0	8	6	27	23	-2	2	7	17	21	-6	5	7	31	29
2	[illegible]	6	21	19	-8	7	6	23	17	1	8	6	26	30	-1	2	7	16	11	-5	5	7	28	24
3	[illegible]	6	39	39	-7	7	6	26	26	-9	9	6	40	39	0	2	7	29	30	-2	5	7	36	31
4	[illegible]	6	28	26	-6	7	6	24	21	-8	9	6	21	11	1	2	7	32	27	0	5	7	24	23
5	[illegible]	6	22	21	-5	7	6	19	16	-6	9	6	44	45	2	2	7	21	17	1	5	7	17	14
-10	[illegible]	6	20	16	-4	7	6	30	23	-5	9	6	29	25	-4	3	7	15	13	-5	6	7	27	31
-9	6	6	47	45	-3	7	6	16	19	-4	9	6	32	26	-3	3	7	58	52	-4	6	7	23	21
-8	6	6	31	32	-1	7	6	26	19	-2	9	6	25	27	-2	3	7	24	19	-3	6	7	35	30
-7	[illegible]	6	23	20	0	7	6	22	23	-1	9	6	23	28	-1	3	7	27	25	-2	6	7	24	19