Short Communications

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Refinement of the crystal structure of Li_2BeF_4*.

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Bragg (1927) determined the positions of the Si and O atoms in phenacite, Be_2SiO_4; then Bragg & Zachariasen (1930) deduced the probable location of the Be atoms. Previously, Zachariasen (1926) had concluded from powder diagrams that Li_2BeF_4 is isotypic with phenacite, but when Thilo & Lehmann (1949) studied the LiF-BeF_2 system, they suggested that Li_2BeF_4 may have the structure of olivine, $(MgFe)_2SiO_4$. Single-crystal studies by Hahn (1953) confirmed the isotypism of Li_2BeF_4 and phenacite. We undertook refinement of the structure in order to obtain details not available from knowledge of the structural type alone.

Experimental

Single crystals of Li_2BeF_4 were grown by slow cooling of a melt of composition 66·7 mole % LiF, 33·3 mole % BeF_2 in a furnace described by Weaver, Ross & Thoma (1963). Two specimens, ground to spherical shape with radii 0·23 and 0·09 mm, were used for data collection. Intensities were measured with a single-crystal orienter and scintillation-counter detector employing zirconium-filtered Mo radiation. All reflections out to $2\theta = 60°$ were measured by the 2θ-scan method. Some difficulty from double reflection was encountered, but was eliminated by reorientation of the crystal. No absorption correction was necessary because of the small absorption coefficient and size of the crystals, but the 34 strongest reflections were omitted from the refinement because they appeared to be extinction-affected.

Table 1. *Positional parameters from least-squares refinement*

Standard deviations ($\times 10^5$) are in parentheses after the values, and the starting parameters from phenacite are in parentheses below.

Atom	*x*	*y*	*z*
Li(1)	−0·02153 (8)	−0·21540 (8)	0·58160 (11)
	(−0·01)	(−0·21)	(0·58)
Li(2)	−0·01634 (8)	−0·20734 (8)	−0·08490 (10)
	(−0·01)	(−0·21)	(−0·08)
Be	−0·01546 (5)	−0·21169 (5)	0·24927 (7)
	(−0·011)	(−0·211)	(0·250)
F(1)	0·11055 (3)	−0·10576 (3)	0·25193 (3)
	(0·120)	(−0·092)	(0·250)
F(2)	−0·00590 (3)	−0·32318 (2)	0·24859 (4)
	(0·000)	(−0·320)	(0·250)
F(3)	−0·07496 (3)	−0·20347 (3)	0·10408 (3)
	(−0·074)	(−0·204)	(0·083)
F(4)	−0·08185 (3)	−0·20918 (3)	0·39227 (3)
	(−0·074)	(−0·205)	(0·417)

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Table 2. *Thermal parameters* ($\times 10^5$) *from the expression* $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)]$, *and their standard deviations* ($\times 10^5$)

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Li(1)	247 (6)	268 (6)	345 (10)	132 (5)	0(6)	−10 (6)
Li(2)	241 (6)	264 (6)	334 (10)	128 (5)	0(6)	3 (6)
Be	159 (4)	182 (4)	237 (6)	87 (3)	5 (4)	6 (4)
F(1)	194 (2)	213 (2)	360 (4)	30 (2)	−18 (2)	5 (2)
F(2)	216 (2)	176 (2)	479 (4)	105 (2)	22 (2)	17 (2)
F(3)	237 (2)	360 (3)	249 (4)	188 (2)	−26 (2)	4 (2)
F(4)	269 (2)	371 (3)	258 (4)	214 (2)	45 (2)	17 (2)

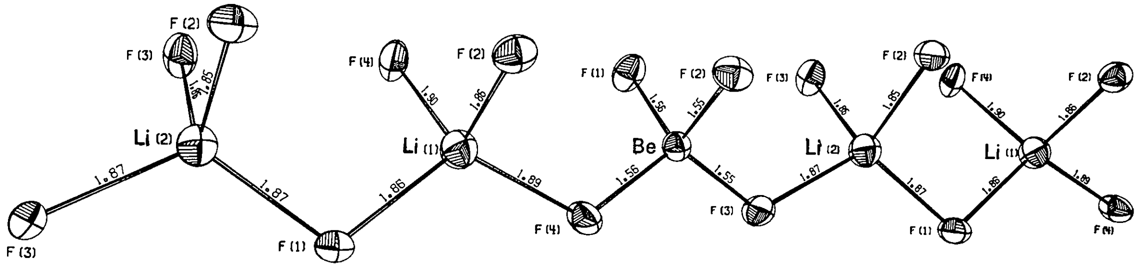

Fig. 1. Chain of tetrahedra along the *c* axis of Li_2BeF_4.

Table 3. *Observed* (F_o) *and calculated* (F_c) *structure factors*
Values marked with an asterisk were affected by extinction

H	K	L	FO	FC
3	0	0	*83	-85
6	0	0	25	24
9	0	0	*155	164
1	1	0	57	-60
4	1	0	*110	-120
7	1	0	92	-94
10	1	0	35	36
13	1	0	37	-37
16	1	0	21	-21
2	2	0	*146	-170
5	2	0	*117	-124
8	2	0	49	48
11	2	0	39	-39
14	2	0	32	-32
3	3	0	*250	341
6	3	0	16	16
9	3	0	10	10
12	3	0	41	41
15	3	0	0	0
1	4	0	*96	97
4	4	0	2	-4
7	4	0	39	-39
10	4	0	10	9
13	4	0	7	-6
2	5	0	81	83
5	5	0	34	-33
8	5	0	68	-69
11	5	0	44	44
14	5	0	16	-16
3	6	0	36	-35
6	6	0	80	80
9	6	0	10	-8
12	6	0	11	11
1	7	0	*109	-113
4	7	0	16	-16
7	7	0	9	-10
10	7	0	11	-11
2	8	0	59	-60
5	8	0	60	61
8	8	0	39	-40
11	8	0	3	3
3	9	0	12	11
6	9	0	40	41
9	9	0	13	13
1	10	0	1	-1
4	10	0	17	-17
7	10	0	9	-9
2	11	0	58	-59
5	11	0	35	-35
8	11	0	14	14
0	12	0	30	-29
3	12	0	25	24
6	12	0	14	13
1	13	0	32	32
4	13	0	26	-26
2	14	0	41	41
5	14	0	8	-9
0	15	0	41	41
3	15	0	20	-20
1	16	0	5	-5
1	0	1	7	6
2	0	-1	6	-5
4	0	1	30	31
5	0	-1	27	-27
7	0	1	21	20
8	0	-1	42	-42
10	0	1	8	-7
11	0	-1	24	24
13	0	1	16	-17
14	0	-1	10	-11
16	0	1	29	30
2	1	1	*73	69
3	1	-1	32	-30
5	1	1	9	9
6	1	-1	63	63
8	1	1	6	6
9	1	-1	16	17
11	1	1	24	25
12	1	-1	12	11
14	1	1	26	26
15	1	-1	12	12
1	2	-1	61	-59
3	2	1	9	-9
4	2	-1	6	-7
6	2	1	90	-92
7	2	-1	20	19
9	2	1	3	-3
10	2	-1	34	-34
12	2	1	2	2
13	2	-1	7	-7
15	2	1	36	-36
1	3	1	6	6
2	3	-1	20	-20
4	3	1	30	-29
5	3	-1	27	28
7	3	1	13	-12
8	3	-1	4	5
10	3	1	32	32
11	3	-1	41	-41
13	3	1	14	-14
14	3	-1	21	21
2	4	1	21	21
3	4	-1	13	12
5	4	1	53	52
6	4	-1	5	6
8	4	1	22	22
9	4	-1	18	18
11	4	1	22	22
12	4	-1	5	2
14	4	1	0	0
1	5	-1	12	12
3	5	1	19	19
4	5	-1	77	-79
6	5	1	6	-6
7	5	-1	4	-3
9	5	1	53	-53
10	5	-1	8	8
12	5	1	2	-2
13	5	-1	19	-19
1	6	1	28	-27
2	6	-1	32	32
4	6	1	40	40
5	6	-1	30	-30
7	6	1	23	-23
8	6	-1	33	32
10	6	1	14	-14
11	6	-1	4	-3
13	6	1	25	25
2	7	1	2	2
3	7	-1	13	13
5	7	1	21	22
6	7	-1	3	-3
8	7	1	11	11
9	7	-1	27	27
11	7	1	24	24
1	8	-1	5	3
3	8	1	50	-50
4	8	-1	7	6
6	8	1	1	0
7	8	-1	41	-41
9	8	1	18	-18
10	8	-1	1	5
1	9	1	32	-32
2	9	-1	36	36
4	9	1	17	-17
5	9	-1	10	11
7	9	1	34	34
8	9	-1	19	-20
10	9	1	17	-17
2	10	1	37	37
3	10	-1	22	22
5	10	1	23	24
6	10	-1	9	-10
8	10	1	24	23
1	11	-1	64	-65
3	11	1	25	-25
4	11	-1	12	12
6	11	1	20	-20
7	11	-1	17	-16
1	12	1	28	29
2	12	-1	9	-7
4	12	1	29	-30
5	12	-1	33	33
7	12	1	8	-8
2	13	1	5	5
3	13	-1	3	3
5	13	1	7	6
1	14	-1	10	-10
3	14	1	4	3
1	15	1	9	-9
2	15	-1	3	1
2	16	1	27	26
0	17	1	29	-28
1	0	-2	55	-52
2	0	2	26	27
4	0	-2	4	-3
5	0	2	58	60
7	0	-2	21	-21
8	0	2	7	-6
10	0	-2	60	-62
11	0	2	6	6
13	0	-2	2	2
14	0	2	21	21
17	0	2	4	4
2	1	-2	34	33
3	1	2	2	2
5	1	-2	12	12
6	1	2	10	10
8	1	-2	3	4
9	1	2	22	-22
11	1	-2	31	31
12	1	2	2	2
14	1	-2	16	15
15	1	2	16	16
1	2	2	35	34
3	2	-2	38	-39
4	2	2	64	-63
6	2	-2	43	42
7	2	2	5	-5
9	2	-2	34	34
10	2	2	3	3
12	2	-2	3	-2
13	2	2	19	-19
16	2	2	4	-4
1	3	-2	4	-5
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13	3	-2	41	-42
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2	4	-2	11	-10
3	4	2	40	-39
5	4	-2	23	22
6	4	2	8	-8
8	4	-2	13	13
9	4	2	10	10
11	4	-2	11	-11
12	4	2	14	-14
1	5	2	30	30
3	5	-2	25	24
4	5	2	11	11
6	5	-2	18	-18
7	5	2	24	-23
9	5	-2	19	19
10	5	2	4	-4
12	5	-2	17	17
13	5	2	6	-5
1	6	-2	8	9
2	6	2	54	54
4	6	-2	28	-28
5	6	2	1	-1
7	6	-2	45	-45
8	6	2	2	-2
10	6	-2	3	0
11	6	2	29	29
2	7	-2	15	13
3	7	2	1	0
5	7	-2	2	-3
6	7	2	35	-35
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9	7	2	2	-1
11	7	-2	16	15
12	7	2	7	8
1	8	2	37	-36
3	8	-2	44	45
4	8	2	25	26
6	8	-2	13	14
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9	8	-2	3	1
10	8	2	7	-7
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4	9	-2	5	-4
5	9	2	29	29
7	9	-2	24	-24
8	9	2	3	4
2	10	-2	18	18
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5	10	-2	4	5
6	10	2	2	1
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9	10	2	26	-26
1	11	2	11	11
3	11	-2	4	4
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6	11	-2	23	22
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1	12	-2	14	-13
2	12	2	4	-3
4	12	-2	26	-26
5	12	2	7	7
2	13	-2	7	-9
3	13	2	38	-38
6	13	2	5	-5
1	14	2	12	12
3	14	-2	6	6
4	14	2	3	3
1	15	-2	6	-7
2	15	2	17	17
0	16	2	8	-8
0	0	3	7	7
3	0	-3	*206	-258
3	0	3	*197	240
6	0	-3	*149	158
6	0	3	*163	-176
9	0	-3	3	-3
9	0	3	15	15
12	0	-3	16	16
12	0	3	19	-18
15	0	-3	13	14
15	0	3	19	-19
1	1	-3	*112	118
1	1	3	*111	-115
4	1	-3	30	30
4	1	3	30	-30
7	1	-3	*164	176
7	1	3	*160	-169
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10	1	3	9	-8
13	1	-3	6	-5
13	1	3	3	3
16	1	3	23	-23
2	2	-3	*97	-105
2	2	3	*105	112
5	2	-3	12	11
5	2	3	7	-7
8	2	-3	54	-55
8	2	3	60	60
11	2	-3	50	-50
11	2	3	45	46
14	2	-3	11	-13
14	2	3	11	11
0	3	-3	*200	240
0	3	3	*210	-258
3	3	-3	48	-47
3	3	3	67	67
6	3	-3	79	-79
6	3	3	67	67
9	3	-3	9	10
9	3	3	20	-19
12	3	-3	21	-21
12	3	3	26	26
15	3	3	6	-6
1	4	-3	*114	120
1	4	3	*114	-118
4	4	-3	9	-4
4	4	3	5	5
7	4	-3	7	6
7	4	3	12	-12
10	4	-3	34	34
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13	4	-3	23	22
13	4	3	17	-18
2	5	-3	31	-31
2	5	3	31	31
5	5	-3	*115	-120
5	5	3	*114	119
8	5	-3	62	62
8	5	3	62	-62
11	5	-3	7	-8
11	5	3	13	13
0	6	-3	*164	-176
0	6	3	*151	158
3	6	-3	*119	123
3	6	3	*130	-132
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9	6	3	18	18
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1	7	3	*110	-112
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8	8	3	61	62
11	8	3	18	-18
3	9	-3	55	-55
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3	12	3	17	-17
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4	13	-3	6	-6
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0	15	-3	18	-19
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3	15	3	7	-7
1	16	3	16	-15
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5	0	-4	21	-21
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10	0	4	36	36
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13	0	4	0	-1
14	0	-4	33	-34
16	0	4	2	2
2	1	4	30	30
3	1	-4	49	49
5	1	4	26	26
6	1	-4	34	33
8	1	4	39	-39
9	1	-4	32	-32
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3	2	4	17	17
4	2	-4	48	47
6	2	4	5	-4
7	2	-4	11	-10
9	2	4	67	-68
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12	2	4	19	19
13	2	-4	30	31
15	2	4	1	-1
1	3	4	19	18
2	3	-4	48	-48
4	3	4	24	23
5	3	-4	9	9
7	3	4	9	-9
8	3	-4	60	-61
10	3	4	28	28
11	3	-4	13	13
13	3	4	42	43
2	4	4	88	-87
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5	4	4	16	16
6	4	-4	33	33
8	4	4	5	-5
9	4	-4	7	6
11	4	4	0	-1
12	4	-4	6	1
14	4	4	0	-2
1	5	-4	62	-61
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4	5	-4	8	8
6	5	4	32	33
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9	5	4	6	-5
10	5	-4	7	-6
12	5	4	32	-33
1	6	4	10	-10
2	6	-4	38	-37
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7	6	4	46	47
8	6	-4	14	15
10	6	4	16	-16
11	6	-4	45	-46
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3	7	-4	18	18
5	7	4	36	-36
6	7	-4	4	5
8	7	4	7	-7
9	7	-4	3	3
11	7	4	23	-23
1	8	-4	52	52
3	8	4	36	-36
4	8	-4	56	-56
6	8	4	25	-25
7	8	-4	10	9
9	8	4	9	8
1	9	4	59	60
2	9	-4	9	8
4	9	4	21	-22
5	9	-4	39	-39
7	9	4	31	31
8	9	-4	5	5
10	9	4	43	44
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3	10	-4	7	7
5	10	4	3	-3
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1	11	-4	9	8
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2	12	-4	5	1
4	12	4	37	38
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2	13	4	7	-7
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5	13	4	7	-7
1	14	-4	35	-35
3	14	4	3	1
1	15	4	12	-12
1	0	-5	2	3
2	0	5	58	-58
4	0	-5	54	54
5	0	5	29	28
7	0	-5	47	-49
8	0	5	26	27
10	0	-5	0	-1
11	0	5	5	-4
13	0	-5	16	16
14	0	5	9	8
2	1	-5	45	46
3	1	5	72	-73
5	1	-5	66	-66
6	1	5	39	38
8	1	-5	12	-12
9	1	5	15	-15
11	1	-5	6	-6
12	1	5	30	-30
14	1	-5	26	-25
15	1	5	2	-0
1	2	5	56	55
3	2	-5	40	39
4	2	5	24	23
6	2	-5	26	26
7	2	5	2	-2
9	2	-5	4	1
10	2	5	13	13
12	2	-5	26	26
13	2	5	0	-1
1	3	-5	45	-45
2	3	5	6	6
4	3	-5	9	10
5	3	5	25	-26
7	3	-5	29	28
8	3	5	0	-1
10	3	-5	18	-17
11	3	5	11	11
13	3	-5	9	7
14	3	5	2	-2
2	4	-5	16	-16
3	4	5	15	-15
5	4	-5	18	19
6	4	5	52	-53
8	4	-5	45	-45
9	4	5	15	15
11	4	-5	11	-11
12	4	5	5	-5
1	5	5	25	-25
3	5	-5	20	-20
4	5	5	25	25
6	5	-5	31	31
7	5	5	19	19
9	5	-5	15	15
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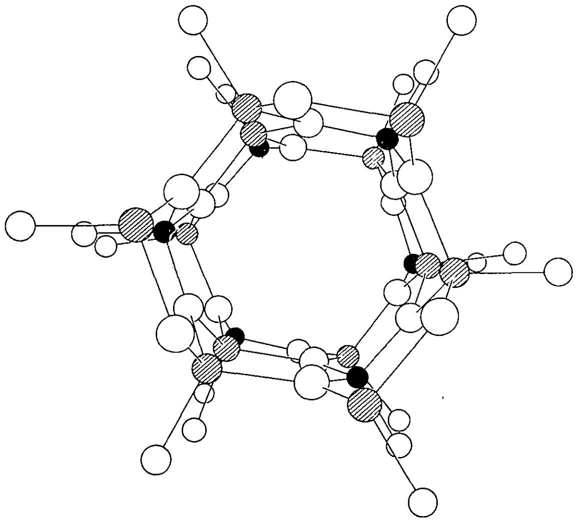

Fig. 2. Perspective view of part of the structure of Li_2BeF_4 down the c axis. Cross-hatched circles represent Li, filled circles Be, open circles F.

The hexagonal unit cell has dimensions: $a = 13{\cdot}29 \pm 0{\cdot}01$, $c = 8{\cdot}91 \pm 0{\cdot}01$ Å and contains 18 formula weights. The space group was determined previously to be $R\bar{3}$.

Refinement and results

The structure of Li_2BeF_4 was refined by iterative least squares employing the Busing, Martin & Levy (1962) computer program. Starting values for atomic positions were obtained from those of Be_2SiO_4 (Bragg & Zachariasen, 1930) by substitution of Li for Be, Be for Si, and F for O. Scattering factors for Li^+, Be^{2+} and F^- were taken from *International Tables for X-ray Crystallography* (1962). The quantity minimized was $\Sigma w|F_o^2 - F_c^2|^2$ with weights, w, equal to the reciprocals of the variances. These were estimated from the empirical equation: $\sigma^2(F_o^2) = s[T + B + 0{\cdot}0009(T-B)^2]/(\mathrm{Lp})^2$, in which s = scale factor, T = total, B = background counts, and Lp = Lorentz-polarization correction (for derivation, see Busing & Levy, 1957). The locations and anisotropic temperature factors of the seven atoms of Li_2BeF_4 in general positions, plus three scale factors, were varied; thus, a total of 66 parameters were adjusted to 975 observations.

The refined positional parameters are given in Table 1, and with them the starting values obtained by transforming the rhombohedral coordinates of phenacite. No very large parameter shifts resulted from the refinement.

Final values for the thermal parameters are presented in Table 2. These numbers correspond to probability ellipsoids of thermal motion which are pictorially represented in Fig. 1 for each kind of atom. The scale of the thermal motion is enlarged 1·8 times relative to interatomic distances. This picture was drawn by an $x-y$ plotter controlled by a computer using the automated graphic arts program by Johnson (1964). Atoms at the centers of the tetrahedra appear to be quite isotropic in motion, while the fluorine atoms show a little more movement perpendicular to their bonds than along them.

In Table 3 are listed the values of $|F_o|$ and F_c on an absolute scale. The residual, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, for these data is 0·025, omitting the extinction-affected reflections.

The structure of Li_2BeF_4 is clearly isotypic with that of Be_2SiO_4, which is described and well illustrated by figures in the paper of Bragg & Zachariasen (1930). Some additional details for Li_2BeF_4 are shown in Figs. 1 and 2. Both the Be^{2+} and Li^+ ions are tetrahedrally coordinated by fluoride ions, and these tetrahedra share all their corners to form a three-dimensional network. Along **c** the tetrahedra are repeated in such a manner that the fluoride ions lie almost on straight lines parallel to **c**, as do columns consisting of LiLiBeLiLiBe ions. One such chain of tetrahedra is illustrated in perspective by Fig. 1, in which the atoms are represented by their thermal ellipsoids. Fig. 2, a view down **c**, shows how the chains are joined.

Bond lengths in the three kinds of tetrahedra are listed in Table 4. The average length for the Be-F bonds is 1·55$_4$ Å, in good agreement with the value of 1·57 ± 0·01 Å in the BeF_4^{2-} ions of $Li_6BeF_4ZrF_8$ (Sears & Burns, 1964). Average Li–F bond lengths of 1·87$_5$ and 1·86$_1$ Å for the two lithium-containing tetrahedra are close to the expected 1·85 Å obtained from the distance in LiF, corrected for ligancy (Pauling, 1960).

Table 4. *Bond distances and standard deviations*

Bond	distance	σ
Be–F(1)	1·559 Å	0·002 Å
F(2)	1·549	0·002
F(3)	1·548	0·002
F(4)	1·560	0·002
Li(1)–F(1)	1·855	0·002
F(2)	1·861	0·002
F(4)	1·899	0·002
F(4′)	1·887	0·002
Li(2)–F(1)	1·871	0·002
F(2)	1·849	0·002
F(3)	1·856	0·002
F(3′)	1·867	0·002

In Be_2SiO_4 the oxygen tetrahedra are all identical, but the inequality of Li–F and Be–F bond lengths does not permit the fluoride tetrahedra to be identical in Li_2BeF_4. The fluoride ions around the Li^+ are not in contact with each other; the average F–F distance around Li(1) is 3·06 Å, and around Li(2) it is 3·03 Å. Consequently these tetrahedra can be somewhat deformed, and the angles around Li(1) range from 104·6 to 116·4° and around Li(2) from 103·9 to 117·3°. Around beryllium, however, the fluoride ions are very tight (average F–F distance, 2·54 Å) and the variation in angle is only from 107·4 to 111·5°.

A remarkable structural feature, not mentioned in the previous work, is the existence of continuous channels through the crystal parallel to **c**, one of which is seen in Fig. 2. When the size of the opening is calculated assuming that the fluorine radius is 1·36 Å, the cylindrical void has a diameter of about 2 Å. These openings should provide paths for rapid diffusion along **c** in these crystals.

We are grateful to R. G. Ross, who prepared the crystals, and to R. E. Thoma for helpful discussions.

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Debye–Waller factors in crystals of the sodium chloride structure.

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Calculation of vibrational properties

In the standard theory of lattice dynamics (*cf.* Maradudin, Montroll & Weiss, 1963) any vibrational property of a lattice can be represented as a sum over the normal lattice modes and, if a reliable model of the interatomic forces is available, may be calculated in a straightforward way by assembling the terms of the 'dynamic matrix' for a mesh of points through the first Brillouin zone and determining the eigenvalues and eigenvectors. This theory is applied here to the calculation of Debye–Waller factors of the individual ions in crystals of the sodium chloride structure. The quantities calculated are the crystallographic B-factors (B_1 for the cation and B_2 for the anion). In the same calculation the lattice specific heat and the two Debye temperatures (Θ_m for diffraction and Θ_c for specific heat) have also been evaluated over a range of temperatures.

Calculations such as this are only possible if a reliable model of the interionic forces is available and, throughout this paper, the 'shell' model (Woods, Cochran & Brockhouse, 1960; Woods, Brockhouse & Cowley, 1963; Cowley, Cochran, Brockhouse & Woods, 1963) has been used exclusively. The above mentioned authors have developed this model and applied it to the interpretation of the dispersion curves of sodium iodide and potassium bromide which they determined experimentally by the method of inelastic neutron diffraction. By using a complex version of the model with nine free parameters they obtained a close fit to the experimentally determined phonon frequencies which were thought to have an accuracy of 1–2 %. For these two crystals it should therefore be possible to calculate the lattice vibrational properties with a similar accuracy. In the case of crystals for which the dispersion curves are not known a simplified version of the 'shell' model can be used for which the parameters can be determined from the elastic and dielectric constants of the material. To assess the accuracy of this derivation it has been applied also to sodium iodide and potassium bromide.

Comparison of calculated and experimental values

Before comparing the calculated B-values with experimental values obtained from diffraction experiments at 300°K an 'expansion correction' was applied to reduce all values to a temperature of 300°K. This correction is described by Paskin (1957). The expansion data of Yates & Panter (1962) were used. (This correction was not applied to the calculated values listed in Table 2.)

Another possible comparison is with the thermodynamic values of Θ_m and Θ_c. The thermodynamic value of Θ_c is, of course, given immediately by the experimental specific heat values; the thermodynamic value of Θ_m is obtainable from the terms of the expansion of the specific heat, C_v, as a power series of the temperature. For this purpose we have followed the theory and the data of Barron, Berg & Morrison (1957) and Barron, Leadbetter, Morrison & Salter (1962).

The comparison of calculated and experimental values of B_1, B_2, Θ_m and Θ_c is shown in Table 1 for sodium iodide, potassium bromide, sodium chloride and lithium fluoride. The B-factors for sodium chloride which were calculated by Buyers & Smith (1964) are also shown. In Table 2 the 'harmonic' values of B_1/B_2, Θ_m and Θ_c are shown as a function of temperature.

The thermal diffuse scattering correction

In assessing the agreement between calculated B-values and those obtained in diffraction experiments it is necessary to take into account the thermal diffuse scattering (TDS) correction. To determine the Debye–Waller factor one must determine the elastic scattering only, at the Bragg positions; but the continuous TDS is peaked at the Bragg positions and one is therefore faced with the problem of subtracting the TDS integrated over that volume of reciprocal space, surrounding the Bragg positions, which is 'seen' by the counter. This is simple enough in principle but laborious in detail (*cf.* Nillson, 1957).

In a simplified approach to this question we have assumed:

(i) that the mode energy is kT and that the modes are acoustic and isotropic with longitudinal velocity c_l and transverse velocity c_t;

(ii) that for single-crystal work the 'seen' volume is a sphere surrounding the Bragg point in reciprocal space, of radius $2\pi\delta\theta/\lambda$, where $2\delta\theta$ is the counter aperture, and that background level lies at the surface of this sphere;