Acta Cryst. (1968). **B24**, 1077

A Reconsideration of the Crystal Structure of β-$Na_2Si_2O_5$

BY A. K. PANT*

Chemistry Department, University of Glasgow, Glasgow, W.2, Scotland

(*Received* 5 *September* 1967)

New data have been used in a refinement of the crystal structure of β-$Na_2Si_2O_5$. This is a sheet structure, the individual sheets being built up from the condensation of the two independent alternating metasilicate chains. The dimensions are: Si(1)–O(bridging) 1·636, 1·634, 1·643 ± 0·003 Å; Si(1)–O(non-bridging) 1·576 ± 0·003 Å; Si(2)–O(bridging) 1·643, 1·637, 1·640 ± 0·003 Å; Si(2)–O(non-bridging) 1·584 ± 0·003 Å. The three Si–O(bridging)–Si angles are: 136·50, 137·11 and 135·11 ± 0·20°. The sheets are held together through sodium atoms; four of the eight sodiums in the unit cell form five Na···O links and the other four form six Na···O links. The structure is interpreted in terms of the Pauling–Zachariasen method of the balancing of valences and in terms of π-bonding effects.

Introduction

The crystal structure of β-$Na_2Si_2O_5$ was determined by Grund (1954) from photographic data for two projections. He showed that this is a sheet structure with two independent silicate tetrahedra in the asymmetric unit. The layers are joined together by the sodium atoms. The Si–O bonds were found to have average lengths: Si–O (bridging) ~1·63 Å and Si–O (non-bridging) ~1·51 Å. Such a large difference is interesting and unusual, but unfortunately the reliability of the results is low; Grund neither gives the number of reflexions used in the refinement nor says anything about the residual *R*.

The present study was undertaken: (*a*) to determine more accurately the Si–O bond lengths and angles, as these are relevant to the discussion of π-bonding in second-row elements (Cruickshank, 1961), (*b*) to test the validity of the Pauling–Zachariasen method of the balancing of valences as an explanation of the variations in all bond lengths (see, for example, datolite, $CaBSiO_4(OH)$; Pant & Cruickshank, 1967), and (*c*) as part of the structure determinations of the different phases of $Na_2Si_2O_5$, which should help in an understanding of the phase transformations. A detailed X-ray study of the α phase has been reported by Pant & Cruickshank (1968) and preliminary studies on the γ and δ phases have been made by Hoffmann & Scheele (1966).

Williamson & Glasser (1966) have done a thorough study of the crystallization of sodium disilicate glass. At one bar pressure α, β, γ and δ phases were obtained in the following temperature ranges: α phase above 700°C; β phase over the range 610–700°C; γ and δ phases below 600°C. At higher pressure (> 100 bars) crystals of phase *C* were also obtained.

Except for the much greater precision of the present work the earlier results of Grund (1954) for the arrangement of sodium, silicon and oxygen atoms have been confirmed.

Crystal data

β-$Na_2Si_2O_5$. $M = 182{\cdot}16$. Monoclinic, $a = 12{\cdot}329 \pm 0{\cdot}004$, $b = 4{\cdot}848 \pm 0{\cdot}004$, $c = 8{\cdot}133 \pm 0{\cdot}003$ Å and $\beta = 104{\cdot}24 \pm 0{\cdot}04°$; $V = 471{\cdot}2$ Å^3, $Z = 4$, $D_o = 2{\cdot}56$ g.cm^{-3} (Grund, 1954), $D_c = 2{\cdot}567$ g.cm^{-3}. $F(000) = 520$. Space group $P2_1/a$ (No. 14). μ for Mo $K\alpha$ radiation $= 8{\cdot}6$ cm^{-1}.

Experimental

Crystals of β-$Na_2Si_2O_5$ were kindly supplied by Dr F. P. Glasser of the Aberdeen University Chemistry Department. The crystals grow in the form of small thin plates normal to [100] and slightly elongated along the *b* axis. For the measurement of intensities a very small crystal of approximate dimensions 0·07 × 0·30 × 0·15 mm was selected and was mounted along the *b* axis on a glass fibre. This was then dipped twice in collodion, which formed a protective coating against moisture and carbon dioxide.

The cell dimensions were redetermined by a method of least squares proposed by Speakman (1966) with data from zero-layer Weissenberg photographs along the *b* and *c* axes taken with Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å) radiation. The values, which are given under crystal data, agree well with those of Grund (1954).

Intensity measurements were made on a Hilger and Watts linear diffractometer (Arndt & Phillips, 1961) using Mo $K\alpha$ radiation; *h*0*l* to *h*6*l* reflexions were measured, all the measurements being on the same scale. The intensities were corrected for Lorentz and polarization factors but absorption was neglected. A small number of weak reflexions observed at values not significantly above the background were included at their observed values and this provided a simple

---

* Present address: Physics Department, McMaster University, Hamilton, Ontario, Canada.

way of treating the 'unobserved' reflexions. This worked well for most of these reflexions, although they were carefully watched at every stage of refinement. Altogether 1564 independent structure amplitudes were obtained initially. Nineteen low angle reflexions could not be observed owing to the beam stop, and are marked by an asterisk in Table 3, where the observed and calculated structure factors are listed.

Least-squares refinement

The structure-factor least-squares program of J. G. F. Smith and D. W. J. Cruickshank for the KDF9 computer was used, with Grund's parameters as the initial values. The form-factors for the neutral atoms were taken from *International Tables for X-ray Crystallography* (1962). Initially unit weight was given to each reflexion. The first structure-factor calculation gave a residual $R=(\Sigma|\Delta|)/(\Sigma|F_o|)$ of ~34% for the 1564 reflexions. Three cycles of full-matrix isotropic refinement followed by three cycles of full-matrix anisotropic refinement with one overall scale factor brought the residual down to 4·37%.

It was noticed at this stage that unit weights were not quite satisfactory; the weighting analysis was poor in the very weak and strong F_o regions, but apparently had no significant $\sin\theta$ dependence. The weighting scheme was therefore changed to

$$\sqrt{w}=|F_o|/p_1 \text{ for } |F_o|\le p_1\text{ , and}$$
$$\sqrt{w}=p_1/|F_o| \text{ for } |F_o|>p_1\text{ ,}$$

where $p_1=10$, and three more cycles of anisotropic refinement were carried out. The R index came down to a final value of 4·27%, with considerable improvement in the estimated standard deviations of the atomic and thermal parameters. In the final two cycles zero weight was given to the 260 reflexion as it had a rather large $\Delta\sqrt{w}$ compared with the other reflexions. The final weighting analysis was quite satisfactory. It may be pertinent to add here that there were no major shifts in the coordinates or vibration parameters after the change of weighting scheme; the actual largest shift was ~0·004 Å in x for O(4) (e.s.d. 0·0014 Å).

The final atomic parameters and their standard deviations are given in Table 1, and the vibration parameters and their standard deviations are given in Table 2. The estimated standard deviations are those given by the inversion of the full matrix. The observed structure amplitudes and those calculated with the parameters of Tables 1 and 2 are given in Table 3.

Table 1. *Final fractional coordinates and e.s.d.'s*

	x	y	z
Na(1)	0·44362 (8)	0·75331 (19)	0·37932 (12)
Na(2)	0·47262 (8)	0·22518 (19)	0·13722 (12)
Si(1)	0·18240 (4)	0·18422 (10)	0·02770 (7)
Si(2)	0·27681 (4)	0·29480 (10)	0·40291 (7)
O(1)	0·21462 (12)	−0·14126 (30)	0·01551 (19)
O(2)	0·26717 (13)	0·62025 (30)	0·45371 (18)
O(3)	0·18097 (12)	0·24614 (32)	0·22574 (19)
O(4)	0·40078 (12)	0·23205 (31)	0·39106 (19)
O(5)	0·06384 (13)	0·24503 (30)	−0·09331 (19)

Estimation of accuracy

The estimated standard deviations in the various bond lengths and angles were obtained from the e.s.d.'s in the fractional coordinates. The e.s.d.'s are: 0·0016 Å in Si–O, 0·0018 Å in Na···O and 0·002 Å in the O···O lengths; and 0·08° in O–Si–O, 0·07° in O–Na–O and 0·10° in Si–O–Si angles. As pointed out by Cruickshank (1964), since the U_{ij}'s for the oxygen atoms are generally greater than those for the silicon atoms, the Si–O lengths will have to be slightly increased to allow for errors due to rotational motions. However, a rigorous analysis, apart from being complicated, is not warranted in the present study, since it is not expected to produce changes of more than 0·004 Å in the Si–O lengths. Also, since the changes, although unequal, are always in the same direction, the differences in the various lengths will remain more or less the same and will not much affect our discussion. To take account of the uncertainties due to (*a*) the rotational motions, and (*b*) the errors in the cell dimensions, the e.s.d.'s in the different bonds and angles have been increased to: 0·003 Å in Si–O and Na···O, and 0·004 Å in the O···O distances; and 0·15° in O–Si–O and O–Na–O, and 0·20° in Si–O–Si angles. These are also shown in Table 4.

Description of the structure and discussion

Crystal structure

The projections of the structure down the [010], [001] and [100] axes are shown in Figs. 1, 2 and 3 respectively. β-$Na_2Si_2O_5$ has a packing arrangement very similar to

Table 2. *Vibration tensor components and e.s.d.'s* (Å^2)

	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{31}$	$2U_{12}$
Na(1)	0·0163 (5)	0·0118 (4)	0·0110 (4)	0·0001 (6)	0·0021 (7)	−0·0016 (6)
Na(2)	0·0129 (4)	0·0119 (4)	0·0151 (4)	0·0017 (6)	0·0098 (7)	0·0004 (6)
Si(1)	0·0065 (2)	0·0046 (2)	0·0057 (2)	−0·0004 (3)	0·0021 (4)	0·0004 (3)
Si(2)	0·0081 (2)	0·0041 (2)	0·0048 (2)	−0·0014 (3)	0·0029 (3)	0·0003 (3)
O(1)	0·0108 (6)	0·0058 (6)	0·0152 (7)	−0·0016 (9)	0·0112 (10)	0·0041 (8)
O(2)	0·0161 (7)	0·0060 (6)	0·0091 (6)	−0·0048 (8)	0·0113 (10)	−0·0008 (9)
O(3)	0·0103 (7)	0·0137 (6)	0·0062 (6)	−0·0042 (9)	0·0016 (10)	−0·0001 (9)
O(4)	0·0094 (7)	0·0113 (6)	0·0112 (7)	−0·0014 (9)	0·0042 (10)	0·0016 (9)
O(5)	0·0109 (7)	0·0112 (6)	0·0077 (6)	0·0017 (8)	0·0016 (10)	0·0020 (9)

Table 3. *Observed and calculated structure factors*

Reflexions marked with an asterisk could not be observed owing to the beam stop.

H	K	L	Fo	Fc
2	0	0	53.1	-57.8
4	0	0	66.4	71.0
6	0	0	22.3	-21.2
8	0	0	53.9	-55.7
10	0	0	3.4	5.4
12	0	0	10.2	-10.5
14	0	0	10.9	-10.3
16	0	0	3.1	-1.9
-16	0	1	22.0	21.8
-14	0	1	32.1	-31.9
-12	0	1	27.4	27.2
-10	0	1	17.2	-17.6
-8	0	1	32.7	-32.3
-6	0	1	36.0	35.4
-4	0	1	83.6	-87.6
-2	0	1	22.4	-21.7
0	0	1*	--	13.1
2	0	1	54.0	51.8
4	0	1	65.0	63.0
6	0	1	99.0	110.0
8	0	1	49.2	-50.2
10	0	1	46.5	46.7
12	0	1	14.5	-14.0
14	0	1	10.2	-10.1
16	0	1	17.5	16.3
-16	0	2	20.6	-20.3
-14	0	2	5.4	5.7
-12	0	2	26.1	-25.8
-10	0	2	10.7	11.4
-8	0	2	70.2	-74.1
-6	0	2	1.6	1.9
-4	0	2	14.1	-14.5
-2	0	2	10.4	-10.6
0	0	2	90.8	93.5
2	0	2	105.5	-110.4
4	0	2	71.7	69.3
6	0	2	40.5	-38.7
8	0	2	35.4	35.8
10	0	2	7.2	6.4
12	0	2	16.8	16.9
14	0	2	1.0	-3.2
-16	0	3	22.2	21.7
-14	0	3	13.4	-13.4
-12	0	3	28.8	28.6
-10	0	3	12.5	-12.1
-8	0	3	11.5	-11.7
-6	0	3	66.3	-67.0
-4	0	3	58.9	-59.3
-2	0	3	105.4	-111.7
0	0	3	40.5	40.1
2	0	3	31.8	27.5
4	0	3	18.4	17.8
6	0	3	45.4	45.2
8	0	3	53.9	-54.9
10	0	3	36.0	36.2
12	0	3	26.7	-26.5
14	0	3	11.4	11.9
-16	0	4	9.9	9.9
-14	0	4	2.2	-0.1
-12	0	4	18.2	18.3
-10	0	4	51.0	51.2
-8	0	4	39.1	-39.0
-6	0	4	86.0	89.3
-4	0	4	56.9	-57.3
-2	0	4	64.0	-62.1
0	0	4	45.3	-45.9
2	0	4	96.6	-99.3
4	0	4	13.2	11.7
6	0	4	14.6	16.2
8	0	4	6.6	6.5
10	0	4	0.9	0.7
12	0	4	13.8	14.4
-16	0	5	9.9	-9.8
-14	0	5	9.6	-10.1
-12	0	5	22.9	26.1
-10	0	5	2.8	4.7
-8	0	5	8.5	8.4
-6	0	5	30.4	29.2
-4	0	5	7.8	8.0
-2	0	5	16.5	-15.1
0	0	5	80.9	80.8
2	0	5	92.1	-93.7
4	0	5	15.6	15.8
6	0	5	34.5	-33.7
8	0	5	38.6	-38.2
10	0	5	29.7	29.5
12	0	5	27.3	-27.9
-16	0	6	5.5	5.1
-14	0	6	12.5	-12.1
-12	0	6	32.3	31.7
-10	0	6	0.8	-1.3
-8	0	6	21.5	21.3
-6	0	6	59.0	59.7
-4	0	6	47.8	-47.4
-2	0	6	21.9	21.6
0	0	6	20.7	-22.7
2	0	6	2.5	-3.8
4	0	6	31.0	30.8
6	0	6	12.0	11.6
8	0	6	21.7	-21.4
10	0	6	15.7	15.1
-16	0	7	27.2	-27.4
-14	0	7	1.0	-3.3
-12	0	7	11.9	-11.7
-10	0	7	6.4	6.7
-8	0	7	0.8	0.1
-6	0	7	50.8	49.6
-4	0	7	24.4	24.5
-2	0	7	30.2	30.0
0	0	7	22.1	21.2
2	0	7	61.7	-59.5
4	0	7	29.4	28.0
6	0	7	30.8	-29.7
8	0	7	24.7	24.3
10	0	7	8.0	9.3
-14	0	8	21.5	-21.3
-12	0	8	2.6	-1.7
-10	0	8	29.4	-29.6
-8	0	8	4.7	-5.5
-6	0	8	0.8	-1.1
-4	0	8	4.0	-3.3
-2	0	8	16.1	17.4
0	0	8	38.3	38.2
2	0	8	7.8	9.7
4	0	8	11.7	11.8
6	0	8	1.0	2.4
-10	0	9	14.5	-14.5
-8	0	9	23.8	-24.8
-6	0	9	30.6	30.8
-4	0	9	39.4	-38.6
-2	0	9	13.6	13.3
0	0	9	7.9	-8.8
2	0	9	23.2	-23.3
4	0	9	30.3	30.2
6	0	9	1.0	-1.2
-10	0	10	21.8	-21.5
-8	0	10	6.6	-6.9
-6	0	10	1.7	-3.2
-4	0	10	14.1	-13.4
-2	0	10	17.3	17.0
0	0	10	17.0	17.6
2	0	10	32.9	-33.0
1	1	0	7.9	8.1
2	1	0	35.7	-37.3
3	1	0	39.9	-41.1
4	1	0	6.2	6.3
5	1	0	37.1	37.2
6	1	0	13.7	-13.4
7	1	0	27.2	-27.1
8	1	0	35.9	-37.5
9	1	0	11.9	11.9
10	1	0	79.1	82.8
11	1	0	4.5	-5.1
12	1	0	4.5	-4.9
13	1	0	4.7	5.3
14	1	0	37.0	37.2
15	1	0	5.1	-4.1
-15	1	1	2.7	3.2
-14	1	1	17.5	17.4
-13	1	1	8.9	-7.6
-12	1	1	11.1	10.8
-11	1	1	19.4	19.0
-10	1	1	50.8	-52.3
-9	1	1	14.0	-14.1
-8	1	1	39.4	-40.3
-7	1	1	8.6	8.3
-6	1	1	40.7	-40.1
-5	1	1	0.7	0.6
-4	1	1	51.8	-56.4
-3	1	1	6.5	-6.3
-2	1	1	76.2	77.3
-1	1	1*	--	1.0
0	1	1*	--	-56.4
1	1	1*	--	12.3
2	1	1	7.3	-5.8
3	1	1	29.7	-28.8
4	1	1	31.3	32.2
5	1	1	11.4	10.9
6	1	1	21.1	-21.8
7	1	1	7.8	-7.6
8	1	1	15.5	15.3
9	1	1	10.4	-10.4
10	1	1	1.7	0.4
11	1	1	15.1	14.1
12	1	1	10.3	-10.6
13	1	1	14.3	-14.2
14	1	1	11.1	10.9
15	1	1	8.6	7.6
-15	1	2	1.0	-1.0
-14	1	2	18.2	17.8
-13	1	2	4.7	0.9
-12	1	2	15.0	14.6
-11	1	2	0.8	1.7
-10	1	2	2.4	1.1
-9	1	2	11.8	11.2
-8	1	2	44.3	44.2
-7	1	2	18.9	-18.2
-6	1	2	47.9	-46.4
-5	1	2	45.7	44.0
-4	1	2	8.4	-8.5
-3	1	2	51.3	-50.2
-2	1	2	44.7	-45.7
-1	1	2	41.2	39.9
0	1	2	8.3	-10.2
1	1	2	15.5	-14.5
2	1	2	51.3	-53.0
3	1	2	4.6	-4.8
4	1	2	31.0	-28.4
5	1	2	15.3	15.2
6	1	2	45.7	-45.5
7	1	2	18.5	-17.8
8	1	2	2.0	1.3
9	1	2	2.2	3.3
10	1	2	37.2	37.7
11	1	2	3.2	-3.8
12	1	2	11.3	-11.4
13	1	2	1.6	0.9
14	1	2	28.4	27.3
-15	1	3	4.6	-4.6
-14	1	3	4.1	-4.2
-13	1	3	0.9	-0.8
-12	1	3	29.2	29.5
-11	1	3	8.6	8.8
-10	1	3	46.1	-47.3
-9	1	3	9.6	-9.5
-8	1	3	19.2	19.5
-7	1	3	8.7	8.6
-6	1	3	13.8	14.1
-5	1	3	5.7	5.8
-4	1	3	17.1	15.6
-3	1	3	4.6	3.3
-2	1	3	38.2	40.9
-1	1	3	1.7	0.1
0	1	3	4.9	-6.8
1	1	3	19.7	18.9
2	1	3	14.2	13.5
3	1	3	29.0	-27.7
4	1	3	31.9	-31.1
5	1	3	29.9	29.2
6	1	3	28.0	-27.2
7	1	3	18.0	-17.0
8	1	3	62.2	-64.5
9	1	3	4.6	4.0
10	1	3	8.9	-8.5
11	1	3	0.9	3.0
12	1	3	14.7	-15.0
13	1	3	9.4	-9.6
14	1	3	13.6	14.1
-15	1	4	1.0	-1.7
-14	1	4	41.2	41.4
-13	1	4	6.3	-5.7
-12	1	4	26.6	26.7
-11	1	4	7.4	6.6
-10	1	4	19.3	19.3
-9	1	4	5.4	-4.5
-8	1	4	3.4	1.6
-7	1	4	6.6	-6.5
-6	1	4	3.4	-3.3
-5	1	4	23.6	23.1
-4	1	4	44.7	-45.0
-3	1	4	35.4	-34.5
-2	1	4	39.8	38.7
-1	1	4	40.4	39.8
0	1	4	30.7	28.8
1	1	4	17.0	-16.0
2	1	4	20.4	-19.2
3	1	4	10.4	9.9
4	1	4	61.3	60.2
5	1	4	5.2	5.0
6	1	4	31.2	-31.5
7	1	4	2.4	-2.8
8	1	4	11.0	9.9
9	1	4	2.1	-0.5
10	1	4	11.3	-11.5
11	1	4	4.8	5.7
12	1	4	35.6	-36.3
-15	1	5	6.3	-6.5
-14	1	5	11.5	-11.8
-13	1	5	1.5	1.7
-12	1	5	22.4	22.6
-11	1	5	0.8	-0.9
-10	1	5	39.7	-40.4
-9	1	5	7.1	-6.5
-8	1	5	94.5	97.6
-7	1	5	2.9	-0.1
-6	1	5	17.3	-17.3
-5	1	5	6.9	6.4
-4	1	5	25.8	25.7
-3	1	5	13.2	-12.4
-2	1	5	21.3	21.4
-1	1	5	7.1	6.6
0	1	5	7.0	-6.6
1	1	5	4.8	4.2
2	1	5	19.2	19.4
3	1	5	14.7	-14.1
4	1	5	16.6	17.5
5	1	5	28.7	27.8
6	1	5	15.1	-15.4
7	1	5	19.1	-18.7
8	1	5	14.1	-13.8
9	1	5	13.7	13.7
10	1	5	24.9	25.5
11	1	5	3.3	-3.2
12	1	5	30.0	-30.2
-15	1	6	1.0	-3.0
-14	1	6	22.5	22.1
-13	1	6	1.6	-1.5
-12	1	6	19.5	-19.6
-11	1	6	6.3	5.5
-10	1	6	15.1	-15.3
-9	1	6	11.6	-11.3
-8	1	6	16.3	-16.1
-7	1	6	1.7	2.2
-6	1	6	7.5	-7.9
-5	1	6	0.7	1.8
-4	1	6	16.8	-15.9
-3	1	6	16.2	-16.4
-2	1	6	63.3	63.2
-1	1	6	19.2	18.3
0	1	6	23.1	-24.0
1	1	6	14.9	-14.6
2	1	6	51.8	53.0
3	1	6	2.3	2.6
4	1	6	36.4	35.2
5	1	6	3.6	3.2
6	1	6	5.7	-5.7
7	1	6	0.9	-2.1
8	1	6	25.9	25.5
9	1	6	1.9	1.3
10	1	6	26.1	-25.5
-13	1	7	1.0	1.7
-12	1	7	1.3	-2.4
-11	1	7	0.9	1.2
-10	1	7	3.1	-2.2
-9	1	7	4.4	-3.9
-8	1	7	36.1	36.4
-7	1	7	1.6	0.8
-6	1	7	56.3	-57.2
-5	1	7	3.8	3.8
-4	1	7	5.6	7.4
-3	1	7	17.3	-16.5
-2	1	7	47.7	-48.1
-1	1	7	12.4	11.9
0	1	7	6.2	5.9
1	1	7	10.1	-9.9
2	1	7	8.0	-7.8
3	1	7	2.6	-2.6
4	1	7	27.7	28.0
5	1	7	9.9	10.0
6	1	7	6.9	6.3
7	1	7	14.1	-14.1
8	1	7	32.2	31.1
9	1	7	9.9	10.2
10	1	7	18.4	18.2
-13	1	8	3.7	4.5
-12	1	8	6.0	-5.8
-11	1	8	3.0	2.1
-10	1	8	30.8	-29.4
-9	1	8	5.1	-4.9
-8	1	8	15.9	15.3
-7	1	8	5.1	5.6
-6	1	8	6.8	6.5
-5	1	8	0.8	0.4
-4	1	8	14.0	-13.7
-3	1	8	6.8	-6.6
-2	1	8	19.0	18.2
-1	1	8	8.5	8.4
0	1	8	49.2	-49.6
1	1	8	10.1	-9.8
2	1	8	14.5	14.7
3	1	8	1.5	-2.2
4	1	8	17.5	-16.8
5	1	8	4.8	4.9
6	1	8	6.2	5.9
-9	1	9	4.2	-4.4
-8	1	9	0.9	0.2
-7	1	9	6.8	7.2
-6	1	9	24.7	-24.8
-5	1	9	0.9	-0.5
-4	1	9	7.8	-7.1
-3	1	9	5.8	-5.9
-2	1	9	0.9	-3.1
-1	1	9	12.4	12.4
0	1	9	8.5	-8.8
1	1	9	9.2	-10.0
2	1	9	22.3	-22.7
3	1	9	3.6	3.2
4	1	9	23.0	23.2
5	1	9	1.0	1.0
6	1	9	26.4	-26.2
-9	1	10	1.0	-1.2
-8	1	10	55.2	55.1
-7	1	10	4.6	4.3
-6	1	10	22.3	-22.4
-5	1	10	3.2	1.6
-4	1	10	17.8	18.8
-3	1	10	4.1	-4.2
-2	1	10	3.6	-4.1
-1	1	10	8.7	9.4
0	1	10	35.5	-35.0
1	1	10	7.4	-7.6
1	2	0	11.1	-11.4
2	2	0	12.7	-10.0
3	2	0	13.7	-13.8
4	2	0	28.2	-28.1
5	2	0	11.7	12.2
6	2	0	7.3	6.7
7	2	0	22.4	-22.2
8	2	0	45.0	45.8
9	2	0	3.2	2.5
10	2	0	1.8	-1.6
11	2	0	5.9	6.0
12	2	0	7.1	7.2
13	2	0	26.4	-26.1
14	2	0	9.9	9.5
15	2	0	22.0	21.4
-15	2	1	11.4	-11.4
-14	2	1	25.1	24.4
-13	2	1	7.7	7.6
-12	2	1	24.2	-24.6
-11	2	1	1.4	1.8
-10	2	1	20.7	20.7
-9	2	1	11.9	-11.6
-8	2	1	14.0	13.9
-7	2	1	37.9	38.3
-6	2	1	14.6	-13.8
-5	2	1	24.0	-23.9
-4	2	1	57.2	56.7
-3	2	1	27.1	25.2
-2	2	1	19.4	19.2
-1	2	1*	--	6.3
0	2	1*	--	-5.8
1	2	1*	--	5.3
2	2	1	36.5	-35.7
3	2	1	1.4	1.0
4	2	1	56.9	-55.6
5	2	1	10.4	10.0
6	2	1	71.1	-73.4
7	2	1	23.2	-23.1
8	2	1	24.6	24.9
9	2	1	9.6	9.2
10	2	1	27.1	-27.0
11	2	1	2.4	-0.3
12	2	1	6.3	6.3
13	2	1	12.2	-12.1
14	2	1	9.8	9.9
15	2	1	9.6	9.4
-15	2	2	20.6	-20.0
-14	2	2	2.9	-1.6
-13	2	2	25.3	24.6
-12	2	2	17.4	16.5
-11	2	2	25.9	-26.0
-10	2	2	3.9	-2.1
-9	2	2	5.5	5.1
-8	2	2	51.1	51.9
-7	2	2	4.1	4.3
-6	2	2	2.2	-2.7
-5	2	2	0.5	-0.3
-4	2	2	23.3	21.8
-3	2	2	9.9	9.2
-2	2	2	23.0	-21.8
-1	2	2	20.0	20.0
0	2	2	26.7	-25.7
1	2	2	7.3	-6.9
2	2	2	45.5	44.1
3	2	2	11.6	11.0
4	2	2	27.3	-25.3
5	2	2	21.0	20.8
6	2	2	19.5	18.3
7	2	2	20.7	-20.3
8	2	2	24.9	-24.3
9	2	2	17.5	17.2
10	2	2	5.9	-6.3
11	2	2	7.4	-7.6
12	2	2	11.9	-12.1
13	2	2	9.1	-9.2
14	2	2	2.6	-0.1
-15	2	3	18.8	-18.5
-14	2	3	6.7	6.9
-13	2	3	14.4	14.6
-12	2	3	22.4	-20.9
-11	2	3	10.1	-10.0
-10	2	3	11.3	10.4
-9	2	3	14.3	-14.3
-8	2	3	4.0	4.9
-7	2	3	25.0	24.1
-6	2	3	60.5	60.1
-5	2	3	44.8	-44.1
-4	2	3	43.3	43.6
-3	2	3	33.4	32.2
-2	2	3	78.4	79.2
-1	2	3	5.4	-10.2
1	2	3	13.6	12.7
2	2	3	27.2	-25.7
3	2	3	0.6	0.1
4	2	3	17.0	-17.0
5	2	3	15.8	15.4
6	2	3	27.9	-27.8
7	2	3	9.5	-9.8
8	2	3	31.7	32.2
9	2	3	15.0	15.5
10	2	3	17.2	-16.8
11	2	3	4.2	2.8
12	2	3	14.4	14.3
13	2	3	11.3	-11.7
14	2	3	6.5	-5.5
-15	2	4	5.7	-6.3
-14	2	4	5.0	4.9
-13	2	4	13.6	12.9
-12	2	4	22.5	-21.7
-11	2	4	21.5	-21.2
-10	2	4	33.9	-33.5
-9	2	4	2.3	1.9
-8	2	4	18.7	18.7
-7	2	4	1.7	1.0
-6	2	4	60.3	-61.2
-5	2	4	12.5	-12.6
-4	2	4	43.4	43.2
-3	2	4	9.1	-8.9
-2	2	4	39.9	38.5
-1	2	4	13.0	12.5
0	2	4	57.5	57.0
1	2	4	26.5	-25.7
2	2	4	56.6	56.1
3	2	4	24.9	24.0
4	2	4	9.0	9.0
5	2	4	0.7	-0.2
6	2	4	24.3	-24.1
7	2	4	10.6	-9.6
8	2	4	2.0	-2.2
9	2	4	16.6	17.0
10	2	4	2.0	-1.8
11	2	4	6.1	-6.0
12	2	4	9.9	-10.3
-15	2	5	19.6	-19.1
-14	2	5	5.5	5.6
-13	2	5	33.2	32.2
-12	2	5	18.2	-17.4
-11	2	5	25.7	-26.0
-10	2	5	6.4	-6.6
-9	2	5	7.8	7.7
-8	2	5	7.8	-6.5
-7	2	5	4.4	3.9
-6	2	5	23.4	-22.7
-5	2	5	32.9	-32.0
-4	2	5	5.7	-5.9
-3	2	5	23.5	23.0
-2	2	5	5.4	4.8
-1	2	5	23.7	-23.2
0	2	5	54.9	-54.5
1	2	5	3.8	2.6
2	2	5	65.1	64.8
3	2	5	10.4	-10.2
4	2	5	6.9	-7.3
5	2	5	13.6	13.3
6	2	5	29.7	29.6
7	2	5	18.1	-17.8
8	2	5	26.0	24.9
9	2	5	19.9	19.8
10	2	5	17.5	-16.5
11	2	5	8.5	-9.1
12	2	5	17.4	16.5
-15	2	6	5.0	5.4
-14	2	6	15.5	14.8
-13	2	6	4.6	5.1
-12	2	6	33.0	-31.9
-11	2	6	2.7	-1.4
-10	2	6	9.2	9.2
-9	2	6	1.8	0.9
-8	2	6	31.2	-29.9
-7	2	6	17.0	16.6
-6	2	6	35.3	-35.1
-5	2	6	24.8	-24.0
-4	2	6	29.7	29.4
-3	2	6	8.4	8.4
-2	2	6	14.3	-14.8
-1	2	6	2.6	-2.0
0	2	6	25.1	24.9
1	2	6	22.9	-22.0
2	2	6	7.9	-7.7
3	2	6	19.3	19.5
4	2	6	17.3	-16.3
5	2	6	20.0	-19.7
6	2	6	16.0	-15.7
7	2	6	0.9	1.0
8	2	6	19.4	18.6
9	2	6	4.9	3.7
-13	2	7	31.7	31.0
-12	2	7	15.6	14.8
-11	2	7	32.7	-31.7
-10	2	7	10.0	-9.5
-9	2	7	30.5	29.3
-8	2	7	2.9	1.2
-7	2	7	9.1	-8.5
-6	2	7	42.8	-41.7
-5	2	7	0.8	2.0
-4	2	7	19.7	-19.6
-3	2	7	10.1	9.5
-2	2	7	30.6	-30.2
-1	2	7	6.8	-6.5
0	2	7	7.7	-6.9
1	2	7	4.7	-3.9
2	2	7	39.9	38.6
3	2	7	1.9	-1.4
4	2	7	13.7	-13.1
5	2	7	4.9	5.2
6	2	7	22.3	21.4
7	2	7	18.1	-18.0
8	2	7	23.7	-23.3
9	2	7	16.7	16.9
-13	2	8	4.9	4.7
-12	2	8	1.0	-1.7
-11	2	8	3.8	-0.6
-10	2	8	30.9	30.4
-9	2	8	0.9	-1.0
-8	2	8	0.9	-3.4
-7	2	8	21.0	20.5
-6	2	8	13.4	12.3
-5	2	8	27.0	-26.4
-4	2	8	8.5	-8.3
-3	2	8	31.6	31.0
-2	2	8	8.4	-8.2
-1	2	8	12.9	-12.9
0	2	8	34.4	-32.8
1	2	8	2.1	1.8
2	2	8	13.2	-13.2
3	2	8	8.5	8.1
4	2	8	5.1	-3.7
5	2	8	10.1	-10.3
6	2	8	3.9	-4.9
-9	2	9	25.6	25.5
-8	2	9	24.1	23.9
-7	2	9	12.4	-13.2
-6	2	9	27.3	-27.2
-5	2	9	9.7	9.9
-4	2	9	33.8	32.6
-3	2	9	2.4	-0.7
-2	2	9	12.8	-13.4
-1	2	9	7.3	7.7
0	2	9	13.7	13.8
1	2	9	10.1	-9.8
2	2	9	11.4	11.3
3	2	9	15.4	15.8
4	2	9	16.4	-16.7
5	2	9	7.4	-6.6
6	2	9	5.7	-5.3
-9	2	10	4.6	4.7
-8	2	10	3.0	0.7
-7	2	10	2.4	3.5
-6	2	10	11.0	10.7
-5	2	10	18.5	-18.2
-4	2	10	1.0	2.3
-3	2	10	27.7	28.0
-2	2	10	9.6	-8.7
-1	2	10	20.5	-20.7
0	2	10	17.7	-18.3
1	2	10	14.3	13.9
1	3	0	4.7	-5.6
2	3	0	16.2	17.4
3	3	0	52.7	57.3
4	3	0	4.5	4.5
5	3	0	49.2	-50.5
6	3	0	8.5	9.0
7	3	0	36.4	36.4
8	3	0	19.7	19.5
9	3	0	11.2	-11.3
10	3	0	49.5	-49.0
11	3	0	2.6	2.2
12	3	0	2.6	-3.2
13	3	0	6.4	-5.9
14	3	0	31.2	-30.3
15	3	0	5.6	4.5
-15	3	1	2.2	-2.3
-14	3	1	20.0	-20.7
-13	3	1	10.7	10.6
-12	3	1	8.9	9.0
-11	3	1	34.6	-35.3
-10	3	1	13.5	13.7
-9	3	1	24.9	25.7
-8	3	1	47.3	51.4
-7	3	1	15.6	-15.9
-6	3	1	6.5	6.4
-5	3	1	2.2	-1.1
-4	3	1	49.1	50.3
-3	3	1	11.5	11.1
-2	3	1	44.7	-45.9
-1	3	1*	--	-2.8
0	3	1*	--	31.6
1	3	1*	--	-14.4
2	3	1	1.8	-2.8
3	3	1	43.4	45.7
4	3	1	22.8	-23.7
5	3	1	13.9	-14.6
6	3	1	21.2	22.5
7	3	1	10.8	11.5
8	3	1	22.9	-25.0
9	3	1	20.7	22.3
10	3	1	17.7	18.8
11	3	1	26.0	-27.8
12	3	1	5.6	-6.3
13	3	1	27.7	27.5
14	3	1	1.9	-1.5
15	3	1	13.9	-13.1
-15	3	2	2.0	-2.0
-14	3	2	4.6	-5.5
-13	3	2	3.8	4.2
-12	3	2	9.0	-9.5
-11	3	2	13.7	-13.9
-10	3	2	5.8	-7.1
-9	3	2	5.8	-7.2
-8	3	2	24.8	-25.5
-7	3	2	13.4	13.6
-6	3	2	29.6	29.8
-5	3	2	56.3	-57.5
-4	3	2	4.8	-4.0
-3	3	2	63.7	64.4
-2	3	2	42.3	42.3
-1	3	2	52.7	-52.1
0	3	2	2.3	2.4
1	3	2	19.3	18.9
2	3	2	40.0	39.0
3	3	2	6.2	6.7
4	3	2	17.5	17.4
5	3	2	20.6	-20.8
6	3	2	29.7	29.7
7	3	2	26.3	26.4
8	3	2	7.2	-7.3
9	3	2	2.4	1.7
10	3	2	17.1	-17.2
11	3	2	2.9	2.6
12	3	2	0.9	-1.7
13	3	2	3.2	2.1
-15	3	3	14.4	14.5
-14	3	3	2.8	-0.5
-13	3	3	4.9	-4.1
-12	3	3	4.1	-5.2
-11	3	3	12.4	-12.3
-10	3	3	9.6	9.2
-9	3	3	13.5	13.6
-8	3	3	16.4	16.9
-7	3	3	12.6	-12.4
-6	3	3	35.2	-35.1
-5	3	3	16.2	-16.2
-4	3	3	9.8	9.6
-3	3	3	0.9	-0.6
-2	3	3	42.6	-42.1
-1	3	3	8.7	-8.6
0	3	3	13.3	13.2
1	3	3	27.0	-26.4
2	3	3	18.5	-17.8
3	3	3	44.1	43.6
4	3	3	28.5	27.6
5	3	3	49.9	-49.7
6	3	3	18.9	17.9
7	3	3	28.7	28.5
8	3	3	39.4	39.4
9	3	3	5.6	-5.0
10	3	3	20.0	19.8
11	3	3	6.7	-6.4
12	3	3	2.8	-2.7
13	3	3	19.9	20.0
-15	3	4	1.7	2.2
-14	3	4	21.2	-21.5
-13	3	4	16.6	16.9
-12	3	4	23.3	-23.8
-11	3	4	21.0	-22.1
-10	3	4	16.4	-16.6
-9	3	4	23.6	23.2
-8	3	4	2.1	3.9
-7	3	4	7.1	-7.2
-6	3	4	4.9	4.9
-5	3	4	20.1	-20.5
-4	3	4	20.4	19.9
-3	3	4	40.1	40.5
-2	3	4	7.2	-6.4
-1	3	4	55.2	-55.6
0	3	4	32.4	-32.6
1	3	4	17.5	17.1
2	3	4	20.7	20.1
3	3	4	14.8	-14.6
4	3	4	44.1	-44.3
5	3	4	10.1	-9.7
6	3	4	20.5	20.9
7	3	4	3.2	2.2
8	3	4	10.4	-10.3
9	3	4	4.2	4.9
10	3	4	15.1	15.8
11	3	4	14.9	-15.5
12	3	4	19.6	19.7
-14	3	5	11.9	11.9
-13	3	5	6.7	-6.5
-12	3	5	7.3	-8.8

Table 3 (*cont.*)

H	K	L	Fo	Fc
-11	3	5	6.9	6.5
-10	3	5	9.3	9.2
-9	3	5	9.3	9.0
-8	3	5	41.4	-42.1
-7	3	5	5.4	5.1
-6	3	5	14.0	-14.1
-5	3	5	18.2	-18.2
-4	3	5	2.3	2.6
-3	3	5	31.8	31.6
-2	3	5	27.3	-27.7
-1	3	5	21.9	-21.8
0	3	5	15.9	16.2
1	3	5	0.7	1.5
2	3	5	22.5	-22.8
3	3	5	17.6	18.2
4	3	5	0.7	-1.0
5	3	5	48.0	-48.4
6	3	5	3.7	4.0
7	3	5	31.8	31.3
8	3	5	9.9	10.2
9	3	5	24.5	-24.4
10	3	5	12.6	-12.1
11	3	5	4.3	4.4
12	3	5	13.2	12.5
-14	3	6	10.8	-10.8
-13	3	6	3.9	3.4
-12	3	6	12.7	12.7
-11	3	6	14.5	-14.6
-10	3	6	6.6	6.3
-9	3	6	30.3	31.0
-8	3	6	17.9	18.5
-7	3	6	16.1	-16.6
-6	3	6	3.2	4.1
-5	3	6	13.5	13.4
-4	3	6	4.1	4.7
-3	3	6	13.8	14.6
-2	3	6	27.8	-28.6
-1	3	6	19.6	-19.7
0	3	6	0.7	0.0
1	3	6	16.4	16.6
2	3	6	25.4	-25.7
3	3	6	0.8	3.2
4	3	6	30.4	-30.5
5	3	6	10.2	-10.2
6	3	6	4.1	5.6
7	3	6	4.5	4.9
8	3	6	21.4	-21.9
9	3	6	3.3	-2.8
-13	3	7	3.9	-2.6
-12	3	7	1.0	-1.8
-11	3	7	3.3	-2.7
-10	3	7	8.8	-9.0
-9	3	7	7.6	7.7
-8	3	7	9.8	-10.1
-7	3	7	2.5	-0.5
-6	3	7	20.4	21.5
-5	3	7	9.8	-9.5
-4	3	7	9.8	10.4
-3	3	7	37.3	37.7
-2	3	7	24.5	25.4
-1	3	7	28.7	-29.2
0	3	7	4.3	4.2
1	3	7	27.6	27.5
2	3	7	3.0	-3.3
3	3	7	2.1	-2.8
4	3	7	8.5	-8.1
5	3	7	12.1	-12.4
6	3	7	17.5	-17.2
7	3	7	21.6	22.6
8	3	7	17.2	-17.6
9	3	7	14.7	-15.9
-13	3	8	13.2	-14.0
-12	3	8	6.8	6.3
-11	3	8	1.0	-2.5
-10	3	8	13.5	13.5
-9	3	8	10.5	10.8
-8	3	8	0.9	-0.1
-7	3	8	15.1	-15.3
-6	3	8	16.2	-16.0
-5	3	8	6.5	5.9
-4	3	8	10.5	10.4
-3	3	8	4.8	4.1
-2	3	8	4.9	-5.1
-1	3	8	7.2	-6.8
0	3	8	23.3	23.2
1	3	8	11.0	11.5
2	3	8	1.8	2.1
3	3	8	12.5	12.5
4	3	8	5.5	5.2
5	3	8	14.5	-15.1
-9	3	9	12.1	12.7
-8	3	9	5.6	5.5
-7	3	9	18.1	-18.6
-6	3	9	9.6	8.7
-5	3	9	4.4	3.5
-4	3	9	12.4	13.1
-3	3	9	10.0	11.1
-2	3	9	1.8	-2.4
-1	3	9	26.0	-27.0
0	3	9	7.8	8.7
1	3	9	23.0	23.5
2	3	9	13.2	13.4
3	3	9	10.5	-11.2
4	3	9	9.2	-9.7
5	3	9	3.6	4.3
-9	3	10	1.0	-1.3
-8	3	10	28.1	-28.9
-7	3	10	7.1	-7.6
-6	3	10	4.2	1.8
-5	3	10	4.5	-3.5
-4	3	10	5.1	-5.1
-3	3	10	5.9	6.2
-2	3	10	3.9	1.3
-1	3	10	15.7	-16.1
0	3	10	20.7	22.5
1	3	10	11.0	11.6
1	4	0	0.6	0.0
2	4	0	32.7	39.6
3	4	0	23.0	25.5
4	4	0	1.0	-0.9
5	4	0	22.0	-23.4
6	4	0	4.5	-5.1
7	4	0	32.4	34.6
8	4	0	19.2	-20.2
9	4	0	10.1	-10.9
10	4	0	6.9	-6.6
11	4	0	0.8	1.0
12	4	0	2.5	-2.3
13	4	0	25.1	25.9
14	4	0	4.7	-5.2
-15	4	1	5.7	5.3
-14	4	1	6.9	-7.0
-13	4	1	3.2	0.4
-12	4	1	13.5	14.1
-11	4	1	8.0	-8.4
-10	4	1	17.6	-18.5
-9	4	1	12.7	13.4
-8	4	1	7.2	7.5
-7	4	1	33.6	-35.5
-6	4	1	8.4	-8.2
-5	4	1	6.7	6.2
-4	4	1	24.2	-24.8
-3	4	1	2.2	3.2
-2	4	1	4.5	-4.9
-1	4	1•	--	-45.2
0	4	1•	--	-12.0
1	4	1•	--	34.9
2	4	1	25.2	25.9
3	4	1	35.5	-36.6
4	4	1	32.9	33.9
5	4	1	15.2	15.9
6	4	1	23.9	24.1
7	4	1	9.6	9.3
8	4	1	6.5	6.1
9	4	1	0.8	-1.7
10	4	1	0.8	0.6
11	4	1	2.2	-1.7
12	4	1	2.4	0.4
13	4	1	10.8	12.0
14	4	1	4.1	-4.4
-15	4	2	22.6	23.1
-14	4	2	1.0	0.7
-13	4	2	26.1	-26.8
-12	4	2	5.8	-5.3
-11	4	2	27.9	28.6
-10	4	2	9.5	-9.7
-9	4	2	3.8	-3.5
-8	4	2	12.0	-12.8
-7	4	2	6.1	-6.1
-6	4	2	8.7	-9.2
-5	4	2	1.5	1.5
-4	4	2	11.2	-11.3
-3	4	2	12.2	-12.1
-2	4	2	31.6	32.0
-1	4	2	17.9	-17.9
0	4	2	19.7	-20.0
1	4	2	0.6	-0.1
2	4	2	9.1	9.4
3	4	2	3.3	-3.0
4	4	2	9.4	-9.1
5	4	2	34.5	-34.6
6	4	2	5.7	-5.3
7	4	2	33.8	34.2
8	4	2	16.7	16.0
9	4	2	29.3	-30.4
10	4	2	2.5	0.6
11	4	2	19.7	19.9
12	4	2	5.4	4.6
13	4	2	1.0	1.7
-15	4	3	12.1	12.4
-14	4	3	4.0	4.4
-13	4	3	3.3	-4.1
-12	4	3	5.8	5.8
-11	4	3	2.2	-1.3
-10	4	3	4.0	-4.1
-9	4	3	25.4	26.8
-8	4	3	4.7	4.2
-7	4	3	30.4	-31.2
-6	4	3	43.8	-44.2
-5	4	3	44.5	45.3
-4	4	3	19.8	-20.3
-3	4	3	22.1	-21.5
-2	4	3	32.4	-32.0
-1	4	3	10.0	-9.8
0	4	3	2.7	-3.7
1	4	3	10.5	10.8
2	4	3	30.8	31.1
3	4	3	24.8	-25.1
4	4	3	7.0	6.9
5	4	3	2.4	3.3
6	4	3	6.3	6.3
7	4	3	5.4	-5.9
8	4	3	2.2	-0.5
9	4	3	7.9	-7.2
10	4	3	10.0	-10.0
11	4	3	9.6	-10.5
12	4	3	2.7	1.3
13	4	3	17.0	16.9
-15	4	4	8.7	8.1
-14	4	4	2.5	-4.0
-13	4	4	13.9	-14.4
-12	4	4	15.1	15.9
-11	4	4	25.8	25.8
-10	4	4	12.3	13.0
-9	4	4	3.5	-3.9
-8	4	4	7.9	7.1
-7	4	4	4.1	4.2
-6	4	4	16.3	16.4
-5	4	4	6.5	7.0
-4	4	4	12.4	-12.6
-3	4	4	18.2	18.2
-2	4	4	17.8	-17.8
-1	4	4	21.0	-20.4
0	4	4	50.2	-50.2
1	4	4	31.7	32.1
2	4	4	8.2	-8.4
3	4	4	26.3	-26.6
4	4	4	22.0	-22.2
5	4	4	3.3	-4.0
6	4	4	22.6	23.1
7	4	4	16.8	17.1
8	4	4	5.5	4.5
9	4	4	26.6	-27.5
10	4	4	2.2	-2.0
11	4	4	15.0	15.2
-15	4	5	12.5	13.1
-14	4	5	1.4	-1.0
-13	4	5	25.7	-26.6
-12	4	5	5.2	4.9
-11	4	5	16.2	16.2
-10	4	5	6.9	6.2
-9	4	5	3.5	5.1
-8	4	5	7.5	7.4
-7	4	5	14.4	-14.2
-6	4	5	6.3	6.1
-5	4	5	42.8	42.7
-4	4	5	6.6	6.9
-3	4	5	26.7	-25.9
-2	4	5	5.0	6.0
-1	4	5	22.2	21.9
0	4	5	13.4	13.5
1	4	5	5.3	5.5
2	4	5	16.9	-16.3
3	4	5	0.7	2.3
4	4	5	9.5	-9.5
5	4	5	5.4	-5.4
6	4	5	16.7	-16.7
7	4	5	10.9	10.7
8	4	5	5.3	-6.1
9	4	5	16.1	-15.7
10	4	5	1.9	-1.4
11	4	5	4.1	5.5
-15	4	6	5.5	-5.9
-14	4	6	8.8	-9.0
-13	4	6	4.6	-6.1
-12	4	6	17.4	18.6
-11	4	6	2.7	1.2
-10	4	6	9.3	-9.2
-9	4	6	4.1	-4.4
-8	4	6	30.8	30.5
-7	4	6	13.8	-13.6
-6	4	6	3.3	3.3
-5	4	6	18.8	18.9
-4	4	6	3.9	-3.5
-3	4	6	3.2	1.9
-2	4	6	2.4	2.2
-1	4	6	7.8	-7.8
0	4	6	22.4	-23.1
1	4	6	34.3	33.8
2	4	6	18.1	18.3
3	4	6	27.6	-27.6
4	4	6	0.8	0.3
5	4	6	25.8	26.4
6	4	6	13.5	13.7
7	4	6	0.9	-1.1
8	4	6	5.8	-6.2
9	4	6	4.0	-6.3
-12	4	7	15.2	-15.3
-11	4	7	24.7	24.8
-10	4	7	8.3	8.4
-9	4	7	22.2	-22.2
-8	4	7	0.9	3.4
-7	4	7	2.1	-1.3
-6	4	7	17.7	17.7
-5	4	7	4.3	4.4
-4	4	7	20.4	20.6
-3	4	7	16.3	-15.5
-2	4	7	19.3	20.1
-1	4	7	9.2	9.7
0	4	7	10.8	-10.7
1	4	7	4.9	5.1
2	4	7	5.5	-6.1
3	4	7	0.9	0.7
4	4	7	11.4	-11.4
5	4	7	4.0	-3.8
6	4	7	5.9	-5.5
7	4	7	17.5	18.3
8	4	7	17.8	18.2
9	4	7	15.7	-16.0
-12	4	8	2.8	-2.1
-11	4	8	1.0	-0.5
-10	4	8	19.2	-19.0
-9	4	8	0.9	-0.5
-8	4	8	6.1	6.6
-7	4	8	20.4	-20.6
-6	4	8	19.7	-19.5
-5	4	8	23.7	23.8
-4	4	8	18.7	18.8
-3	4	8	27.6	-27.8
-2	4	8	0.9	-1.9
-1	4	8	3.5	5.0
0	4	8	19.7	19.1
1	4	8	5.8	6.1
2	4	8	18.4	18.7
3	4	8	15.3	-15.8
4	4	8	8.4	-9.2
5	4	8	17.1	17.5
-8	4	9	16.6	-15.7
-7	4	9	4.2	5.4
-6	4	9	12.8	12.4
-5	4	9	4.2	-5.3
-4	4	9	11.0	-11.8
-3	4	9	4.9	-4.0
-2	4	9	4.4	3.7
-1	4	9	6.9	-6.4
0	4	9	12.8	-13.3
1	4	9	8.8	9.4
2	4	9	3.9	3.3
3	4	9	16.9	-18.3
4	4	9	4.1	-3.1
5	4	9	6.9	7.4
-8	4	10	1.0	2.3
-7	4	10	2.3	-1.3
-6	4	10	14.9	-15.0
-5	4	10	15.9	16.7
-4	4	10	8.9	9.5
-3	4	10	28.0	-27.5
-2	4	10	1.0	0.5
-1	4	10	16.7	17.0
0	4	10	12.8	13.5
1	4	10	9.4	-9.8
1	5	0	0.6	-1.2
2	5	0	1.4	-2.9
3	5	0	29.8	-32.4
4	5	0	10.5	-11.3
5	5	0	24.1	24.6
6	5	0	8.2	-8.5
7	5	0	15.7	-16.1
8	5	0	3.7	0.5
9	5	0	1.5	-0.8
10	5	0	10.1	10.3
11	5	0	3.7	4.0
12	5	0	17.1	17.0
13	5	0	1.6	1.3
14	5	0	14.5	14.1
-14	5	1	14.4	14.2
-13	5	1	3.5	-2.3
-12	5	1	12.8	-12.9
-11	5	1	26.5	26.2
-10	5	1	0.8	0.5
-9	5	1	19.1	-19.2
-8	5	1	29.8	-30.9
-7	5	1	15.5	15.7
-6	5	1	10.7	-11.1
-5	5	1	6.1	-6.4
-4	5	1	7.8	-7.4
-3	5	1	0.7	-1.4
-2	5	1	6.0	7.4
-1	5	1•	--	-0.9
0	5	1•	--	-7.0
1	5	1•	--	7.8
2	5	1	9.1	9.5
3	5	1	27.5	-28.2
4	5	1	2.2	0.4
5	5	1	0.8	1.2
6	5	1	4.4	-4.5
7	5	1	3.1	-3.5
8	5	1	14.0	13.8
9	5	1	20.5	-20.8
10	5	1	19.2	-18.9
11	5	1	22.1	21.7
12	5	1	9.0	8.9
13	5	1	21.5	-21.3
14	5	1	3.2	1.2
-14	5	2	1.4	0.3
-13	5	2	9.2	-9.2
-12	5	2	2.3	-2.8
-11	5	2	19.4	19.9
-10	5	2	18.9	19.1
-9	5	2	4.1	-4.5
-8	5	2	0.7	0.0
-7	5	2	6.0	6.2
-6	5	2	9.4	-9.4
-5	5	2	27.0	26.4
-4	5	2	6.4	6.3
-3	5	2	32.8	-32.3
-2	5	2	24.0	-24.7
-1	5	2	27.7	28.8
0	5	2	2.4	-2.8
1	5	2	12.5	-12.5
2	5	2	7.9	-7.8
3	5	2	2.1	1.8
4	5	2	22.6	-22.8
5	5	2	6.2	5.5
6	5	2	7.1	-7.3
7	5	2	11.7	-11.9
8	5	2	7.7	7.7
9	5	2	11.2	-10.4
10	5	2	0.9	-2.5
11	5	2	1.8	1.4
12	5	2	17.1	16.3
13	5	2	4.7	-4.8
-14	5	3	1.4	0.9
-13	5	3	10.5	10.6
-12	5	3	7.5	-7.9
-11	5	3	4.0	3.5
-10	5	3	8.0	8.6
-9	5	3	5.9	-5.3
-8	5	3	23.3	-23.7
-7	5	3	8.1	8.0
-6	5	3	19.3	18.9
-5	5	3	13.1	12.3
-4	5	3	6.8	6.8
-3	5	3	4.1	4.5
-2	5	3	5.4	5.7
-1	5	3	6.6	6.2
0	5	3	7.3	7.8
1	5	3	17.7	17.3
2	5	3	8.8	8.3
3	5	3	27.8	-26.7
4	5	3	19.7	-18.9
5	5	3	31.3	30.8
6	5	3	4.7	-5.0
7	5	3	14.7	-14.7
8	5	3	21.1	-21.3
9	5	3	0.9	-0.2
10	5	3	21.5	-21.3
11	5	3	5.9	4.9
12	5	3	12.4	11.9
13	5	3	17.5	-17.0
-14	5	4	4.9	5.2
-13	5	4	20.6	-20.3
-12	5	4	16.4	15.8
-11	5	4	26.6	26.2
-10	5	4	17.1	16.6
-9	5	4	30.1	-30.1
-8	5	4	13.7	-13.5
-7	5	4	22.8	22.3
-6	5	4	2.5	-1.2
-5	5	4	4.1	-4.5
-4	5	4	7.9	-7.6
-3	5	4	11.6	-10.8
-2	5	4	6.7	-6.5
-1	5	4	28.5	27.7
0	5	4	21.1	20.6
1	5	4	6.3	-3.2
2	5	4	4.6	-3.0
3	5	4	15.0	12.0
4	5	4	11.7	11.2
5	5	4	3.3	2.8
6	5	4	2.1	3.5
7	5	4	4.9	5.6
8	5	4	0.9	-0.0
9	5	4	10.8	-9.7
10	5	4	13.3	-12.4
11	5	4	17.7	17.7
-14	5	5	9.8	-10.0
-13	5	5	9.3	9.0
-12	5	5	1.6	-1.0
-11	5	5	12.5	-12.2
-10	5	5	10.9	10.5
-9	5	5	1.2	-2.3
-8	5	5	6.0	6.2
-7	5	5	8.7	-8.9
-6	5	5	18.8	18.2
-5	5	5	17.4	17.4
-4	5	5	2.7	-3.0
-3	5	5	28.0	-26.9
-2	5	5	5.2	5.3
-1	5	5	20.3	19.0
0	5	5	0.7	-1.5
1	5	5	5.3	-6.8
2	5	5	9.6	9.6
3	5	5	4.4	-5.1
4	5	5	0.8	-2.8
5	5	5	32.1	31.1
6	5	5	1.7	1.3
7	5	5	16.1	-15.8
8	5	5	5.5	-4.6
9	5	5	15.3	15.1
10	5	5	2.4	-0.6
11	5	5	1.0	-1.1
-14	5	6	1.0	0.6
-13	5	6	2.6	-3.2
-12	5	6	5.6	-5.8
-11	5	6	15.3	14.9
-10	5	6	2.8	2.3
-9	5	6	33.6	-32.9
-8	5	6	18.8	-18.5
-7	5	6	25.4	24.1
-6	5	6	0.8	-0.7
-5	5	6	29.5	-28.5
-4	5	6	4.3	3.3
-3	5	6	8.1	7.7
-2	5	6	2.6	1.9
-1	5	6	2.7	-2.4
0	5	6	10.9	10.3
1	5	6	1.5	-0.6
2	5	6	12.6	12.0
3	5	6	11.0	-10.2
4	5	6	11.4	11.4
5	5	6	9.7	8.9
6	5	6	6.0	7.1
7	5	6	4.2	-0.9
8	5	6	6.6	6.3
-12	5	7	4.5	4.1
-11	5	7	1.7	1.6
-10	5	7	17.6	16.4
-9	5	7	3.9	-4.5
-8	5	7	7.6	-7.5
-7	5	7	2.8	-1.4
-6	5	7	2.9	0.9
-5	5	7	8.6	8.5
-4	5	7	12.2	-11.9
-3	5	7	34.2	-33.1
-2	5	7	19.2	-18.3
-1	5	7	25.3	24.7
0	5	7	0.8	0.4
1	5	7	28.7	-27.9
2	5	7	0.9	2.2
3	5	7	10.9	10.9
4	5	7	1.3	-2.5
5	5	7	0.9	-0.9
6	5	7	20.4	20.0
7	5	7	8.3	-9.1
8	5	7	8.0	7.3
-12	5	8	4.1	-4.2
-11	5	8	2.8	-0.8
-10	5	8	3.4	-0.5
-9	5	8	7.6	-8.5
-8	5	8	10.2	-10.2
-7	5	8	16.2	15.9
-6	5	8	22.0	20.5
-5	5	8	12.2	-12.0
-4	5	8	4.0	-4.9
-3	5	8	8.7	9.1
-2	5	8	5.8	-6.7
-1	5	8	9.1	-8.9
0	5	8	2.6	-1.0
1	5	8	0.9	1.6
2	5	8	11.9	-11.3
3	5	8	21.9	-20.8
4	5	8	3.9	-1.7
-1	5	9	22.8	21.9
0	5	9	1.0	-0.8
1	5	9	21.2	-20.5
2	5	9	10.2	-10.0
3	5	9	13.8	13.9
4	5	9	1.0	1.9
-1	5	10	7.9	7.7
0	5	10	8.2	-8.8
1	5	10	2.6	-2.8
1	6	0	1.2	5.0
2	6	0	17.6	-26.9
3	6	0	18.0	-20.1
4	6	0	1.5	-0.1
5	6	0	14.2	14.4
6	6	0	14.0	14.1
7	6	0	22.0	-21.9
8	6	0	0.7	0.5
9	6	0	8.5	8.4
10	6	0	10.9	10.7
11	6	0	6.9	-6.7
12	6	0	1.8	0.7
13	6	0	12.4	-12.3
14	6	0	1.4	-1.2
-14	6	1	8.0	-8.6
-13	6	1	10.7	-10.8
-12	6	1	2.0	-0.6
-11	6	1	12.2	11.6
-10	6	1	7.6	7.5
-9	6	1	7.4	-7.3
-8	6	1	9.5	-10.0
-7	6	1	17.7	18.0
-6	6	1	11.1	11.6
-5	6	1	5.6	6.4
-4	6	1	11.0	11.3
-3	6	1	10.9	-11.8
-2	6	1	2.7	-3.7
-1	6	1•	--	38.9
0	6	1•	--	17.9
1	6	1•	--	-31.1
2	6	1	17.0	-19.1
3	6	1	33.2	35.3
4	6	1	18.2	-18.5
5	6	1	24.2	-23.9
6	6	1	1.6	-0.8
7	6	1	4.1	3.9
8	6	1	12.6	-13.2
9	6	1	5.4	-5.5
10	6	1	6.7	6.1
11	6	1	0.9	1.4
12	6	1	0.9	3.5
13	6	1	4.5	-3.4
-14	6	2	7.2	-6.8
-13	6	2	13.0	12.6
-12	6	2	3.4	3.7
-11	6	2	16.8	-16.8
-10	6	2	11.9	11.1
-9	6	2	0.8	1.7
-8	6	2	10.0	-9.8
-7	6	2	1.2	-0.6
-6	6	2	22.1	22.0
-5	6	2	5.4	5.3
-4	6	2	7.1	-7.1
-3	6	2	6.4	6.5
-2	6	2	15.2	-16.2
-1	6	2	7.8	10.2
0	6	2	15.7	18.1
1	6	2	3.7	4.7
2	6	2	14.4	-14.0
3	6	2	1.3	-0.9
4	6	2	7.9	7.6
5	6	2	25.7	25.2
6	6	2	9.5	9.5
7	6	2	23.5	-22.8
8	6	2	15.4	-15.9
9	6	2	21.7	21.9
10	6	2	5.2	5.7
11	6	2	21.0	-20.2
12	6	2	1.0	0.2
-14	6	3	10.9	-10.8
-13	6	3	9.0	-9.6
-12	6	3	4.0	5.4
-11	6	3	11.3	11.5
-10	6	3	4.6	-3.9
-9	6	3	24.1	-23.9
-8	6	3	4.7	-4.9
-7	6	3	19.5	18.8
-6	6	3	27.8	27.4
-5	6	3	26.2	-25.9
-4	6	3	8.5	9.1
-3	6	3	8.3	8.2
-2	6	3	6.3	6.5
-1	6	3	12.0	12.1
0	6	3	16.3	16.3
1	6	3	11.3	-10.8
2	6	3	33.0	-32.4
3	6	3	23.9	23.4
4	6	3	1.6	1.1
5	6	3	11.8	-11.6
6	6	3	1.1	1.1
7	6	3	15.5	15.6
8	6	3	10.1	-10.2
9	6	3	2.8	-2.6
10	6	3	17.2	16.6
11	6	3	12.1	12.0
12	6	3	2.6	-2.7
-14	6	4	7.4	-7.4
-13	6	4	3.7	3.7
-12	6	4	0.9	0.3
-11	6	4	14.6	-14.7
-10	6	4	10.4	-9.7
-9	6	4	0.8	1.9
-8	6	4	13.5	-13.1
-7	6	4	8.1	-8.3
-6	6	4	6.7	7.0
-5	6	4	3.9	3.3
-4	6	4	10.1	-10.2
-3	6	4	21.0	-20.6
-2	6	4	17.8	17.9
-1	6	4	17.2	16.6
0	6	4	26.6	25.2
1	6	4	21.9	-21.5
2	6	4	2.3	-0.1
3	6	4	18.8	18.0
4	6	4	11.4	10.7
5	6	4	4.6	3.2
6	6	4	9.0	-8.9
7	6	4	11.7	-11.0
8	6	4	13.6	-12.9
9	6	4	19.9	19.3
10	6	4	7.6	8.2
-13	6	5	8.6	9.1
-12	6	5	0.9	0.2
-11	6	5	2.0	0.6
-10	6	5	2.0	-3.0
-9	6	5	13.0	-12.5
-8	6	5	8.5	-8.7
-7	6	5	11.6	11.1
-6	6	5	5.2	5.1
-5	6	5	29.3	-28.4
-4	6	5	8.7	-8.2
-3	6	5	15.7	14.8
-2	6	5	6.6	-7.5
-1	6	5	14.3	-14.0
0	6	5	6.6	6.4
1	6	5	5.9	-4.8
2	6	5	8.7	-9.1
3	6	5	1.3	-1.0
4	6	5	18.5	17.5
5	6	5	0.8	-0.1
6	6	5	0.9	3.8
7	6	5	0.9	0.0
8	6	5	1.6	-0.3
9	6	5	6.0	4.7
10	6	5	3.7	4.9
-13	6	6	1.7	-1.1
-12	6	6	4.7	5.2
-11	6	6	4.5	5.8
-10	6	6	4.3	-5.8
-9	6	6	0.9	2.5
-8	6	6	14.7	-14.3
-7	6	6	6.8	6.2
-6	6	6	4.7	4.5
-5	6	6	5.9	-5.9
-4	6	6	7.0	-6.0
-3	6	6	11.6	-11.3
-2	6	6	6.6	6.1
-1	6	6	10.7	11.0
0	6	6	14.1	13.6
1	6	6	27.5	-26.5
2	6	6	12.3	-11.9
3	6	6	21.4	20.4
4	6	6	2.4	-1.7
5	6	6	22.3	-21.8
6	6	6	0.9	-1.9
7	6	6	4.2	3.4
8	6	6	9.5	-9.0
-11	6	7	4.3	-6.6
-10	6	7	1.0	-1.5
-9	6	7	6.8	7.0
-8	6	7	11.9	-11.6
-7	6	7	6.4	6.0
-6	6	7	4.6	4.8
-5	6	7	3.1	-1.7
-4	6	7	27.4	-26.2
-3	6	7	9.6	9.3
-2	6	7	4.7	-3.9
-1	6	7	7.3	-7.0
0	6	7	11.5	11.7
1	6	7	3.5	-2.8
2	6	7	6.8	-6.4
3	6	7	0.9	-2.8
4	6	7	21.3	20.3
5	6	7	2.5	2.9
6	6	7	2.9	-3.8
7	6	7	10.4	-10.9
8	6	7	10.7	-10.5
-11	6	8	7.5	7.7
-10	6	8	3.4	-3.6
-9	6	8	4.6	-2.8
-8	6	8	6.6	6.4
-7	6	8	14.5	14.4
-6	6	8	8.5	8.1
-5	6	8	11.5	-11.3
-4	6	8	12.5	-12.3
-3	6	8	13.2	12.6
-2	6	8	2.2	1.1
-1	6	8	5.9	4.2
0	6	8	5.4	-6.4
1	6	8	8.9	-8.3
2	6	8	18.4	-17.9
3	6	8	13.3	13.2
-1	6	9	5.9	5.7
0	6	9	2.6	0.7
1	6	9	4.1	-5.5
2	6	9	2.2	-1.6
3	6	9	12.1	12.1
-1	6	10	6.2	-6.3
0	6	10	2.1	-3.0

that of α-$\mathrm{Na_2Si_2O_5}$ (Pant & Cruickshank, 1968). α-$\mathrm{Na_2Si_2O_5}$ consists of two-dimensional corrugated layers of tetrahedra, of the formula $[\mathrm{Si_2O_5}]_n^{2n-}$, with channels running parallel to the short axis ($c=4{\cdot}90$ Å). Each layer can be thought of as being built up from symmetry-related metasilicate chains running parallel to the c axis and joined together through the oxygen atoms O(1) on the twofold axes; the angles Si–O(1)–Si joining the metasilicate chains were ~160°. These layers contain rings of six $[\mathrm{SiO_4}]^{4-}$ tetrahedra, formed by the condensation of the metasilicate chains. β-$\mathrm{Na_2Si_2O_5}$ is also a sheet structure consisting of two-dimensional corrugated layers of tetrahedra of the formula $[\mathrm{Si_2O_5}]_n^{2n-}$ extending in the plane normal to **a***, with the channels running along the short axis ($b=4{\cdot}85$ Å). There are, however, two different metasilicate chains in β-$\mathrm{Na_2Si_2O_5}$ which are not symmetry related and are differently oriented in the unit cell. This can be clearly understood from Figs. 1 and 3. One metasilicate chain (hereafter referred to as 'metasilicate chain I') runs along the twofold screw axis at $(\frac{1}{4},y,0)$ whereas the other metasilicate chain (hereafter referred to as 'metasilicate chain II') runs along the twofold screw axis at $(\frac{1}{4},y,\frac{1}{2})$. Each layer is thus built up from alternating metasilicate chains I and II condensed together through the oxygen atoms O(3); these oxygen atoms, however, lie in general positions, and the angles Si–O(3)–Si ~135° as against ~160° in α-$\mathrm{Na_2Si_2O_5}$. These layers also contain rings of six $[\mathrm{SiO_4}]^{4-}$ tetrahedra, formed by the condensation of the metasilicate

Table 4. *Bond lengths and angles*

Bonds		Bonds	
Si(1)–O(1)	1·636 ± 0·003 Å	Si(2)–O(2)	1·643 ± 0·003 Å
Si(1)–O(1′)	1·634	Si(2)–O(2′)	1·637
Si(1)–O(3)	1·643	Si(2)–O(3)	1·640
Si(1)–O(5)	1·576	Si(2)–O(4)	1·584
O(1) –O(1′)	2·609 ± 0·004 Å	O(2) –O(2′)	2·604 ± 0·004 Å
O(1) –O(3)	2·640	O(2) –O(3)	2·624
O(1) –O(5)	2·634	O(2) –O(4)	2·632
O(1′)–O(3)	2·655	O(2′)–O(3)	2·600
O(1′)–O(5)	2·705	O(2′)–O(4)	2·732
O(3) –O(5)	2·641	O(3) –O(4)	2·714

Angles		Angles	
O(1) –Si(1)–O(1′)	105·86 ± 0·15°	O(2) –Si(2)–O(2′)	105·08 ± 0·15°
O(1) –Si(1)–O(3)	107·27	O(2) –Si(2)–O(3)	106·14
O(1) –Si(1)–O(5)	110·14	O(2) –Si(2)–O(4)	109·28
O(1′)–Si(1)–O(3)	108·21	O(2′)–Si(2)–O(3)	104·96
O(1′)–Si(1)–O(5)	114·78	O(2′)–Si(2)–O(4)	115·94
O(3) –Si(1)–O(5)	110·25	O(3) –Si(2)–O(4)	114·60

Si–O–Si angles at the bridging oxygen atoms	
Si(1)–O(1)–Si(1′)	136·50 ± 0·20°
Si(2)–O(2)–Si(2′)	137·11
Si(1)–O(3)–Si(2)	135·11

Bonds		Bonds	
Na(1)–O(2)	2·482 ± 0·003 Å	Na(2)–O(1′)	2·425 ± 0·003 Å
Na(1)–O(4)	2·588	Na(2)–O(3′)	2·495
Na(1)–O(4′)	2·387	Na(2)–O(4)	2·439
Na(1)–O(4″)	2·326	Na(2)–O(5′)	2·570
Na(1)–O(5′)	2·306	Na(2)–O(5″)	2·381
		Na(2)–O(5‴)	2·416

Angles		Angles	
O(2)—Na(1)–O(4)	62·50 ± 0·15°	O(1′) –Na(2)–O(3′)	156·30 ± 0·15°
O(2)—Na(1)–O(4′)	91·55	O(1′) –Na(2)–O(4)	86·09
O(3)—Na(1)–O(4″)	114·29	O(1′) –Na(2)–O(5′)	63·57
O(2)—Na(1)–O(5′)	114·93	O(1′) –Na(2)–O(5″)	93·63
O(4)—Na(1)–O(4′)	153·97	O(1′) –Na(2)–O(5‴)	98·78
O(4)—Na(1)–O(4″)	97·80	O(3′) –Na(2)–O(4)	108·51
O(4)—Na(1)–O(5′)	93·57	O(3′) –Na(2)–O(5′)	96·77
O(4′) –Na(1)–O(4″)	94·88	O(3′) –Na(2)–O(5″)	103·93
O(4′) –Na(1)–O(5′)	95·91	O(3′) –Na(2)–O(5‴)	65·04
O(4″)–Na(1)–O(5′)	129·12	O(4)—Na(2)–O(5′)	90·96
		O(4)—Na(2)–O(5″)	92·63
		O(4)—Na(2)–O(5‴)	172·46
		O(5′) –Na(2)–O(5″)	156·63
		O(5′) –Na(2)–O(5‴)	86·13
		O(5″)–Na(2)–O(5‴)	92·80

chains (Fig. 3). In each tetrahedron one oxygen atom has a silicon coordination number of one, and three oxygen atoms have silicon coordination numbers of two. The various layers are held together in the structure through sodium atoms.

There are striking similarities between the symmetries of the metasilicate chains in Na_2SiO_3 (McDonald & Cruickshank, 1967), α-$Na_2Si_2O_5$ (Pant & Cruickshank, 1968) and in β-$Na_2Si_2O_5$. All metasilicate chains possess either perfect or nearly perfect mirror and glide planes and a twofold screw axis. Whereas in Na_2SiO_3 ($mc2_1$) and α-$Na_2Si_2O_5$ (nearly $cm2_1$) the symmetries are correlated with the crystallographic axes, in β-$Na_2Si_2O_5$, however, the mirror and the glide planes do not lie perpendicular to the crystallographic axes. Metasilicate chain I has a perfect twofold screw axis ($\frac{1}{4},y,0$), a mirror plane almost passing through the silicon atoms Si(1) and Si(1″) and the bridging oxygen atoms O(1) and O(1′) and parallel to the b axis, and a b-glide plane roughly normal to the line passing through Si(1) and Si(1″). Metasilicate chain II has also a perfect twofold screw axis ($\frac{1}{4},y,\frac{1}{2}$), a mirror plane almost passing through the silicon atoms Si(2) and Si(2′) and the bridging oxygen atoms O(2′) and O(2″) and parallel to the b axis, and a b-glide plane roughly normal to the line passing through Si(2) and Si(2′). The angles at the bridging oxygen atoms within each of these metasilicate chains are very close to 135°: $\sim$134° in Na_2SiO_3, $\sim$139° in α-$Na_2Si_2O_5$, and $\sim$137° in both the chains in β-$Na_2Si_2O_5$. In each case the chains run parallel to the short axis of length $\sim$4·9 Å. These observations suggest that the metasilicate chains have reasonably fixed dimensions and that it is the orientations of the individual chains, and the alterations in the coordination of the sodium atoms, which are the important differences between α- and β-$Na_2Si_2O_5$. $Na_2Si_3O_7$ (Jamieson, 1967), which has an order–disorder structure, also has a short axis of 4·9 Å and contains metasilicate chains running parallel to the short axis; these chains are condensed to form $[Si_3O_7]_n^{2n-}$ sheets.

The sodium coordination

There are two independent sodium atoms in the asymmetric unit. Na(1) is surrounded by five oxygen atoms at distances varying between 2·306 and 2·588 Å. Two of these distances (2·306 and 2·326 Å) are marginally smaller than the expected sum of ionic radii, $0·95+1·40=2·35$ Å. This polyhedron of five oxygen atoms is a distorted trigonal bipyramid. Na(2) is coordinated to six oxygen atoms in the form of a distorted octahedron; the Na(2)···O distances vary between 2·381 and 2·570 Å. Table 4 shows the bond lengths and angles at the sodium atoms.

The silicate sheet

The bond lengths and angles in the silicate sheet are given in Table 4, and are in close agreement with those found in α-$Na_2Si_2O_5$ (Pant & Cruickshank, 1968).

The bridging Si–O bonds of mean length 1·639 ± 0·002 Å are appreciably different from the non-bridging bonds of mean length 1·580 ± 0·003 Å; such a difference is expected in terms of $d-p$ π-bonding theory suggested by Cruickshank (1961); this has been discussed in detail by McDonald & Cruickshank (1967) and by Pant & Cruickshank (1967, 1968). In the present

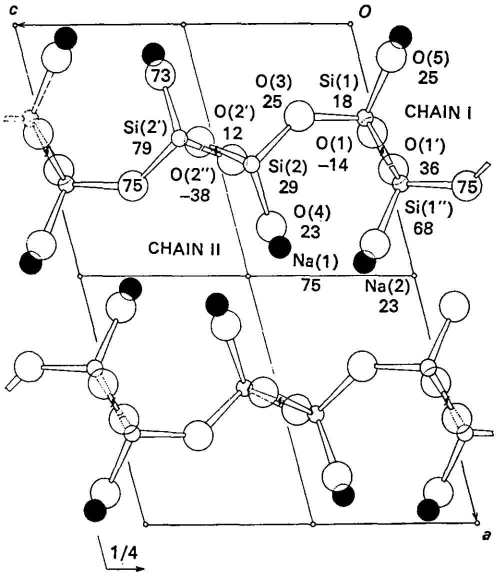

Fig. 1. Projection of the structure along [010]. Numbers give the heights of the atoms in hundredths of the cell edge. Bonds are shown broken where the actual links are between atoms one of which differs by a cell translation from that illustrated.

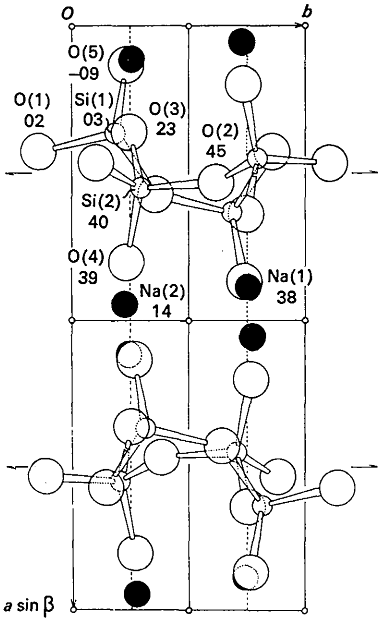

Fig. 2. Projection of the structure along [001]. Numbers give the heights of the atoms in hundredths of the cell edge.

case, the spread of the individual Si–O(bridging) lengths is from 1·634 to 1·643 ± 0·003 Å while the two Si–O(non-bridging) lengths differ by 0·008 Å. These spreads to not appear to be very significant; this is consistent with the fact that the Si–O(bridging)–Si angles at O(1), O(2) and O(3) are almost equal, the actual values being 136·5, 137·1 and 135·1 ± 0·20° respectively. In α-$Na_2Si_2O_5$, where the Si–O(bridging)–Si angles are 138·9 (twice) and 160·0 ± 0·15°, the Si–O-(bridging) lengths are 1·643, 1·638 and 1·609 ± 0·004 Å and the Si–O(non-bridging) is 1·578 ± 0·004 Å. The overall mean Si–O lengths in α- and β-$Na_2Si_2O_5$, which are expected to be equal (Smith & Bailey, 1963), are 1·617 ± 0·002 and 1·624 ± 0·002 Å respectively. The difference, 0·007 Å, appears to be significant and is probably due to the slight differences in the sodium coordination in the two structures.

There are appreciable distortions of the angles at Si: in the Si(1) tetrahedra the largest angle is O(1′)–Si(1)–O(5) = 114·8° and the smallest is O(1)–Si(1)–O(1′) = 105·9°; in the Si(2) tetrahedra the largest and smallest angles are O(2′)–Si(2)–O(4) = 115·9° and O(2′)–Si(2)–O(3) = 105·0° respectively. It may be useful to add that the larger angles always involve the non-bridging oxygen atoms whereas the smaller ones involve the bridging oxygen atoms. This agrees with the results for datolite, $CaBSiO_4(OH)$ (Pant & Cruickshank, 1967) and α-$Na_2Si_2O_5$ (Pant & Cruickshank, 1968); the distortions are attributed to the repulsions between the charged non-bridging oxygen atoms. Plots of the mean length of any pair of bonds forming an angle at Si against the corresponding O···O distance fit the general curve given by McDonald & Cruickshank (1967).

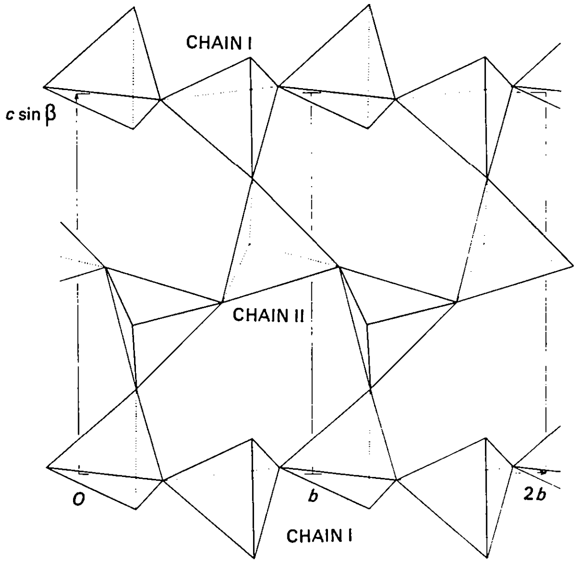

Fig. 3. Projection of the structure along [100] showing sheets formed by condensation of alternate metasilicate chains I and II. For clarity only one sheet is projected. The sheets contain rings of six $[SiO_4]^{4-}$ tetrahedra.

As in datolite and in α-$Na_2Si_2O_5$, the variations in the various bond distances can also be explained on the basis of the Pauling–Zachariasen method of the balancing of valences.*

If we assign bond strengths of 1·00 to tetrahedral Si–O bonds, $\frac{1}{5}$ to an Na(1)···O link and $\frac{1}{6}$ to an Na(2)···O link, we see that O(1) (~2·17), O(2) (2·2) and O(3) (~2·17) are '*overbonded*' and O(4) (~1·77) and O(5) (~1·71) are '*underbonded*'. The strengths are balanced in the actual structure by the lengthening of the two Si–O(1), two Si–O(2) and two Si–O(3) bonds and by the shortening of the Si–O(4) and Si–O(5) bonds and by variations in the various Na···O links. As the Si–O(bridging)–Si angles are all nearly equal, the slight difference in Si–O(4) (1·584 Å) and Si–O(5) (1·576 Å) may be correlated with the slightly stronger bonds from Na to O(4) (O(4) ~1·77 and O(5) ~1·71).

The average, 2·375 Å, of the four nearly equal Na(1)···O distances is significantly less than the average, 2·431 Å, of the five nearly equal Na(2)···O distances. This is consistent with the idea of the balancing of valences.

I am indebted to Professor D. W. J. Cruickshank for suggesting the problem and for his encouragement and continued interest in the work; he also read the manuscript critically and made many useful suggestions. My thanks are also due to Mrs Lois A. Wood (née Beattie) for her help in the collection of the intensity data. The award of the Turner and Newall Research Fellowship by Glasgow University is gratefully acknowledged.

References

Arndt, U. W. & Phillips, D. C. (1961). *Acta Cryst.* **14**, 807.
Cruickshank, D. W. J. (1961). *J. Chem. Soc.* 5486.
Cruickshank, D. W. J. (1964). *Acta Cryst.* **17**, 672.
Grund, A. (1954). *Bull. Soc. franç. Minér. Crist.* **77**, 775.
Hoffmann, W. & Scheele, H. J. (1966). Private communication.
International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.
Jamieson, P. B. (1967). *Nature, Lond.* **214**, 794.
McDonald, W. S. & Cruickshank, D. W. J. (1967). *Acta Cryst.* **22**, 37.
Pant, A. K. & Cruickshank, D. W. J. (1967). *Z. Kristallogr.* **125**, 286.
Pant, A. K. & Cruickshank, D. W. J. (1968). *Acta Cryst.* B**24**, 13.
Smith, J. V. & Bailey, S. W. (1963). *Acta Cryst.* **16**, 801.
Speakman, J. C. (1966). Private communication.
Williamson, J. & Glasser, F. P. (1966). *Physics and Chemistry of Glasses*, **7**, 127.

---

* It may however be pointed out that the two theories ($d-p$ π-bonding theory and the method of balancing of valences) for the Si–O bonds are not exclusive. π-bonding in Si–O bonds may be part of the mechanism whereby valency balance is achieved.