Acta Cryst. (1974). B30, 921

A Refinement of the Crystal Structure of Gypsum $CaSO_4.2H_2O$

BY W. F. COLE AND C. J. LANCUCKI

Division of Building Research, Commonwealth Scientific and Industrial Research Organization, Melbourne, Australia

(*Received* 3 *September* 1973; *accepted* 12 *October* 1973)

With the use of three-dimensional X-ray diffraction data the crystal structure of gypsum has been refined by least-squares methods. Initial parameters used were those found by Atoji & Rundle [*J. Chem. Phys.* (1958), **29**, 1306] from neutron-diffraction data. Significant changes were made in the x and z parameters of the oxygen atoms of the sulphate ion and the oxygen atom of the water molecule. Bond lengths around the sulphate ion show equal sulphur-to-oxygen distances of mean value 1·459 Å, but one pair of oxygen-to-oxygen distances of 2·323 Å and the corresponding pair of oxygen–sulphur–oxygen bond angles of 105·5° are significantly different from the others, which have mean values of 2·411 Å and 111·5°, respectively. As a result the symmetry of the sulphate ion is lowered from a tetrahedron to a sphenoid. The new oxygen parameters indicate that there are two distinctly different hydrogen-bond lengths of 2·816 and 2·896 Å rather than one only of mean value 2·820 Å as found by Atoji & Rundle. A re-working of the data of Atoji & Rundle produced refinement beyond that which they reported and clearly indicated the two different hydrogen-bond lengths (difference $0{\cdot}065 \pm 0{\cdot}018$ Å) shown by the X-ray work. The re-refining of the neutron data also confirmed the lowering of the symmetry of the sulphate ion, although this did not show up in Atoji & Rundle's refinement. On the basis of the new parameters for the hydrogen atoms from the re-worked neutron data and the parameters for the water oxygen found from the X-ray data, the two O–H distances in the water molecule are calculated as 0·962 and 0·944 Å but the difference is not statistically significant. The details of the refined structure are in agreement with conclusions drawn by other workers from spectroscopic data. The anisotropic thermal parameters are discussed with respect to the structure.

Introduction

The crystal structure of gypsum, $CaSO_4.2H_2O$ was determined by Wooster (1936) from two-dimensional X-ray diffraction data with Fourier methods, which gave an R index of 13·6% on observed data. It was further refined by Atoji & Rundle (1958) from $0kl$, $hk0$ and $hk\bar{h}$ neutron-diffraction data by means of both Fourier and least-squares refinement methods to an R index of 15·5% on observed data. The neutron-diffraction work permitted the fixing of the positions of the hydrogen atoms and indicated small but significant changes in the positions of all of the oxygen atoms from those established by Wooster. Denne & Jones (1969) re-examined the neutron-diffraction data of Atoji & Rundle by an occupation-factor approach and found that the distribution of the hydrogen atoms was centrosymmetric.

By modern standards the crystal structure of gypsum is only poorly refined and the present study was undertaken to refine the structure of this important industrial and building material by using three-dimensional X-ray data collected on a modern semi-automatic counter diffractometer. The study has shown (Cole & Lancucki, 1972*a*, *b*) that the symmetry of the SO_4 ion in gypsum is lower than tetrahedral, confirming the earlier deductions of Rousset & Lochet (1945) from Raman, and Hass & Sutherland (1956) from infrared spectra. It has also been found (Cole & Lancucki, 1973) that the water molecule is asymmetrical, confirming the deductions of Seidl, Knop & Falk (1969) from infrared spectra of partially deuterated gypsum.

Experimental

The gypsum used was from Monte San Derato Bologna, Italy. It had the following composition: CaO 32·5, SO_3 46·4, H_2O 21·0, SiO_2+ other insolubles 0·01, $R_2O_3<0{\cdot}01$, $MgO<0{\cdot}005$, $Na_2O<0{\cdot}01$, SrO 0·025, $BaO<0{\cdot}005$, $CO_2<0{\cdot}01$, and Cl 0·01%. It was shaped into a sphere of about 0·3 mm diameter, and ellipsoids of 0·3 mm on the minor axis and 0·37 mm on the major axis as described by Cole & Lancucki (1965). This involved spinning cut cubes of the crystals to ellipsoids by circulating kerosine in a Bond cell, and hand shaping the ellipsoids to spheres, followed by etching in running water. The crystals used in the analysis showed some surface streaking for many low-angle reflexions.

The unit-cell dimensions were determined by the θ method, as described by Weiss, Cochran & Cole (1948), with a Unicam single-crystal goniometer. The values of a^*, b^*, c^* and β^* were obtained directly from $h00$, $0k0$ and $00l$ reflexions by extrapolating the regression equations on $\cos^2\theta$ to $\theta=90°$. The new unit-cell parameters and those found by Atoji & Rundle are reported below together with other relevant crystallographic data relating to the Bragg cell (Bragg, 1937).

	This study	Atoji & Rundle
Space group	$I2/a$	$I2/a$
a	5·670 ± 0·002 Å	5·68 ± 0·008 Å
b	15·201 ± 0·002	15·18 ± 0·009
c	6·533 ± 0·002	6·52 ± 0·008
β	118° 36′ ± 4′	118° 23′ ± 20′
Cell volume	494·37 Å^3	494·59 Å^3
Cell contents	4($CaSO_4.2H_2O$)	4($CaSO_4.2H_2O$).

The spherically shaped crystal was rotated about the b axis and the ellipsoidal crystal was rotated about the a axis and initially Weissenberg photographs were taken with Mo $K\alpha$ radiation and multiple-film packs with Sn foil (0·025 mm thick) as an absorber. The intensities of the reflexions were estimated by eye with a multiple-film scale prepared under the same conditions as for the films. Of these data use was made of only the b-axis intensities and these were corrected for both Lorentz–polarization and absorption. The latter correction was small since $\mu r = 0{\cdot}54$. Data from the same crystals rotated about the same axes were subsequently collected on a computer-controlled Buerger–Supper equi-inclination X-ray diffractometer as described by Freeman, Guss, Nockolds, Page & Webster (1970). A constant slow scan speed of 0·05° sec^{-1} was used with filtered Mo $K\alpha$ radiation, although some data about the b axis were collected with radiation monochromatized with a plane graphite crystal. For each level of reciprocal space the varying indices were allowed to take both positive and negative values so that reflexions with a multiplicity of two were measured twice and those with a multiplicity of four were measured four times.

The counter-diffractometer data were processed in the normal manner for application of Lorentz–polarization factors and calculations of I_{hkl}, $\sigma(I_{hkl})$, F_{hkl} and $\sigma(F_{hkl})$. Because of streaking, many low-angle reflexions suffered a background imbalance, *i.e.* they did not satisfy the test $|B_1 - B_2| < (BI) . \sigma(B) + (IC)$ where $\sigma(B) = \sqrt{(B_1 + B_2)}$, $BI = 10{\cdot}0$ and $IC = 0{\cdot}01$. In these instances the lowest background value was assumed for both B_1 and B_2 and the data processed in the normal way. In the merging of the two sets of data from a and b axes all levels were scaled manually to the $2kl$ level on the basis of the sums of the F values of common reflexions, thereby yielding finally only one scale factor (Sq) between observed and calculated F values. This was necessitated by the large amount of data being handled compared with the memory limitations of available computer programs. 2193 non-equivalent reflexions were measured as present and a further 2158 were recorded as being too weak to be observed ($I < I\text{min} = \text{RIM} . \sigma(B)/\sqrt{2}$ where RIM = 3·5). For these I was set equal to 0·33Imin and $\sigma(I)$ was set equal to 0·29Imin.

Structure analysis

A least-squares refinement was made on the counter-diffractometer data using the Busing, Martin & Levy

Table 1. *Isotropic temperature coefficients* (B), *fractional atomic parameters* (x/a, y/b, z/c) *from X-ray film and counter data of the present work and the neutron counter data of Atoji & Rundle* (1958), *as refined by them, and as re-refined in the present work*

(Numbers in parentheses are standard deviations in the least significant digits.)

	B (Å^2)				x/a			
	X-ray		Neutron		X-ray		Neutron	
	Film	Counter	Counter Atoji & Rundle	Counter Re-refined	Film	Counter	Counter Atoji & Rundle	Counter Re-refined
Ca	0·88 (5)	0·51 (1)	1·66	1·72 (25)	0·5000 (0)	0·5000 (0)	0·5000 (0)	0·5000 (0)
S	0·66 (6)	0·63 (1)	1·84	1·40 (36)	0·0000 (0)	0·0000 (0)	0·0000 (0)	0·0000 (0)
O(1)	1·49 (7)	1·24 (2)	2·13	1·67 (17)	0·9623 (10)	0·9607 (3)	0·9665 (11)	0·9642 (16)
O(11)	1·41 (6)	1·18 (2)	2·18	1·94 (18)	0·7586 (10)	0·7592 (2)	0·7602 (13)	0·7602 (17)
O(*W*)	2·19 (10)	1·90 (3)	2·41	2·50 (20)	0·3784 (12)	0·3778 (3)	0·3797 (15)	0·3779 (22)
H(1)			3·82	4·05 (33)			0·2360 (40)	0·2447 (55)
H(2)			3·56	3·98 (35)			0·4100 (50)	0·3936 (38)

	y/b				z/c			
	X-ray		Neutron		X-ray		Neutron	
	Film	Counter	Counter Atoji & Rundle	Counter Re-refined	Film	Counter	Counter Atoji & Rundle	Counter Re-refined
Ca	0·0787 (6)	0·0797 (0)	0·0800 (7)	0·0783 (8)	0·2500 (0)	0·2500 (0)	0·2500 (0)	0·2500 (0)
S	0·0784 (7)	0·0772 (0)	0·0782 (10)	0·0778 (12)	0·7500 (0)	0·7500 (0)	0·7500 (0)	0·7500 (0)
O(1)	0·1314 (5)	0·1312 (1)	0·1352 (8)	0·1327 (4)	0·5515 (9)	0·5518 (2)	0·5506 (14)	0·5495 (16)
O(11)	0·0216 (5)	0·0227 (1)	0·0220 (3)	0·0221 (4)	0·6674 (8)	0·6661 (2)	0·6735 (14)	0·6674 (16)
O(*W*)	0·1824 (6)	0·1820 (1)	0·1831 (6)	0·1826 (6)	0·4597 (11)	0·4588 (2)	0·4500 (17)	0·4553 (20)
H(1)			0·1650 (15)	0·1601 (10)			0·4890 (40)	0·4974 (50)
H(2)			0·2460 (15)	0·2430 (12)			0·4880 (40)	0·4896 (29)

(1962) computer program *ORFLS* with isotropic temperature factors and the initial atomic parameters and temperature factors found by Atoji & Rundle (1958). The *f* curves for S^{6+}, O, and H were taken from Mirkin (1964), Ca^{2+} from *International Tables for X-ray Crystallography* (1962) and O^{2-} from the example on quartz featured in *ORFLS*. With structure factors having unit weights (w) and hkl reflexions for k between 0 and 3, an overall disagreement index $R=\sqrt{\sum w(F_o-\mathrm{Sq}F_c)^2}/\sqrt{\sum wF_o^2}=0{\cdot}089$ was achieved, excluding hydrogen atoms, after four cycles of refinement for 365 non-equivalent reflexions. With anisotropic temperature factors, $R=0{\cdot}074$. For the full data set of 2193 non-equivalent reflexions refined with the use of a weighting function $w=[\sigma(F_o)]^{-2}$ an R value $=0{\cdot}055$ was obtained with isotropic temperature factors after three cycles of refinement; with anisotropic temperature factors, $R=0{\cdot}048$ after three cycles of refinement. When hydrogen atoms were introduced into the isotropic refinements with the parameters found by Atoji & Rundle, R became 0·059. Attempts to refine the hydrogen parameters with the full data set were unsuccessful, the temperature factors assuming unrealistic values. Some refinement of the positional parameters for hydrogen was achieved by using reflexions with $\sin\theta<0{\cdot}4$ and keeping the thermal parameters constant, as recommended by Huber-Buser (1971). The final parameters gave values of bond lengths within the water molecule considerably different from acceptable values. Difference Fourier maps based on $\Delta F=(F_o-\mathrm{Sq}F_c)$ and excluding hydrogen atoms from the calculated structure factors were computed in the form of projected sections in the vicinity of the hydrogen atoms for both sets of data. Weak electron density maxima were found in the vicinity of the expected values and the positional parameters deduced from the peaks [for H(1) $x/a=0{\cdot}2500$, $y/b=0{\cdot}1463$, $z/c=0{\cdot}4680$; for H(2) $x/a=0{\cdot}3917$, $y/b=0{\cdot}2166$, $z/c=0{\cdot}5033$] were in closer agreement with the least-squares refinement than with the values found by Atoji & Rundle from neutron-diffraction data. The hydrogen positions are discussed further in a later paragraph.

The positional and thermal parameters for O(1), O(11), O(W), Ca and S are given in Table 1 with their standard deviations for the isotropic refinement of the 2193 non-equivalent reflexions. They are compared with the previous values found by Atoji & Rundle (1958). The thermal parameters arising from the anisotropic refinement of the same 2193 reflexions are given in Table 2.

Table 2. *Refined anisotropic thermal parameters* ($\times 10^4$)

The anisotropic temperature factor has the form

$$T=\exp\left[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2kl\beta_{23}+2hl\beta_{13})\right].$$

(Numbers in parentheses are standard deviations in the least significant digit.)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ca	69 (1)	9 (0)	59 (1)	0	23 (1)	0
S	52 (2)	7 (0)	46 (1)	0	13 (1)	0
O(1)	115 (4)	15 (0)	89 (3)	−3 (1)	42 (3)	4 (1)
O(11)	81 (4)	14 (0)	92 (3)	−8 (1)	15 (3)	4 (1)
O(W)	225 (6)	16 (1)	204 (5)	3 (2)	149 (5)	−7 (1)

Because the positional parameters for O(1), O(11) and O(W) differed significantly from those found by Atoji & Rundle using neutron methods, the film data collected from the rotation about the b axis were also subjected to a least-squares refinement. In this case each level of reciprocal space was scaled independently to the calculated structure factors and the scale factors and atomic parameters were refined with isotropic temperature factors to an R value of 0·011 with a unit weighting function. The parameters (Table 1) showed similar differences from the neutron-diffraction data reported by Atoji & Rundle as occurred with the X-ray counter diffraction data.

In view of these differences a re-refinement was made of the neutron-diffraction data with the computer program *ORFLS* using isotropic temperature factors and initial atomic parameters and temperature factors as found by Atoji & Rundle. The scattering lengths of 0·49, 0·31, 0·58 and −0·38 in Fermi units (10^{-11} mm) for Ca, S, O, and H, respectively were the same as those used by Atoji & Rundle. In four cycles of refinement R was lowered from 0·154 to 0·092, to give atomic parameters and temperature factors nearly identical with those in Table 1. The values in Table 1 relate to refinements made with the more recent scattering lengths of 0·490, 0·280, 0·577, and −0·378 for Ca, S, O, and H, respectively. These gave a minimum R value of 0·091. The new scattering lengths mainly influenced the temperature factors, particularly that for S. The atomic parameters for O(1), O(11) and O(W) have approached those found from the X-ray work and H(1) and H(2) are in positions considerably different from those found by Atoji & Rundle. Attempts to refine the neutron-diffraction data anisotropically were only partially successful. Atoms O(1), Ca and S were not positive-definite after the first cycle and if these were left isotropic, atom H(1) became not positive-definite after the second cycle of refinement. The R index was lowered to a minimum value of 0·081.

The observed and calculated X-ray structure factors based on the anisotropic X-ray refinement parameters for Ca, S, O(1), O(11) and O(W) and the isotropic neutron re-refined parameters for hydrogen are given in Table 3. The observed and calculated neutron structure factors based on the re-refined isotropic parameters of Atoji & Rundle's observed data are given in Table 4.

Discussion

In the crystal structure of gypsum (Wooster, 1936; Atoji & Rundle, 1958) there are two crystallographically distinct sulphate oxygen atoms [O(1) and O(11)]. The new refinements have produced significant changes in the x and z parameters (Table 1) of the oxygen atoms O(1) and O(11) and the oxygen atom O(W) of the water molecule from those given in previous studies. As a result a clearer picture has emerged of the details of the sulphate ion and of the hydrogen-bond distances in gypsum. Bond lengths and angles calculated by means of *ORFFE* (Busing, Martin & Levy, 1964) for the present X-ray study are given in Table 5 and are compared with those obtained by Atoji & Rundle from their neutron-diffraction study. The most striking differences lie in the O(1)–O(11) and O(1′)–O(11′) bond lengths of 2·323 Å and the related O(1)–S–O(11) and O(1′)–S–O(11′) bond angles of 105·5°. The four other oxygen–oxygen distances around the sulphate

Table 3. *Observed and calculated X-ray structure factors for* $CaSO_4.2H_2O$ (× 10)

Unobserved reflexions are indicated by an asterisk.

H	L	FO	SQ FC
	K = 0		
2	0	893	885
4	0	838	792
6	0	345	337
8	0	385	-371
10	0	133	120
12	0	112	118
0	2	439	-354
2	2	438	-442
2	-2	389	-384
4	2	623	-587
4	-2	957	-978
6	2	239	-225
6	-2	620	-590
8	2	273	-265
8	-2	361	-351
10	2	123	-120
10	-2	248	-241
12	2	87	-84
12	-2	152	-147
0	4	795	754
2	4	648	635
2	-4	1043	1102
4	4	437	442
4	-4	314	282
6	4	383	376
6	-4	334	353
8	4	222	216
8	-4	234	224
10	4	120	129
10	-4	251	267
12	4	88	96
12	-4	96	93
14	-4	66	74
0	6	412	-401
2	6	542	-527
2	-6	687	-668
4	6	193	-188
4	-6	524	-510
6	6	217	-211
6	-6	726	-708
8	6	75	-73
8	-6	320	-311
10	-6	240	-234
12	-6	113	-110
14	-6	100	-98
0	8	228	221
2	8	273	265
2	-8	385	374
4	8	177	172
4	-8	327	318
6	8	186	181
6	-8	247	249
8	8	74	45
8	-8	222	232
10	-8	221	242
12	-8	134	173
14	-8	63	95
0	10	333	329
2	10	218	-211
2	-10	284	-276
4	10	165	-162
4	-10	325	-314
6	10	86	-63
6	-10	258	-244
8	-10	294	-266
10	-10	113	-101
12	-10	74	-94
14	-10	31	-54
0	12	154	154
2	12	75	71
2	-12	124	136
4	12	70	58
4	-12	254	249
6	-12	188	185
8	-12	193	191
10	-12	120	137
12	-12	122	133
14	-12	44	41
0	14	124	-114
2	-14	106	-100
4	-14	111	-103
6	-14	92	-90
8	-14	112	-100
10	-14	90	-87
12	-14	38	-61
4	-16	84	80
6	-16	105	110
8	-16	80	79
10	-16	61	49
	K = 1		
1	0*	22	65
3	0	104	78
5	0	83	78
7	0	65	-82
9	0*	39	-19
11	0*	57	-55
13	0*	29	-34
0	1*	9	-37
2	1	469	-476
2	-1	609	-545
4	1	62	-56
4	-1	225	-212
6	1*	36	-44
6	-1*	25	23
8	1	46	-49
8	-1*	33	-13
10	1*	48	-46
10	-1*	37	-5
12	1*	38	-8
12	-1*	38	8
1	2	620	662
1	-2	317	-248
3	2	86	75
3	-2	516	504
5	2	176	175
5	-2	99	-100
7	2*	36	-11
7	-2	86	75
9	2*	62	46
9	-2	89	-89
11	2*	43	-6
11	-2	41	41
13	-2*	34	-28
0	3	69	77
2	3*	24	-8
2	-3	593	-602
4	3	68	52
4	-3	378	-364
6	3*	34	16
6	-3*	78	9
8	3*	39	-21
8	-3*	27	9
10	3*	39	-8
10	-3*	33	-15
12	-3*	37	7
14	-3*	31	9
1	4	149	-139
1	-4	93	38
3	4	191	193
3	-4	373	-366
5	4	39	-63
5	-4	55	42
7	4	60	63
7	-4	136	-136
9	4	52	-47
9	-4*	46	-50
11	4*	29	-16
11	-4*	83	-57
13	-4*	32	-9
0	5	52	-38
2	5	53	56
2	-5	173	-168
4	5*	44	35
4	-5	196	-173
6	5*	38	14
6	-5*	24	18
8	5*	48	-26
8	-5	94	112
10	5*	35	-26
10	-5*	28	33
12	-5*	32	22
14	-5*	32	18
1	6*	54	36
1	-6	58	-48
3	6*	47	40
3	-6	122	-129
5	6*	49	64
5	-6*	40	11
7	6*	40	20
7	-6*	33	-34
9	6*	31	32
9	-6*	29	22
11	-6*	38	-11
13	-6*	28	40
0	7*	38	34
2	7	56	66
2	-7	31	-17
4	7	67	72
4	-7	138	-106
6	7*	48	22
6	-7*	43	4
8	7*	36	9
8	-7*	79	75
10	-7*	37	36
12	-7*	28	-11
14	-7*	34	2
1	8*	37	13
1	-8	145	-162
3	8	70	-76
3	-8*	55	-37
5	8*	37	15
5	-8	151	140
7	8*	34	19
7	-8*	37	43
9	-8	78	-69
11	-8*	37	11
13	-8*	35	-21
0	9*	36	23
2	9*	38	17
2	-9	55	60
4	9*	40	14
4	-9*	41	21
6	9*	23	8
6	-9*	33	27
8	-9	92	81
10	-9	72	63
12	-9*	35	5
14	-9*	33	-3
1	10*	42	-43
1	-10*	40	32
3	10*	54	34
3	-10	57	56
5	10*	34	-21
5	-10	51	44
7	10*	37	28
9	10	77	62
11	-10*	41	19
13	-10*	39	29
0	11*	41	-7
2	11*	38	19
2	-11*	45	75
4	11*	34	11
4	-11*	39	23
6	11*	38	-16
8	-11*	39	15
10	-11*	39	14
12	-11*	39	12
14	11*	32	-32
1	12*	37	-29
1	-12*	42	-26
3	12*	33	-17
3	-12*	55	-35
5	-12*	37	-7
7	12*	48	-6
9	-12*	33	21
11	-12*	45	-15
13	-12*	40	7
0	13*	36	-21
2	13*	32	12
2	-13*	38	41
4	-13*	41	33
6	-13*	39	13
8	-13*	40	4
10	-13*	40	18
12	-13*	39	20
1	14*	31	37
1	-14*	35	5
3	-14*	37	40
5	-14*	38	9
7	-14*	38	49
9	-14*	42	19
11	-14*	44	27
13	14*	30	19
0	15*	29	11
2	-15*	33	9
4	-15*	35	-3
6	-15*	35	13
8	-15*	39	23
10	-15*	38	9
12	-15*	42	-17
3	-16*	31	27
5	16*	34	11
7	-16*	33	0
9	-16*	33	2
11	-16*	30	-30
	K = 2		
2	0	95	55
4	0	630	651
6	0	154	143
8	0	214	210
10	0	70	64
12	0	84	91
1	1	1083	1141
3	1	602	600
3	-1	707	720
5	1	259	251
5	-1	667	-693
7	1	204	196
7	-1	425	-418
9	1	144	147
9	-1	256	249
11	1	103	95
11	-1	124	-118
13	-1*	60	-61
0	2	991	1101
2	2	210	203
2	-2	564	511
4	2	336	343
4	-2	332	-316
6	2	157	-146
6	-2	190	-199
8	2	198	-197
8	-2	208	-205
10	2*	45	-45
10	-2	125	-127
12	2	69	-48
12	-2*	63	-60
1	3	184	-188
1	-3	505	504
3	3	443	-465
3	3	480	491
5	3	348	355
5	-3	403	405
7	3	280	-281
7	3	202	213
9	3	158	-155
9	-3	235	248
11	3	95	-105
11	-3	150	166
13	-3	74	144
0	4	205	188
2	4	411	418
2	-4	427	422
4	4	199	205
4	-4	289	294
6	4	160	156
6	-4	427	433
8	4	95	94
8	-4	120	114
10	4	67	68
10	-4	145	154
12	-4*	35	51
14	-4*	54	53
1	5	602	628
1	-5	747	-795
3	5	405	420
3	-5	519	-523
5	5	235	242
5	-5	429	-423
7	5	173	177
7	-5	350	-358
9	5	78	84
9	-5	217	-216
11	-5	97	-105
13	-5	42	-66
0	6	148	-147
2	6	280	-287
2	-6	509	-515
4	6	98	-96
4	-6	163	-158
6	6	174	-173
6	-6	259	-247
8	6*	38	-43
8	-6	103	-109
10	-6	172	183
12	-6*	40	-61
14	6*	31	-58
1	7	219	-233
1	-7	239	246
3	7	185	-189
3	-7	396	425
5	7	149	-148
5	-7	428	439
7	7	101	-100
7	7	330	338
9	7	69	-41
9	-7	212	221
11	-7	165	196
0	8	173	175
2	8	205	205
2	-8	223	220
4	8	88	80
4	8	169	173
6	8	102	103
6	-8	253	241
8	8*	21	8
8	-8	184	173
10	-8	87	87
12	8*	39	68
14	-8*	23	48
1	9	259	261
1	9	271	264
3	9	175	181
3	-9	273	-260
5	9	153	153
5	-9	148	-144
7	9	80	60
7	9	183	-180
9	-9	164	160
11	9	111	-119
0	10	141	-143
2	10	70	81
2	-10	178	-122
4	10	85	85
4	-10	221	-213
6	10*	43	30
6	10	111	-98
8	-10	134	129
10	10	82	-77
12	-10	86	95
14	-10*	22	28
1	11	150	-157
1	-11	182	187
3	11	92	96
3	-11	227	235
5	11	66	-44
5	-11	263	259
7	11	246	227
9	-11	146	138
11	11	87	95
0	12	120	117
2	12*	34	42
2	12	86	68
4	12	66	46
4	12	124	121
6	12	76	71
8	-12	127	123
10	-12*	40	57
12	-12*	46	49
14	-12*	21	14
1	13	82	68
1	13	87	-90
3	13	66	34
3	-13	95	96
5	-13	99	104
7	-13	81	-94
9	-13	107	-117
11	-13	91	99
0	14	63	63
2	-14	61	-55
4	-14	86	77
6	14	73	-72
8	-14*	50	-56
10	14*	31	-47
12	14*	40	44
1	-15	91	71
3	15	89	81
5	-15	82	87
7	-15	79	75
9	-15*	54	59
11	15*	33	37
4	16*	42	29
6	-16*	47	50
8	-16*	30	37
10	-16*	28	36
	K = 3		
1	0*	24	-52
3	0	391	-362
5	0	96	62
7	0*	30	9
9	0	71	69
11	0*	36	-5
13	0*	27	21
0	1	133	123
2	1	181	193
2	-1	267	294
4	1	55	-41
4	-1	111	-108
6	1	132	-140
6	-1*	26	-23
8	1*	35	34
8	-1*	46	-24
10	1*	37	-56
10	-1*	36	33
12	1*	38	-10
12	1*	46	16
1	2	112	100
1	2	204	-218
3	2	432	-420
3	-2	170	156
5	2*	32	21
5	-2	268	258
7	2	52	47
7	2	133	147
9	2*	38	26
9	-2*	32	9
11	2*	36	9
11	-2*	51	60
13	-2*	39	-19
0	3	333	355
2	3	159	153
2	-3	257	-262
4	3*	35	7
4	-3	162	-158
6	3*	40	15
6	-3	103	-89
8	3*	38	-3
8	3	57	67
10	3*	37	13
10	3*	32	7
12	-3*	38	-14
14	-3*	27	33
1	4	257	248
1	-4	443	423
3	4*	31	-23
3	-4*	23	6
5	4	128	-126
5	-4	74	60
7	4*	37	38
7	-4*	24	2
9	4*	59	-49
9	-4*	121	112
11	4*	27	18
11	-4*	32	-3
13	-4*	32	3
0	5	49	37
2	5	77	81
2	-5	116	107
4	5*	32	-39
4	-5	112	104
6	5*	38	6
6	5*	31	-18
8	5*	38	36
8	5*	35	62
10	5*	33	-41
10	-5*	32	31
12	5*	54	55
14	-5*	43	26
1	6*	43	-33
1	-6	144	143
3	6	72	61
3	-6	183	167
5	6*	40	10
5	6	52	50
7	6*	38	38
7	6	44	41
9	6*	30	2
9	-6	72	75
11	-6*	29	3
13	6*	28	1
0	7	122	128
2	7*	42	43
2	-7*	49	31
4	7	76	79
4	-7*	28	33
6	7*	40	18
6	-7*	30	36
8	7*	35	19
8	-7*	36	-27
10	-7*	30	4
12	7*	31	-7
14	7*	31	2
1	8	70	74
1	8*	36	17
3	8*	39	31
3	-8	234	218
5	8*	43	30
5	8*	34	-25
7	8*	32	24
7	-8*	31	18
9	8*	22	37
11	-8*	44	40
13	-8*	28	32
0	9*	39	17
2	9*	36	7
2	9*	32	34
4	9*	37	7
4	9	68	66
6	9*	32	3
6	9	86	91
8	-9	56	50
10	-9*	34	43
12	-9*	36	23
14	-9*	31	15
1	10*	42	-14
1	-10	64	69
3	10*	60	50
3	10*	45	23
5	10*	32	-17
5	10*	64	47
7	10	77	75
9	-10*	36	25
11	-10*	35	8
13	-10*	38	6
0	11*	42	15
2	11*	37	30
2	-11*	37	24
4	11*	32	6
4	11*	36	19
6	11*	38	4
8	-11*	38	5
10	-11*	37	34
12	11*	39	14
14	11*	29	-34
1	12*	34	17
1	-12*	41	14
3	12*	31	15
3	12*	40	6
5	12*	42	13
7	12*	44	-49
9	-12*	39	29
11	-12*	37	14
13	12*	32	10
2	13*	31	-21
2	-13	46	44
4	13*	37	30
6	-13*	61	44
8	-13*	39	21
10	13*	45	12
12	13*	40	14
1	14*	29	17
1	-14*	32	-20
3	-14*	35	6
5	14*	42	27
7	-14*	38	8
9	14*	39	39
11	14*	36	3
13	-14*	28	5
2	15*	32	5
4	-15*	33	-13
6	15*	33	14
8	15*	37	21
10	-15*	36	-13
12	15*	29	-43
3	16*	29	-19
5	16*	31	2
7	16*	31	-10
9	16*	30	6
11	16*	28	-5
	K = 4		
0	0	590	564
2	0	1015	-996
4	0	191	170
6	0	266	-266
8	0	52	-39
10	0	76	79
12	0	31	9
1	1	401	371
1	1	1282	-1311
3	1	594	591
3	1	840	825
5	1	466	495
5	-1	468	-484
7	1	338	340
7	-1	244	245
9	1	182	187
9	-1	244	263
11	1	114	115
11	-1	129	-133
13	-1	64	73
0	2	188	-187
2	2	194	189
2	-2	328	318
4	2*	36	0
4	2	215	245
6	2	138	148
6	2	255	266
8	2*	46	35
8	-2	175	180
10	2	88	97
10	-2	120	118
12	2*	27	10
12	-2	71	78
1	3	757	766
1	-3	947	993
3	3	583	-582
3	3	323	320
5	3	253	256
5	-3	592	601
7	3	257	269
7	-3	376	398
9	3	127	132
9	3	274	285
11	3	95	93
11	3	106	120
13	3	802	109
0	4	424	-435
2	4	243	244
2	4	132	-114
4	4	250	265
4	-4	229	220
6	4	154	157
6	-4*	30	18
8	4	100	102
8	-4	119	119
10	4*	49	57
10	4*	29	15
12	4*	44	-69
14	4*	28	6
1	5	309	331
1	5	473	506
3	5	415	415
3	5	636	-650
5	5	245	254
5	5	588	-560
7	5	188	200
7	5	265	-283
9	5	99	95
9	-5	218	232
11	-5	160	187
13	-5	75	-107
0	6	309	337
2	6	74	69
2	-6	171	190
4	6	136	142
4	-6	408	430
6	6*	13	1
6	6	198	200
8	6*	51	56
8	6	227	218
10	6	61	64
12	6*	44	69
14	-6*	29	16
1	7	376	397
1	-7	424	439
3	7	230	-246
3	7	382	410
5	7	195	199
5	7	240	254
7	7	118	127
7	-7	336	357
9	7	231	244
11	-7	142	160
13	7	50	75
0	8	92	97
2	8	42	46
2	-8	52	44
4	8	102	107
4	-8	86	86
6	8	57	-43
6	-8	51	70
8	8	60	50
8	-8	93	95
10	-8	82	101
12	8*	31	67
14	8*	30	52
1	9	253	264
1	9	210	217
3	9	152	160
3	9	379	344
5	9	143	142
5	9	322	325
7	9	62	36
7	-9	296	291
9	9	134	-141
11	-9	132	-149
13	9	68	94
0	10	119	119
2	10	121	123
2	10	179	178
4	10	49	59
4	-10	109	101
6	10*	36	31
6	10	144	136
8	10*	56	39
10	10	61	54
12	-10*	31	5
14	10*	79	26
1	11	151	160
1	-11	176	184
3	11	110	-104
3	-11	217	271
5	11	85	61
5	-11	162	169
7	11	162	168
9	11	186	173
11	-11	118	129
13	-11	53	72
0	12*	78	12
2	12	66	44
2	-12	74	-84
4	12*	27	9
4	-12	68	-58
6	12	122	115
8	12	68	-72
10	-12	89	-89
12	12	50	45
14	12*	31	-24
1	13	99	95
1	13	120	-127
3	13	75	44
3	13	114	-123
5	-13	154	156
7	13	146	137
9	13	102	110
11	-13	48	63
13	13	53	59
0	14	44	36
2	14	46	41
4	14*	45	25
6	14*	42	24
8	14*	39	24
10	14*	36	20
12	14*	31	24
1	-15	81	59
3	15	74	78
5	15	99	94
7	-15	66	72
9	15	77	81
11	15	64	68
4	16	48	-46
6	-16*	33	39
8	16	48	44
10	-16*	35	-14
	K = 5		
1	0	391	-379
3	0	66	74
5	0	117	110
7	0*	62	-14
9	0	44	54
11	0*	37	15
0	1	138	104
2	1	58	-56
2	1	698	679
4	1	166	158
4	1	109	99
6	1	94	-32
6	-1	140	104
8	1	88	80
8	-1*	41	12
10	1*	38	13
10	1*	62	45
12	1*	30	11
12	-1*	38	3
1	2	137	-137
1	2	890	-909
3	2	148	142
3	2	135	118
5	2*	32	4
5	-2*	35	-21
7	2	98	-100
7	-2	56	67
9	2*	36	9
9	2	77	75
11	2*	37	10
11	-2*	36	27
13	-2*	33	16
0	3	88	-64
2	3*	25	5
2	-3	350	325
4	3*	38	-31
4	-3	192	185
6	3*	33	41
6	-3	42	40
8	3*	42	27
8	-3*	31	-40
10	3*	38	40
10	-3*	34	2
12	-3*	38	-31
1	4	96	-91
1	4*	36	37
3	4	120	121
3	-4	86	53
5	4	83	-75
5	-4	293	292
7	4*	44	40
7	4	61	73
9	4*	37	21
9	4*	47	49
11	-4*	35	20
13	4*	32	27
0	5	195	-165
2	5*	29	-14
2	5	73	61
4	5	102	-102
4	5	253	243
6	5*	35	10
6	5	40	-73
8	5*	48	14
8	5*	30	-4
10	5*	34	-7
10	-5*	58	49
12	5*	35	14
14	5*	31	-6
1	6*	45	10
1	6	67	-46
3	6*	45	37
3	6	91	78
5	6*	49	-42
5	-6	108	116
7	6	45	53
7	6*	39	35
9	6*	32	12
9	6*	30	11
11	6	53	58
13	6*	35	3
0	7*	34	29
2	7	105	98
2	7	81	74
4	7*	38	0
4	7*	29	-20
6	7*	36	39
6	7*	28	4
8	7*	38	14
8	7	122	114
10	7*	38	37
12	7*	32	26
14	7*	32	4
1	8	113	123
1	8*	65	11
3	8*	39	3
3	8	86	87
5	8*	50	35
5	8*	34	24
7	8*	33	16
7	8	156	145
9	8*	32	8
11	-8*	34	13
13	8	38	6
0	9*	34	-10
2	9*	37	34
2	9*	34	19
4	9*	39	40
4	-9	61	22
6	9*	33	11
6	9*	32	13
8	-9	57	-60
10	-9*	36	-16
12	9*	34	1
14	9*	32	16
1	10*	49	21
1	10*	62	36
3	10*	39	18
3	-10	61	-59
5	10*	33	-25
5	-10*	38	-10
7	-10*	41	-16
9	-10*	35	-17
11	10	57	-56
13	-10*	40	-29
0	11*	36	4
2	11*	38	21
2	-11	83	74
4	11*	33	-22
4	-11*	38	21
6	11	78	53
8	11*	40	-17
10	11*	48	-42
12	11*	36	10
14	11*	31	-11
1	12	49	31
1	12*	57	40
3	12*	33	12
3	12*	40	12
5	12*	48	12
7	12*	45	10
9	12*	38	30
11	12*	38	12
13	-12*	40	-17
0	13*	36	22
2	13*	32	10
2	-13*	33	7
4	13*	40	27
6	13*	44	14
8	-13*	42	2
10	13*	39	12
12	13*	37	9
1	14*	31	17
1	14*	34	24
3	-14*	36	-9
5	-14*	42	-49
7	-14*	45	-17
9	-14*	37	-24
11	14*	38	-9
13	-14*	30	-39
2	-15*	34	-10
4	15*	37	-15
6	-15*	36	0
8	15*	40	17
10	-15*	37	10
12	15*	38	-16
3	-16*	30	18
5	-16*	33	2
7	-16*	33	-6
9	16*	32	18
	K = 6		
0	0	215	155
2	0	974	965
4	0	555	-560
6	0	491	477
8	0	223	-218
10	0	197	-204
12	0	84	-109
1	1	172	157
1	-1*	32	10
3	1	308	304
3	-1	349	337
5	1	93	108
5	-1	54	-62
7	1	127	120
7	-1*	26	30
9	1*	57	76
9	-1*	55	-51
11	1*	34	38
11	1*	78	7
13	-1*	23	31
0	2	1024	1076
2	2	742	724
2	-2	1040	1027
4	2	396	389
4	-2	482	462
6	2	415	412
6	-2	403	392
8	2	213	206
8	2	326	325
10	2	160	163
10	-2	195	195
12	2	107	120
1	3*	20	7
1	-3	605	609
3	3	225	278
3	-3	338	314
5	3*	78	2
5	3	335	378
7	3	58	61
7	-3*	23	1
9	3*	41	33
9	-3	98	83
11	3*	26	-16
11	3*	27	5
13	-3*	24	22
0	4	609	614
2	4	512	509
2	-4	458	-445
4	4	397	400
4	4	736	-749
6	4	240	-236
6	-4	494	-482
8	4	167	-166
8	-4	361	355
10	4	89	121
10	4	163	-167
12	-4	142	159
14	4*	33	-38
1	5*	37	-50
1	5	54	49
3	5	42	39
3	5	146	129
5	5*	32	19
5	-5*	22	-35
7	5	64	69
7	5	86	104
9	5*	33	12
9	5	108	-103
11	5*	25	54
13	-5*	23	-31
0	6	517	522
2	6	275	278
2	6	472	478
4	6	326	332
4	-6	533	519
6	6	178	178
6	6	242	243
8	6	145	150
8	-6	314	320
10	6	201	215
12	6	132	152
14	-6	57	62
1	7	156	155
1	7	74	61
3	7	86	98
3	-7	169	158
5	7	79	82
5	-7	73	39
7	7*	38	30
7	7	46	32
9	7*	49	61
11	7*	25	23
13	-7*	22	4
0	8	384	-375
2	8	274	-264
2	-8	331	327
4	8	221	215
4	8	364	-358
6	8	89	-111
6	8	382	-375
8	8	89	-59
8	8	288	-275
10	-8	159	183
12	-8	90	-106
14	-8	62	-86
1	9	52	62
1	-9*	29	-25
3	9*	42	-34
3	-9	142	-143
5	9*	37	28
5	-9*	37	40
7	9*	22	-22
7	-9	140	132
9	9	69	-71
11	-9	59	66
13	9*	22	2
0	10	182	183
2	10	178	176
2	-10	281	279
4	10	120	119
4	10	273	260
6	10	58	55
6	-10	265	255
8	-10	167	163
10	10	191	192
12	10	97	116
14	10	66	63
1	11*	36	39
1	11*	32	9
3	11*	35	-17
3	11*	33	0
5	11*	41	-28
5	11*	32	-4
7	-11*	32	17
9	11*	40	0
11	11*	35	12
13	11*	30	28
0	12	136	133
2	12	137	-128
2	12	194	-187
4	12	70	-36
4	12	143	-141
6	-12	180	181
8	-12	167	-151
10	-12	123	-124
12	-12	42	-66
14	-12*	32	36
1	13*	25	24
1	-13	64	-56
3	-13	70	-46
5	-13*	57	-58
7	-13*	34	13
9	-13*	35	-29
11	-13*	29	-49
13	-13*	24	-2
0	14	89	89
2	14	120	107
4	-14	136	124
6	-14	140	125
8	-14	106	101
10	-14	85	79
12	-14	69	72
1	15*	22	5
3	-15*	25	-5
5	-15*	25	21
7	-15*	25	16
9	15*	25	34
11	15*	27	11
4	-16	72	-54
6	-16	59	-65
8	16	60	-75
10	16	52	40
	K = 7		
1	0	503	494
3	0	157	140
5	0	90	70
7	0*	43	-8
9	0*	37	21
11	0*	48	-19
0	1	222	218
2	1	346	-323
2	1	31	31
4	1	204	220
4	-1	137	-127
6	1*	45	32
6	1	157	150
8	1	96	99
8	1*	33	-25
10	1*	37	-17
10	-1*	42	2
12	1*	34	41
12	-1*	36	-25
1	2	286	281
1	-2*	24	-36
3	2*	31	20
3	2	110	92
5	2	95	81
5	2	139	-162
7	2*	47	-18
7	-2*	31	-27
9	2*	39	-8
9	-2	112	-95
11	2*	39	-13
11	-2*	40	-21
13	2*	30	37
0	3	327	-310
2	3	150	-152
2	3	45	46
4	3*	33	-12
4	-3*	30	-28
6	3*	41	29
6	3	140	158
8	3*	37	26
8	-3	65	49
10	3*	36	10
10	3*	34	22
12	-3*	36	-18
1	4*	28	11
1	4	190	160
3	4	158	145
3	4	87	90
5	4*	48	40
5	-4	36	46
7	4	85	88
7	4	82	83
9	4*	38	6
9	-4*	32	5
11	4*	37	1
13	-4*	30	8
0	5	250	237
2	5	45	43
2	-5	128	-126
4	5*	47	19
4	5*	34	26
6	5*	62	56
6	-5	84	-88
8	5*	37	-7
8	5	87	77
10	5*	32	34
10	5	66	-78
12	5*	35	13
14	5*	32	36
1	6	42	-41
1	-6	78	-73
3	6*	34	10
3	6	132	130
5	6*	41	21
5	6	121	97
7	6*	37	0
7	6	122	-116
9	6*	32	5
9	-6*	32	26
11	-6*	54	-31
13	-6*	30	33
0	7	64	48
2	7	112	-110
2	-7	156	141
4	7*	42	16
4	-7	103	-111
6	7*	56	-61
6	-7	39	25
8	7*	34	13
8	-7*	32	22
10	7*	34	29
12	-7*	33	-24
14	-7*	32	6
1	8	44	10
1	8	88	86
3	8*	38	14
3	-8*	32	-1
5	8*	42	38
5	-8	83	-64
7	8*	34	5
7	8*	32	26
9	8*	34	3
11	8*	45	65
13	8*	40	23
0	9	38	-2
2	9	65	15
2	-9*	35	0
4	9*	41	-3
4	-9*	75	-90
6	9*	33	4
6	-9	80	78
8	-9*	35	-31
10	-9*	38	5
12	-9*	36	-39
14	9*	32	12
1	10	74	76
1	-10*	56	-46
3	10*	38	-19
3	-10	78	68
5	10*	33	-21
5	10*	50	13
7	-10*	36	-27
9	10*	38	1
11	10*	40	6
13	-10*	37	4
0	11	84	-39
2	11*	36	10
2	-11*	39	11
4	11*	34	-26
4	-11*	40	22
6	-11	75	-61
8	11*	37	31
10	-11*	38	13
12	-11*	37	22
14	11*	32	-27
1	12*	26	-54
1	12*	43	5
3	-12*	33	-11
3	-12*	38	12
5	12	69	47
7	-12*	38	36
9	-12*	47	46
11	-12*	52	23
13	-12*	37	27
0	13*	35	35
2	13*	32	3
2	13*	38	4
4	13*	42	40
6	-13*	54	26
8	-13*	39	31
10	-13*	38	13
12	-13*	37	0
1	14*	30	36
1	-14*	34	18
3	-14*	36	7
5	14*	42	3
7	-14*	38	16
9	-14*	48	7
11	-14*	40	5
2	15*	32	3
4	-15*	35	5
6	15*	36	7
8	-15*	34	2
10	15*	35	19
3	-16*	30	42
5	16*	32	30
7	-16*	33	16
9	-16*	32	26
	K = 8		
0	0	460	421
2	0	420	403
4	0	119	119
6	0	294	295
8	0	206	208
10	0	152	150
12	0	70	-84
1	1	602	596
1	1	446	435
3	1	373	-376
3	-1	584	588
5	1	391	381
5	-1	236	216
7	1	230	230
7	-1	269	280
9	1	160	-153
9	-1	117	120
11	1	76	-90
11	1	126	138
13	-1*	21	21
0	2	474	466
2	2	778	730
2	-2	550	517
4	2	435	450
4	-2	509	511
6	2	303	291
6	-2	314	293
8	2	132	127
8	-2	145	129
10	2	105	107
10	2	88	79
12	-2	66	74
1	3	699	709
1	-3	363	346
3	3	253	240
3	3	669	-654
5	3	319	319
5	-3	273	274
7	3	110	110
7	-3	367	-366
9	3	148	142
9	-3	132	129
11	3*	34	22
11	-3	128	-136
13	3*	25	54
0	4	467	-472
2	4	164	167
2	-4	555	569
4	4	170	-170
4	-4	456	-460
6	4	137	-142
6	4	250	262
8	4	98	96
8	4	311	323
10	4	69	-73
10	4	174	-179
12	4	97	111
14	4*	33	-17
1	5	322	-341
1	-5	263	278
3	5	194	-198
3	5	423	438
5	5	231	237
5	5	318	310
7	5	103	-98
7	-5	263	256
9	5	113	115
9	-5	182	189
11	-5	132	135
13	5	66	83
0	6	325	313
2	6	267	262
2	-6	110	99
4	6	246	248
4	-6	244	237
6	6	144	136
6	-6	238	234
8	6	116	116
8	-6	180	182
10	-6	80	86
12	-6	74	97
14	-6*	46	53
1	7	242	242
1	-7	348	358
3	7	275	279
3	-7	279	227
5	7	129	136
5	-7	284	-293
7	7	103	101
7	7	174	173
9	7	192	197
9	-7	70	76
11	-7	57	84
0	8	270	269
2	8	165	176
2	-8	356	357
4	8	145	149
4	-8	367	-351
6	8	75	-71
6	-8	230	-211
8	8	156	144
10	-8	149	-145
12	8	67	74
14	8*	32	30
1	9	130	-119
1	9	255	253
3	9	165	-164
3	9	192	183
5	9	63	-58
5	-9	302	293
7	9	78	-51
7	-9	159	154
9	-9	179	170
11	9	74	88
13	-9	62	81
0	10	117	106
2	10	104	100
2	-10	126	132
4	10	72	66
4	-10	102	102
6	10	56	30
6	10	187	195
8	-10	167	174
10	10	175	133
12	10	56	69
14	-10	51	51
1	11	89	93
1	-11	147	146
3	11	102	99
3	-11	120	-126
5	11	50	25
5	11	133	138
7	-11	129	-128
9	-11	123	-120
11	11	76	88
13	-11*	48	61
0	12	110	100
2	12	111	101
2	12	154	134
4	12	137	120
6	12	124	107
8	12*	43	47
10	12*	47	58
12	12	46	55
1	13	90	89
1	13	88	83
3	-13	125	118
5	13	92	96
7	-13	127	112
9	13*	53	61
11	-13*	40	64
13	13*	24	24
0	14	42	57
2	-14	83	77
4	14	86	88
6	14	78	91
8	-14	101	101
10	14	79	74
12	14*	38	34
1	-15*	22	-20
3	-15	81	77
5	15	57	53
7	-15	80	73
9	-15*	51	-58
11	15	52	-47
4	16*	22	23
6	16	32	-33
8	16*	35	32
10	16*	21	11
	K = 9		
1	0	227	222
3	0	52	-60
5	0*	30	27
7	0	52	-15
9	0*	52	6
11	0*	35	25
0	1	494	490
2	1*	26	13
2	1	118	103
4	1	75	81
4	-1	262	258
6	1	153	-148
6	-1	84	-100
8	1*	43	49
8	-1	131	121
10	1*	42	34
10	-1*	34	5
12	1*	30	61
12	-1*	39	20
1	2	196	199
1	2	180	182
3	2*	30	8
3	2	80	72
5	2*	43	54
5	-2	97	-93
7	2*	41	28
7	-2*	29	28
9	2*	35	11
9	2*	38	9
11	2*	32	3
11	-2*	34	16
13	-2*	19	17
0	3	206	185
2	3	84	87
2	-3*	22	4
4	3	70	-84
4	3*	22	20
6	3	60	-52
6	3	56	27
8	3	53	70
8	-3*	32	-32
10	3*	35	-18
10	3	65	72
12	3*	33	23
1	4	45	42
1	4	135	114
3	4*	29	7
3	4*	45	56
5	4*	31	5
5	4	98	118
7	4*	35	31
7	4	74	66
9	4*	34	-8
9	4*	31	-7
11	-4*	34	9
13	4*	28	16
0	5	131	118
2	5	199	202
2	-5	282	-263
4	5*	32	-4
4	-5	97	103
6	5	65	68
6	-5	128	-127
8	5*	35	-7
8	-5*	29	12
10	5*	21	51
10	-5*	32	41
12	5*	40	39
14	-5*	28	-46
1	6	51	6
1	-6*	64	48
3	6*	33	8
3	-6	44	7
5	6*	44	33
5	6	54	50
7	6*	34	13
7	6	74	63
9	6*	30	5
9	6*	30	28
11	-6*	32	1
13	-6*	28	7
0	7	149	125
2	7*	35	-43
2	-7*	39	55
4	7*	44	52
4	-7	43	45
6	7*	35	39
6	7	146	146
8	7*	32	12
8	7*	36	17
10	7	67	69
12	7*	31	40
14	-7*	29	45
1	8*	64	-25
1	-8	74	-53
3	8*	37	-27
3	-8*	31	6
5	8*	35	8
5	-8	83	-76
7	8*	31	-5
7	-8	51	44
9	-8*	32	-12
11	8*	33	23
13	8*	78	2
0	9	84	57
2	9	46	50
2	9*	34	30
4	9*	43	36
4	-9*	31	18
6	9	37	29
6	-9	73	66
8	9*	33	21
10	-9*	35	-8
12	-9*	33	-18
14	-9*	29	-17
1	10*	50	-24
1	10*	55	-50
3	10*	36	5
3	10*	34	4
5	10*	30	1
5	10*	34	6
7	10*	33	17
9	10*	34	8
11	10*	35	29
13	10*	35	11
0	11*	98	65
2	11*	34	1
2	11*	37	14
4	11*	30	15
4	-11	107	104
6	11	58	55
8	11	84	73
10	11*	36	12
12	11*	34	26
14	11*	28	25
1	12*	33	17
1	12*	45	13
3	12*	30	-7
3	12*	37	8
5	-12*	35	12
7	12*	44	14
9	12*	35	5
11	12*	35	10
13	12*	34	14
0	13*	33	17
2	13*	29	13
2	13*	35	17
4	-13*	36	-18
6	13*	35	14
8	13*	37	22
10	-13*	36	-29
12	13*	33	25
1	14*	28	-8
1	-14*	31	-1
3	14*	34	13
5	-14*	34	10
7	-14*	36	13
9	14*	34	1
11	14*	34	14
2	15	33	31
4	-15*	32	10
6	15*	32	19
8	15*	35	6
10	15*	33	1
5	16*	29	12
7	16	42	7
9	16*	29	4
	K = 10		
0	0	261	195
2	0*	32	57
4	0	63	58
6	0	71	68
8	0	75	81
10	0	63	46
12	0*	27	26
1	1	938	920
1	1	340	324
3	1	591	-590
3	1	449	478
5	1	462	-444
5	1	312	292
7	1	308	-305
7	-1	373	361
9	1	230	223
9	1	147	136
11	1	116	128
11	-1	141	156
0	2	183	162
2	2	207	-194
2	2	121	114
4	2	181	-172
4	-2	170	-149
6	2	63	-66
6	2	135	96
8	2	54	54
8	2	54	-21
10	2*	32	-20
10	2*	43	-31
12	2*	28	14
1	3	692	685
1	3	596	596
3	3	353	343
3	-3	1033	-1034
5	3	433	420
5	3	466	433
7	3	147	141
7	3	409	-386
9	3	158	152
9	-3	179	179
11	3*	33	16
11	-3	168	178
13	3	58	64
0	4	108	108
2	4	53	52
2	-4	240	229
4	4*	30	40
4	4	132	109
6	4*	50	40
6	-4	124	104
8	4*	34	33
8	-4	74	77
10	4*	30	15
10	4	72	74
12	4*	28	23
1	5	465	446
1	-5	370	355
3	5	233	218
3	-5	352	343
5	5	267	262
5	-5	313	314
7	5	148	138
7	5	404	396
9	5	143	155
9	5	268	280
11	-5	151	162
13	-5	82	117
0	6	59	64
2	6	98	-102
2	6	40	-37
4	6*	34	-59
4	6*	25	-31
6	6	69	-54
6	6	107	88
8	6*	33	-31
8	-6	44	55
10	6*	29	30
12	6*	33	30
14	6*	24	18
1	7	341	322
1	7	435	416
3	7	340	330
3	7	401	-370
5	7	207	198
5	-7	464	423
7	7	143	130
7	-7	202	-167
9	7	182	-177
11	-7	95	101
13	-7	81	108
0	8	90	79
2	8	68	63
2	-8	127	113
4	8	52	40
4	8	116	122
6	8*	78	29
6	8*	33	51
8	8	45	41
10	-8*	30	30
12	8*	27	31
14	-8*	24	2
1	9	159	-153
1	-9	348	338
3	9	173	-176
3	-9	255	249
5	9	75	67
5	9	325	320
7	-9	241	239
9	-9	289	276
11	9	119	128
13	9	83	92
0	10	57	42
2	10*	35	21
2	10*	33	-29
4	10*	78	-21
4	10*	37	-43
6	-10*	49	48
8	10	89	77
10	10*	40	38
12	10*	29	27
14	-10*	24	-12
1	11	138	127
1	11	172	159
3	11	145	130
3	11	142	-138
5	11	194	181
7	11	154	153
9	11	101	-108
11	11	84	98
13	11	64	90
0	12	57	36
2	12*	28	27
2	12*	35	30
4	12*	35	40
6	12*	37	28
8	-12*	34	11
10	12*	33	13
12	-12*	30	19
1	13	121	118
1	13	135	122
3	13	189	170
5	13	147	129
7	13	148	134
9	13	109	96
11	13	94	92
13	13*	23	14
0	14*	36	-17
2	-14*	38	-29
4	14*	39	28
6	14*	37	-32
8	14*	34	27
10	14	50	-29
12	14*	27	6
1	15*	35	16
3	-15	80	-84
5	15	72	-69
7	15	102	-100
9	15	70	-80
11	15	62	44
4	16*	23	4
6	16*	25	13
8	16*	25	9
	K = 11		
1	0	434	426
3	0	89	81
5	0*	26	-10
7	0	50	59
9	0*	39	-12
11	0*	30	4
0	1	241	220
2	1	156	-168
2	1	111	109
4	1	90	88
4	-1	140	-144
6	1	98	-100
6	-1*	40	30
8	1*	44	51
8	-1*	64	57
10	1*	39	41
10	-1*	33	7
12	1*	25	54
12	1*	29	6
1	2	128	123
1	2	238	229
3	2*	37	24
3	2	65	77
5	2*	28	-8
5	-2	152	173
7	2*	34	1
7	-2	82	84
9	2*	32	16
9	2*	36	48
11	2*	35	30
13	2*	25	45
0	3*	28	43
2	3*	35	40
2	3*	25	28
4	3*	29	-19
4	-3	74	-85
6	3*	33	8
6	3*	31	3
8	3*	35	-38
8	-3*	31	-28
10	3*	27	12
10	-3*	32	35
12	-3*	29	7
1	4	82	-99
1	-4	203	-193
3	4	50	-62
3	-4	50	29
5	4	98	-97
5	4	115	120
7	4	61	-69
7	4	66	60
9	4*	31	-32
9	-4*	29	-33
11	4*	29	6
13	-4*	26	-8
0	5	69	65
2	5	107	104
2	5	144	-140
4	5*	45	-35
4	-5	55	77
6	5*	43	43
6	-5	99	-99
8	5*	34	-18
8	-5*	39	59
10	-5*	27	38
12	5*	29	27
1	6	89	82
1	-6*	68	58
3	6*	35	37
3	6*	37	59
5	6*	34	4
5	6	189	194
7	6*	34	-8
7	-6	129	130
9	6*	26	25
9	-6*	39	39
11	-6*	28	1
13	-6*	26	14
0	7	91	87
2	7*	35	-40
2	7*	36	56
4	7*	41	55
4	7	88	-55
6	7*	45	36
6	-7*	40	44
8	7*	31	3
8	-7*	31	7
10	-7*	27	42
12	-7*	29	8
14	-7*	28	32
1	8	66	25
1	-8*	44	10
3	8*	46	-15
3	-8	40	21
5	8*	34	30
5	-8*	30	18
7	8*	27	-20
7	-8*	48	33
9	-8*	30	-41
11	-8*	40	-62
13	8*	27	-25
0	9*	32	17
2	9*	41	27
2	-9*	33	7
4	9*	31	7
4	9*	32	-4
6	9*	27	16
6	9*	40	21
8	9*	33	-15
10	-9*	61	23
12	9*	29	-11
14	9*	26	-16
1	10	71	70
1	10	98	71
3	10	53	39
3	10*	42	41
5	10*	27	20
5	10*	47	24
7	10	60	57
9	10*	32	7
11	-10*	30	-15
13	10*	26	-14
0	11*	33	-35
2	11*	31	19
2	11*	35	15
4	11*	27	-22
4	11*	35	58
6	11*	35	-9
8	11*	44	39
10	-11*	28	-6
12	11*	38	25
1	12*	30	-1
1	-12*	43	1
3	12*	26	12
3	12*	38	-36
5	12	49	47
7	12*	36	-39
9	12*	32	24
11	12*	38	-45
13	12*	38	-37
0	13*	29	16
2	13*	26	14
2	-13*	32	18
4	-13*	35	-9
6	13*	36	14
8	13*	36	-14
10	13*	28	-3
12	-13*	29	-6
1	14*	28	7
3	14*	31	6
5	14*	31	-9
7	14*	36	0
9	14*	32	13
11	-14*	28	2
2	15*	37	28
4	15*	29	-1
6	-15*	36	10
8	15*	33	8
10	15*	26	12
5	-16	42	40
7	-16*	27	-30
9	16*	25	24
	K = 12		
0	0	507	484
2	0	434	434
4	0	327	318
6	0	317	326
8	0	227	234
10	0	153	170
12	0	75	72
1	1	177	-171
1	-1	250	243
3	1	53	-55
3	1	448	463
5	1	164	165
5	-1	87	85
7	1	67	-77
7	1	147	155
9	1*	47	-39
9	1*	45	40
11	1*	33	-40
11	1	75	81
0	2	583	-594
2	2	610	625
2	-2	595	-598
4	2	471	-468
4	2	470	472
6	2	302	307
6	2	358	-336
8	2	190	-185
8	2	180	180
10	2	126	-111
10	-2	128	-138
12	2	60	81
1	3	361	374
1	-3*	21	17
3	3	54	37
3	3	133	131
5	3	152	162
5	3	55	-10
7	3*	41	36
7	-3	218	-221
9	3	96	96
9	-3*	48	44
11	3	58	74
13	3*	23	12
0	4	449	458
2	4	298	301
2	-4	522	533
4	4	244	239
4	-4	443	465
6	4	172	173
6	4	373	385
8	4	137	129
8	-4	289	315
10	4	74	54
10	4	187	205
12	-4	98	115
1	5	191	188
1	-5	120	116
3	5	112	105
3	5	309	300
5	5	151	148
5	5	170	176
7	5*	32	19
7	-5	66	58
9	5	62	-57
9	5*	42	41
11	5*	41	45
13	5*	24	40
0	6	337	-333
2	6	319	306
2	-6	283	-269
4	6	264	-261
4	-6	301	-306
6	6	179	-174
6	-6	262	-259
8	6	121	-134
8	-6	202	-208
10	-8	117	-135
12	-8	96	-120
1	7	83	63
1	-7	192	-191
3	7	81	70
3	-7	68	-52
5	7*	34	33
5	-7	126	-129
7	7*	21	41
7	-7	94	-92
9	-7	188	-180
11	-7*	27	-29
13	-7*	29	-48
0	8	301	309
2	8	218	220
2	-8	356	355
4	8	185	183
4	-8	385	369
6	8	99	98
6	-8	252	254
8	-8	275	220
10	-8	133	147
12	-8	115	96
14	-8	64	22
1	9	48	-36
1	-9	107	109
3	9	108	-109
3	-9*	31	22
5	9*	26	-22
5	-9	148	149
7	-9*	37	27
9	-9*	37	45
11	-9*	28	18
13	-9*	30	53
0	10	151	-147
2	10	119	-120
2	10	148	160
4	10	98	-91
4	10	172	-181
6	-10	190	-206
8	-10	172	-188
10	-10	117	138
12	10	80	-98
1	11	44	37
1	-11	91	-92
3	11	54	48
3	-11	88	-83
5	-11	110	-70
7	-11*	47	-52
9	11	74	64
11	-11	55	-47
13	-11*	30	-6
0	12	136	127
2	12	112	117
2	-12	160	151
4	-12	151	142
6	-12	133	125
8	12	92	87
10	12	69	86
12	-12	45	68
1	13	44	-34
1	13*	27	14
3	13	46	40
5	13*	34	26
7	-13	62	68
9	13*	40	23
11	-13*	28	35
0	14	63	-43
2	14	96	96
4	14	99	98
6	-14	111	115
8	14	100	101
10	14	83	91
12	-14	50	-30
3	15	36	-39
5	-15*	25	-21
7	-15*	26	-29
9	15*	25	-10
6	16	55	79
6	-16*	33	24
	K = 13		
1	0*	18	1
3	0	121	-102
5	0*	49	-65
7	0*	34	-14
9	0*	34	-8
11	0*	32	-13
0	1	50	-5
2	1	256	-254
2	1	174	176
4	1	120	119
4	1*	40	53
6	1*	32	-24
6	-1	202	198
8	1	68	65
8	-1*	34	40
10	1*	34	-36
10	-1*	34	35
12	1*	31	1
1	2*	22	-22
1	-2	146	139
3	2*	35	-29
3	2*	29	-24
5	2*	33	23
5	2*	41	5
7	2*	35	43
7	-2*	38	18
9	2*	35	6
9	-2*	43	62
11	2*	29	42
11	2*	32	13
13	-2*	28	52
0	3	113	-109
2	3*	33	-33
2	-3*	24	18
4	3*	32	41
4	-3*	31	-36
6	3	73	86
6	-3	88	76
8	3*	36	21
8	3*	32	-29
10	3*	32	44
10	3*	33	-16
12	-3*	32	-49
1	4*	28	-26
1	-4*	24	0
3	4	99	-92
3	-4*	31	47
5	4*	36	-18
5	-4	101	-85
7	4*	37	-35
7	-4*	36	5
9	4*	33	-9
9	-4*	33	9
11	-4*	32	7
13	-4*	31	24
0	5	275	274
2	5	56	-54
2	5	66	17
4	5	101	-94
4	5	120	111
6	5*	36	6
6	-5*	29	17
8	5*	41	-28
8	-5	102	91
10	-5*	33	-49
12	5*	32	9
1	6*	30	-4
1	-6*	45	63
3	6*	45	9
3	-6	74	80
5	6*	38	14
5	-6*	31	25
7	6*	36	12
7	-6*	37	6
9	-6*	41	47
11	-6*	32	32

Table 3 (*cont.*)

H	L	FO	SQFC
13	-6*	31	1
0	7*	30	13
2	7	74	-70
2	-7	75	47
4	7*	39	37
4	-7	139	-142
6	7*	36	-34
6	-7	48	-46
8	7*	29	28
8	-7	55	-58
10	-7*	33	-36
12	-7*	41	-45
1	8	61	-39
1	-8*	33	5
3	8*	37	-11
3	-8*	33	14
5	8*	39	-22
5	-8*	43	8
7	8*	29	-36
7	-8*	56	-56
9	-8*	33	-10
11	-8*	32	-12
13	-8*	31	2
0	9	74	43
2	9*	44	-37
2	-9*	36	36
4	9*	34	-41
4	-9	74	47
6	9*	29	-20
6	-9*	41	-22
8	-9*	34	-13
10	-9*	42	25
12	-9*	33	-15
1	10*	35	37
1	-10*	42	17
3	10*	34	12
3	-10	76	62
5	10*	29	40
5	-10*	47	30
7	-10*	38	19
9	-10*	42	-4
11	-10*	44	28
13	-10*	30	5
0	11*	34	3
2	11	41	35
2	-11	52	-88
4	11*	29	-10
4	-11*	38	-34
6	-11	107	-98
8	-11*	36	-6
10	-11*	35	-21
12	-11*	34	3
1	12*	33	-12
1	-12*	35	-9
3	12*	28	-35
3	-12*	37	-13
5	-12*	39	-5
7	-12*	37	29
9	-12*	35	-31
11	-12*	32	-18
13	-12*	28	-30
0	13*	28	18
2	-13*	34	9
4	-13*	38	-17
6	-13*	37	2
8	-13*	38	5
10	-13*	41	37
12	-13*	30	18
1	-14*	30	13
3	-14*	32	9
5	-14*	34	19
7	-14*	33	7
9	-14*	32	2
11	-14*	30	13
2	-15*	28	-14
4	-15*	31	-16
6	-15*	31	-6
8	-15*	32	-8
10	-15*	36	13
7	-16*	28	-32
K = 14			
0	0	387	314
2	0	526	529
4	0	409	387
6	0	300	291
8	0	128	121
10	0	110	118
12	0*	48	24
1	1	213	207
1	-1	337	-340
3	1	319	315
3	-1	158	-143
5	1	243	246
5	-1	208	-208
7	1	183	193
7	-1	50	-55
9	1	123	121
9	-1	133	-132
11	1*	48	66
11	-1*	45	-41
0	2	448	-446
2	2	292	-304
2	-2	487	-485
4	2	192	-190
4	-2	289	-280
6	2	220	-225
6	-2	291	-283
8	2	148	-140
8	-2	218	-232
10	2	95	-103
10	-2	155	-161
12	-2	61	-87
1	3	242	-248
1	-3	509	519
3	3	319	-319
3	-3	227	234
5	3	88	-84
5	-3	374	358
7	3	137	-137
7	-3	158	156
9	3*	31	-31
9	-3	158	160
11	-3*	40	44
13	-3*	32	34
0	4	340	343
2	4	387	385
2	-4	247	245
4	4	313	298
4	-4	361	360
6	4	183	173
6	-4	288	274
8	4	125	128
8	-4	184	171
10	4	67	38
10	-4	86	96
12	-4	63	93
1	5	100	93
1	5	170	-174
3	5	188	179
3	-5	158	-170
5	5*	65	87
5	-5	218	-216
7	5	119	119
7	-5	144	-165
9	5	53	33
9	-5	117	-126
11	-5	103	-110
13	-5	38	-59
0	6	340	-334
2	6	178	-178
2	-6	396	-370
4	6	189	-188
4	-6	380	-364
6	6	90	-102
6	-6	196	-186
8	6	87	-92
8	-6	217	-223
10	-6	132	-141
12	-6	84	-96
1	7	735	-736
1	-7	218	199
3	7	138	-144
3	-7	261	247
5	7	142	-123
5	-7	105	94
7	7	72	-74
7	-7	189	151
9	-7	45	58
11	-7	78	81
13	-7*	22	24
0	8	203	206
2	8	168	154
2	-8	141	148
4	8	132	133
4	-8	195	193
6	8	83	88
6	-8	214	217
8	-8	200	198
10	-8	86	102
12	-8	68	86
1	9	133	137
1	9	63	85
3	9*	33	39
3	-9	190	-198
5	9*	62	72
5	-9	136	-147
7	-9	191	-198
9	-9	98	-93
11	-9	99	-89
13	-9*	22	-45
0	10	156	-147
2	10	141	-128
2	-10	204	-192
4	10	97	-97
4	-10	204	-189
6	-10	139	-141
8	-10	81	-88
10	-10	92	-102
12	-10*	46	-69
1	11	90	-83
1	-11*	57	68
3	11	42	-56
3	11	99	85
5	-11*	57	65
7	-11	56	56
9	11*	50	67
11	-11	60	56
13	-11*	38	36
0	12	93	80
2	12	81	76
2	-12	127	117
4	-12	101	98
6	12	140	134
8	-12	129	119
10	-12	95	96
12	-12*	28	47
1	13*	40	39
1	-13	90	-84
3	-13	69	-70
5	13	107	-97
7	13	88	-64
9	-13	80	67
11	-13	79	-27
0	14	58	24
2	-14	72	-74
4	-14	69	-64
6	-14	73	-70
8	-14*	38	-47
10	-14	51	-55
3	15*	22	14
5	-15*	55	52
7	15*	24	39
9	-15*	42	40
K = 15			
1	0	174	176
3	0	101	106
5	0	78	40
7	0*	39	15
9	0*	36	15
11	0*	34	-3
0	1	82	68
2	1	36	-44
2	-1	287	266
4	1*	35	30
4	-1*	28	33
6	1	122	-119
6	-1*	48	47
8	1*	35	20
8	-1*	33	14
10	1*	35	-40
10	-1*	43	47
12	-1*	30	30
1	2*	45	21
1	-2	115	114
3	2	99	92
3	-2	53	-87
5	2*	36	-2
5	-2*	32	-18
7	2*	48	32
7	-2	75	-87
9	2*	36	22
9	-2*	36	-17
11	2*	31	18
11	-2*	45	-45
0	3	127	103
2	3	108	96
2	-3	46	63
4	3*	33	1
4	-3*	28	17
6	3	45	44
8	-3	44	-37
8	3*	35	15
8	-3	81	-84
10	3*	32	40
10	-3*	35	6
12	-3*	31	-24
1	4	130	123
1	-4*	32	-1
3	4*	40	35
3	-4*	33	28
5	4	74	91
5	-4	96	-91
7	4*	43	14
7	-4*	37	-7
9	4*	33	38
9	-4*	35	42
11	-4*	36	4
13	-4*	28	-22
0	5	107	-86
2	5*	33	10
2	-5*	26	10
4	5	88	96
4	-5	216	205
6	5*	38	-9
6	5*	32	17
8	5*	34	-29
8	-5	52	40
10	6*	35	2
12	-5*	39	46
1	6*	38	-34
1	-6*	53	-57
3	6*	35	4
3	6	104	-99
5	6*	41	11
5	-6	97	-104
7	6*	34	20
7	-6*	64	-57
9	-6*	34	-23
11	-6*	36	-4
13	-6*	29	-1
0	7	94	102
2	7*	38	-19
2	-7*	32	-4
4	7*	54	48
4	-7*	32	-15
6	7*	34	-7
6	-7*	34	2
8	-7	79	-89
10	-7*	35	-38
12	-7*	32	-16
1	8*	50	-41
1	-8*	41	-6
3	8*	37	14
3	-8	60	-62
5	8*	35	-1
5	-8*	37	-17
7	8*	29	1
7	-8*	58	-29
9	-8*	36	38
11	-8*	36	7
13	-8*	29	22
0	9*	33	-23
2	9*	45	-38
2	-9*	42	28
4	9*	34	-32
4	-9	68	41
6	9*	29	-40
6	-9	81	73
8	-9*	35	-15
10	-9*	35	13
12	-9*	32	9
1	10	42	-22
1	-10*	60	-59
3	10	43	-36
3	-10*	37	-13
5	10*	29	19
5	-10*	72	-41
7	-10*	42	12
9	-10*	36	7
11	10*	36	28
13	-10*	37	11
0	11*	36	3
2	11*	34	31
2	-11	61	-65
4	11*	29	28
4	-11*	38	-8
6	-11*	38	-36
8	11*	35	-16
10	-11	67	-57
12	-11*	34	-1
1	12*	33	-12
1	-12*	35	3
3	-12*	38	7
5	-12*	41	18
7	-12*	43	21
9	12*	37	26
11	-12*	35	24
0	13*	32	3
2	13*	35	21
4	13*	35	3
6	-13*	39	30
8	13*	35	15
10	-13*	41	3
12	-13*	29	27
1	-14*	30	15
3	-14*	33	-3
5	14*	34	19
7	-14*	34	5
9	14*	32	10
11	-14*	32	15
4	-15*	31	37
6	15*	31	8
8	-15*	31	-21
K = 16			
0	0	107	97
2	0	133	143
4	0	87	94
6	0	48	35
8	0	53	-37
10	0*	26	4
1	1	376	381
1	-1	600	-601
3	1	374	376
3	-1	471	-465
5	1	292	288
5	-1	441	-420
7	1	205	202
7	-1	221	-221
9	1	130	135
9	-1	217	-216
11	1	70	62
11	-1	86	88
0	2	195	206
2	2*	31	23
2	-2	87	73
4	2*	46	65
4	-2*	29	-18
6	2*	31	20
6	-2	59	-58
8	2*	37	43
8	-2*	30	9
10	2*	25	-14
10	-2*	27	-14
12	-2*	24	-7
1	3	334	-335
1	-3	439	451
3	3	395	-392
3	-3	275	235
5	3	204	-208
5	-3	374	373
7	3	223	-225
7	-3	237	240
9	3	110	-109
9	-3	216	215
11	-3	99	110
0	4	69	63
2	4*	28	-27
2	-4*	36	8
4	4*	37	34
4	-4	42	-52
6	4*	33	20
6	-4	117	-136
8	4*	31	17
8	-4*	28	-16
10	-4*	27	-30
12	-4*	24	-1
1	5	323	319
1	-5	438	-424
3	5	336	379
3	-5	428	-420
5	5	198	187
5	-5	355	-341
7	5	163	157
7	-5	227	-273
9	5	64	30
9	-5	153	-155
11	-5	117	-128
13	-5	67	-42
0	6	62	-53
2	6*	28	35
2	-6	78	68
4	6*	33	-3
4	-6	60	80
6	6*	40	53
6	4	49	43
8	6*	28	3
8	-6*	47	57
10	-6*	26	38
12	-6*	24	5
1	7	260	-256
1	-7	257	252
3	7	161	157
3	-7	287	311
5	7	133	135
5	-7	241	233
7	7	93	94
7	7	313	301
9	-7	180	179
11	-7	143	144
13	-7	55	53
0	8	50	-35
2	8*	39	-49
2	-8*	37	-51
4	8*	33	10
4	-8*	30	-14
6	8*	25	-8
6	-8	74	-76
8	-8*	46	-29
10	-8*	28	6
12	-8*	24	16
1	9	211	209
1	-9	160	-161
3	9	135	128
3	-9	245	239
5	9	178	134
5	-9	181	-180
7	-9	181	-177
9	-9	110	-103
11	-9	103	-112
13	-9	58	-56
0	10*	30	-18
2	10*	28	-20
2	-10*	33	-24
4	10*	25	1
4	-10*	33	22
6	-10*	33	-13
8	-10*	32	6
10	-10*	27	14
12	10*	25	33
1	11	141	-129
1	-11	170	154
3	11	88	-79
3	11	199	178
5	-11	172	163
7	-11	162	146
9	-11	147	135
11	-11	84	78
0	12*	26	-34
2	12*	23	-7
2	12*	27	1
4	-12*	34	-10
6	12*	33	27
8	12*	32	-15
10	-12*	26	15
12	-12*	26	8
1	13	65	30
1	-13	97	-94
3	13	83	-79
5	-13	124	-115
7	13	99	91
9	-13	98	-97
11	13	50	54
2	14*	24	0
4	-14*	25	20
6	14*	25	17
8	-14*	29	14
10	-14*	25	4
5	-15	82	56
7	-15	58	40
9	-15	48	34
K = 17			
1	0	44	15
3	0	105	120
5	0	87	76
7	0*	45	38
9	0*	37	11
11	0*	35	23
0	1	84	88
2	1	119	-116
2	-1	72	-80
4	1*	35	13
4	-1	121	133
6	1	67	-77
6	-1*	34	9
8	1*	37	10
8	-1*	36	-26
10	1*	45	44
10	-1*	39	-2
12	-1*	37	36
1	2	137	-135
1	-2	73	-60
3	2*	41	51
3	2	86	-99
5	2	63	-67
5	-2	58	55
7	2*	44	-15
7	-2	69	-93
9	2*	36	-41
9	-2*	36	-17
11	-2*	44	-45
0	3*	41	40
2	3*	36	19
2	-3	104	-103
4	3*	38	3
4	-3	131	-132
6	3*	37	9
6	-3*	32	-4
8	3*	46	-33
8	-3*	35	-27
10	3*	34	28
10	-3*	39	18
12	-3*	31	-4
1	4	121	124
1	-4*	58	58
3	4*	41	34
3	-4	94	96
5	4	91	80
5	-4	59	57
7	4*	38	-5
7	-4	91	78
9	4*	32	38
9	4*	35	-16
11	-4*	37	29
0	5	57	-2
2	5	72	82
2	-5	122	-119
4	5*	40	5
4	-5*	41	-26
6	5*	38	15
6	-5*	51	-38
8	5*	35	-9
8	-5	69	78
10	5*	38	12
12	-5*	31	26
1	6*	39	-30
1	6	59	-80
3	6*	46	-16
3	-6	68	-84
5	6*	43	-36
5	-6*	37	25
7	6*	34	-13
7	-6*	35	-17
9	6*	45	63
11	-6*	47	-29
13	6*	31	28
0	7	72	59
2	7*	36	24
2	7*	33	13
4	7*	71	64
4	7	43	40
6	7*	34	1
6	-7*	36	19
8	-7*	43	37
10	-7*	39	30
12	-7*	32	6
1	8*	45	20
1	-8*	69	57
3	8*	47	53
3	-8*	34	-27
5	8*	34	6
5	-8*	68	74
7	8*	36	28
9	-8*	45	38
11	-8*	38	-11
13	-8*	31	35
0	9*	40	2
2	9*	38	16
2	-9*	43	41
4	9*	35	10
4	-9*	40	18
6	-9*	38	43
8	-9*	43	29
10	-9*	60	50
12	-9*	32	-8
1	10*	37	-2
1	-10*	57	-56
3	-10*	37	-34
5	-10	87	-62
7	-10*	37	5
9	-10*	37	-34
11	-10*	38	-22
13	-10*	30	-27
0	11*	36	-20
2	11*	34	13
2	-11*	37	8
4	-11	49	43
6	11*	39	-8
8	-11*	53	19
10	-11*	38	-3
12	11*	34	-4
1	12*	33	9
1	-12*	35	19
3	-12*	37	11
5	-12*	43	12
7	12*	46	33
9	-12*	37	25
11	-12*	36	10
0	13*	31	-22
2	13*	34	31
4	-13*	36	21
6	-13*	35	15
8	13*	36	2
10	-13*	36	-4
1	14*	30	-18
3	14*	33	-23
5	-14*	34	-8
7	14*	33	16
9	-14*	33	4
4	15*	30	-26
6	-15*	31	-20
8	-15*	31	-40
K = 18			
0	0	527	527
2	0	316	-312
4	0	370	364
6	0	153	-166
8	0	179	-181
10	0	66	63
1	1	269	266
1	-1	267	-243
3	1	208	204
3	-1	129	-145
5	1	87	78
5	-1	265	-264
7	1*	40	58
7	-1	142	-145
9	1	56	63
9	1	105	111
11	1*	28	8
11	-1*	27	-40
0	2	318	379
2	2	227	224
2	-2	257	268
4	2	245	257
4	-2	341	334
6	2	160	137
6	-2	238	249
8	2	150	149
8	-2	200	201
10	2	55	69
10	-2	108	123
12	2	68	59
1	3	46	-39
1	-3	185	186
3	3	189	-179
3	-3	170	161
5	3	127	-121
5	-3	165	152
7	3	117	-119
7	-3*	34	44
9	3	44	-58
9	-3	90	95
11	-3	41	62
0	4	277	-275
2	4	303	-303
2	-4	332	-342
4	4	235	-218
4	-4	212	211
6	4	150	181
6	-4	200	-218
8	4	102	-103
8	-4	119	-117
10	-4	120	-134
12	-4	46	68
1	5	215	217
1	-5	267	260
3	5	157	162
3	5	154	-151
5	5*	63	74
5	5	141	-131
7	5	172	78
7	5	161	-157
9	-5	79	-76
11	-5*	27	-43
0	6	229	211
2	6	252	249
2	6	339	334
4	6	104	108
4	-6	229	227
6	6	90	123
6	-6	285	289
8	6	52	19
8	-6	149	153
10	-6	131	140
12	6*	34	61
1	7	86	-87
1	7*	36	55
3	7	63	-65
3	-7	172	173
5	7	56	-58
5	-7	140	148
7	7*	32	-21
7	-7	131	133
9	-7	54	58
11	-7	80	90
13	-7*	22	24
0	8	178	-178
2	8	153	-152
2	8	178	-185
4	8	102	93
4	8	164	-165
6	8	174	-175
8	-8	134	128
10	-8	115	118
12	8	59	-91
1	9	123	113
1	9	108	96
3	9	57	59
3	-9	127	108
5	9	66	58
5	-9*	34	28
7	9	73	-69
9	-9*	48	63
11	9	37	-42
0	10	167	155
2	10	108	105
2	-10	156	145
4	10	89	70
4	-10	163	161
6	-10	105	110
8	10	125	123
10	10	60	68
12	-10*	36	61
1	11	64	-59
1	-11	62	68
3	11*	23	-17
3	-11	75	84
5	-11	127	112
7	11	98	88
9	-11	48	55
11	-11*	27	34
0	12	95	-91
2	12	51	-20
2	-12	76	-75
4	-12	137	-126
6	-12	109	100
8	-12	115	-110
10	-12	65	-65
1	-13	49	-43
3	-13*	25	-29
5	-13*	37	-40
7	-13*	25	-20
9	-13*	25	-55
11	-13*	25	-24
2	-14	50	33
4	14	64	66
6	-14*	25	56
8	-14*	35	56
10	-14*	32	31
K = 19			
1	0*	15	3
3	0	65	-59
5	0*	25	-33
7	0	41	58
9	0*	30	29
11	0*	27	53
0	1	82	86
2	1*	29	7
2	-1*	37	-51
4	1*	64	75
4	-1	50	-66
6	1	55	14
6	-1	36	-27
8	1*	30	37
8	-1*	29	-31
10	1*	28	3
10	-1*	30	-24
1	2	132	148
1	-2	58	66
3	2	75	86
3	-2	80	-123
5	2	118	-114
5	-2*	24	-2
7	2*	31	0
7	2	39	37
9	2	41	-37
9	-2	42	56
11	-2*	28	-15
0	3	54	55
2	3	51	-53
2	-3*	45	43
4	3*	46	-47
4	-3*	35	16
6	3*	31	-12
6	3	66	63
8	3*	36	30
8	-3*	29	7
10	-3*	35	27
12	-3*	25	-5
1	4*	28	42
1	-4*	24	26
3	4	58	-94
3	-4	109	135
5	4*	33	30
5	-4*	23	-13
7	4*	31	-29
7	-4	74	88
9	4*	25	51
9	-4*	30	49
11	-4*	36	48
0	5*	28	11
2	5*	45	53
2	-5	87	-92
4	5*	33	19
4	-5*	35	-35
6	5*	43	29
6	-5	56	-55
8	5*	26	10
8	-5*	29	-7
10	-5*	30	-36
12	-5*	26	-9
1	6	54	47
1	-6*	28	31
3	6*	39	-42
3	-6	62	67
5	6*	28	-47
5	6*	25	-13
7	6*	27	-9
7	-6*	29	9
9	-6*	30	-4
11	6*	29	4
0	7	42	-22
2	7*	41	-42
2	-7*	38	36
4	7*	33	-5
4	-7*	32	7
6	7*	32	-27
6	-7*	31	34
8	-7*	35	35
10	-7*	30	12
12	-7*	27	17
1	8*	25	7
1	-8	96	104
3	8*	32	46
3	-8	72	65
5	8*	28	-12
5	-8	88	89
7	-8*	35	-24
9	-8	38	47
11	-8*	29	3
0	9*	32	29
2	9*	29	21
2	-9*	43	-22
4	9*	27	17
4	-9	61	-52
6	-9*	31	-12
8	-9*	30	-20
10	-9*	30	0
12	-9*	26	-21
1	10*	30	22
1	-10*	28	-18
3	-10*	42	37
5	-10*	28	-26
7	-10*	37	-32
9	-10*	46	53
11	-10*	29	-7
0	11	36	-25
2	11*	27	-4
2	-11*	34	8
4	11*	35	25
6	-11*	32	8
8	11*	30	35
10	-11*	29	14
12	11*	28	6
1	12*	26	34
1	-12	33	22
3	-12*	29	23
5	12*	28	13
7	12*	31	4
9	12*	38	17
11	-12*	27	21
0	13*	24	7
2	-13*	27	10
4	13*	29	-13
6	-13*	28	-12
8	-13	28	-3
10	13*	27	-1
3	-14*	26	-44
5	-14*	27	-6
7	-14*	28	-31
9	-14*	25	-41
K = 20			
0	0	519	-522
2	0	284	-285
4	0	315	-323
6	0	154	-150
8	0	176	-180
10	0	56	-63
1	1	212	-211
1	-1	151	143
3	1	133	-133
3	-1	161	160
5	1*	42	-55
5	-1	137	147
7	1	64	-53
7	-1	149	146
9	1*	31	-34
9	1*	48	53
11	-1*	33	43
0	2	268	271
2	2	216	212
2	-2	230	235
4	2	256	256
4	-2	319	328
6	2	174	118
6	2	223	233
8	2	178	137
8	-2	166	172
10	2	49	32
10	-2	96	117
1	3	65	82
1	-3*	48	-69
3	3	81	89
3	-3	162	-157
5	3	117	123
5	-3	67	-83
7	3	67	70
7	-3*	48	-65
9	3	51	55
9	-3*	45	-63
11	3	42	-57
0	4	287	-279
2	4	275	-276
2	-4	345	-345
4	4	192	-197
4	-4	187	-172
6	4	172	173
6	4	196	197
8	4	101	-110
8	-4	114	-116
10	-4	110	-128
12	-4	38	30
1	5	191	-177
1	-5	190	184
3	5	98	100
3	-5	109	112
5	5	92	-81
5	-5	100	98
7	5*	39	-30
7	-5	71	86
9	-5	76	74
11	-5*	26	16
0	6	165	178
2	6	232	239
2	-6	275	288
4	6	91	99
4	-6	210	219
6	6	116	117
6	-6	293	295
8	-6	179	138
10	-6	119	128
12	-6	35	61
1	7*	32	48
1	-7	69	-74
3	7*	51	59
3	-7	92	-94
5	7	37	38
5	-7	162	-156
7	-7	77	-87
9	-7	76	-74
11	7*	27	-46
0	8	130	-124
2	8	145	141
2	-8	191	-186
4	8	100	86
4	-8	148	-145
6	8	97	-58
6	-8	132	-130
8	8	99	116
10	-8	101	-113
12	-8	42	-75
1	9	60	-59
1	-9	91	88
3	9	68	-62
3	-9	61	57
5	9	33	-30
5	9*	31	36
7	-9*	32	33
9	9*	42	54
11	-9*	26	39
0	10	155	150
2	10	102	98
2	-10	139	129
4	10	75	48
4	-10	170	158
6	10	143	124
8	-10	133	128
10	-10*	42	51
12	-10*	25	34
1	11	60	49
1	-11	67	-56
3	-11	73	-70
5	11	84	-74
7	-11	91	-78
9	11*	32	-30
11	-11*	30	-27
0	12	82	-88
2	-12	63	-65
4	-12	118	-118
6	-12	70	-79
8	-12	86	93
10	-12	60	-73
1	-13*	22	13
3	-13	41	38
5	-13	24	24
7	-13*	24	34
9	-13*	23	31
4	-14	63	40*
6	-14	58	44
8	-14*	38	37
K = 21			
1	0*	32	-54
3	0*	24	0
5	0*	29	-22
7	0*	31	-3
9	0	36	-26
0	1	51	53
2	1	92	101
2	1	53	59
4	1	76	82
4	-1*	32	20
6	1*	39	46
6	-1*	41	-29
8	1	44	59
8	-1*	30	-8
10	1*	29	36
10	1*	31	-17
1	2*	35	35
1	-2	50	64
3	2	78	87
3	-2*	35	-41
5	2*	30	-17
5	2	71	89
7	2*	37	28
7	-2*	31	-34
9	2*	28	-3
9	-2*	35	33
11	-2*	28	-14
0	3	59	-68
2	3*	30	-45
2	-3	160	167
4	3	48	-60
4	-3	123	124
6	3*	34	-18
6	-3	62	67
8	3*	29	-12
8	3*	30	12
10	3*	39	35
1	4*	39	38
1	-4	97	102
3	4*	35	-53
3	-4*	24	4
5	4*	31	28
5	4*	43	43
7	4*	30	-38
7	4*	30	23
9	-4*	30	30
11	-4*	29	1
0	5*	25	15
2	5*	34	15
2	-5*	30	4
4	5*	35	0
4	5*	44	33
6	5*	41	20
6	-5*	47	-57
8	5*	26	46
8	-5	48	-65
10	-5*	38	-47
12	-5*	25	-34
1	6*	29	19
1	-6*	27	3
3	6*	40	19
3	-6*	27	3
5	6*	30	-2
5	-6*	30	7
7	6*	27	1
7	-6*	30	43
9	-6*	29	-3
11	-6*	29	13
0	7	57	-48
2	7	65	-70
2	-7*	55	52
4	7	53	-49
4	-7	63	71
6	7*	28	-32
6	7*	39	15
8	7*	30	-12
10	-7*	37	-9
12	-7*	31	29
1	8*	30	-35
1	-8*	29	21
3	8*	30	11
3	-8	55	-60
5	8*	28	-26
5	-8*	30	21
7	-8*	31	-19
9	-8*	30	27
11	-8*	29	-25
0	9*	31	36
2	9*	30	5
2	9*	47	-43
4	9*	33	0
4	-9*	55	-50
6	9*	33	35
8	-9	65	-76
10	9*	32	-38
12	9*	25	33
1	10*	30	26
1	-10*	30	8
3	10*	27	-19
3	-10*	30	26
5	-10*	32	-12
7	-10*	39	37
9	-10*	29	8
11	10*	28	12
0	11*	29	-16
2	11*	27	-31
2	-11*	30	-6
4	11*	36	10
6	-11*	33	11
8	-11*	30	6
10	11*	31	4
1	12*	26	18
1	-12*	28	8
3	-12*	30	3
5	12*	30	-10
7	-12*	30	6
9	-12*	29	-7
2	-13*	27	-39
4	-13*	29	-23
6	-13*	29	-17
8	-13*	28	8
5	-14*	28	3
7	-14*	26	-23
K = 22			
0	0*	22	-3
2	0	90	69
4	0	57	-111
6	0*	29	15
8	0*	30	-47
10	0*	37	-4
1	1	307	-302
1	-1	317	326
3	1	257	257
3	-1	326	324
5	1	183	-184
5	-1	246	260
7	1	159	-146
7	-1	221	207
9	1	79	-85
9	-1	123	125
11	-1	83	55
0	2	173	162
2	2*	30	23
2	-2	85	64
4	2	32	73
4	-2*	39	7
6	2*	30	13
6	2*	28	-18
8	2	52	49
8	-2*	31	16
10	-2*	32	6
1	3	268	249
1	-3	267	-257
3	3	275	224
3	-3	245	-233
5	3	188	183
5	-3	212	-205
7	3	143	139
7	3	173	-165
9	3	89	63
9	-3	128	-138
11	3	67	-90
0	4*	25	23
2	4	53	54
2	-4	66	42
4	4*	33	4
4	4*	44	-47
6	4*	30	0
6	-4	137	-127
8	4*	28	-1
8	-4*	30	5
10	-4*	42	36
1	5	266	254
1	-5	285	281
3	5	202	-206
3	-5	272	259
5	5	154	-149
5	-5	266	257
7	5	91	-104
7	-5	180	168
9	-5	138	131
11	-5	64	77
0	6*	27	-30
2	6*	42	50
2	-6	87	84
4	6*	40	-3
4	6*	37	-46
6	6	62	54
6	6*	29	0
8	-6*	30	-24
10	-6*	40	46
12	6*	27	5
1	7	156	146
1	-7	197	-187
3	7	177	123
3	-7	216	-193
5	7	102	95
5	-7	194	-194
7	7	162	-156
9	7	143	-143
11	-7	85	-103
0	8*	29	-35
2	8	67	-53
2	-8*	49	-45
4	8*	38	73
6	8	78	-59
8	8*	31	28
10	-8*	33	9
12	8*	27	12
1	9	153	-136
1	-9	163	147
3	9	124	-113
3	-9	158	143
5	9	157	131
7	9	135	125
9	-9	100	85
11	9	55	73
0	10*	31	5
2	10*	29	6
2	-10*	35	-6
4	-10	71	43
6	-10*	30	-5
8	10*	30	24
10	-10*	32	15
1	11	91	90
1	-11	107	-99
3	11	142	130
5	-11	135	-120
7	11	128	-114
9	-11	85	-80
11	11	79	54
0	12	39	26
2	-12*	29	0
4	-12	38	-13
6	12*	30	14
8	-12*	29	-21
10	-12*	30	13
3	-13	77	63
5	-13	61	68
7	-13	69	74
9	13	54	41
6	-14*	26	11
K = 23			
1	0*	24	19
3	0*	25	9
5	0	45	38
7	0*	44	27
9	0*	38	-51
0	1*	22	-14
2	1*	40	29
2	-1	67	69
4	1*	33	4
4	-1*	32	-15
6	1*	32	24
6	-1*	31	2
8	1*	32	0
8	1*	32	9
10	1*	28	37
10	-1*	31	-7
1	2*	43	49
1	-2	118	130
3	2	137	147
3	-2*	24	18
5	2*	31	42
5	-2	85	95
7	2*	37	56
7	-2*	37	-30
9	2*	30	8
9	-2*	31	30
11	-2*	28	-9
0	3*	31	-28
2	3*	37	26
2	-3*	29	-22
4	3*	35	1
4	-3*	48	-36
6	3*	33	2
6	-3	35	37
8	3*	30	-2
8	-3*	32	19
10	-3*	33	14
1	4*	31	19
1	-4	95	-112
3	4*	29	-42
3	4*	26	33
5	4*	32	30
5	4	83	93
7	4*	32	-34
7	-4*	36	-50
9	-4	43	-68
11	-4*	29	20
0	5*	31	-12
2	5*	36	4
2	5*	31	-12
4	5*	36	25
4	-5*	54	-45
6	5*	32	5
6	-5*	31	3
8	5*	32	14
10	-5*	33	-1
1	6*	41	37
1	6*	33	3
3	6	58	52
3	6*	28	10
5	6*	35	37
5	-6*	31	4
7	-6*	36	26
9	-6*	31	-9
11	-6*	30	26
0	7*	39	-31
2	7*	38	3
2	-7*	35	13
4	7*	32	-4
4	-7*	35	1
6	7*	28	32
6	-7*	31	-8
8	-7*	33	42
10	-7*	32	8
1	8*	56	-69
1	8*	40	-41
3	8*	33	-9
3	-8	105	-107
5	8*	29	-33
5	-8*	32	-20
7	-8*	57	58
9	8*	31	8
11	8*	29	27
0	9*	33	7
2	9*	32	8
2	9*	46	15
4	9*	29	37
4	-9*	36	-19
6	-9*	32	-13
8	-9*	32	4
10	-9*	32	10
1	10*	32	22
1	-10*	33	-14
3	10*	29	-3
3	-10*	31	20
5	-10*	33	10
7	-10*	37	47
9	10*	47	22
11	10*	35	26
0	11*	31	1
2	11*	33	19
4	-11*	33	8
6	11*	32	-3
8	-11*	37	3
10	-11*	30	21
1	-12*	30	27
3	12*	32	-19
5	-12*	32	-18
7	12*	32	7
9	12*	30	-9
2	-13*	39	32
4	-13*	30	-6
6	-13*	30	-18
8	-13*	29	-28
K = 24			
0	0	173	146
2	0	272	273
4	0	153	159
6	0	162	171
8	0	48	58
10	0	68	55
1	1	138	-133
1	-1	172	177
3	1	165	-164
3	-1	156	149
5	1	138	-149
5	-1	84	94
7	1	119	123
7	-1	71	68
9	1	48	69
9	-1	53	66
0	2	163	-168
2	2	165	-168
2	-2	206	-216
4	2	75	82
4	-2	123	-139
6	2	178	-130
6	2	128	-137
8	2*	63	56
8	-2	112	-122
10	2	73	84
1	3	201	195
1	-3	209	-217
3	3	149	156
3	-3	145	-148
5	3	93	76
5	-3	159	-177
7	3	67	69
7	-3	106	-117
9	-3	85	-83
11	-3*	29	-9
0	4	190	199
2	4	166	167
2	-4	115	116
4	4	153	154
4	4	188	189
6	4	95	94
6	-4	113	107
8	4	64	47
8	4	97	113
10	-4*	32	35
1	5	89	-74
1	5	81	113
3	5	81	-97
3	-5	124	133
5	5	71	-75
5	5	140	144
7	5	64	-46
7	5	88	80
9	-5	89	94
11	5	47	58
0	6	165	-179
2	6	64	-74
2	-6	129	-147
4	6	106	-112
4	-6	198	206
6	6*	30	-43
6	-6	77	-97
8	-6	118	-127
10	-6	67	70
1	7	132	128
1	-7	139	137
3	7	91	93
3	-7	92	-102
5	7	74	76
5	7	80	79
7	-7	84	84
9	-7	57	62
11	-7*	29	-33
0	8	118	112
2	8	91	74
2	-8	172	81
4	8	86	83
4	-8	77	89
6	-8	94	99
8	-8	88	90
10	-8	50	65
1	9	78	-71
1	-9	81	72
3	9	50	-47
3	-9	122	114
5	-9	120	110
7	-9	97	99
9	-9	47	49
11	-9	52	40
0	10	77	-71
2	10	77	-67
2	-10	119	-112
4	10	101	92
6	-10	107	-101
8	-10*	57	41
10	-10	66	-62
1	11	49	28
1	11	55	-51
3	11	53	-55
5	-11*	32	-32
7	11	54	51
9	-11	49	-52
2	12	65	67
4	12	46	48
6	-12	58	74
8	12*	60	57
3	-13	58	29
5	-13	54	39
7	-13	48	30
K = 25			
1	0*	20	-17
3	0	53	50
5	0	70	-59
7	0*	30	4
9	0*	30	-12
0	1*	27	-42
2	1*	30	18
2	-1*	28	-2
4	1	58	-72
4	-1*	31	22
6	1*	34	-41
6	-1*	41	25
8	1*	41	-45
8	-1*	34	15
10	-1*	29	9
1	2*	23	2
1	-2	103	113
3	2*	26	30
3	-2*	24	17
5	2*	32	-5
5	-2*	35	46
7	2*	35	39
7	-2*	30	3
9	2*	27	38
9	-2*	51	56
0	3	71	89
2	3*	52	56
2	-3	64	-75
4	3*	34	24
4	-3	58	-65
6	3*	34	9
6	-3*	33	47
8	3*	31	-3
8	3*	43	35
10	3*	30	13
1	4*	26	2
1	-4*	24	-28
3	4	83	79
3	-4*	25	13
5	4*	31	3
5	4	62	71
7	4*	30	27
7	4*	30	12
9	-4*	31	13
11	-4*	28	-32
0	5	40	27
2	5*	34	12
2	-5*	37	9
4	5*	34	-1
4	-5*	37	10
6	5*	30	27
6	-5*	33	42
8	5*	35	13
10	-5*	31	35
1	6*	28	20
1	6	51	48
3	6*	34	18
3	6	68	66
5	6*	31	6
5	-6*	30	-1
7	-6*	30	24
9	6*	31	13
11	-6*	29	46
0	7	54	38
2	7	47	53
2	-7	58	-62
4	7*	31	24
4	-7*	33	-3
6	-7*	40	13
8	-7*	35	10
10	-7*	31	-17
1	8*	46	-47
1	-8*	29	11
3	8*	31	5
3	-8*	29	28
5	8*	32	6
7	-8	59	-63
9	-8*	30	-4
11	-8*	28	-39
0	9*	31	-10
2	9*	30	13
2	-9*	32	25
4	-9*	35	31
6	-9*	55	52
8	-9*	34	31
10	-9*	30	21
1	10*	30	19
1	-10*	32	7
3	10*	35	39
5	-10*	32	8
7	10*	31	5
9	-10*	30	-5
0	11*	29	4
2	-11*	31	-2
4	-11*	31	-5
6	11*	31	12
8	11*	30	6
3	-12*	30	-7
5	12*	30	-13
7	-12*	30	-16
6	-13*	28	1
K = 26			
0	0	170	138
2	0	217	220
4	0	147	136
6	0	167	165
8	0	94	88
1	1*	52	41
1	-1	85	-79
3	1*	34	18
3	-1	106	-116
5	1	67	55
5	1*	41	44
7	1*	32	18
7	-1*	40	-43
9	1*	28	16
9	1*	30	27
0	2	228	230
2	2	258	-251
2	2	236	-236
4	2	143	162
4	-2	170	-173
6	2	157	-158
6	-2	134	-137
8	2	72	-77
8	-2	102	-107
10	-2	61	-43
1	3	90	-93
1	-3*	40	12
3	3*	35	-23
3	-3*	28	21
5	3*	48	-46
5	3*	35	5
7	3*	29	-18
7	-3	63	66
9	-3*	32	11
0	4	195	196
2	4	131	136
2	-4	176	178
4	4	137	123
4	4	237	235
6	4	83	82
6	4	149	149
8	-4	148	149
10	-4	67	80
1	5*	52	57
1	-5*	42	-41
3	5*	31	42
3	5	108	-104
5	5*	31	45
5	-5	68	-57
7	5*	32	-31
9	-5*	33	-7
0	6	183	-174
2	6	106	-109
2	-6	87	115
4	6	95	-128
4	-6	154	-147
6	6	78	-38
6	-6	97	91
8	-6	110	-117
10	-6	48	78
1	7*	37	23
1	7*	47	47
3	7*	31	-17
3	7*	31	19
5	7*	28	-9
5	-7*	37	73
7	-7*	33	40
9	-7*	39	51
0	8	150	140
2	8	111	97
2	8	144	142
4	8	163	151
6	-8	138	132
8	-8	93	85
10	-8	64	69
1	9*	30	21
1	9*	37	-35
3	9*	36	36
3	-9*	31	15
5	-9*	55	-51
7	9*	32	-7
9	9*	30	-11
0	10	69	72
2	-10	105	95
4	-10	86	77
6	10	109	98
8	-10	77	80
10	10	80	-60
1	11*	29	33
3	11*	30	26
5	11*	30	30
7	11*	30	17
9	11	45	36
2	12	87	46
4	12	57	46
6	12	72	60
8	12*	28	20
K = 27			
1	0*	40	49
3	0*	27	11
5	0*	33	1
7	0*	34	17
9	0*	28	19
0	1	54	-74
2	1*	36	-3
2	-1*	41	48
4	1*	50	-57
4	1*	67	76
6	1*	34	-17
6	-1*	34	17
8	1*	31	-26
8	-1*	40	47
1	2	61	-81
1	-2*	33	-39
3	2*	28	-4
3	-2*	39	-47
5	2*	34	-39
5	-2*	42	47
7	2*	30	-11
7	2*	35	15
9	-2*	29	10
0	3	44	46
2	3*	39	43
2	-3*	31	19
4	3*	37	37
4	3*	35	-27
6	3*	30	25
6	-3*	34	-44
8	3*	39	-32
10	3*	27	-29
1	4*	31	25
1	-4*	38	-34
3	4*	30	-24
3	-4*	28	33
5	4*	30	5
5	-4*	33	41
7	4*	28	48
7	-4*	42	45
9	4*	30	9
0	5*	32	-19
2	5*	44	-53
2	-5*	52	73
4	5*	31	-21
4	5*	35	32
6	5*	27	-38
6	-5*	47	39
8	5*	33	-7
10	-5*	28	30
1	6*	33	4
1	-6*	32	-9
3	6*	31	-7
3	-6*	29	9
5	6*	29	-72
5	-6*	39	16
7	-6*	43	41
9	-6*	30	-12
0	7*	33	18
2	7*	31	37
2	-7*	54	-51
4	7*	29	2
4	-7*	37	-10
6	-7*	49	-55
8	-7*	33	-28
10	-7*	33	-34
1	8*	31	8
1	-8*	31	44
3	8*	29	18
3	8*	31	2
5	-8*	43	41
7	-8*	40	12
9	-8*	30	24
0	9*	30	-16
2	9*	29	-29
2	9*	31	21
4	-9*	31	25
6	9*	35	22
8	-9*	32	8
10	-9*	27	26
1	10*	28	41
1	-10*	30	-4
3	-10*	30	9
5	-10*	30	8
7	-10*	30	0
9	-10*	29	10
2	-11*	29	-18
4	-11*	30	-23
6	-11*	30	-5
8	-11*	28	-37
5	12*	28	-30
K = 28			
0	0	56	43
2	0	84	68
4	0*	32	1
6	0	42	51
8	0*	30	30
1	1	185	206
1	-1	126	-141
3	1	144	167
3	-1	121	-142
5	1	140	150
5	-1	97	-105
7	1	91	100
7	-1	95	-111
9	-1	62	-47
0	2*	55	-39
2	2	97	-92
2	-2	73	-61
4	2*	44	-51
4	2	72	-71
6	2	41	-52
6	2	49	-42
8	2*	27	6
8	-2*	31	-22
1	3	177	-196
1	-3	160	169
3	3	120	122
3	3	219	236
5	3	117	-129
5	3	134	141
7	3	48	-47
7	3	119	131
9	3	60	69
0	4	60	70
2	4*	34	17
2	4*	54	53
4	4*	30	26
4	4	56	62
6	4*	29	27
6	-4*	30	17
8	-4	56	61
10	-4*	27	8
1	5	114	133
1	-5	109	-120
3	5	79	83
3	-5	119	-134
5	5	81	99
5	5	86	-106
7	-5	119	-128
9	5	76	88
0	6	66	-56
2	6*	35	31
2	-6*	33	-3
4	6*	30	52
4	-6	53	50
6	6*	29	30
8	-6	38	26
10	6*	28	8
1	7	117	114
1	-7	119	130
3	7	108	-116
3	7	114	115
5	7	112	128
7	-7	75	74
9	7	59	70
0	8*	30	39
2	8*	29	25
2	-8	51	54
4	-8	55	48
6	-8	33	31
8	-8*	37	22
1	9	68	63
1	-9	110	108
3	-9	107	-94
5	-9	114	-112
7	-9	75	-78
9	-9	78	-79
0	10*	28	-3
2	-10*	29	-28
4	10*	29	-4
6	-10*	29	-41
8	-10*	29	-15
3	11	60	41
5	-11	63	88
7	11	50	42
K = 29			
1	0*	36	56
3	0*	43	51
5	0*	33	21
7	0	45	32
0	1*	45	-58
2	1*	30	-4
2	-1*	29	-18
4	1*	28	-16
4	-1*	34	52
6	1*	29	35
6	-1*	32	25
8	1*	27	-35
8	-1*	36	23
1	2*	28	-48
1	-2*	27	-13
3	2*	34	-19
3	-2*	52	-57
5	2*	29	-31
5	-2*	37	-27
7	2*	28	-16
7	-2*	29	-49
9	-2*	27	11
0	3*	32	-27
2	3*	33	16
2	-3*	31	-2
4	3*	29	20
4	-3*	27	-2
6	3*	29	4
6	-3*	32	13
8	-3*	29	7
1	4*	37	49
1	-4*	29	27
3	4*	29	21
3	-4*	39	45
5	4*	34	42
5	-4*	33	18
7	-4*	29	16
9	-4*	28	19
0	5*	46	-31
2	5*	36	-48
2	-5*	33	49
4	5*	29	2
4	5*	27	-17
6	-5*	40	35
8	-5*	29	0
1	6*	44	-34
1	-6*	46	-46
3	6*	29	-27
3	-6*	41	-27
5	-6*	51	-46
7	-6*	29	-22
9	-6*	28	-31
0	7*	50	-32
2	7*	29	7
2	-7*	29	14
4	-7*	29	-10
6	-7*	29	-37
8	-7*	29	9
1	8*	29	7
1	-8*	29	28
3	-8*	30	12
5	-8*	46	39
7	8*	29	11
9	-8*	28	27
0	9*	28	-5
2	9*	31	12
4	-9*	29	-8
6	-9*	29	-16
8	-9*	34	5
1	-10*	29	-26
3	-10*	29	-18
5	-10*	28	-14
7	-10*	28	-13
4	-11*	27	-47
6	-11*	27	-39
K = 30			
0	0	113	-113
2	0	47	-62
4	0*	61	-66
6	0*	39	-56
8	0	58	-55
1	1	123	141
1	-1	72	-100
3	1	89	106
3	-1	103	-120
5	1	80	100
5	-1	74	-77
7	1	42	73
7	-1	69	-87
0	2	85	104
2	2	91	114
2	-2	78	92
4	2	101	114
4	-2	89	97
6	2	45	58
6	-2	86	74
8	-2*	37	32
1	3	117	140
1	3	90	103
3	3	58	-74
3	-3	133	157
5	3	80	-95
5	-3	73	81
7	-3	84	97
9	-3*	30	24
0	4	74	-107
2	4	33	-57
2	-4	116	-125
4	4*	35	-42
4	-4	67	-77
6	4*	32	-26
6	-4	81	-85
8	-4	58	-62
1	5	100	103
1	-5	77	-80
3	5	63	80
3	-5	88	-98
5	5	61	47
5	-5	87	-79
7	-5	70	81
9	-5*	37	-30
0	6	52	56
2	6	68	77
2	6	48	57
4	6*	42	41
4	-6*	56	43
6	-6	68	68
8	-6*	33	48
1	7	72	-70
1	-7	91	98
3	7	57	-67
3	-7	92	89
5	-7	92	97
7	-7	52	48
9	-7*	37	38
0	8	69	-88
2	8	47	-41
2	-8	90	-81
4	-8	90	-84
6	8	47	-46
8	-8*	32	-42
1	-9	78	-81
3	-9	43	-62
5	-9	67	-83
7	-9	51	56
2	-10*	21	20
4	-10*	40	47
6	-10*	31	38
K = 31			
1	0*	40	67
3	0*	30	40
5	0*	28	17
7	0	29	21
0	1*	17	11
2	1	48	67
2	-1*	29	-41
4	1*	28	-9
4	-1*	24	-7
6	1*	27	28
8	-1*	30	-48
8	-1*	28	6
1	2*	25	-9
1	-2*	23	8
3	2*	25	-9
3	-2*	34	-37
5	2*	27	-12
5	-2*	25	-30
7	-2*	27	-30
0	3*	20	-4
2	3*	25	-13
2	-3*	36	27
4	3	31	-18
4	-3*	24	37
6	3*	28	-10
6	-3*	27	6
8	-3*	27	17
1	4*	38	40
1	-4*	28	38
3	4*	27	25
3	-4*	39	19
5	4*	27	40
5	-4*	25	-1
7	-4*	27	7
0	5	48	60
2	5*	27	9
2	-5*	25	-7
4	5*	27	28
4	-5*	26	-28
6	-5*	27	6
8	-5*	27	-36
1	6*	27	-24
1	-6*	28	-29
3	6*	27	-12
3	-6	40	-27
5	-6	45	-56
7	-6*	27	-27
0	7*	26	-27
2	7*	27	4
2	-7*	27	-3
4	-7*	28	44
6	-7*	27	17
8	-7*	27	13
1	8*	27	13
1	-8*	27	8
3	8*	27	4
5	-6*	27	8
7	-8*	27	-3
0	9*	28	-3
2	-9*	27	-17
4	-9*	27	-8
6	-9*	27	-1
3	-10*	28	-38
5	-10*	28	-34
K = 32			
0	0	137	-121
2	0	114	-118
4	0	108	-114
6	0	74	-96
1	1*	17	-12
1	-1*	17	4
3	1	32	-34
3	-1	33	-37
5	1*	28	-9
5	-1*	25	13
7	-1*	28	-12
0	2	141	144
2	2	98	120
2	-2	115	142
4	2	103	104
4	-2	88	107
6	2	61	81
6	-2	83	90
8	-2	67	37
1	3*	23	-13
1	-3	40	-67
3	3*	26	33
3	-3*	47	-24
5	3*	26	-8
5	-3	38	-43
7	-3*	28	14
0	4	91	-107
2	4	101	-102
2	-4	61	-114
4	4	78	-89
4	-4	80	-104
6	-4	90	-108
8	-4	62	-66
1	5*	28	9
1	-5*	24	7
3	5*	28	-4
3	-5*	19	-23
5	-5*	25	5
7	-5*	28	15
0	6	73	88
2	6	84	97
2	-6	87	105
4	-6	61	94
6	-6	65	74
8	-6	48	40
1	-7*	26	-1
3	-7*	28	-28
5	-7*	28	1
7	-7*	28	-2
0	8	72	-88
2	-8	86	-88
4	-8	69	-93
6	-8	64	-74
1	-9	56	8
3	-9*	25	28
5	-9*	26	-2

ion have a mean value of 2·411 Å, and the corresponding angles a mean value of 111·5°. The sulphur–oxygen distances are essentially identical at 1·459 Å and can be compared with an average distance of 1·49 Å in other inorganic structures (*International Tables for X-ray Crystallography*, 1962). The new values of bond lengths and angles for the sulphate ion in gypsum lower its symmetry from a tetrahedron in the point group $\bar{4}3m$ (hexatetrahedral) to a sphenoid in the point group $\bar{4}2m$ (tetragonal bisphenoidal). The fact that the symmetry of the sulphate ion must be lower than tetrahedral has long been established from both Raman (Rousset & Lochet, 1945) and infrared spectra (Hass & Sutherland, 1956), both of which show

Table 4. *Observed and calculated neutron structure factors for* $CaSO_4.2H_2O$

Based on an isotropic re-refinement of Atoji & Rundle's observed data. Structure factors are scaled to 100*F* in Fermi units, where *F* is calculated for one $CaSO_4.{}_2H_2O$.

h	*k*	*l*	FO	SQFC
2	0	0	52·9	53·2
4	0	0	61·4	52·8
6	0	0	9·7	12·5
0	2	0	81·7	78·4
0	4	0	44·4	−37·5
0	6	0	61·4	54·2
0	8	0	21·0	−20·9
0	10	0	51·3	49·7
0	12	0	32·4	−31·5
0	14	0	15·6	13·6
0	16	0	31·9	30·0
0	18	0	66·2	−65·7
0	0	2	31·7	−37·6
0	0	4	8·6	−2·2
0	0	6	25·5	−26·6
1	1	0	16·3	14·3
1	3	0	6·4	−5·4
1	5	0	44·3	−40·2
1	7	0	52·3	50·0
1	9	0	47·4	44·0
1	11	0	81·3	−78·0
1	13	0	15·2	10·3
1	15	0	24·9	26·2
1	17	0	6·5	−8·1
2	2	0	39·4	−39·0
2	4	0	125·1	−118·2
2	6	0	16·9	−17·5
2	8	0	21·0	−13·6
2	10	0	23·7	−29·8
2	12	0	13·4	9·5
2	14	0	53·1	52·4
2	16	0	27·1	27·2
3	1	0	24·3	20·9
3	3	0	64·2	−63·3
3	5	0	3·0	3·4
3	7	0	29·1	31·2
3	9	0	10·6	−8·7
3	11	0	11·3	−8·8
3	13	0	23·3	−21·9
3	15	0	20·6	24·9
4	2	0	70·2	62·8
4	4	0	25·6	26·4
4	6	0	50·3	−49·4
4	8	0	63·6	60·8
4	10	0	11·6	−12·3
4	12	0	9·5	−8·6
4	14	0	32·3	31·5
5	1	0	22·0	22·4
5	3	0	21·8	−19·6
5	5	0	21·4	18·3
5	7	0	21·6	20·6
5	9	0	< 4·0	−4·6
5	11	0	8·6	4·8
6	2	0	21·6	−19·8
6	4	0	32·6	−32·8
0	1	1	< 5·0	3·1
0	3	1	20·8	20·2
0	5	1	19·3	17·3
0	7	1	18·5	16·3
0	9	1	65·2	67·2
0	11	1	36·0	41·4
0	13	1	13·9	12·7
0	15	1	25·0	26·1
0	17	1	19·1	19·2
0	2	2	28·1	−31·1
0	4	2	61·6	−61·8
0	6	2	59·3	56·9
0	8	2	2·3	−6·0
0	10	2	27·5	23·1
0	12	2	57·0	−66·8
0	14	2	10·2	−8·7
0	16	2	47·9	46·9
0	1	3	5·0	7·7
0	3	3	34·7	34·9
0	5	3	5·9	−7·0
0	7	3	51·3	−49·7
0	9	3	49·6	48·1
0	11	3	3·8	−2·1
0	13	3	37·7	−39·6
0	15	3	22·9	19·5
0	2	4	11·3	13·4
0	4	4	49·6	−49·0
0	6	4	26·3	−23·4
0	8	4	39·9	−40·1
0	10	4	26·7	25·3
0	12	4	< 2·0	−2·0
0	1	5	< 2·0	−2·1
0	3	5	11·8	8·5
0	5	5	36·5	−34·8
0	7	5	70·0	−67·7
0	9	5	33·5	35·3
0	11	5	15·8	−17·8
0	2	6	35·1	35·3
0	4	6	43·3	40·4
2	0	2	48·2	40·1
2	0	4	45·1	27·9
1	2	$\bar{1}$	70·2	−75·9
2	2	$\bar{2}$	18·4	−21·9
3	2	$\bar{3}$	23·8	19·4
4	2	$\bar{4}$	< 4·0	−5·9
5	2	$\bar{5}$	42·1	−35·7
1	4	$\bar{1}$	33·2	−36·5
2	4	$\bar{2}$	25·8	−24·9
3	4	$\bar{3}$	43·6	−40·4
4	4	$\bar{4}$	21·0	14·4
5	4	$\bar{5}$	34·2	−31·0
1	6	$\bar{1}$	15·4	13·0
2	6	$\bar{2}$	90·0	102·7
3	6	$\bar{3}$	28·2	27·7
4	6	$\bar{4}$	86·7	−86·0
5	6	$\bar{5}$	15·9	16·9
1	8	$\bar{1}$	23·3	−24·1
3	8	$\bar{3}$	31·1	−36·2
4	8	$\bar{4}$	23·8	−22·8
1	10	$\bar{1}$	23·9	−22·6
2	10	$\bar{2}$	14·3	−11·6
3	10	$\bar{3}$	120·1	−139·3
4	10	$\bar{4}$	11·3	6·0
1	12	$\bar{1}$	26·4	29·4
2	12	$\bar{2}$	27·5	−24·8
4	12	$\bar{4}$	20·5	30·7
1	14	$\bar{1}$	42·0	−40·5
2	14	$\bar{2}$	32·0	−24·3
3	14	$\bar{3}$	< 3·0	5·6
1	16	$\bar{1}$	43·0	−44·9

splitting of fundamental frequencies associated with the SO_4 ion. The lower symmetry was not revealed by Atoji & Rundle from their neutron diffraction results but the re-refining of their observations shows (Table 5) that it was present in their data. The reduced symmetry probably arises because of the different environment surrounding the two crystallographically distinct sulphate oxygens O(1) and O(11). The symmetry-related pair of atoms O(1) and O(1′) are each hydrogen bonded to two water molecules towards which they face whereas the symmetry-related pair O(11) and O(11′) form no hydrogen bonds but have close Ca^{2+} neighbours. Atoms O(1), O(11) and O(1′), O(11′) are drawn closer together and atoms O(1), O(1′) and O(11), O(11′) spread slightly apart with respect to the values found by Atoji & Rundle to produce the observed distortion from tetrahedral symmetry.

Each calcium atom in gypsum is surrounded by three pairs of oxygen atoms [one of O(1), O(1′) and two of O(11), O(11′)] belonging to SO_4 groups and by a pair of water molecules (Fig. 1) with oxygen atoms O(*W*), O(*W′*). For atoms O(1) and O(11) of the same SO_4 group the Ca–O(1) pair and the Ca–O(11) pair have bond lengths that are significantly shorter (Table 5) than those found by Atoji & Rundle. This arises from the shortening of the O(1)–O(11) bond distance and the decreasing of the O(1)–S–O(11) bond angle. The second shorter Ca–O(11) bond length (Table 5) links the Ca of the one cell to the symmetry-related pair of O(11) and O(11′) atoms in the next cell and this is slightly lengthened, as is the distance between Ca and the O(*W*) atoms in the same cell with respect to the values found by Atoji & Rundle.

The changes in the *x* and *z* parameters of atoms O(1) and O(*W*) (Table 1) from those found by Atoji & Rundle affect the hydrogen-bond distances given by O(*W*)–O(1) [or O(1′)] through H(1) and O(*W*)–O(1) [or O(1′)] through H(2) (Fig. 1). These distances, as well as the two distances O(*W*)–H(1) and O(*W*)–H(2) in each water molecule, are non-equivalent and in principle need not be of the same length (Seidl, Knop & Falk, 1969). In fact Seidl, Knop & Falk have shown that appreciable asymmetry of the water molecule is indicated by the large splittings in gypsum of the three isolated HDO frequencies: 90 cm^{-1} for O–H stretching, 65 cm^{-1} for O–D stretching, and 14 cm^{-1} for the bending. They argue that it would be necessary to determine the positional parameters of O(*W*) and O(1) with standard deviations of the order of 0·001 Å to verify the asymmetry found by the spectroscopic results. The new X-ray results indicate that the two distances O(*W*)–O(1) [or O(1′)] through H(1) and O(*W*)–O(1) [or O(1′)] through H(2) of the water molecule differ by $0{\cdot}080 \pm 0{\cdot}003$ Å (Table 5) while the refined neutron data indicate a difference of $0{\cdot}065 \pm 0{\cdot}018$ Å, both results being statistically significant. The original refinement of Atoji & Rundle gave no difference in these bond lengths.

If the true hydrogen positions are taken as those

Table 5. *Interatomic distances and bond angles*

	X-ray, isotropic and anisotropic	Neutron, isotropic	
	This study	Atoji & Rundle	Re-refined
Sulphate ion			
S——O(1)	1·457±0·001 Å	1·497±0·014 Å	1·483±0·014 Å
S——O(11)	1·461±0·002	1·479±0·010	1·468±0·014
O(1)—O(1′)	2·409±0·002	2·442±0·013	2·452±0·020
O(1)—O(11)=O(1′)-O(11′)	2·323±0·002	2·421±0·014	2·370±0·013
O(11)-O(11′)	2·407±0·003	2·415±0·010	2·398±0·018
O(1)—O(11′)=O(1′)-O(11)	2·414±0·002	2·438±0·011	2·434±0·011
O(1)—S-O(1′)	111·5±0·1°	109·4±1·4°	111·5±1·3°
O(11)-S-O(11′)	111·0±0·1	109·4±1·0	109·5±1·3
O(1)—S-O(11)=O(1)-S-O(11′)	105·5±0·1	108·9±1·3	106·8±0·5
O(1)—S-O(11′)=O(1′)-S-O(11)	111·7±0·1	110·1±1·2	111·1±0·6
Water molecule			
O(*W*)-H(1)	0·962±0·012 Å	1·002±0·030 Å	0·981±0·040 Å
O(*W*)-H(2)	0·944±0·021	0·981±0·024	0·939±0·023
H(1)—H(2)	1·531±0·030	1·580±0·036	1·531±0·030
H(1)—O(*W*)-H(2)	106·9±1·0°	105·6±4·5°	105·7±1·8°
Hydrogen bond			
O(*W*)-O(1) [or O(1′) through H(1)]	2·816±0·002 Å	2·816±0·014 Å	2·799±0·013 Å
O(*W*)-O(1) [or O(1′) through H(2)]	2·896±0·002	2·824±0·015	2·865±0·011
O(1)—H(1)=O(1′)-H(1)	1·860±0·013	1·814	1·826±0·038
O(1)—H(2)=O(1′)-H(2)	1·955±0·006	1·845	1·932±0·019
O(1)—H(1)-O(*W*)=O(1′)-H(1)-O(*W*)	172·3±1·0°	177·7°	171·0±1·8°
O(1)—H(2)-O(*W*)=O(1′)-H(2)-O(*W*)	174·1±1·0	178·1	172·3±2·1
Calcium-oxygen distances			
Ca-O(1)	2·528±0·002 Å	2·566 Å	2·552±0·009 Å
Ca-O(11)	2·544±0·002	2·588	2·548±0·010
Ca-O(11)	2·378±0·001	2·353	2·357±0·012
Ca-O(*W*)	2·380±0·001	2·341	2·383±0·014

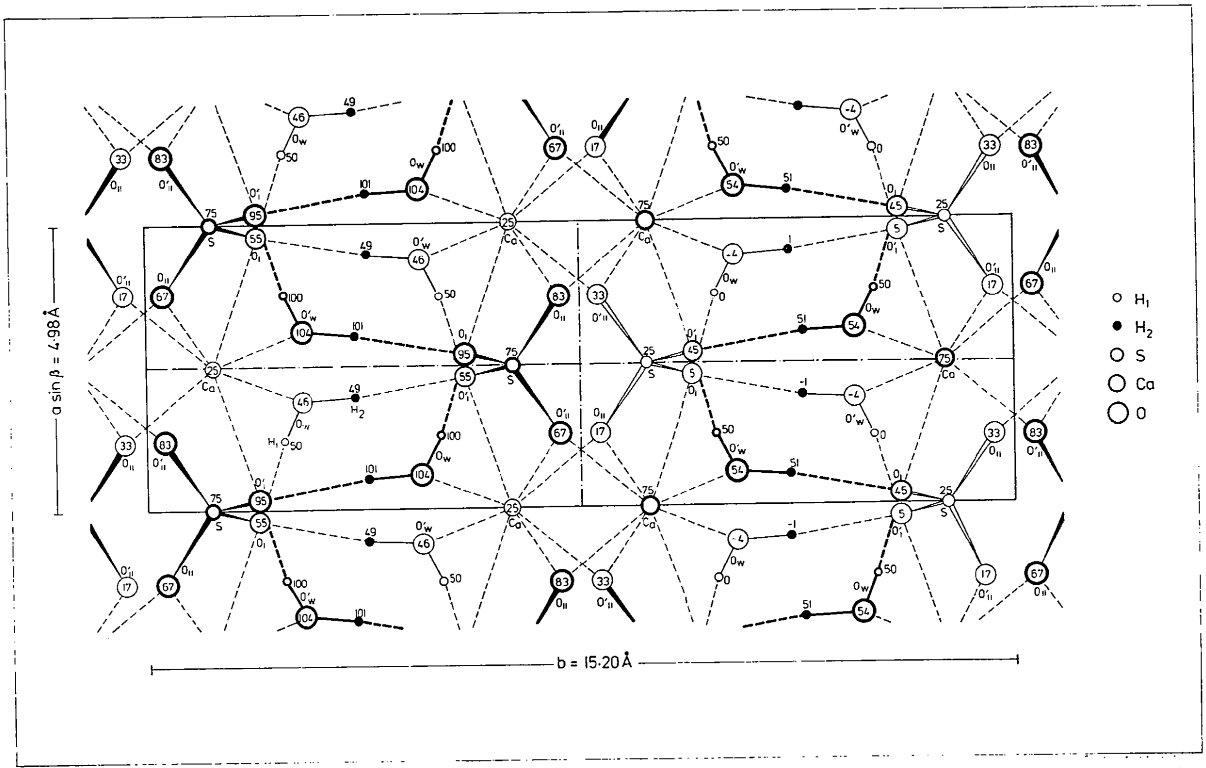

Fig. 1. One-half of the unit cell of gypsum projected on the (001) plane [after Atoji & Rundle (1958)]. The fractional coordinates have been multiplied by 100.

given from the re-refined neutron data (Table 1) and if they are combined with the O(*W*) parameters given by the X-ray refinement, then the O(*W*)–H(1) distance is 0·962 Å, and the O(*W*)–H(2) distance 0·944 Å, the H(1)–O(*W*)–H(2) bond angle 106·9°, and the H(1)–H(2) distance 1·531 Å (Table 5). The O(*W*)–H and O(*W*)–H–O(1) distances correlate well with those from hydrates given in Fig. 8 of Atoji & Rundle. The location of the two hydrogen atoms is essentially along the lines joining O(*W*)–O(1) and O(*W*)–O(1′) (Table 5 and Fig. 1) as reported earlier by Atoji & Rundle. Thus the shorter O(*W*)–H(2) distance is associated with the longer O(*W*)–H(2)–O(1) [or O(1′)] distance and the longer O(*W*)–H(1) with the shorter O(*W*)–H(1)–O(1) [or O(1′)] as expected. The ratio of the distance O(*W*)–H(2) to the distance O(*W*)–H(1) is 0·979 which can be compared with the ratio of 0·966 reported by Seidl, Knop & Falk (1969) as being derivable by R. W. Green from spectroscopic data.

In the attempts to re-refine the neutron-diffraction data with mixed isotropic–anisotropic temperature factors the hydrogen positional parameters, after one cycle of refinement, gave higher values for the O(*W*)–H(1) (1·042 Å) and O(*W*)–H(2) (0·937 Å) distances, using the O(*W*) positional parameters from the neutron refinement as also when using the X-ray positional parameters for O(*W*) [O(*W*)–H(1) 1·022 Å and O(*W*)–H(2) 0·951 Å]. Thus, although the hydrogen positional parameters are known with less certainty than the others, those obtained in the present work, when combined with O(*W*) positions from either neutron or X-ray data, yield values of bond lengths consistent with two hydrogen bonds of different length and strength.

In the structure of gypsum the water molecules form two parallel sheets in the direction of the prominent cleavage of the crystal (Fig. 1), and the H(2) atoms are all located within the double layer whereas the H(1) atoms are always outside it. This means that an electrical repulsion between the sheets would lengthen hydrogen bonds involving the H(2) atom relative to those involving the H(1) atom, as is observed.

In the neutron-diffraction refinement of Atoji & Rundle the parameters were refined with isotropic temperature factors, since it was observed from Fourier methods that the thermal motions were isotropic or nearly isotropic. The root-mean square amplitudes of the thermal motion along the principal axes set out in Table 6 show that the thermal motions of Ca and S are nearly isotropic, but those of O(1), O(11) and O(*W*) show some anisotropy, particularly O(*W*). The locations of the thermal ellipsoids for Ca and S are very similar and are shown in Fig. 2 with respect to the atom projections on the *ac* plane. Greatest thermal movement of

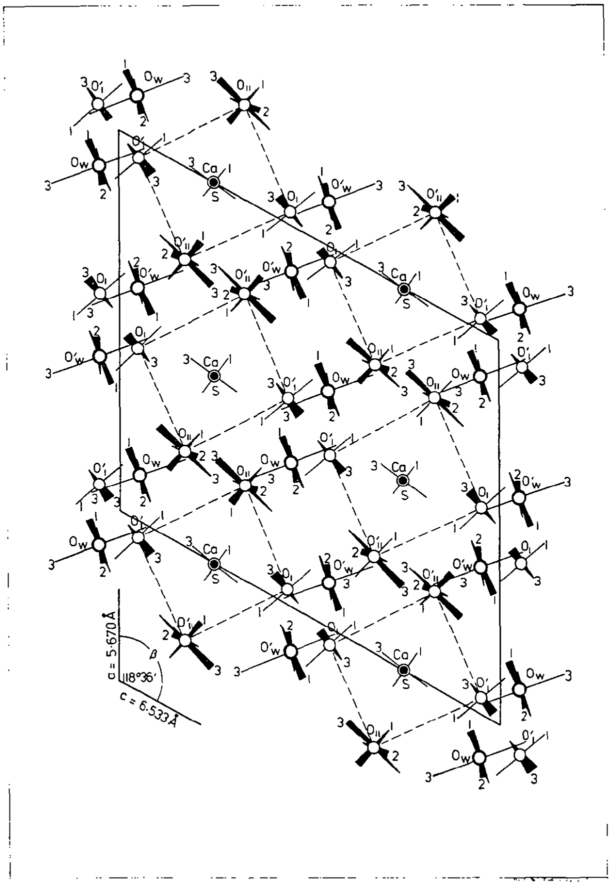

Fig. 2. Position of principal axes of thermal ellipsoids (1, 2 and 3) with respect to the *ac* plane of gypsum. The lengths of the axes are proportional to the magnitude of the r.m.s. amplitudes of thermal motion (Table 6) projected into the *ac* plane. The thicknesses of the wedges indicate the magnitude of the angle of inclination (*I*) of the principal axes to the *ac* plane. The directions that the wedges point to are the angles φ (Table 6) that the principal axes make with the *a* axis. For atoms O(1) and O(1′) the principal axis 2 nearly superimposes on axis 3 and is not shown. Its inclination to the plane is opposite to that of axis 3.

Table 6. *Root-mean-square (r.m.s.) amplitudes of thermal motion along the principal axes, angle of principal axes to the a axis (φ) and inclination of principal axes to ac plane (I)*

(Numbers in parentheses are standard deviations in the least significant digit.)

	Axis 1			Axis 2			Axis 3		
	φ	*I*	r.m.s.	φ	*I*	r.m.s.	φ	*I*	r.m.s.
Ca	45°	0°	0·092 (1) Å	—	90°	0·105 (1) Å	135°	0°	0·108 (1) Å
S	37	0	0·077 (2)	—	90	0·091 (1)	127	0	0·100 (1)
O(1)	50	0	0·118 (2)	320°	32	0·118 (2)	142	58	0·140 (2)
O(11)	42	9	0·093 (2)	293	66	0·118 (2)	135	22	0·154 (2)
O(*W*)	157	26	0·121 (3)	347	64	0·150 (2)	249	3	0·191 (2)

Ca and S takes place approximately in the direction of the *c* axis. The intermediate axis of these ellipsoids lies in the direction of the *b* axis. The directions of the ellipsoids for O(1) and O(11) are similar to those for Ca and S except that the intermediate axis is inclined to the *b* axis (Table 6). For atom O(*W*) the directions of the ellipsoid are different from those of the other atoms and the greatest thermal motion is more nearly in line with the least thermal motion of atoms O(1), O(11), Ca and S. Its intermediate axis is inclined to the *b* axis (Table 6).

The authors wish to thank Professor H. Freeman and staff of the Chemistry Department of the University of Sydney for instructing them in the use of the Supper equi-inclination Weissenberg diffractometer and for supplying them with copies of the crystallographic computer programs used in the work.

References

ATOJI, M. & RUNDLE, R. E. (1958). *J. Chem. Phys.* **29**, 1306–1311.

BRAGG, W. L. (1937). *Atomic Structure of Minerals*, p. 130. New York: Cornell Univ. Press.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*. Report ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1964). *ORFEE*. Report ORNL-TM-306, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

COLE, W. F. & LANCUCKI, C. J. (1965). *Rev. Sci. Instrum.* **36**, 1669–1670.

COLE, W. F. & LANCUCKI, C. J. (1972*a*). *Nature, Phys. Sci.* **238**, 95–96.

COLE, W. F. & LANCUCKI, C. J. (1972*b*). *Nature, Phys. Sci.* **240**, 48.

COLE, W. F. & LANCUCKI, C. J. (1973). *Nature, Phys. Sci.* **242**, 104–105.

DENNE, W. A. & JONES, D. W. (1969). *Z. Kristallogr.* **130**, 314–317.

FREEMAN, H. C., GUSS, J. M., NOCKOLDS, C. E., PAGE, R. & WEBSTER, A. (1970). *Acta Cryst.* A**26**, 149–152.

HASS, M. & SUTHERLAND, G. B. B. M. (1956). *Proc. Roy. Soc.* A**236**, 427–445.

HUBER-BUSER, E. (1971). *Z. Kristallogr.* **133**, 150–167.

International Tables for X-ray Crystallography (1962). Vol. III, pp. 204–205 and p. 272. Birmingham: Kynoch Press.

MIRKIN, L. I. (1964). *Handbook of X-ray Analysis of Polycrystalline Materials*, pp. 326, 327. New York: Consultants Bureau.

ROUSSET, A. & LOCHET, R. (1945). *J. Phys. Radium*, **6**, 57–61.

SEIDL, V., KNOP, O. & FALK, M. (1969). *Canad. J. Chem.* **47**, 1361–1368.

WEISS, O., COCHRAN, W. & COLE, W. F. (1948). *Acta Cryst.* **1**, 83–88.

WOOSTER, W. A. (1936). *Z. Kristallogr.* **94**, 375–396.

Acta Cryst. (1974). B**30**, 929

Electron Diffraction and the Structure of α-N_2

BY J. A. VENABLES AND C. A. ENGLISH*

School of Mathematical and Physical Sciences, University of Sussex, Brighton, BN1 9QH, England

(*Received* 11 *June* 1973; *accepted* 18 *September* 1973)

Electron diffraction patterns have been obtained from annealed single crystals of α-N_2. The {100} patterns were found to be particularly suitable for resolving the controversy as to whether α-N_2 has the *Pa*3 or $P2_13$ structure. A quantitative comparison of these patterns with calculated intensities was used to set a (conservative) upper limit of 0·05 Å for the displacement of the centre of the N_2 molecule from the *Pa*3 structure. This and other more qualitative evidence strongly suggests that the structure is in fact *Pa*3. Twins on {111} planes were observed and were shown to give rise to some reflexions which are forbidden by *Pa*3 symmetry. The possibility is discussed that twinning could explain a previous X-ray observation of isolated reflexions which were not consistent with the *Pa*3 structure.

1. Introduction

The exact structure of the low temperature α-phase of solid nitrogen has been under discussion since the first X-ray work of Vegard (1929) and Ruhemann (1932). The structure proposed by Ruhemann was *Pa*3 cubic, in which the centres of the N_2 molecules are on a f.c.c. lattice, but each molecule points in a different ⟨111⟩ direction. The Vegard structure is essentially similar but the centre of a molecule is displaced by a small distance, *r*, along the ⟨111⟩ direction parallel to the axis of that molecule. This displacement lowers the symmetry to $P2_13$, which is a non-centrosymmetric structure.

Many diffraction experiments have been performed in an attempt to decide which structure is correct. X-ray powder patterns (Bolz, Boyd, Mauer & Peiser,

---

* Present address: A.E.R.E., Harwell, Didcot, Berkshire, England.