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The Crystal Structure of α,α-Trehalose Dihydrate from Three Independent X-ray Determinations*

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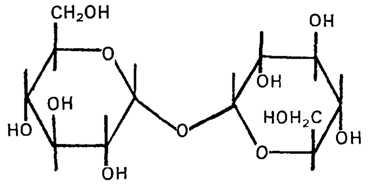
The structure of the dihydrate of the nonreducing disaccharide α,α-trehalose (α-D-glucopyranosyl α-D-glucopyranoside) has been determined independently by direct methods in three different laboratories. There are four units $C_{12}H_{22}O_{11}.2H_2O$ in an orthorhombic cell ($P2_12_12_1$) with $a = 12{\cdot}230$ (2), $b = 17{\cdot}890$ (3), and $c = 7{\cdot}596$ (1) Å. The discrepancy indices $R(F)$ are: 0·057 (based on 3293 Mo $K\alpha$ diffractometer data); 0·041 (1611 Cu $K\alpha$ diffractometer data); 0·055 (2149 Cu $K\alpha$ photographic data). Comparison of coordinates suggests that their standard errors may have been underestimated by a factor of ~2. The α,α-trehalose molecule has approximate C_2 symmetry, but there are some significant structural differences between the two chemically equivalent halves. The angles at the ring oxygen atoms are 114·0 and 114·2°; the angle at the glycosidic oxygen is 115·8°. The two rings have *C*l conformations; the conformations about the linking C–O bonds are stabilized by the conformational 'anomeric effect' and also by a complex system of hydrogen bonds involving all of the hydroxyl groups, both water molecules, and one ring oxygen. By hydrogen bonding each glucopyranosyl moiety is linked to the other in the same molecule indirectly through two different water molecules. The helical arrangement of hydrogen bonds about the screw axes parallel to **c** suggests the possibility of observing ferroelectric behavior.

Introduction

α,α-Trehalose (I), or α-D-glucopyranosyl α-D-glucopyranoside, is one of three isomeric D-glucopyranosyl D-glucopyranosides collectively known as the trehaloses (Birch, 1963). It is a nonreducing disaccharide composed of two α-D-glucosyl units linked by a glycosidic oxygen bridge between their two anomeric carbon atoms, C(1) and C′(1) in the usual numbering system. The isomeric α,β-trehalose and β,β-trehalose have been synthesized, but only the α,α isomer occurs naturally. Known also as mycose or mushroom sugar, α,α-trehalose is widespread in nature, where it is found in bacteria, insect blood, fungi, algae, lichens, and some higher plants. It accounts for as much as 15% of the weight of mushrooms and dried yeast, but apparently it is not present in more basic foodstuffs. As the major blood sugar of many, but not all, insects (Wyatt & Kalf, 1957), it is important in insect metabolism. It is specifically hydrolyzed by the enzyme trehalase isolated from the wax moth (Kalf & Rieder, 1958).



(I)

This paper reports the results of three X-ray crystal-structure determinations of α,α-trehalose dihydrate carried out independently and simultaneously in our three separate laboratories. This is the first structure reported of a carbohydrate oligomer containing a glycosidic oxygen atom which is axial with respect to two sugar rings. A comparison of the two nonequivalent D-glucosyl moieties of the molecule in the crystal is interesting because the significant differences between the two must result from the packing of the molecules, which in isolation have chemically equivalent moieties and inherent twofold axes of symmetry.

Experimental

α,α-Trehalose dihydrate (m.p. 96–97 °C) is very soluble in water and in aqueous ethanol, but nearly insoluble in anhydrous ethanol. It can be crystallized in anhydrous form from dry pyridine, but from aqueous ethanol

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it comes out as a beautifully crystalline dihydrate. Groth (1910) described the dihydrate as orthorhombic bisphenoidal and gave the axial ratios $a:b:c=0{\cdot}6814:1:0{\cdot}4171$, on the basis of goniometric observations dating back to 1857.

X-ray photography and diffractometry confirm that the dihydrate is orthorhombic and establish $P2_12_12_1$ as the space group, the observed extinctions being reflections $h00$, $0k0$, and $00l$ for odd values of h, k, and l respectively. The largest of the crystals available at Edinburgh showed a feeble piezoelectric response.

The three sets of unit-cell translations are in remarkably good agreement (see Table 1, which presents a synopsis of the experimental work). The Oak Ridge cell parameters were derived by the least-squares method (Busing & Levy, 1967; Busing, 1970) from the 2θ angles of 12 resolved Mo $K\alpha_1$ reflections in the range 40·8° to 44·4° 2θ recorded with the Oak Ridge computer-controlled diffractometer (Busing, Ellison, Levy, King & Roseberry, 1968). The 12 reflections were 6 pairs of Friedel mates; the 2θ angles of the two reflections of each pair were measured in opposite senses to nullify any possible error in the zero of the 2θ scale of the diffractometer. The Pittsburgh parameters were derived by a least-squares method using 2θ angles for 20 general Cu $K\alpha$ reflections in the 2θ range 45 to 60°. The 2θ values were obtained on a Picker FACS-I diffractometer from measurements on both the positive and negative sides of the 2θ circle. The Edinburgh translations were derived by extrapolation procedures from angle data obtained with a knife-edged camera which provides a standard high angle.

The recording of intensity data (see Table 1) with the Oak Ridge computer-controlled diffractometer and preliminary data reduction followed procedures virtually identical with those used in a study of 6-mercaptopurine monohydrate (Brown, 1969). In particular, the ω step-scan technique devised by Levy (1966) and described briefly in the 6-mercaptopurine paper was used for reflections below 22° 2θ to provide more reliable background determinations on the low-angle sides of the Bragg peaks than is possible with θ–2θ scans. The recording of reflections in the highest angle range, 60 to 65° 2θ, was not completed, because the crystal spontaneously split into two pieces, possibly as the effect of contraction of a thin film of glue on the base of the crystal upon cracks produced when the crystal was cut from a larger one. There had been no indication in the intensity values recorded periodically (every 20 reflections) for a reference reflection that deterioration of the crystal was occurring.

For each reflection a statistical standard error $\sigma_c(|F^2|)$ was calculated according to the equation

$$\sigma_c^2(|F^2|)=(AS/Lp)^2(T+k^2B)\,,$$

where S is the scale factor on the intensities, A is the correction factor for absorption, L is the Lorentz factor, p is the polarization factor, T is the total count B is the background count, and k is the ratio of times spent measuring T and B. The standard errors were used in calculating the weights in the subsequent least-squares refinement (see below). However, the low-angle background measurements were not considered reliable even in the ω-scan method for $2\theta<12°$. Accordingly, the 34 reflections of lowest angle were later given zero weights in the final refinement cycles, along with two other reflections for which the intensities were discovered to have been improperly recorded. Otherwise, all reflections were considered as observed.

Table 1. *Experimental data for α,α-trehalose dihydrate*

Orthorhombic, space group $P2_12_12_1$; asymmetric unit $C_{12}H_{22}O_{11}.2H_2O$, formula weight 378·2; cell volume 1662 Å³, observed density 1·512, calculated density 1·511 g.cm^{-3}, $Z=4$; μ(Cu $K\alpha$)$=12.2$, μ(Mo $K\alpha$)$=1{\cdot}49$ cm^{-1}.

Cell parameters	Oak Ridge	Pittsburgh	Edinburgh
a	12·229 (2) Å	12·230 (2) Å	12·233 (3) Å
b	17·890 (3)	17·890 (3)	17·889 (4)
c	7·597 (1)	7·595 (1)	7·596 (2)
λ	0·70926	1·54178	1·5405, 1·5443
Temperature	23·5 ± 0·5 °C	1[illegible]·0 ± 1·0 °C	18·0 ± 1·0 °C
Intensity data			
Crystal source	Mann Research*	Dr D. French†	Dr G. G. Birch‡
shape	Polyhedron	Polyhedron	Spheres
size (mm)	0·3 × 0·3 × 0·4	0·3 × 0·4 × 0·4	0·3–0·4 radii
Data collection technique	Diffractometry, ω and θ–2θ scans	Diffractometry, θ–2θ scans	Weissenberg photography
Radiation	Mo $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
$(\sin\theta/\lambda)_{\max}$ (Å^{-1})	0·758	0·599	0·645
Independent data	3329	1634	2149
Absorption correction	Yes§	No	Yes

* Mann Research Laboratories, 136 Liberty Street, New York, U.S.A.
† Iowa State University, Ames, Iowa, U.S.A.
‡ National College of Food Technology, Weybridge, Surrey, England.
§ The range of correction factors was 1·033 to 1·056.

The least-squares method of Thiessen, Levy & Brown (1970*a*, *b*) provided normalized structure factors (Hauptman & Karle, 1953), the scale factor, and a preliminary over-all anisotropic temperature factor. Statistical tests clearly indicated the centric distribution for the zonal intensities and the acentric one for the general intensities.

The Pittsburgh intensity data were measured on a Picker FACS-I diffractometer up to $2\theta = 130°$, using the θ–2θ scan mode with a scan speed of 2° 2θ per minute. The scan width used for each intensity measurement was 1·7° plus a dispersion term for Ni-filtered Cu $K\alpha$ radiation. Background counts of 10 sec duration were recorded at the beginning and end points of each scan. Three reference reflections recorded every 49 reflections varied less than 2·5% over the period of the data collection. Therefore, it seems that no crystal deterioration was occurring.

The intensity data were reduced to structure factors and normalized to E's by the programs of Shiono (1971). Using the criterion that a measured intensity less than two standard deviations be considered unobserved, 23 of the 1634 independent reflections were considered unobserved and assigned weights of zero. No corrections for absorption were made.

The Edinburgh intensity data were obtained by the equiinclination Weissenberg method. Photographs were taken with the crystal rotating about the *a* axis ($h = 0$–9), the *b* axis ($k = 0$–14), and the *c* axis ($l = 0$–5). Multiple-film packs were used, and multiple exposures were made. The intensity comparisons and the interfilm and interlayer scaling were done very carefully for a total of 2149 independent reflections. This total, which includes 52 unobserved reflections, is no less than 98·5% of the accessible reflections for Cu $K\alpha$ radiation. A few 'Renninger' reflections were noticed.

Absorption corrections appropriate for spherical crystals (*International Tables for X-ray Crystallography*, 1959, p. 299) were applied. The data generally had an internal consistency characterized by a 5% standard deviation, except for the very small and very large F's, which were less reliably determined. The three axial projections were confirmed as centrosymmetrical by intensity statistics.

Solution

In each of the three determinations the solution was achieved by direct methods. At Oak Ridge the tangent formula (Karle & Hauptman, 1956; Karle & Karle, 1966) was used in reiterative phasing, with the aid of Drew's program *PHASEM* (see Drew, Templeton & Zalkin, 1969; Drew, 1969). The starting set of phases (Table 2) included four phases set arbitrarily to specify the origin and enantiomorph (Karle & Hauptman, 1956) and seven others for which values were indicated with tentatively acceptable probabilities of correctness by a calculation with the $\sum_1$ formula (Hauptman & Karle, 1953; Karle & Hauptman, 1956). The phasing process converged for the 258 reflections with $|E| < 1·66$ in 20 cycles. Of the highest 26 peaks in the E map computed with 258 phased E's, 25 peaks were found to represent quite well the 25 carbon and oxygen atoms of the asymmetric unit, the 24th peak in order of decreasing height being spurious.

The acceptance of seven phases from the $\sum_1$ calculation was perhaps not cautious; but since the chemical structure of α,α-trehalose is well known, no difficulty was expected in recognizing a false solution. As it turned out, for the intensity invariants with $|E| \geq 1·50$ for which the $\sum_1$ calculation was made, the 11 phase indications with highest probabilities of correctness ($P \geq 0·717$) were all correct.

The tangent formula and the phase extension method of Hall (1967, 1970) were used to solve the structure in Pittsburgh. Six zonal reflections were used as the starting phase set* (Table 2). These were extended to 227 phases with a minimum $|E|$ of 1·4. The E map calculated using these phases showed only 25 major peaks corresponding to the entire trehalose molecule and the two water oxygens. No spurious peaks of significant height were generated.

At Edinburgh a prolonged attempt was made to solve the structure from Patterson projections and by three-dimensional Patterson methods. One ring (primed atoms in our numbering system) was reasonably accurately located, but the position of the other was off by about 0·5 Å (as seen in retrospect), so that a sucessful refinement was not possible.

After Patterson methods were abandoned in favor of direct methods, the solution was achieved by the symbolic addition procedure (Karle & Karle, 1966) and by the method of phasing with the tangent formula described by Germain, Main & Woolfson (1970, 1971), as implemented in the program *MULTAN* (Main, Woolfson & Germain, 1971). Readily interpretable E maps were obtained using 291 reflections with $|E| \geq 1·38$ phased by the first procedure and 265 reflections with $|E| \geq 1·50$ phased by the second procedure. The starting phases for both procedures are given in Table 2. The two sets of phases were about equally good, with about 90% of the zonal phases correct and with an average error of about 35° in the others. As at Oak Ridge, the $\sum_1$ relation was found to work very well; although only two signs were indicated with high probability, they were both correct, as were the next half-dozen less probable indications.

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* The indices of these reflections have been transformed and the phases shifted appropriately from the original values, which were based on a unit cell with the translations **a** and **b** interchanged from the assignment specified in Table 1. Phase shifts are required because for space group $P2_12_12_1$ the set of permissible origins (Hauptman & Karle, 1956) for one cell description does not coincide with the set for the other description, given that both determinations used the same form for the structure-factor expression. The origin shifts is $m/4$, $n/4$, $p/4$, where m, n, and p are odd integers whose particular values depend on the phase assignments made to fix the origin.

Table 2. *Starting sets of phases* φ_{tr} *and* φ_{sa} *used in solving the structure by the tangent-refinement and symbolic addition methods, respectively*

	h	k	l	$\|E\|$	φ_{tr}	φ_{sa}
Oak Ridge	5	0	2	4·05	0	
	9	5	0	3·41	$\pi/2$	
	0	17	1	3·34	$\pi/2$	
	14*	0*	7*	3·78	$\pi/2$	
	10	0	0	2·11	π	
	4	6	0	2·43	π	
	0*	12*	10*	1·94	π	
	0	14	0	2·39	0	
	12*	0*	8*	2·49	π	
	0	4	8	2·15	0	
	2*	26*	0*	2·19	π	
Pittsburgh	5	0	2	2·95	0	
	9	5	0	2·95	$\pi/2$	
	0	4	3	2·20	π	
	4	9	0	2·27	0 (π)†	
	0	17	1	2·98	a ($\pi/2$)‡	
	0	9	2	2·85	b ($\pi/2$)‡	
Edinburgh	5	0	2	3·65	0	0
	9	5	0	3·20	$\pi/2$	
	0	17	1	3·14	$\pi/2$	
	11	4	0	2·32	$\pi/2$	
	10	0	0	2·07	π	
	0	18	6	1·61	0	0
	0	4	3	2·78	0, π‡	
	1	8	1	2·13	$\pi/4$, $-\pi/4$ $3\pi/4$, $-3\pi/4$‡	
	0	9	2	2·54		$\pi/2$
	6	8	3	2·82		a (0·11π)‡
	4	13	4	2·41		b (−0·37π)‡

* Reflection beyond the Cu $K\alpha$ limiting sphere.
† Phase shifted from 0 to π.
‡ Phases established for symbols and phases selected for reflections for which more than one starting phase was entered.

Refinement

In the three determinations, (I), (II), and (III), denoting Oak Ridge, Pittsburgh, and Edinburgh, respectively, all 26 hydrogen atoms were located approximately by difference syntheses following some preliminary cycles of least-squares refinement. In the final cycles of each determination anisotropic thermal parameters were used for the carbon and oxygen atoms and isotropic parameters for the hydrogen atoms. In determination (I), the hydrogen thermal parameters were adjusted; in (II), held fixed at values for the parent C and O atoms reached in preliminary refinement; in (III), held fixed at 2·5 Å^2. Hydrogen coordinates were adjusted in all three determinations. The scattering factors were from the following sources: (I) Hanson, Herman, Lea & Skillman (1964) for C and O and Stewart, Davidson & Simpson (1965) for H; (II) Cromer & Waber (1965) for C and O and Stewart *et al.* for H; (III) Berghuis *et al.* (1955) for C, Freeman (1959) for O, and McWeeny (1951) for H.

The full-matrix least-squares method was used in (I), with minimization of $\sum w(\Delta|F|^2)^2$; the block-diagonal method was used in (II) and (III), with minimization of $\sum w(\Delta|F|)^2$. For (I), except for zero weights noted already, the weights were set according to the equation

$$w(|F_o^2|)=1/[\sigma_c^2(|F_o|^2)+(0{\cdot}03|F_o|^2)^2]\,,$$

where $\sigma_c^2(|F_o|^2)$ is the purely statistical variance already defined and the term $(0{\cdot}03|F_o|^2)^2$ is an empirical correction term (Peterson & Levy, 1957). For (II), the basis of the weighting was essentially the same as for (I), except that the factor 0·03 was replaced by 0·05 and the equation appropriate for $w(|F_o|)$ is

$$w(|F_o|)=4|F_o|^2/[\sigma_c^2(|F_o|^2)+(0{\cdot}05|F_o|^2)^2]\,.$$

The scheme used in (III) was:

$$\begin{aligned} w(|F_o|)&=1\,, & |F_o|&<14\,;\\ w(|F_o|)&=14/|F_o|\,, & 14\le|F_o|&\le 50\,;\\ w(|F_o|)&=700/|F_o|^2\,, & |F_o|&>50\,. \end{aligned}$$

The final measures of goodness of fit[*] were: (I) $R(F)=0{\cdot}057$ (excluding only data with zero weights), $R_w(F^2)=0{\cdot}081$, and $\sigma_1=1{\cdot}209$; (II) $R(F)=0{\cdot}041$ for observed data only and 0·057 for all data, $R_w(F^2)=0{\cdot}087$, and $\sigma_1=1{\cdot}401$; (III) $R(F)=0{\cdot}055$ (all data).

The final parameters and standard errors from all three determinations are shown in Table 3, which also includes a set of weighted-average coordinates and standard errors. The weight used for each coordinate was the reciprocal of the square of its standard error; the standard error reported for each average is the square root of the reciprocal of the sum of weights for that average. The coordinates describe the α,α-trehalose molecule in correct absolute configuration.

The observed and calculated structure factors (×10) for all three determinations are given in Table 4. For a given reflection hkl the first entry gives the Oak Ridge data; the second, if present, gives the Edinburgh data; and the third, if present, gives the Pittsburgh data.[†] The Table also includes in each entry for Oak Ridge either the standard error $\sigma(|F_o|)\times 100$ [$\sigma(|F_o|)$ being calculated as $\sigma(|F_o^2|)/2|F_o|$], or, if $|F_o|^2\le\sigma(|F_o^2|)$, the error $\sigma(|F_o^2|)\times 10$ (in which case a minus sign precedes the error). The 34 low-angle reflections given zero weight in final refinement are indicated by negative signs on the $|F_o|$ values. Two other reflections given zero weights because they were not properly determined are marked with U's. The 'unobserved' data among the entries for Pittsburgh are also marked with U's. The unobserved Edinburgh data are represented by zero $|F_o|$ values.

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[*] These measures of goodness-of-fit are explicitly defined by Brown (1969), among others.

[†] Since the space group is noncentrosymmetric, it is important, at least in principle, to note that the Pittsburgh data are actually for reflections $\bar{h}kl$ rather than for hkl. The negative sign on $\bar{h}$ arises in the index transformation mentioned in an earlier footnote.

Table 3. *Structure parameters and their standard errors*

The four entries on successive lines for each atom give the Oak Ridge, Pittsburgh, Edinburgh, and average parameters (see text). The parameters β_{ij} are those of the temperature factor exp $[-\beta_{11}h^2-\beta_{22}k^2-\beta_{33}l^2-2\beta_{12}hk-2\beta_{13}hl-2\beta_{23}kl]$; the parameter B is that of the factor exp $[-B\lambda^{-2}\sin^2\theta]$.

ATOM	10^5X	10^5Y	10^5Z	$10^5\beta_{11}$	$10^5\beta_{22}$	$10^5\beta_{33}$	$10^5\beta_{12}$	$10^5\beta_{13}$	$10^5\beta_{23}$
C(1)	4551(15)	16629(9)	35309(25)	210(10)	111(4)	762(28)	13(5)	-67(14)	-40(9)
	4533(21)	16635(14)	35318(41)	252(15)	123(7)	1024(44)	5(8)	-64(22)	-65(15)
	4559(26)	16634(17)	35301(45)	296(18)	121(8)	919(51)	5(11)	-59(27)	-58(16)
AV	4547(11)	16631(7)	35310(19)						
C(2)	13137(16)	19093(10)	22034(25)	369(13)	107(4)	720(27)	18(6)	5(16)	-10(9)
	13115(22)	19100(15)	21983(40)	343(15)	136(7)	829(42)	-9(9)	34(23)	-18(14)
	13071(27)	19085(17)	21988(44)	370(19)	133(8)	711(48)	11(11)	-30(26)	2(17)
AV	13119(12)	19093(7)	22014(19)						
C(3)	24382(15)	18361(10)	30500(26)	256(10)	109(4)	781(27)	-18(6)	62(15)	0(9)
	24367(21)	18339(14)	30421(40)	290(14)	117(6)	959(41)	1(9)	87(22)	-26(14)
	24351(26)	18347(17)	30407(45)	305(18)	123(8)	787(49)	-7(11)	94(28)	-12(17)
AV	24373(11)	18352(7)	30463(20)						
C(4)	24606(15)	22962(10)	47333(25)	230(10)	119(4)	800(27)	-20(6)	7(15)	-17(9)
	24616(20)	22984(15)	47434(37)	194(12)	136(7)	1000(44)	-26(8)	77(21)	-5(15)
	24681(26)	22974(17)	47344(43)	259(17)	138(8)	817(50)	-23(11)	13(26)	-33(17)
AV	24622(11)	22970(7)	47361(19)						
C(5)	14990(14)	21339(10)	59560(24)	236(10)	99(4)	720(26)	-12(5)	9(14)	-1(9)
	14944(20)	21338(14)	59570(37)	269(14)	105(7)	874(42)	-28(8)	51(22)	10(14)
	15017(25)	21295(17)	59563(43)	292(18)	125(8)	786(49)	-19(11)	28(27)	-9(18)
AV	14982(10)	21331(7)	59563(18)						
C(6)	14001(17)	27052(10)	74245(25)	357(12)	137(5)	671(27)	-27(6)	-18(16)	-17(10)
	13965(23)	27025(16)	74417(37)	405(15)	144(7)	808(43)	-23(9)	-9(24)	-24(16)
	14004(29)	27063(18)	74292(45)	403(21)	145(9)	815(51)	-24(12)	0(30)	-43(19)
AV	13991(12)	27048(8)	74298(19)						
C'(1)	-1332(15)	5110(10)	48529(24)	257(10)	134(5)	603(25)	-21(6)	43(14)	-63(9)
	-1371(20)	5105(16)	48614(38)	223(13)	164(7)	805(41)	-23(8)	12(22)	-50(15)
	-1386(25)	5134(18)	48424(42)	270(17)	165(9)	589(45)	-8(11)	76(26)	-72(18)
AV	-1354(11)	5113(8)	48529(18)						
C'(2)	3507(15)	-2598(10)	52691(23)	280(11)	155(5)	527(25)	-24(6)	-2(14)	28(9)
	3459(21)	-2581(16)	52658(37)	273(13)	162(7)	882(44)	-52(9)	15(22)	13(15)
	3480(26)	-2565(18)	52730(41)	296(18)	178(9)	604(45)	-26(11)	16(26)	21(18)
AV	3489(11)	-2588(8)	52691(18)						
C'(3)	5779(16)	-6788(10)	35733(25)	293(11)	126(4)	671(26)	18(6)	-62(14)	18(9)
	5814(23)	-6803(15)	35727(40)	302(14)	148(7)	831(42)	15(9)	-54(22)	49(15)
	5767(27)	-6813(18)	35652(43)	331(19)	162(9)	613(46)	37(11)	5(26)	57(18)
AV	5786(12)	-6796(8)	35716(19)						
C'(4)	-4191(16)	-6898(10)	23848(25)	275(11)	107(4)	786(28)	-1(6)	-74(15)	-32(9)
	-4179(21)	-6930(14)	23695(39)	306(15)	137(7)	847(43)	10(9)	-22(22)	-52(15)
	-4158(26)	-6903(17)	23751(45)	320(19)	136(8)	808(51)	15(11)	-44(28)	-26(18)
AV	-4181(11)	-6908(7)	23794(19)						
C'(5)	-9084(15)	882(9)	21549(24)	211(10)	116(4)	704(25)	-5(5)	-58(14)	-31(9)
	-9074(20)	890(15)	21544(40)	232(14)	129(7)	978(44)	-1(8)	-30(23)	-26(15)
	-9007(25)	873(17)	21512(43)	240(17)	143(8)	755(48)	-2(10)	-27(26)	-34(18)
AV	-9067(11)	882(7)	21541(19)						
C'(6)	-20099(16)	529(11)	12532(32)	261(11)	150(5)	1201(36)	17(6)	-187(17)	-69(12)
	-20147(24)	508(15)	12507(47)	327(15)	140(7)	1392(51)	4(9)	-179(26)	-5(16)
	-20090(28)	532(19)	12497(52)	325(20)	171(9)	1154(62)	20(12)	-158(31)	-26(21)
AV	-20109(12)	524(8)	12518(24)						
O(1)	7041(10)	9135(7)	39699(18)	216(7)	105(3)	941(21)	-16(4)	3(11)	-44(7)
	7046(14)	9146(10)	39754(27)	198(10)	105(5)	1035(35)	-17(6)	-15(16)	-1(11)
	7043(17)	9142(12)	39735(31)	242(12)	116(6)	823(36)	-26(7)	29(20)	-20(13)
AV	7043(7)	9139(5)	39720(13)						
O(2)	12687(14)	14725(9)	6396(20)	453(11)	196(5)	754(22)	18(6)	-58(13)	-60(8)
	12685(18)	14739(12)	6494(30)	443(12)	189(6)	781(31)	24(7)	-149(19)	-28(12)
	12701(21)	14719(14)	6354(33)	421(16)	204(7)	825(38)	35(10)	-69(22)	-56(15)
AV	12689(10)	14728(6)	6412(15)						
O(3)	32883(13)	21113(9)	19564(23)	427(11)	191(4)	1216(27)	-98(6)	335(15)	-139(10)
	32828(17)	21097(12)	19566(31)	377(13)	191(6)	1292(37)	-94(7)	218(19)	-137(13)
	32865(21)	21091(15)	19510(37)	424(17)	210(7)	1147(44)	-91(10)	280(25)	-122(17)
AV	32863(9)	21104(6)	19554(17)						
O(4)	34141(13)	21500(11)	57459(23)	236(9)	298(6)	1098(27)	-29(6)	-59(14)	24(11)
	34223(15)	21507(13)	57363(32)	214(11)	272(7)	1083(33)	-4(7)	-52(17)	10(14)
	34171(20)	21523(16)	57356(36)	260(14)	296(9)	955(40)	-14(10)	-62(21)	43(16)
AV	34175(9)	21507(7)	57411(17)						
C(5)	4797(10)	21402(7)	50226(18)	212(7)	133(3)	830(20)	11(4)	-37(11)	-89(7)
	4800(14)	21431(10)	50250(29)	214(10)	129(5)	1009(30)	9(6)	26(15)	-114(11)
	4805(18)	21424(12)	50227(32)	266(13)	137(6)	866(36)	16(8)	-27(20)	-79(14)
AV	4799(7)	21414(5)	50231(14)						
O(6)	14820(14)	34548(8)	68429(22)	540(11)	127(4)	1125(26)	1(6)	-207(15)	-49(8)
	14827(18)	34534(11)	68400(31)	479(13)	123(5)	1190(38)	10(7)	-167(19)	-56(11)
	14786(23)	34549(13)	68414(36)	525(18)	133(6)	1101(43)	8(10)	-210(25)	-73(15)
AV	14816(10)	34544(6)	68418(16)						
O'(2)	13101(13)	-1918(9)	63102(19)	368(10)	268(5)	600(21)	-24(6)	-91(12)	35(9)
	13065(16)	-1895(13)	63182(29)	321(11)	267(7)	657(29)	5(8)	-119(16)	-2(12)
	13122(21)	-1918(15)	63075(31)	383(15)	285(9)	534(34)	-2(10)	-119(21)	18(15)
AV	13093(9)	-1912(7)	63116(14)						
C'(3)	9177(15)	-14203(8)	39899(22)	679(13)	157(4)	923(25)	132(6)	-224(16)	-19(9)
	9165(19)	-14182(12)	39798(29)	608(15)	178(6)	928(37)	119(8)	-196(21)	3(12)
	9219(25)	-14190(14)	39829(35)	649(20)	179(7)	921(41)	128(11)	-186(27)	21(16)
AV	9181(11)	-14195(6)	39856(16)						
O'(4)	-1315(14)	-9897(9)	6990(21)	421(11)	195(4)	960(25)	52(6)	-163(14)	-183(9)
	-1325(17)	-9884(12)	6971(30)	416(12)	180(6)	956(33)	48(7)	-151(19)	-156(12)
	-1238(21)	-9866(14)	6911(34)	434(16)	193(7)	952(41)	50(10)	-213(24)	-170(15)
AV	-1302(10)	-9887(6)	6969(15)						
O'(5)	-10804(10)	4499(7)	38138(18)	200(7)	148(3)	886(21)	-11(4)	17(11)	-94(8)
	-10804(13)	4470(11)	38080(26)	152(9)	155(5)	910(32)	-27(6)	-12(16)	-71(11)
	-10761(17)	4487(13)	38154(32)	204(12)	165(6)	878(37)	-11(8)	-1(19)	-76(14)
AV	-10796(7)	4490(5)	38125(13)						
O'(6)	-23748(13)	7726(9)	7166(23)	409(10)	190(5)	1075(27)	109(6)	-46(14)	-23(9)
	-23739(16)	7756(12)	7119(31)	330(11)	189(6)	1104(32)	87(7)	-43(18)	-16(13)
	-23785(21)	7739(14)	7080(35)	413(16)	196(7)	988(41)	82(10)	-90(23)	-2(15)
AV	-23752(9)	7737(6)	7134(16)						
O(W1)	16542(15)	-97(10)	-2079(24)	504(11)	228(5)	831(25)	38(6)	28(15)	-60(10)
	16497(19)	-47(13)	-2058(30)	489(13)	237(6)	763(35)	31(7)	59(18)	-82(12)
	16539(22)	-66(15)	-2094(34)	455(17)	247(8)	829(40)	22(10)	103(24)	-72(16)
AV	16528(10)	-76(7)	-2076(16)						
O(W2)	-7179(16)	15369(12)	-9882(31)	500(13)	271(6)	2036(42)	26(8)	-105(20)	306(14)
	-7245(19)	15376(14)	-9913(40)	445(14)	260(8)	1935(54)	33(8)	-80(25)	272(17)
	-7197(25)	15420(17)	-9884(47)	518(20)	280(10)	1790(60)	17(12)	-75(32)	269(22)
AV	-7205(11)	15383(8)	-9891(22)						

ATOM	10^4X	10^4Y	10^4Z	10B
H(C1)	-286(17)	1701(11)	3013(29)	11(4)
	-292(25)	1683(18)	3137(46)	16
	-253(46)	1698(31)	3139(80)	25
AV	-285(14)	1696(9)	3057(24)	
H(C2)	1180(18)	2441(12)	1912(30)	11(4)
	1156(28)	2377(19)	1895(49)	17
	1083(49)	2417(31)	1835(85)	25
AV	1165(15)	2423(9)	1901(25)	
H(C3)	2541(18)	1321(11)	3387(28)	11(4)
	2481(26)	1264(20)	3384(45)	17
	2610(49)	1305(32)	3331(79)	25
AV	2530(14)	1307(9)	3381(23)	
H(C4)	2452(19)	2816(13)	4363(32)	19(5)
	2379(24)	2830(19)	4424(46)	17
	2498(48)	2833(32)	4488(81)	25
AV	2431(14)	2822(10)	4393(25)	
H(C5)	1590(20)	1677(14)	6516(32)	20(5)
	1687(26)	1595(18)	6600(46)	15
	1604(47)	1635(32)	6560(83)	25
AV	1624(15)	1645(10)	6544(25)	
H(C6)	675(21)	2617(12)	7980(35)	19(5)
	695(28)	2536(19)	8116(52)	20
	705(48)	2521(32)	8073(82)	25
AV	685(16)	2586(10)	8029(28)	
H'(C6)	1978(20)	2627(13)	8243(35)	19(5)
	2068(28)	2597(18)	8283(47)	20
	2041(50)	2610(31)	8368(87)	25
AV	2012(16)	2616(10)	8268(27)	
H(C'1)	-329(18)	748(12)	5901(33)	14(4)
	-349(24)	726(18)	6037(50)	16
	-356(46)	685(31)	5851(86)	25
AV	-338(14)	736(10)	5933(26)	
H(C'2)	-155(20)	-503(13)	5925(33)	16(4)
	-176(27)	-520(19)	6050(48)	18
	-199(47)	-508(32)	5961(85)	25
AV	-166(15)	-508(10)	5965(26)	
H(C'3)	1138(18)	-420(12)	2984(31)	12(4)
	1151(25)	-396(18)	2844(47)	17
	1139(47)	-430(32)	2984(82)	25
AV	1142(14)	-415(10)	2944(25)	
H(C'4)	-950(21)	-1033(13)	2902(33)	19(5)
	-932(26)	-1016(20)	2946(49)	20
	-918(48)	-1027(31)	3042(83)	25
AV	-941(15)	-1028(10)	2928(26)	
H(C'5)	-435(17)	394(12)	1444(29)	11(4)
	-386(25)	393(19)	1468(47)	15
	-451(48)	448(32)	1519(82)	25
AV	-421(14)	398(9)	1456(24)	
H(C'6)	-1962(19)	-249(13)	180(33)	18(5)
	-1886(27)	-216(19)	357(48)	21
	-1987(46)	-198(32)	139(77)	25
AV	-1942(15)	-234(10)	226(26)	
H'(C'6)	-2547(23)	-190(13)	2076(34)	20(5)
	-2554(28)	-223(18)	2164(49)	21
	-2412(51)	-220(31)	2235(78)	25
AV	-2535(17)	-203(10)	2120(26)	
H(O2)	735(30)	1540(18)	169(47)	41(8)
	780(29)	1503(20)	205(53)	23
	582(47)	1575(31)	-64(82)	25
AV	729(19)	1532(12)	147(32)	
H(O3)	3384(21)	1846(14)	1216(36)	18(5)
	3365(27)	1847(23)	1069(56)	25
	3482(46)	1810(32)	1198(87)	25
AV	3389(16)	1842(11)	1177(29)	
H(O4)	3827(24)	2261(17)	5271(43)	30(7)
	3981(26)	2124(19)	4947(51)	22
	4050(50)	2350(35)	5380(85)	25
AV	3914(17)	2220(12)	5169(31)	
H(O6)	1053(27)	3548(18)	6109(45)	39(7)
	984(27)	3568(20)	6215(52)	21
	938(47)	3556(33)	6012(85)	25
AV	1007(18)	3557(12)	6134(32)	
H(O'2)	1811(30)	-55(21)	5681(52)	53(9)
	1988(28)	-128(20)	5575(52)	22
	1960(50)	-90(35)	5510(85)	25
AV	1913(19)	-94(13)	5609(34)	
H(O'3)	1125(21)	-1591(14)	3106(36)	17(5)
	1147(29)	-1629(21)	3149(55)	25
	1080(50)	-1600(35)	2950(85)	25
AV	1127(16)	-1602(11)	3100(29)	
H(O'4)	364(32)	-818(20)	466(54)	52(10)
	445(26)	-748(19)	440(51)	22
	470(50)	-690(35)	360(85)	25
AV	421(19)	-768(13)	438(34)	
H(O'6)	-2642(24)	967(15)	1467(38)	28(6)
	-2864(27)	1036(19)	1634(49)	22
	-2774(48)	988(30)	1701(77)	25
AV	-2744(17)	993(11)	1552(28)	
H(W1)	1524(24)	394(17)	91(41)	27(6)
	1519(29)	483(22)	84(52)	24
	1515(48)	446(32)	-40(79)	25
AV	1521(17)	429(12)	70(30)	
H'(W1)	1603(27)	-36(17)	-1167(46)	33(7)
	1622(31)	-2(22)	-1338(56)	24
	1640(48)	-27(33)	-1264(80)	25
AV	1616(19)	-24(12)	-1240(33)	
H(W2)	-925(28)	1890(18)	-1378(47)	38(7)
	-1020(33)	1862(25)	-1369(63)	33
	-976(47)	1976(32)	-1340(84)	25
AV	-967(20)	1897(13)	-1369(34)	
H'(W2)	-1178(28)	1323(19)	-385(48)	43(8)
	-1202(32)	1407(24)	-291(60)	33
	-1220(50)	1320(35)	-430(85)	25
AV	-1193(20)	1351(14)	-362(34)	

Table 4. *Observed and calculated structure factors*

See text for explanation.

K	FO	FC	SIG**
****	0 K	0	******
2	-173	158	29**
	163	160	**
	163	163	**
4	-727	701	110**
	646	707	**
	643	685	**
6	563	568	87**
	529	541	**
	567	572	**
8	108	112	39**
	107	115	**
	110	107	**
10	113	112	43**
	113	110	**
	118	118	**
12	201	206	45**
	205	203	**
	225	208	**
14	653	659	101**
	580	621	**
	639	638	**
16	342	345	64**
	308	314	**
	328	341	**
18	126	127	54**
	124	123	**
	118	127	**
20	106	102	54**
	93	94	**
	93	100	**
22	80	84	47**
	77	72	**
24	50	46	79**
26	32	27	119**
****	1 K	0	******
1	-287	247	45**
	271	253	**
	230	259	**
2	-187	170	32**
	185	173	**
	172	170	**
3	-899	860	136**
	824	858	**
	819	860	**
4	-535	516	82**
	498	527	**
	511	519	**
5	-1096	1077	165**
	961	1049	**
	1025	1064	**
6	169	160	33**
	176	176	**
	166	156	**
7	245	238	43**
	231	238	**
	244	262	**
8	225	238	42**
	207	214	**
	224	247	**
9	536	528	84**
	482	512	**
	530	516	**
10	206	202	39**
	192	178	**
	207	178	**
11	00	51	-25**
	54	49	**
	55	57	**
12	28	7	83**
	35	2	**
	52	18	**
13	112	106	36**
	111	98	**
	107	103	**
14	80	87	46**
	82	83	**
	73	72	**
15	99	98	42**
	88	82	**
	92	90	**
16	126	130	46**
	123	124	**
	128	127	**
17	96	101	58**
	89	89	**
	92	95	**
18	183	191	38**
	165	175	**
	172	181	**
19	0	26	-74**
	33	24	**
	25	20	**
20	0	13	-70**
	0	4	**
	70	9	**
21	0	19	-69**
	22	17	**
22	0	25	-59**
	22	23	**
23	82	81	77**
	27	37	**
24	155	148	39**
25	130	132	44**
26	171	169	35**
27	0	3	-76**
****	2 K	0	******
0	-588	533	89**
	530	555	**
	507	534	**
1	-454	420	70**
	409	415	**
	388	427	**
2	-716	682	109**
	632	668	**
	616	682	**
3	-437	433	68**
	418	418	**
	399	413	**
4	-806	795	122**
	750	764	**
	730	774	**
5	596	579	92**
	574	586	**
	568	564	**
6	264	267	45**
	275	264	**
	262	272	**
7	546	526	85**
	507	495	**
	538	551	**
8	268	263	47**
	269	245	**
	268	264	**
9	408	402	66**
	379	395	**
	399	370	**
10	319	315	53**
	289	299	**
	310	312	**
11	326	320	54**
	299	295	**
	321	315	**
12	27	42	92**
	43	39	**
	36	40	**
13	104	105	39**
	104	96	**
	107	98	**
14	130	130	38**
	128	118	**
	128	121	**
15	40	1	81**
	0	10	**
	70	3	**
16	174	172	43**
	152	160	**
	163	174	**
17	134	139	48**
	128	130	**
	132	138	**
18	12	6	-58**
	0	8	**
	70	2	**
19	68	69	55**
	69	65	**
	71	69	**
20	85	88	85**
	73	79	**
	76	77	**
21	48	43	79**
	40	38	**
22	102	96	35**
	85	85	**
23	0	17	-60**
24	20	1	-73**
25	85	80	52**
26	122	116	35**
****	3 K	0	******
1	-552	517	85**
	491	505	**
	487	504	**
2	-84	86	26**
	85	80	**
	79	78	**
3	115	115	33**
	131	140	**
	114	132	**
4	811	800	123**
	789	774	**
	731	784	**
5	171	169	34**
	192	181	**
	194	159	**
6	394	393	68**
	370	368	**
	369	384	**
7	110	108	31**
	115	109	**
	107	138	**
8	26	20	57**
	19	21	**
	17	30	**
9	184	192	38**
	183	184	**
	186	205	**
10	310	308	52**
	296	295	**
	302	302	**
11	197	199	39**
	191	183	**
	190	176	**
12	237	244	65**
	219	235	**
	232	219	**
13	161	165	39**
	152	152	**
	158	156	**
14	125	127	39**
	123	118	**
	121	117	**
15	152	152	43**
	141	140	**
	145	151	**
16	73	61	53**
	65	66	**
	62	63	**
17	291	299	49**
	262	271	**
	271	280	**
18	114	108	37**
	106	96	**
	106	102	**
19	46	42	72**
	47	43	**
	38	35	**
20	107	103	41**
	103	99	**
	99	101	**
21	108	105	34**
	100	96	**
22	66	62	46**
	63	57	**
23	0	23	-70**
24	31	40	119**
25	34	33	95**
26	79	74	45**
****	4 K	0	******
0	829	793	124**
	805	764	**
	736	792	**
1	204	200	37**
	195	198	**
	186	183	**
2	340	349	55**
	320	339	**
	310	350	**
3	299	304	50**
	298	302	**
	278	315	**
4	261	256	45**
	252	238	**
	248	231	**
5	330	318	55**
	318	300	**
	318	312	**
6	903	891	137**
	857	850	**
	819	882	**
7	457	438	73**
	430	415	**
	438	431	**
8	428	412	68**
	399	387	**
	410	383	**
9	640	652	99**
	580	613	**
	619	631	**
10	181	186	38**
	177	178	**
	181	177	**
11	299	302	51**
	285	205	**
	296	289	**
12	186	200	40**
	174	195	**
	183	195	**
13	46	46	67**
	49	44	**
	46	41	**
14	243	252	46**
	221	239	**
	232	258	**
15	118	118	46**
	115	112	**
	116	112	**
16	131	125	46**
	124	116	**
	122	129	**
17	74	82	47**
	81	77	**
	78	80	**
18	48	45	65**
	48	41	**
	43	37	**
19	60	61	57**
	63	56	**
	55	52	**
20	169	175	40**
	162	158	**
	162	167	**
21	36	48	82**
	49	47	**
22	28	7	103**
23	75	59	50**
24	3	14	-75**
25	135	128	33**
26	27	30	126**
****	5 K	0	******
1	488	476	77**
	456	444	**
	445	452	**
2	370	368	60**
	349	363	**
	343	363	**
3	332	328	55**
	321	320	**
	308	319	**
4	18	12	83**
	35	23	**
	26	2	**
5	274	278	48**
	269	240	**
	259	260	**
6	108	106	33**
	104	109	**
	101	102	**
7	6	2	-39**
	29	18	**
	60	5	**
8	156	154	35**
	160	157	**
	156	152	**
9	205	215	40**
	195	193	**
	194	204	**
10	28	23	-100**
	35	27	**
	45	33	**
11	126	127	37**
	124	120	**
	127	122	**
12	129	136	38**
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4	309	298	52**
	304	282	**
	298	303	**
5	658	648	102**
	598	617	**
	614	619	**
6	366	363	61**
	338	334	**
	357	349	**
7	162	151	34**
	161	146	**
	159	154	**
8	190	187	38**
	191	179	**
	188	178	**
9	212	216	41**
	205	198	**
	213	207	**
10	113	114	35**
	109	112	**
	111	107	**
11	86	87	39**
	83	88	**
	86	81	**
12	272	275	49**
	253	253	**
	261	256	**
13	47	54	68**
	56	52	**
	49	55	**
14	94	85	45**
	90	73	**
	91	81	**
15	84	87	53**
	84	87	**
	82	82	**
16	135	137	35**
	126	130	**
	129	134	**
17	56	47	56**
	56	51	**
	51	50	**
18	27	37	113**
	43	36	**
	36	31	**
19	0	32	-65**
	33	31	**
	30	28	**
20	45	47	60**
	54	44	**
21	103	92	34**
	87	83	**
22	73	73	44**
23	59	58	63**
24	62	62	65**
25	58	66	59**
26	69	74	52**
****	5 K	2	******
0	1054	1401	219**
	1243	1315	**
	1271	1356	**
1	300	296	51**
	282	276	**
	281	297	**
2	197	194	39**
	193	182	**
	185	190	**
3	205	192	40**
	206	183	**
	199	195	**
4	21	37	85**
	54	49	**
	34	39	**
5	309	295	52**
	298	287	**
	294	291	**
6	252	245	45**
	235	233	**
	237	248	**
7	352	345	58**
	328	330	**
	331	325	**
8	249	240	45**
	234	235	**
	238	244	**
9	168	157	37**
	152	157	**
	157	154	**
10	83	94	41**
	100	93	**
	100	89	**
11	76	70	43**
	77	68	**
	75	72	**
12	76	83	47**
	86	84	**
	79	80	**
13	198	197	43**
	183	182	**
	190	185	**
14	198	205	44**
	186	196	**
	197	206	**
15	53	49	54**
	57	47	**
	56	45	**
16	148	153	36**
	142	143	**

Table 4 (*cont.*)

K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**
	147	146	**		258	275	**	7	86	97	44**	3	113	112	41**
17	81	83	45**		282	281	**		94	88	**	4	128	129	40**
	78	74	**	9	155	161	41**		98	87	**	5	25	30	-74**
	81	79	**		151	150	**	8	169	170	37**	6	34	37	113**
18	69	65	49**		158	154	**		150	153	**	7	124	116	39**
	62	58	**	10	180	183	44**		163	160	**	8	64	55	60**
	64	57	**		174	173	**	9	188	185	39**	****	0 K	3	******
19	58	63	65**		180	175	**		177	177	**	1	298	296	50**
	63	55	**	11	169	169	42**		183	179	**		278	298	**
	64	63	**		155	152	**	10	92	90	42**		304	303	**
20	44	48	65**		164	153	**		86	84	**	2	162	155	34**
	47	42	**	12	137	138	35**		88	86	**		157	159	**
21	80	78	41**		131	126	**	11	59	69	61**		170	149	**
	71	70	**		134	132	**		64	62	**	3	391	379	63**
22	26	33	-69**	13	170	174	37**		67	71	**		380	368	**
23	43	39	84**		155	158	**	12	166	164	39**		400	395	**
24	21	35	-62**		167	172	**		153	151	**	4	1193	1172	181**
25	58	56	58**	14	59	64	57**		160	154	**		1005	1130	**
****	6 K	2	******		59	59	**	13	131	129	38**		1130	1115	**
0	94	94	34**		63	67	**		109	118	**	5	687	656	106**
	99	81	**	15	36	32	88**	14	152	151	34**		644	621	**
	89	80	**		41	37	**		128	142	**		684	635	**
1	527	513	82**		37	35	**	15	60	58	51**	6	26	24	62**
	502	481	**	16	46	39	72**		49	52	**		33	27	**
	495	503	**		49	38	**	16	88	86	40**		28	37	**
2	560	551	87**		38	36	**	17	55	59	67**	7	210	195	39**
	519	512	**	17	133	138	40**	18	74	68	55**		198	188	**
	519	536	**		123	126	**	19	89	88	40**		209	195	**
3	619	606	95**	18	95	91	36**	20	63	68	54**	8	349	345	57**
	567	579	**		81	78	**	21	75	67	46**		321	312	**
	580	603	**	19	85	80	39**	****	12 K	2	******		348	326	**
4	225	222	41**		63	70	**	0	86	91	42**	9	85	89	38**
	221	212	**	20	0	13	-67**		93	90	**		84	88	**
	221	225	**	21	44	53	82**		93	95	**		84	94	**
5	120	113	33**	22	26	23	121**	1	121	119	36**	10	238	234	44**
	120	109	**	23	75	76	45**		122	117	**		226	224	**
	119	100	**	24	46	35	72**		122	126	**		235	223	**
6	224	218	42**	****	9 K	2	******	2	143	145	36**	11	333	332	56**
	218	217	**	0	214	223	43**		184	138	**		315	311	**
	215	214	**		205	221	**		141	147	**		56	33	**
7	267	264	47**		211	214	**	3	42	51	75**		338	326	**
	255	249	**	1	168	171	39**		51	48	**	12	31	42	109**
	255	254	**		155	158	**		45	48	**		41	31	**
8	90	90	38**		161	162	**	4	112	112	36**		38	36	**
	86	82	**	2	134	137	36**		100	104	**	13	246	245	46**
	88	85	**		124	136	**		103	110	**		223	230	**
9	167	167	39**		128	129	**	5	71	77	50**		239	226	**
	167	163	**	3	143	143	38**		76	73	**	14	78	73	53**
	164	167	**		137	142	**		74	76	**		74	76	**
10	191	195	41**		139	138	**	6	123	127	38**		76	74	**
	185	188	**	4	181	182	40**		114	125	**	15	138	129	42**
	189	188	**		167	168	**		126	124	**		123	118	**
11	187	192	41**		176	181	**	7	184	186	40**		128	120	**
	173	174	**	5	231	242	46**		176	179	**	16	8	10	-54**
	181	184	**		226	226	**		184	186	**		0	2	**
12	49	50	70**		243	237	**	8	45	39	72**		17	9	**
	53	48	**	6	179	179	42**		37	38	**	17	84	77	40**
	50	48	**		168	171	**		36	35	**		78	69	**
13	62	65	63**		178	162	**	9	41	37	82**		72	68	**
	65	61	**	7	93	99	50**		40	35	**	18	81	79	46**
	65	68	**		97	91	**		38	40	**		77	76	**
14	76	77	54**		97	96	**	10	51	51	66**		75	72	**
	72	69	**	8	240	246	47**		43	32	**	19	103	95	41**
	71	75	**		223	227	**		42	41	**		103	87	**
15	61	63	51**		238	235	**	11	46	43	73**		97	91	**
	64	64	**	9	104	100	46**		40	36	**	20	65	70	60**
	62	64	**		91	92	**	12	95	96	36**		67	66	**
16	162	162	36**		96	105	**		85	87	**	21	58	58	52**
	148	148	**	10	66	73	64**	13	71	77	46**		59	53	**
	153	155	**		66	65	**		64	67	**	22	62	57	51**
17	155	154	37**		68	73	**	14	29	36	102**	23	80	84	50**
	138	145	**	11	254	263	45**		31	33	**	24	55	36	67**
	146	152	**		228	251	**	15	0	31	-70**	25	58	44	56**
18	91	94	45**		251	258	**	16	79	82	51**	26	64	54	53**
	89	81	**	12	25	21	-61**	17	33	33	115**	****	1 K	3	******
	90	83	**		29	28	**	18	73	71	46**	0	468	448	74**
19	62	52	46**		27	26	**	19	54	55	62**		430	437	**
	56	52	**	13	173	169	38**	20	101	99	39**		440	439	**
20	108	107	35**		150	161	**	****	13 K	2	******	1	329	314	54**
	97	96	**		163	172	**	0	53	44	63**		325	313	**
21	61	51	50**	14	133	131	38**		55	44	**		302	307	**
22	64	65	59**		120	125	**		52	48	**	2	271	276	47**
23	71	66	55**		129	130	**	1	36	27	85**		261	268	**
24	73	72	46**	15	167	169	39**		27	24	**		263	261	**
25	77	76	46**		149	156	**		31	31	**	3	25	26	53**
****	7 K	2	******		159	165	**	2	40	29	78**		33	22	**
0	36	31	64**	16	91	91	46**		38	29	**		30	26	**
	49	40	**		75	78	**		37	30	**	4	463	452	73**
	55	53	**	17	56	55	52**	3	115	112	38**		442	437	**
1	268	263	47**		48	49	**		109	109	**		459	446	**
	257	251	**	18	49	44	61**		111	109	**	5	341	331	57**
	256	255	**		41	41	**	4	47	48	71**		334	334	**
2	401	386	65**	19	0	11	-67**		52	47	**		338	325	**
	385	360	**	20	96	94	44**		51	48	**	6	511	514	81**
	380	378	**	21	107	111	43**	5	77	73	48**		486	508	**
3	133	127	35**	22	0	11	-63**		73	75	**		512	497	**
	129	117	**	23	28	37	116**		77	81	**	7	145	136	33**
	132	123	**	****	10 K	2	******	6	86	91	48**		144	138	**
4	64	72	48**	0	44	45	78**		86	92	**		148	125	**
	69	77	**		48	46	**		93	91	**	8	134	129	33**
	65	66	**		63	56	**	7	171	171	39**		134	127	**
5	360	365	59**	1	75	80	55**		161	158	**		136	129	**
	341	348	**		77	83	**		168	171	**	9	396	397	64**
	348	343	**		83	84	**	8	97	102	46**		369	372	**
6	76	77	41**	2	85	80	49**		91	97	**		390	386	**
	76	79	**		80	79	**	9	59	79	58**	10	197	194	39**
	72	75	**		87	70	**		81	77	**		180	182	**
7	102	107	37**	3	62	52	59**	10	0	10	-58**		191	181	**
	106	96	**		62	49	**		0	9	**	11	194	199	40**
	117	100	**		59	54	**	11	87	92	40**		182	191	**
8	290	289	51**	4	241	245	47**		77	83	**		195	192	**
	268	270	**		215	231	**	12	33	20	88**	12	209	209	43**
	277	284	**		230	239	**		25	27	**		192	200	**
9	47	38	61**	5	182	184	43**	13	0	32	-70**		207	203	**
	44	33	**		172	176	**	14	45	42	79**	13	244	243	46**
	44	42	**		180	181	**	15	11	22	-73**		205	228	**
10	148	149	39**	6	30	21	123**	16	47	45	67**		230	234	**
	139	138	**		38	18	**	17	55	61	60**	14	48	48	79**
	141	146	**		29	28	**	18	63	56	54**		52	45	**
11	191	199	43**	7	194	197	44**	****	14 K	2	******		55	50	**
	188	192	**		177	188	**	0	16	27	-72**	15	59	59	66**
	191	195	**		190	197	**		33	28	**		60	56	**
12	157	155	42**	8	242	243	43**		33	26	**		58	51	**
	139	152	**		220	227	**	1	51	45	69**	16	191	196	38**
	151	150	**		234	241	**		47	48	**		179	179	**
13	43	37	89**	9	97	94	39**	2	40	40	88**		181	184	**
	37	36	**		96	92	**		41	32	**	17	87	91	41**
	38	37	**		97	95	**	3	29	27	119**		84	85	**
14	127	133	36**	10	147	148	36**		31	31	**		83	83	**
	120	124	**		130	132	**	4	102	105	35**	18	54	57	61**
	131	126	**		142	138	**		106	99	**		63	56	**
15	86	96	44**	11	229	230	42**	5	132	124	33**		56	61	**
	92	91	**		203	215	**		114	112	**	19	33	21	96**
	92	89	**		223	225	**	6	32	50	96**		29	23	**
16	42	53	82**	12	61	59	55**		49	44	**		24	20	**
	59	48	**		56	56	**	7	0	28	-58**	20	115	109	41**
	51	49	**		58	61	**		29	24	**		112	98	**
17	127	133	39**	13	135	137	38**	8	103	102	37**	21	0	17	-56**
	128	122	**		120	122	**		91	96	**		19	18	**
	127	134	**		129	127	**	9	32	14	91**	22	137	132	34**
18	68	73	57**	14	128	129	39**		25	21	**	23	71	67	54**
	67	66	**		112	117	**	10	53	52	66**	24	40	46	97**
19	114	113	34**		122	130	**	11	52	44	68**	25	43	36	74**
	108	103	**	15	61	58	49**	12	65	68	59**	26	24	26	-67**
20	78	77	42**		61	57	**	13	105	104	42**	****	2 K	3	******
	59	68	**	16	87	91	39**	14	48	40	65**	0	913	917	139**
21	94	88	43**		73	79	**	15	21	21	-63**		816	891	**
22	46	45	81**	17	135	135	34**	16	54	47	62**		819	886	**
23	0	25	-61**		93	119	**	17	75	66	47**	1	142	135	33**
24	29	32	110**	18	104	106	40**	****	15 K	2	******		145	134	**
****	8 K	2	******	19	36	29	102**	0	63	57	49**		134	135	**
0	7	8	-50**	20	51	44	75**		54	47	**	2	265	256	46**
	52	17	**	21	0	30	-64**	1	47	45	64**		265	237	**
	30	16	**	22	10	12	-66**		47	39	**		242	240	**
1	286	292	50**	****	11 K	2	******	2	123	119	34**	3	665	662	102**
	278	279	**	0	53	58	74**		105	106	**		623	635	**
	283	276	**		65	61	**	3	77	75	43**		617	607	**
2	200	201	40**		60	63	**		70	67	**	4	157	163	35**
	184	196	**	1	117	116	45**	4	0	4	-58**		164	158	**
	193	195	**		114	110	**		0	8	**		153	171	**
3	148	153	37**		114	107	**	5	65	67	50**	5	420	405	68**
	150	153	**	2	237	236	47**		56	66	**		404	380	**
	146	141	**		236	229	**	6	0	19	-62**		403	402	**
4	220	224	42**		228	237	**	7	124	120	38**	6	601	599	93**
	208	216	**	3	51	51	74**	8	110	114	41**		556	555	**
	214	226	**		57	46	**	9	4	11	-72**		588	575	**
5	274	275	49**		48	50	**	10	74	67	53**	7	175	175	36**
	255	258	**	4	0	23	-75**	11	78	77	52**		171	159	**
	265	258	**		29	23	**	12	0	17	-62**		174	179	**
6	244	252	46**		38	24	**	13	75	70	46**	8	226	227	42**
	230	236	**	5	97	97	38**	14	83	72	43**		216	214	**
	238	242	**		90	91	**	15	61	53	57**		229	206	**
7	116	124	40**		96	94	**	****	16 K	2	******	9	164	166	36**
	120	116	**	6	118	119	36**	0	28	15	126**		153	159	**
	120	126	**		107	110	**	1	72	65	52**		161	169	**
8	291	295	52**		115	114	**	2	50	44	71**	10	49	46	54**

K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**
	53	35	**	****	5 K	3	******	14	74	76	47**		30	28	**
	47	46	**	0	60	65	39**		74	70	**	13	144	146	38**
11	105	98	38**		62	57	**		76	74	**		130	134	**
	98	106	**		58	83	**	15	157	157	37**		136	133	**
	101	96	**	1	344	326	56**		146	141	**	14	112	112	34**
12	268	258	48**		331	295	**		146	146	**		107	109	**
	241	244	**		321	303	**	16	136	130	37**	15	75	69	41**
	254	243	**	2	299	297	50**		124	125	**		68	63	**
13	286	288	52**		286	270	**		125	122	**	16	68	63	46**
	255	266	**		273	268	**	17	36	24	93**		62	57	**
	273	271	**	3	407	394	65**		31	21	**	17	78	78	49**
14	293	297	53**		398	373	**	18	90	94	38**	18	75	78	53**
	263	280	**		385	386	**		86	87	**	19	0	9	-73**
	283	291	**	4	210	208	40**	19	116	118	35**	20	28	23	110**
15	122	124	44**		267	199	**		105	105	**	21	56	49	59**
	112	110	**		202	217	**	20	76	75	55**	****	11 K	3	******
	113	113	**	5	79	86	37**	21	85	78	47**	0	46	66	66**
16	64	69	50**		80	77	**	22	41	32	74**		59	75	**
	63	62	**		72	67	**	23	53	51	61**		56	63	**
	62	63	**	6	17	30	-45**	24	51	46	66**	1	77	83	45**
17	153	148	36**		43	39	**	****	8 K	3	******		85	75	**
	136	136	**		30	31	**	0	187	186	40**		82	79	**
	143	142	**	7	76	75	42**		193	190	**	2	40	49	75**
18	68	74	52**		84	70	**		184	181	**		53	54	**
	68	65	**		212	216	**	1	142	149	38**		47	50	**
	68	69	**		77	72	**		147	145	**	3	122	123	36**
19	62	55	54**	8	376	379	62**		141	136	**		117	116	**
	52	49	**		344	362	**	2	15	28	-56**		118	122	**
	49	52	**		358	368	**		38	29	**	4	32	19	89**
20	63	57	46**	9	206	213	42**		40	36	**		25	19	**
	64	57	**		199	199	**	3	89	79	42**		21	20	**
21	32	33	88**		204	195	**		86	70	**	5	62	59	52**
	38	29	**	10	311	309	54**		83	76	**		73	57	**
22	67	72	55**		289	273	**	4	49	53	63**		62	58	**
23	51	43	71**		296	298	**		79	49	**	6	69	72	48**
24	38	15	96**	11	350	359	59**		85	54	**		69	68	**
25	31	40	104**		329	343	**	5	56	49	54**		69	67	**
26	0	9	-66**		339	343	**		56	49	**	7	100	106	40**
****	3 K	3	******	12	255	256	48**		47	49	**		100	93	**
0	219	212	41**		237	251	**	6	41	41	79**		97	102	**
	211	207	**		246	252	**		53	42	**	8	90	91	42**
	210	210	**	13	40	53	98**		46	44	**		89	85	**
1	444	446	71**		56	53	**	7	254	258	48**		87	89	**
	429	418	**		52	52	**		238	239	**	9	141	142	37**
	414	434	**	14	70	77	47**		252	255	**		136	128	**
2	320	321	54**		77	68	**	8	268	274	50**		137	131	**
	317	312	**		72	68	**		245	258	**	10	79	88	50**
	295	312	**	15	41	43	75**		258	270	**		83	88	**
3	457	446	73**		53	40	**	9	159	164	42**		82	89	**
	449	425	**		47	41	**		153	151	**	11	116	124	42**
	425	420	**	16	34	41	96**		158	152	**		118	114	**
4	103	103	33**		46	36	**	10	155	155	42**		115	121	**
	104	98	**		39	32	**		144	138	**	12	148	147	40**
	97	112	**	17	175	178	39**		148	146	**		145	138	**
5	487	480	76**		178	161	**	11	26	25	112**	13	67	69	47**
	462	450	**		171	175	**		40	27	**		68	64	**
	463	450	**	18	91	90	44**		29	28	**	14	69	65	46**
6	223	216	41**		89	84	**	12	210	205	40**		59	60	**
	229	215	**		88	87	**		190	194	**	15	72	65	45**
	214	216	**	19	69	72	42**		204	193	**	16	13	27	-69**
7	184	176	36**		70	66	**	13	167	163	37**	17	77	83	53**
	179	172	**	20	33	35	81**		147	149	**	18	62	55	63**
	172	166	**		27	28	**		157	149	**	19	47	46	68**
8	29	30	79**	21	51	36	67**	14	22	25	-66**	20	56	68	61**
	33	24	**	22	60	64	63**		37	28	**	****	12 K	3	******
	32	25	**	23	0	5	-73**		30	26	**	0	100	88	38**
9	261	256	47**	24	0	18	-63**	15	73	75	51**		97	86	**
	244	249	**	25	122	115	35**		76	69	**		94	89	**
	252	250	**	****	6 K	3	******		73	70	**	1	85	87	44**
10	293	295	51**	0	133	124	39**	16	52	51	69**		93	86	**
	272	277	**		128	102	**		51	50	**		89	81	**
	279	280	**		124	120	**	17	55	43	51**	2	145	140	37**
11	203	207	41**	1	105	103	34**		43	40	**		149	135	**
	190	189	**		111	99	**	18	90	94	38**		142	141	**
	196	204	**		102	96	**		80	83	**	3	44	53	80**
12	91	90	46**	2	257	257	46**	19	20	24	-66**		57	48	**
	93	81	**		253	238	**	20	60	62	63**		51	50	**
	91	83	**		247	242	**	21	74	75	54**	4	87	89	43**
13	353	354	60**	3	102	93	39**	22	38	25	80**		86	81	**
	320	328	**		108	96	**	23	29	33	114**		86	87	**
	330	335	**		109	103	**	****	9 K	3	******	5	94	98	42**
14	274	267	50**	4	179	177	37**	0	117	122	39**		94	92	**
	246	244	**		165	166	**		120	121	**		94	95	**
	253	250	**		172	172	**		120	121	**	6	48	54	75**
15	228	227	47**	5	176	172	37**	1	33	41	96**		54	53	**
	211	215	**		173	171	**		40	42	**		55	54	**
	213	211	**		170	168	**		36	43	**	7	12	11	-67**
16	75	74	46**	6	289	284	50**	2	180	183	42**		0	14	**
	77	67	**		274	272	**		176	180	**		17	12	**
	72	70	**		278	271	**		181	172	**	8	118	121	40**
17	47	48	71**	7	287	280	50**	3	69	72	67**		126	115	**
	47	41	**		274	262	**		71	71	**		120	125	**
	46	47	**		273	281	**		72	69	**	9	103	102	44**
18	0	17	-68**	8	607	610	94**	4	100	106	45**		109	98	**
	0	14	**		542	579	**		101	101	**		106	96	**
	17	15	**		580	578	**		102	101	**	10	92	91	36**
19	54	55	66**	9	238	241	46**	5	105	107	43**		76	85	**
	51	50	**		221	234	**		104	105	**	11	44	52	67**
	48	50	**		232	229	**		102	107	**		52	45	**
20	61	53	48**	10	70	64	54**	6	28	15	129**	12	52	49	58**
	57	51	**		74	63	**		22	9	**		48	47	**
21	35	37	87**		69	72	**		17	11	**	13	32	42	95**
	40	34	**	11	123	124	43**	7	41	50	95**		35	38	**
22	17	17	-68**		118	115	**		49	47	**	14	37	54	98**
23	64	71	59**		121	124	**		47	52	**	15	63	63	62**
24	0	5	-63**	12	90	85	49**	8	79	87	58**	16	83	81	49**
25	66	67	52**		84	82	**		87	88	**	17	68	68	49**
****	4 K	3	******		81	78	**		83	83	**	18	43	41	77**
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	289	263	**		38	15	**		276	295	**	****	13 K	3	******
	281	261	**		25	15	**		300	291	**	0	75	72	50**
1	593	573	92**	14	106	106	37**	10	153	157	36**		73	63	**
	542	544	**		106	104	**		141	145	**		71	74	**
	551	570	**		104	104	**		148	146	**	1	94	91	43**
2	186	183	38**	15	146	149	36**	11	113	119	37**		93	91	**
	194	184	**		142	141	**		107	111	**		93	83	**
	172	181	**		141	146	**		115	115	**	2	39	34	87**
3	112	113	31**	16	189	188	39**	12	0	17	-63**		44	32	**
	110	103	**		179	169	**		22	16	**		37	35	**
	102	107	**		177	174	**		16	19	**	3	27	37	125**
4	555	552	86**	17	50	56	69**	13	79	80	48**		41	38	**
	520	535	**		59	50	**		74	69	**		35	38	**
	528	527	**		51	55	**		76	76	**	4	61	65	57**
5	154	138	34**	18	147	139	39**	14	118	113	38**		66	64	**
	149	135	**		140	130	**		101	105	**		65	67	**
	145	140	**	19	59	63	49**		108	113	**	5	50	44	72**
6	380	372	61**		60	55	**	15	67	66	60**		52	44	**
	354	360	**	20	45	47	66**		71	67	**		50	42	**
	360	358	**		44	39	**	16	78	72	41**	6	207	201	42**
7	267	271	47**	21	65	58	56**		72	69	**		195	193	**
	260	261	**	22	107	104	42**	17	133	136	34**	7	86	90	42**
	254	271	**	23	31	25	99**		118	120	**		91	85	**
8	304	300	52**	24	41	29	80**	18	14	35	-68**	8	62	64	50**
	289	292	**	****	7 K	3	******	19	42	37	83**		71	66	**
	291	287	**	0	19	25	-49**	20	49	37	75**	9	139	138	34**
9	98	104	39**		40	42	**	21	22	6	-61**		129	127	**
	106	102	**		23	21	**	22	53	51	62**	10	70	65	47**
	101	117	**	1	65	64	42**	****	10 K	3	******		61	61	**
10	239	236	45**		76	62	**	0	168	162	42**	11	91	92	40**
	222	222	**		62	56	**		160	155	**		69	84	**
	228	217	**	2	242	241	44**		161	165	**	12	71	73	53**
11	283	284	50**		248	237	**	1	269	269	50**	13	43	46	83**
	262	262	**		232	231	**		260	258	**	14	33	46	114**
	274	276	**	3	312	310	53**		264	272	**	15	59	60	55**
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	271	278	**		304	308	**		51	31	**	17	60	63	57**
	275	273	**	4	272	270	48**		56	33	**	****	14 K	3	******
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	349	362	**		265	251	**		135	131	**		54	53	**
	367	378	**	5	258	263	47**		131	139	**	1	32	33	84**
14	110	112	45**		251	248	**	4	206	214	44**		40	35	**
	99	102	**		249	250	**		193	198	**	2	100	98	35**
	105	105	**	6	48	50	62**		199	200	**		96	92	**
15	91	88	39**		57	49	**	5	186	190	43**	3	126	120	33**
	87	81	**		59	54	**		182	182	**		109	110	**
	84	83	**	7	112	120	41**		179	188	**	4	65	65	48**
16	148	149	36**		120	119	**	6	212	214	40**		69	61	**
	140	136	**		114	117	**		202	200	**	5	169	168	35**
	140	143	**	8	260	263	48**		207	209	**		151	155	**
17	231	237	43**		247	247	**	7	167	171	36**	6	117	115	36**
	227	215	**		256	256	**		158	161	**		113	110	**
	218	222	**	9	301	305	54**		163	164	**	7	154	148	35**
18	117	121	40**		275	295	**	8	50	50	62**		129	129	**
	116	113	**		291	292	**		47	39	**	8	26	32	120**
	115	118	**	10	167	169	43**		49	40	**	9	105	100	41**
19	49	49	76**		160	162	**	9	101	101	39**	10	56	54	66**
	55	45	**		163	171	**		98	90	**	11	28	24	131**
20	75	70	41**	11	20	38	-76**		98	94	**	12	146	143	38**
	74	67	**		37	32	**	10	138	140	37**	13	65	57	50**
21	37	39	78**		37	31	**		137	136	**	14	48	27	67**
	41	38	**	12	58	56	51**		135	133	**	15	87	87	41**
22	42	35	82**		60	46	**	11	101	101	40**	16	11	30	-67**
23	30	22	117**		54	53	**		91	100	**	****	15 K	3	******
24	56	55	57**	13	126	127	35**		95	101	**	0	41	24	69**
25	0	18	-66**		114	118	**	12	0	29	-68**	1	27	14	108**
			**		118	123	**		38	30	**	2	89	85	81**

K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**	K	FO	FC	SIG**
3	137	131	35**		180	178	**	23	64	66	52**		75	77	**		34	35	**
4	88	84	46**		183	179	**	24	25	21	-66**	16	0	9	-67**	1	81	73	43**
5	83	74	47**	7	222	224	42**	****	5 K	4	******		0	8	**		61	68	**
6	125	125	39**		205	220	**	0	91	94	35**	17	99	104	36**		78	68	**
7	0	12	-74**		218	206	**		97	100	**		91	90	**	2	107	108	38**
8	114	117	42**	8	350	353	58**		84	95	**	18	45	39	64**		101	106	**
9	18	37	-76**		321	336	**	1	105	113	37**		37	37	**		104	108	**
10	103	97	44**		346	337	**		116	114	**	19	39	43	89**	3	133	125	36**
11	34	42	96**	9	280	287	49**		110	113	**	20	102	106	43**		119	116	**
12	108	114	37**		240	277	**	2	96	88	35**	21	38	11	95**		129	128	**
13	66	65	53**		273	261	**		101	83	**	22	66	68	50**	4	26	16	117**
14	4	34	-67**	10	146	144	38**		86	83	**	23	39	22	83**		9	16	**
****	16 K	3	******		129	131	**	3	166	167	37**	****	8 K	4	******		23	25	**
0	85	79	46**		139	141	**		164	168	**	0	101	115	43**	5	38	38	81**
1	45	48	82**	11	22	29	-58**		160	157	**		102	113	**		33	33	**
2	69	70	57**		35	32	**	4	145	148	36**		99	110	**		33	36	**
3	45	33	84**		36	35	**		139	142	**	1	205	204	42**	6	50	51	65**
4	81	78	50**	12	223	228	45**		138	147	**		193	191	**		53	54	**
5	92	91	47**		198	216	**	5	318	319	54**		195	187	**		51	55	**
6	42	40	91**		217	215	**		279	305	**	2	159	170	40**	7	73	78	53**
****	0 K	4	******	13	143	162	44**		299	303	**		154	163	**		77	72	**
0	260	266	47**		139	149	**	6	415	424	67**		160	160	**		80	78	**
	244	243	**		148	144	**		364	404	**	3	220	229	45**	8	81	76	46**
	250	254	**	14	135	139	44**		397	403	**		211	219	**		72	67	**
1	224	225	43**		118	126	**	7	106	111	38**		219	226	**		77	71	**
	210	194	**		127	130	**		101	107	**	4	123	122	42**	9	44	46	80**
	230	221	**	15	105	108	37**		99	98	**		120	121	**		47	42	**
2	312	300	52**		91	104	**	8	116	121	40**		123	116	**		48	43	**
	280	280	**		100	102	**		120	119	**	5	116	123	46**	10	87	91	49**
	317	282	**	16	81	76	44**		120	115	**		118	116	**		85	83	**
3	446	435	70**		65	67	**	9	335	339	57**		123	124	**	11	69	62	43**
	397	397	**		73	73	**		292	318	**	6	81	73	50**		61	63	**
	450	411	**	17	51	54	67**		318	329	**		75	77	**	12	89	87	39**
4	568	566	88**		46	42	**	10	56	48	66**		75	77	**		78	82	**
	505	533	**		47	49	**		48	53	**	7	131	141	44**	13	83	77	41**
	570	548	**	18	128	133	39**		50	54	**		129	142	**		68	75	**
5	218	214	41**		121	121	**	11	260	261	49**		139	139	**	14	65	79	44**
	201	191	**		124	127	**		231	246	**	8	107	117	52**	15	36	34	100**
	223	189	**	19	47	47	58**		248	249	**		103	111	**	16	40	48	96**
6	117	127	35**		44	43	**	12	119	121	45**		107	111	**	17	28	33	-62**
	118	118	**	20	99	91	35**		107	117	**	9	152	151	36**	18	10	30	-63**
	122	133	**		87	81	**		114	111	**		135	139	**	19	20	21	-65**
7	117	112	33**	21	0	27	-60**	13	32	31	92**		148	145	**	****	12 K	4	******
	112	111	**	22	51	57	73**		33	29	**	10	90	92	41**	0	22	11	-64**
	116	99	**	23	54	55	71**		31	26	**		87	93	**		29	13	**
8	29	18	79**	24	41	39	79**	14	112	117	38**		89	95	**		70	18	**
	35	27	**	25	99	95	39**		102	104	**	11	68	62	49**	1	70	79	51**
	32	24	**	****	3 K	4	******		111	109	**		59	66	**		75	74	**
9	200	193	40**	0	259	261	45**	15	137	143	38**		61	63	**		77	75	**
	118	164	**		246	259	**		129	132	**	12	152	150	38**	2	162	158	38**
	203	179	**		247	244	**		138	135	**		131	134	**		163	148	**
10	188	182	40**	1	306	305	51**	16	226	234	43**		143	138	**		159	151	**
	177	173	**		286	291	**		205	212	**	13	109	109	39**	3	11	39	-66**
	187	180	**		284	281	**		217	222	**		93	101	**		35	39	**
11	27	10	105**	2	115	113	33**	17	88	94	49**		103	106	**		36	37	**
	25	15	**		117	109	**		82	78	**	14	38	43	88**	4	176	176	39**
	25	27	**		110	103	**		86	83	**		43	38	**		173	172	**
12	88	95	50**	3	244	243	43**	18	145	147	33**		40	37	**		170	179	**
	90	90	**		288	238	**		134	131	**	15	48	44	73**	5	74	66	51**
	96	96	**		227	234	**	19	63	61	48**		48	45	**		62	62	**
13	55	54	74**	4	154	152	35**		62	56	**	16	49	38	59**		63	60	**
	66	65	**		154	147	**	20	59	57	59**		35	35	**	6	132	127	38**
	62	60	**		149	138	**	21	77	71	49**	17	131	122	34**		118	115	**
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	40	19	**		175	166	**	23	48	42	65**	18	98	101	42**	7	133	129	40**
	20	14	**		176	169	**	24	26	26	126**	19	84	77	46**		125	125	**
15	101	104	37**	6	170	179	37**	****	6 K	4	******	20	7	33	-74**	8	163	168	36**
	97	96	**		167	175	**	0	287	288	60**	21	38	26	87**		152	157	**
	104	93	**		166	177	**		270	286	**	22	76	69	45**	9	31	30	91**
16	130	126	37**	7	137	134	36**		275	285	**	****	9 K	4	******		33	30	**
	115	122	**		139	130	**	1	125	124	36**	0	0	14	-68**	10	24	5	118**
	125	119	**		134	148	**		129	118	**		25	14	**		16	11	**
17	113	109	39**	8	209	216	42**		121	115	**		70	11	**	11	75	65	43**
	104	103	**		194	202	**	2	282	282	50**	1	48	43	78**		59	61	**
	107	104	**		204	206	**		268	276	**		48	51	**	12	90	84	42**
18	66	67	53**	9	124	125	37**		271	275	**		49	46	**	13	84	86	47**
	64	65	**		115	122	**	3	191	187	39**	2	111	112	45**	14	42	35	88**
	59	58	**		122	126	**		185	189	**		104	110	**	15	0	23	-76**
19	0	6	-70**	10	178	178	40**		184	172	**		107	109	**	16	81	74	42**
	0	6	**		167	172	**	4	209	213	42**	3	101	109	46**	17	53	49	62**
20	92	81	37**		173	177	**		198	209	**		95	111	**	18	90	87	42**
	81	81	**	11	208	209	42**		202	216	**		99	112	**	****	13 K	4	******
21	108	100	34**		186	187	**	5	35	37	79**	4	15	24	-69**	0	48	50	75**
	88	91	**		193	192	**		47	47	**		33	29	**		46	50	**
22	30	18	113**	12	155	163	42**		46	39	**		28	23	**	1	111	104	40**
23	46	38	83**		142	152	**	6	78	69	44**	5	92	92	52**		100	102	**
24	64	65	52**		150	159	**		77	68	**		98	87	**	2	32	35	106**
25	27	34	125**	13	291	297	53**		74	66	**		97	91	**		35	31	**
****	1 K	4	******		246	271	**	7	195	203	42**	6	93	93	37**	3	41	41	69**
0	119	122	32**		270	279	**		179	193	**		89	79	**		43	46	**
	122	123	**	14	194	193	38**		189	196	**		92	89	**	4	108	108	35**
	118	113	**		173	185	**	8	134	132	39**	7	49	50	61**		106	102	**
1	157	153	36**		185	195	**		125	131	**		44	40	**	5	52	52	56**
	150	163	**	15	82	78	42**		135	126	**		46	43	**		48	47	**
	145	151	**		66	69	**	9	226	229	45**	8	80	79	41**	6	81	81	41**
2	114	115	32**		72	68	**		198	216	**		73	72	**		79	80	**
	113	116	**	16	104	109	40**		217	218	**		73	72	**	7	75	67	43**
	114	116	**		100	94	**	10	150	153	44**	9	66	68	50**		63	62	**
3	300	296	50**		100	102	**		138	149	**		69	68	**	8	173	168	36**
	267	282	**	17	95	96	43**		146	153	**		67	63	**		144	153	**
	290	284	**		95	86	**	11	120	122	45**	10	37	33	83**	9	10	22	-63**
4	153	137	35**		92	91	**		113	118	**		38	40	**		25	25	**
	145	127	**	18	105	108	42**		120	119	**		35	36	**	10	54	40	66**
	155	121	**		96	95	**	12	130	132	35**	11	110	110	40**	11	53	52	70**
5	282	267	48**		96	97	**		122	126	**		103	104	**	12	15	14	-72**
	257	258	**	19	80	72	38**		127	131	**		108	108	**	13	47	49	84**
	279	254	**		78	73	**	13	215	225	41**	12	124	129	39**	14	73	75	47**
6	207	197	40**	20	76	78	43**		196	206	**		117	123	**	15	101	94	37**
	187	181	**		73	70	**		208	206	**		121	129	**	16	79	73	46**
	206	180	**	21	6	6	-65**	14	110	109	38**	13	59	54	57**	****	14 K	4	******
7	41	45	57**	22	80	82	49**		94	98	**		49	44	**	0	94	94	38**
	51	51	**	23	15	25	-61**		105	102	**		51	47	**		83	89	**
	55	44	**	24	89	83	40**	15	184	187	39**	14	76	72	41**	1	73	72	43**
8	39	26	65**	25	52	52	67**		167	171	**		69	60	**		67	65	**
	37	30	**	****	4 K	4	******		180	174	**	15	59	61	51**	2	44	37	65**
	35	25	**	0	357	357	58**	16	117	117	40**		56	60	**		38	32	**
9	77	79	44**		331	379	**		104	112	**	16	36	32	82**	3	37	37	80**
	81	80	**		341	353	**		114	108	**		31	30	**		33	36	**
	88	81	**	1	315	312	53**	17	00	121	-16**	17	90	85	43**	4	44	42	69**
10	128	139	38**		292	313	**		102	112	**	18	49	46	74**		40	39	**
	125	135	**		297	300	**	18	55	57	54**	19	56	59	67**	5	133	129	35**
	129	134	**	2	164	158	37**		51	47	**	20	0	26	-62**		92	118	**
11	83	92	47**		165	158	**	19	121	122	35**	21	50	54	68**	6	21	26	-70**
	84	83	**		154	146	**		101	111	**	****	10 K	4	******	7	77	77	52**
	88	90	**	3	162	166	37**	20	89	84	44**	0	138	148	35**	8	50	39	74**
12	104	105	43**		167	171	**	21	75	71	52**		130	145	**	9	80	74	51**
	98	95	**		158	162	**	22	56	46	57**		134	154	**	10	102	100	44**
	98	95	**	4	104	105	50**	23	54	52	60**	1	127	139	35**	11	117	112	41**
13	193	194	44**		107	99	**	****	7 K	4	******		130	135	**	12	81	74	84**
	167	184	**		103	101	**	0	15	16	-52**		126	134	**	13	62	65	55**
	184	191	**	5	73	79	43**		33	7	**	2	47	61	63**	14	83	89	45**
14	170	178	44**		88	74	**		70	4	**		56	60	**	15	34	42	103**
	157	165	**		77	72	**	1	135	129	37**		51	55	**	****	15 K	4	******
	163	168	**	6	103	105	39**		133	117	**	3	107	107	36**	0	0	6	-70**
15	52	48	58**		105	94	**		130	126	**		101	100	**	1	64	64	60**
	53	47	**		103	99	**	2	119	123	38**		107	110	**	2	0	20	-71**
	46	51	**	7	100	101	38**		117	116	**	4	149	150	35**	3	41	44	92**
16	91	94	41**		104	96	**		113	119	**		141	138	**	4	160	154	38**
	81	87	**		103	95	**	3	96	100	41**		142	133	**	5	89	93	49**
	86	87	**	8	127	130	39**		99	97	**	5	156	166	36**	6	98	97	46**
17	79	83	46**		120	122	**		95	97	**		147	149	**	7	88	93	49**
	71	80	**		122	118	**	4	180	176	40**		150	161	**	8	89	89	49**
	74	83	**	9	47	50	69**		168	159	**	6	78	80	44**	9	146	143	33**
18	57	48	59**		63	47	**		176	158	**		73	78	**	10	58	49	56**
	48	44	**		54	51	**	5	177	172	40**		82	81	**	11	99	102	39**
	46	47	**	10	203	206	43**		169	164	**	7	29	19	101**	12	59	58	60**
19	39	52	90**		193	192	**		172	156	**		0	14	**	****	0 K	5	******
	44	45	**		199	194	**	6	204	202	42**		25	19	**	1	139	140	35**
20	49	51	59**	11	375	382	63**		186	188	**	8	72	71	46**		139	143	**
	52	44	**		330	367	**		196	193	**		67	65	**		144	137	**
21	91	93	40**		360	362	**	7	312	316	55**		71	69	**	2	79	77	37**
	69	86	**	12	212	218	46**		282	298	**	9	102	106	41**		73	66	**
22	71	68	53**		190	206	**		301	295	**		94	105	**		74	73	**
23	60	52	63**		201	202	**	8	169	175	43**		103	105	**	3	77	80	39**
24	28	40	114**	13	350	362	60**		154	167	**	10	38	15	82**		80	69	**
25	64	62	54**		322	339	**		166	166	**		0	8	**		78	73	**
****	2 K	4	******		334	333	**	9	315	321	56**		15	9	**	4	0	3	-49**
0	7	10	-41**	14	9	24	-61**		275	296	**	11	76	75	50**		25	17	**
	35	30	**		25	23	**		304	301	**		72	76	**		15	13	**
	49	41	**		27	27	**	10	133	132	43**		77	81	**	5	303	310	56**
1	345	350	56**	15	50	59	67**		119	119	**	12	90	79	44**		296	301	**
	317	339	**		61	53	**		124	121	**		75	76	**		314	306	**
	323	331	**		56	56	**	11	88	86	40**	13	78	78	42**	6	30	19	88**
2	367	367	60**	16	124	121	38**		86	80	**		73	73	**		44	25	**
	350	351	**		103	113	**		89	83	**	14	41	46	71**		36	35	**
	342	351	**		111	119	**	12	164	165	36**		40	40	**	7	157	163	37**
3	128	128	32**	17	24	26	-79**		148	147	**	15	33	48	95**		156	147	**
	123	117	**		27	24	**		158	150	**		35	42	**		156	157	**
	120	108	**		26	27	**	13	55	46	60**	16	54	53	67**	8	34	20	78**
4	421	402	67**	18	27	36	-73**		53	45	**	17	27	43	-74**		35	30	**
	382	399	**		40	36	**		49	46	**	18	54	37	68**		34	31	**
	397	386	**	19	112	112	35**	14	60	41	55**	19	0	14	-62**	9	275	263	50**
5	196	194	38**		108	106	**		47	44	**	20	33	20	99**		246	251	**
	183	175	**	20	20	12	-60**		43	40	**	****	11 K	4	******		268	243	**
	188	178	**	21	44	50	81**	15	80	84	48**	0	44	38	68**	10	0	17	-73**
6	187	191	38**	22	48	38	75**		77	76	**		37	47	**		0	13	**

Table 4 (*cont.*)

K	FO	FC	SIG**
			**
	70	3	**
11	348	355	60**
	310	339	**
	343	346	**
12	163	168	43**
	153	155	**
	157	161	**
13	97	104	38**
	93	97	**
	95	96	**
14	28	29	105**
	31	29	**
	30	27	**
15	47	62	72**
	63	57	**
	58	53	**
16	32	47	107**
	43	42	**
	42	40	**
17	85	78	46**
	79	66	**
	72	71	**
18	123	119	33**
	117	110	**
19	65	70	49**
	64	70	**
20	115	108	35**
21	25	7	-71**
22	55	55	72**
23	49	53	66**
24	54	48	64**
****	1 K	5	******
0	139	132	34**
	138	127	**
	132	139	**
1	181	179	37**
	173	181	**
	168	175	**
2	122	120	34**
	113	118	**
	112	105	**
3	177	178	37**
	172	166	**
	173	163	**
4	159	170	38**
	157	164	**
	162	163	**
5	160	160	36**
	150	161	**
	154	155	**
6	102	104	39**
	107	102	**
	106	104	**
7	159	158	37**
	145	148	**
	155	138	**
8	206	209	42**
	188	208	**
	204	201	**
9	119	111	40**
	108	111	**
	112	110	**
10	91	97	46**
	86	92	**
	87	92	**
11	163	162	42**
	148	150	**
	155	145	**
12	28	46	-80**
	48	48	**
	45	47	**
13	86	95	40**
	81	82	**
	82	82	**
14	69	83	49**
	70	76	**
	71	73	**
15	83	78	44**
	77	72	**
	75	77	**
16	92	91	43**
	92	87	**
	90	87	**
17	0	14	-67**
	0	11	**
	14	17	**
18	134	129	33**
	129	122	**
19	91	86	37**
	88	80	**
20	118	113	35**
21	90	89	45**
22	46	53	85**
23	36	26	87**
24	75	68	47**
****	2 K	5	******
0	59	65	43**
	62	63	**
	75	81	**
1	60	54	45**
	63	51	**
	54	51	**
2	215	215	41**
	199	221	**
	201	207	**
3	251	256	46**
	237	237	**
	238	221	**
4	158	155	37**
	151	158	**
	151	138	**
5	188	193	40**
	179	184	**
	184	181	**
6	80	83	42**
	80	86	**
	79	71	**
7	88	84	42**
	84	78	**
	83	82	**
8	189	195	41**
	182	184	**
	186	182	**
9	84	86	47**
	90	91	**
	87	84	**
10	187	192	43**
	177	183	**
	185	192	**
11	158	167	43**
	147	154	**
	152	163	**
12	157	165	43**
	144	152	**
	151	149	**
13	322	327	53**
	279	308	**
	301	310	**
14	95	93	39**
	8	89	**
	83	82	**
15	70	73	50**
	68	67	**
	67	73	**
16	96	98	41**
	91	93	**
	87	93	**
17	83	87	48**
	82	77	**
	75	78	**
18	85	85	38**
	82	80	**
19	37	28	78**
	31	27	**
20	56	36	62**
21	91	90	46**
22	55	54	70**
23	63	60	52**
24	36	35	93**
****	3 K	5	******
0	142	140	36**
	139	130	**
	139	130	**
	132	131	**
1	294	293	51**
	286	283	**
	277	275	**
2	177	167	38**
	174	171	**
	162	157	**
3	327	336	55**
	316	320	**
	307	319	**
4	179	180	38**
	167	173	**
	165	164	**

K	FO	FC	SIG**
			**
5	160	155	38**
	148	142	**
	149	146	**
6	221	228	43**
	211	214	**
	213	220	**
7	145	144	38**
	143	135	**
	138	130	**
8	95	103	44**
	97	102	**
	95	97	**
9	113	115	44**
	109	117	**
	105	104	**
10	193	198	43**
	181	188	**
	181	184	**
11	139	145	43**
	131	137	**
	136	144	**
12	81	81	40**
	73	78	**
	74	78	**
13	112	115	36**
	100	104	**
	100	101	**
14	53	52	63**
	47	58	**
	50	53	**
15	44	61	78**
	62	49	**
	50	53	**
16	140	147	38**
	139	133	**
	133	137	**
17	85	81	47**
	77	75	**
18	91	84	36**
	87	79	**
19	90	85	38**
	81	80	**
20	91	91	43**
21	43	29	86**
22	103	94	36**
23	47	46	69**
24	41	37	82**
****	4 K	5	******
0	95	96	38**
	94	99	**
	88	91	**
1	279	290	49**
	270	275	**
	263	269	**
2	271	272	48**
	260	261	**
	258	264	**
3	134	134	37**
	133	136	**
	127	133	**
4	454	458	73**
	413	438	**
	433	436	**
5	371	377	62**
	334	359	**
	352	364	**
6	226	232	44**
	214	226	**
	217	221	**
7	189	191	41**
	173	173	**
	175	176	**
8	87	81	47**
	84	82	**
	79	78	**
9	267	277	50**
	249	269	**
	256	256	**
10	168	169	41**
	160	165	**
	162	165	**
11	88	86	50**
	77	81	**
	77	82	**
12	36	38	76**
	33	37	**
	32	28	**
13	139	138	35**
	124	134	**
	130	138	**
14	14	31	-63**
	27	32	**
	27	30	**
15	102	104	80**
	95	97	**
	97	99	**
16	116	119	41**
	119	117	**
	113	119	**
17	43	45	65**
	38	35	**
18	57	61	54**
	64	58	**
19	52	40	57**
20	63	59	58**
21	88	87	49**
22	44	49	75**
23	54	40	63**
****	5 K	5	******
0	28	38	-88**
	48	39	**
	54	47	**
1	365	363	61**
	345	354	**
	344	346	**
2	109	111	40**
	109	97	**
	103	103	**
3	106	105	41**
	109	109	**
	106	108	**
4	526	536	83**
	467	510	**
	498	499	**
5	385	400	64**
	357	372	**
	365	378	**
6	399	404	66**
	353	384	**
	379	385	**
7	134	135	43**
	132	125	**
	128	134	**
8	311	312	55**
	284	289	**
	296	291	**
9	92	86	50**
	88	77	**
	85	89	**
10	147	156	45**
	147	145	**
	148	146	**
11	116	118	36**
	114	115	**
	115	119	**
12	89	93	42**
	82	82	**
	85	81	**
13	36	42	88**
	49	42	**
	40	43	**
14	76	82	52**
	73	80	**
	77	77	**
15	61	59	61**
	60	54	**
	53	54	**
16	52	58	71**
	55	52	**
17	23	31	-56**
	38	28	**
18	54	55	57**
	51	51	**
19	133	131	37**
20	75	74	53**
21	92	90	47**
22	30	24	111**
23	48	53	73**
****	6 K	5	******
0	50	47	69**
	54	41	**
	49	47	**
1	460	466	74**
	419	451	**
	437	449	**
2	198	203	42**

K	FO	FC	SIG**
			**
	192	198	**
	191	198	**
3	238	250	46**
	221	241	**
	230	229	**
4	189	189	43**
	178	177	**
	179	177	**
5	98	100	45**
	94	94	**
	94	92	**
6	29	18	121**
	35	20	**
	18	14	**
7	108	114	45**
	106	110	**
	107	111	**
8	139	146	43**
	132	148	**
	138	144	**
9	166	167	42**
	152	156	**
	153	147	**
10	143	140	35**
	127	130	**
	135	135	**
11	78	78	42**
	77	72	**
	73	72	**
12	151	149	36**
	135	135	**
	137	138	**
13	155	159	38**
	152	150	**
	150	150	**
14	101	94	41**
	92	87	**
	93	89	**
15	86	87	46**
	82	77	**
	80	84	**
16	87	81	37**
	77	80	**
17	8	20	-58**
	33	20	**
18	60	56	51**
19	40	56	92**
20	113	112	42**
21	54	63	61**
22	52	45	66**
****	7 K	5	******
0	214	217	45**
	205	213	**
	203	208	**
1	102	100	43**
	99	96	**
	96	88	**
2	180	178	43**
	176	172	**
	174	176	**
3	199	202	43**
	190	196	**
	189	195	**
4	92	93	51**
	100	92	**
	90	86	**
5	273	278	51**
	257	258	**
	266	257	**
6	190	200	44**
	183	187	**
	186	187	**
7	64	58	62**
	66	70	**
	62	67	**
8	171	171	36**
	161	161	**
	168	164	**
9	49	53	62**
	63	53	**
	57	53	**
10	130	136	36**
	121	127	**
	127	125	**
11	16	17	-61**
	0	8	**
	16	14	**
12	42	38	76**
	46	36	**
	41	38	**
13	88	91	44**
	84	85	**
	88	92	**
14	0	14	-66**
	0	5	**
	13	3	**
15	71	62	42**
	63	61	**
16	29	22	100**
	27	30	**
17	150	143	34**
	109	130	**
18	0	7	-70**
19	48	44	78**
20	74	64	44**
21	75	68	45**
22	43	49	79**
****	8 K	5	******
0	86	91	56**
	93	84	**
	92	94	**
1	148	163	43**
	150	163	**
	146	147	**
2	202	212	44**
	190	202	**
	196	199	**
3	80	85	56**
	87	88	**
	80	89	**
4	205	216	45**
	190	206	**
	198	203	**
5	46	49	62**
	43	45	**
	44	45	**
6	59	48	49**
	52	45	**
	51	44	**
7	78	76	43**
	80	73	**
	79	75	**
8	18	25	-60**
	43	30	**
	37	35	**
9	108	109	38**
	100	104	**
	106	105	**
10	57	51	56**
	59	52	**
	48	49	**
11	56	44	58**
	48	40	**
	47	43	**
12	123	123	39**
	122	118	**
	118	113	**
13	65	62	57**
	59	58	**
14	123	123	33**
	111	114	**
15	41	28	71**
	25	31	**
16	118	116	36**
	88	107	**
17	29	29	121**
18	78	79	53**
19	26	53	-79**
20	17	36	-64**
21	72	65	48**
****	9 K	5	******
0	154	156	35**
	144	157	**
	185	184	**
1	66	52	48**
	62	52	**
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	87	84	**
	83	78	**
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	38	37	**
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K	FO	FC	SIG**
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5	180	186	37**
	168	174	**
	175	180	**
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	77	67	**
	78	70	**
7	55	60	59**
	67	60	**
	63	62	**
8	92	97	41**
	86	92	**
	86	94	**
9	54	51	60**
	54	47	**
	50	51	**
10	56	52	62**
	55	47	**
	53	48	**
11	149	143	38**
	136	136	**
	137	139	**
12	135	133	33**
	129	127	**
13	70	69	44**
	64	65	**
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	60	62	**
15	25	26	121**
16	27	46	134**
17	56	55	67**
18	34	18	108**
19	57	53	58**
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	81	71	**
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	53	49	**
	51	49	**
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	46	28	**
	43	38	**
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	127	134	**
	129	140	**
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	97	99	**
	103	108	**
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	60	53	**
	59	56	**
7	98	110	43**
	102	112	**
	104	102	**
8	113	96	39**
	102	87	**
	98	85	**
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	29	24	**
	26	24	**
10	101	102	44**
	100	95	**
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	65	54	**
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	76	78	**
13	63	63	50**
	56	58	**
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16	53	52	72**
17	29	32	109**
18	44	48	74**
19	56	57	60**
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	137	133	**
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	53	50	**
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	46	43	**
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	35	29	**
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	47	51	**
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13	0	25	-70**
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15	35	18	108**
16	56	63	59**
17	0	18	-66**
18	150	150	35**
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	80	72	**
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	85	75	**
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	51	48	**
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	77	70	**
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	44	38	**
9	106	101	37**
	86	87	**
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	49	52	**
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8	24	24	-71**
9	132	130	38**
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12	61	61	53**
13	92	95	41**
14	44	49	77**
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5	28	34	-77**
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K	FO	FC	SIG**
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9	150	152	34**
10	94	85	38**
11	30	43	110**
12	72	72	49**
13	0	9	-68**
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3	91	81	47**
4	64	66	62**
6	157	143	36**
7	125	118	36**
8	51	45	69**
9	52	44	68**
10	46	33	77**
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	181	180	**
	177	164	**
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	210	235	**
	232	234	**
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	53	54	**
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	182	193	**
	197	194	**
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	248	266	**
	277	264	**
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	166	186	**
	179	176	**
6	234	247	50**
	217	226	**
	238	227	**
7	155	157	42**
	148	160	**
	156	151	**
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	113	126	**
	120	127	**
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	54	48	**
12	33	37	86**
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	21	31	**
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	75	71	**
	74	75	**
15	34	49	106**
	54	44	**
	42	46	**
16	67	64	43**
	66	60	**
17	190	181	36**
	172	174	**
18	113	114	36**
	107	102	**
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20	27	22	133**
21	20	1	-62**
22	35	31	95**
23	0	24	-68**
****	1 K	6	******
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	40	29	**
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	122	121	**
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	177	185	**
	182	183	**
3	183	181	40**
	173	178	**
	179	180	**
4	188	198	41**
	175	178	**
	183	182	**
5	135	141	39**
	123	139	**
	134	131	**
6	85	76	48**
	82	76	**
	80	74	**
7	150	148	41**
	135	137	**
	140	140	**
8	134	149	43**
	131	138	**
	136	141	**
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	92	87	**
	92	91	**
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	48	48	**
	47	44	**
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	64	69	**
	60	68	**
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	120	129	**
	120	126	**
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	86	90	**
	83	91	**
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	27	23	**
16	113	110	33**
	110	105	**
17	128	129	34**
	125	121	**
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	29	23	**
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22	63	54	53**
23	38	28	89**
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	62	56	**
	55	49	**
4	152	155	39**
	147	145	**
	144	148	**
5	191	196	42**
	172	192	**
	179	181	**
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	94	108	**
	92	91	**
7	119	115	42**
	123	112	**
	117	107	**
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	130	133	**
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	95	106	**
	97	101	**
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	106	108	**
	105	105	**
12	189	193	38**
	175	176	**

K	FO	FC	SIG**
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	173	174	**
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	102	100	**
	101	96	**
14	62	57	56**
	55	55	**
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15	36	42	98**
	44	44	**
	38	31	**
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22	57	55	58**
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	173	170	**
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	205	204	**
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5	150	155	41**
	150	144	**
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6	96	85	51**
	91	94	**
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7	123	123	42**
	117	114	**
	112	108	**
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	129	135	**
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9	98	98	38**
	94	89	**
	88	82	**
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	19	13	**
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	33	37	**
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	51	44	**
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	75	71	**
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21	110	107	36**
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3	293	308	53**
	278	300	**
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	171	172	**
	163	168	**
5	165	171	42**
	167	167	**
	161	156	**
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	91	78	**
	87	76	**
7	76	84	58**
	87	87	**
	77	80	**
8	194	201	38**
	194	198	**
	183	190	**
9	106	109	37**
	108	111	**
	104	112	**
10	112	112	36**
	109	107	**
	105	108	**
11	116	114	37**
	115	113	**
	111	112	**
12	165	169	38**
	161	157	**
	158	154	**
13	109	109	40**
	106	102	**
	101	101	**
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	29	31	**
	32	30	**
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	73	66	**
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	73	60	**
17	104	106	36**
	92	96	**
18	93	87	42**
19	17	22	-72**
20	25	14	-76**
21	144	143	34**
22	104	102	39**
****	5 K	6	******
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	51	47	**
	45	42	**
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	229	236	**
	226	226	**
2	363	363	62**
	342	355	**
	336	343	**
3	309	322	55**
	284	302	**
	290	300	**
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	118	121	**
	111	112	**
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	173	169	**
	169	174	**
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	37	33	**
7	218	227	40**
	210	211	**
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	57	58	**
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9	92	90	40**
	93	82	**
	88	80	**
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	108	110	**
	106	112	**
12	38	41	82**
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13	112	104	40**
	112	108	**
	103	103	**

K	FO	FC	SIG**
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	52	45	**
15	47	58	61**
	60	53	**
16	60	56	48**
	56	49	**
17	63	65	59**
18	45	54	82**
19	40	32	95**
20	28	11	115**
21	148	147	35**
****	6 K	6	******
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	249	272	**
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	114	114	**
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	112	107	**
	108	109	**
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****	7 K	6	******
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	76	74	**
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	91	90	**
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	260	262	**
	258	253	**
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	44	48	**
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	51	37	**
	41	40	**
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	123	126	**
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	46	47	**
	41	49	**
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	64	59	**
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17	77	77	52**
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19	46	41	70**
20	58	59	60**
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	108	114	**
	104	108	**
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	73	74	**
	71	72	**
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	98	93	**
	99	98	**
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	77	78	**
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	107	108	**
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	38	37	**
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14	75	77	45**
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16	41	38	89**
17	54	49	70**
18	31	39	100**
19	0	17	-66**
****	9 K	6	******
0	0	13	-67**
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	22	26	**
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	77	81	**
	79	79	**
2	34	24	90**
	27	25	**
	26	23	**
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	80	86	**

K	FO	FC	SIG**
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	164	164	**
	161	171	**
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	120	112	**
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	82	81	**
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	112	109	**
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16	72	67	47**
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	47	42	**
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14	52	41	60**
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	73	71	**
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6	20	4	-69**
7	54	57	67**
8	63	62	60**
9	116	112	41**
10	87	72	47**
11	26	38	-74**
12	72	74	48**
13	45	40	72**
14	13	19	-67**
15	25	30	-69**
****	13 K	6	******
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3	65	61	56**
4	17	11	-70**
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6	47	32	77**
7	64	62	61**
8	56	51	68**
9	51	55	64**
10	95	92	38**
11	86	81	42**
12	93	90	41**
13	47	49	73**
****	14 K	6	******
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3	77	74	53**
4	97	97	46**
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6	51	50	64**
7	31	30	101**
8	41	28	79**
9	27	34	128**
10	83	81	45**
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6	29	32	135**
7	110	103	41**
****	0 K	7	******
1	116	121	50**
	112	101	**
	112	109	**
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	178	186	**
	184	180	**
3	42	51	93**
	56	48	**
	54	52	**
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	209	215	**
	208	200	**
5	107	107	44**
	93	104	**
	95	100	**
6	11	3	-59**
	38	6	**
	22	8	**
7	108	113	43**
	102	105	**
	98	103	**
8	113	103	37**
	108	112	**
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	57	44	**
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	31	22	**
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11	73	75	51**

K	FO	FC	SIG**
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	77	68	**
	71	75	**
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	184	171	**
	159	162	**
13	94	94	45**
	101	87	**
	83	87	**
14	25	3	104**
	16	8	**
15	0	0	-55**
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16	52	54	59**
	55	46	**
17	35	37	99**
18	23	7	-71**
19	63	43	61**
20	80	76	45**
21	36	23	94**
****	1 K	7	******
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	150	157	**
	147	152	**
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	326	352	**
	310	335	**
2	133	139	43**
	120	131	**
	123	127	**
3	152	160	43**
	150	160	**
	145	145	**
4	165	174	44**
	165	161	**
	159	158	**
5	122	132	35**
	121	124	**
	118	118	**
6	87	95	39**
	88	91	**
	84	85	**
7	78	84	42**
	83	86	**
	78	84	**
8	36	22	85**
	31	26	**
	25	26	**
9	63	64	52**
	72	61	**
	61	67	**
10	59	53	56**
	64	50	**
	54	47	**
11	72	69	48**
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	62	65	**
12	33	45	103**
	43	40	**
	39	38	**
13	92	91	43**
	93	90	**
14	24	20	107**
	16	19	**
15	15	28	-57**
	19	27	**
16	17	22	-59**
	19	23	**
17	41	39	86**
18	90	79	45**
19	73	75	56**
20	38	27	87**
21	79	69	45**
****	2 K	7	******
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	84	82	**
	76	76	**
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	49	44	**
	40	38	**
2	97	98	48**
	100	94	**
	91	100	**
3	195	205	45**
	185	200	**
	181	190	**
4	121	121	46**
	105	99	**
5	86	85	39**
	88	87	**
	80	80	**
6	62	60	49**
	54	53	**
	52	56	**
7	153	153	36**
	147	153	**
	140	147	**
8	170	169	37**
	169	168	**
	157	148	**
9	158	152	37**
	152	145	**
	143	140	**
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11	63	56	54**
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	55	51	**
12	34	36	96**
	29	39	**
	30	35	**
13	57	53	64**
	56	51	**
14	27	26	97**
	29	31	**
15	30	37	94**
	38	39	**
16	50	38	59**
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18	83	75	47**
19	62	59	52**
20	57	68	59**
21	57	56	60**
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	54	53	**
	55	51	**
1	118	121	46**
	120	125	**
	110	114	**
2	140	137	43**
	132	128	**
	123	123	**
3	64	66	49**
	74	63	**
	63	65	**
4	181	186	37**
	167	172	**
	163	164	**
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	33	28	**
	20	20	**
6	122	128	35**
	121	121	**
	113	125	**
7	87	87	40**
	83	83	**
	76	81	**
8	42	50	75**
	52	58	**
	46	53	**
9	148	148	36**
	142	139	**
	128	137	**
10	106	105	39**
	102	104	**
	95	105	**
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	60	57	**
	57	59	**
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	54	45	**
	46	48	**
13	75	70	39**
	70	72	**
14	38	42	74**
	46	44	**
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	25	26	**
16	43	48	79**
17	48	46	78**
18	71	65	56**
19	100	101	38**
20	108	108	37**
21	40	41	87**
			**

K	FO	FC	SIG**
			**
****	4 K	7	******
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	56	52	**
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	92	91	**
	84	82	**
2	89	91	39**
	91	84	**
	78	76	**
3	104	106	38**
	104	102	**
	97	111	**
4	126	125	36**
	123	127	**
	115	116	**
5	146	147	36**
	148	148	**
	136	141	**
6	203	206	39**
	197	202	**
	185	182	**
7	111	103	39**
	114	107	**
	106	97	**
8	75	81	49**
	81	78	**
	74	65	**
9	16	30	-64**
	33	30	**
	26	29	**
10	54	38	61**
	47	38	**
	37	32	**
11	25	25	-65**
	29	22	**
	25	20	**
12	67	61	53**
	59	56	**
13	50	57	56**
	56	55	**
14	42	33	66**
	41	34	**
15	85	77	38**
	73	80	**
16	130	126	37**
17	130	132	40**
18	109	107	43**
19	80	76	44**
20	88	85	44**
****	5 K	7	******
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	38	20	**
	46	25	**
1	93	93	38**
	96	96	**
	94	89	**
2	57	61	56**
	75	68	**
	61	60	**
3	67	68	49**
	73	70	**
	67	66	**
4	128	136	37**
	128	131	**
	124	118	**
5	211	218	40**
	201	213	**
	199	208	**
6	91	86	42**
	95	90	**
	89	81	**
7	185	189	39**
	182	180	**
	169	171	**
8	100	105	41**
	103	107	**
	98	100	**
9	113	112	39**
	111	112	**
	104	102	**
10	167	168	39**
	169	168	**
	156	166	**
11	30	39	115**
	38	38	**
12	37	41	75**
	44	41	**
13	125	120	34**
	117	112	**
14	78	74	41**
	66	67	**
15	99	94	41**
16	48	45	77**
17	58	59	66**
18	73	76	46**
19	14	16	-66**
20	84	89	44**
****	6 K	7	******
0	5	4	-61**
	35	20	**
	58	36	**
1	138	144	36**
	132	136	**
	126	128	**
2	84	84	73**
	43	42	**
	40	35	**
3	29	35	108**
	43	29	**
	28	29	**
4	127	133	37**
	123	118	**
	118	117	**
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	63	55	**
	56	53	**
6	70	62	49**
	69	61	**
	63	58	**
7	86	79	43**
	85	74	**
	79	74	**
8	55	42	60**
	48	45	**
	42	44	**
9	59	51	58**
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	49	52	**
10	37	23	89**
	22	22	**
11	62	55	46**
	62	60	**
12	30	23	91**
	29	22	**
13	52	61	58**
	54	56	**
14	66	55	55**
15	123	124	39**
16	51	37	72**
17	119	125	35**
18	156	155	34**
19	70	69	50**
****	7 K	7	******
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	123	120	**
	120	113	**
1	114	115	43**
	115	109	**
	107	107	**
2	74	76	50**
	77	75	**
	74	73	**
3	81	79	48**
	84	86	**
	81	79	**
4	57	54	61**
	63	53	**
	56	54	**
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	25	14	**
	19	14	**
6	128	131	39**
	122	124	**
	119	123	**
7	68	65	61**
	63	58	**
	59	58	**
8	21	22	-71**
	22	19	**
	18	17	**
9	6	10	-53**
	22	16	**
10	66	60	46**
	64	62	**
11	120	110	35**

K	FO	FC	SIG**
			**
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12	70	67	46**
	59	64	**
13	87	79	43**
14	48	53	79**
15	69	75	60**
16	46	45	81**
17	39	26	82**
18	0	15	-67**
****	8 K	7	******
0	92	105	45**
	99	104	**
	95	95	**
1	0	34	-67**
	31	24	**
	28	21	**
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	41	33	**
	33	40	**
3	183	187	40**
	200	186	**
	178	180	**
4	27	22	124**
	22	22	**
	22	28	**
5	140	137	38**
	145	130	**
	130	123	**
6	77	82	49**
	80	71	**
7	23	30	-53**
	33	23	**
8	59	56	49**
	55	50	**
9	54	50	54**
	52	53	**
10	42	34	69**
	37	32	**
11	108	106	36**
	93	104	**
12	28	30	123**
13	118	113	38**
14	28	12	128**
15	54	60	74**
16	44	30	71**
17	94	97	40**
18	32	24	105**
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	84	85	**
1	110	107	41**
	106	102	**
2	71	72	54**
	71	65	**
3	106	105	43**
	101	105	**
4	78	76	41**
	80	69	**
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	60	50	**
6	44	52	66**
	53	52	**
7	83	83	40**
	77	83	**
8	23	21	-57**
	27	16	**
9	40	34	75**
	37	33	**
10	64	60	56**
11	31	32	109**
12	69	67	55**
13	58	57	66**
14	56	58	56**
15	13	24	-62**
16	29	19	111**
17	47	47	72**
****	10 K	7	******
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	63	60	**
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	81	77	**
2	70	74	46**
	77	66	**
3	66	67	47**
	68	62	**
4	71	62	45**
	65	61	**
5	83	85	41**
	79	76	**
6	202	196	38**
	179	185	**
7	68	58	46**
8	97	92	41**
9	30	48	121**
10	58	43	62**
11	28	24	128**
12	31	23	120**
13	62	59	52**
14	83	82	75**
15	23	30	-66**
****	11 K	7	******
0	80	79	44**
	68	73	**
1	85	87	42**
2	105	103	37**
3	159	156	36**
4	67	65	56**
5	62	57	58**
6	6	33	-72**
7	41	44	91**
8	94	86	43**
9	69	59	56**
10	81	80	51**
11	43	20	71**
12	0	14	-63**
13	80	82	44**
14	45	34	74**
****	12 K	7	******
0	95	88	45**
1	75	72	53**
2	60	49	63**
3	90	92	46**
4	112	113	42**
5	110	107	41**
6	57	57	68**
7	18	7	-73**
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9	75	70	45**
10	60	64	56**
11	42	40	79**
12	44	46	77**
****	13 K	7	******
0	103	102	45**
1	75	68	56**
2	58	50	56**
3	39	55	85**
4	107	111	36**
5	53	48	61**
6	86	97	71**
7	15	25	-66**
8	58	62	59**
9	45	35	75**
10	0	14	-68**
****	14 K	7	******
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3	47	56	74**
4	43	29	77**
5	33	34	101**
6	65	63	59**
****	0 K	8	******
0	138	132	38**
	132	120	**
	123	118	**
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	86	87	**
	86	85	**
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	201	212	**
	194	199	**
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	70	6	**
4	232	236	43**
	234	227	**
	215	219	**
5	131	132	39**
	135	128	**
	125	125	**
6	47	19	67**
	0	8	**
	21	11	**
7	144	145	38**
	149	143	**
	132	131	**

K	FO	FC	SIG**
			**
8	31	25	119**
	31	33	**
	29	30	**
9	58	58	68**
	64	54	**
	52	56	**
10	39	39	72**
	47	46	**
11	47	34	57**
	40	30	**
12	53	52	54**
	47	44	**
13	73	72	45**
	71	69	**
14	30	29	114**
15	110	120	41**
16	58	50	66**
17	140	138	34**
18	79	74	45**
19	84	82	45**
****	1 K	8	******
0	88	94	43**
	94	87	**
	86	86	**
1	49	52	75**
	47	49	**
	44	46	**
2	150	155	37**
	141	149	**
	135	134	**
3	102	99	40**
	94	101	**
	92	97	**
4	120	123	40**
	121	123	**
	115	112	**
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	88	90	**
	79	78	**
6	55	54	62**
	56	51	**
	50	50	**
7	135	131	38**
	133	133	**
	118	117	**
8	77	84	51**
	83	88	**
	73	78	**
9	117	122	41**
	122	119	**
	102	111	**
10	49	41	55**
	47	36	**
11	90	88	37**
	93	88	**
12	71	60	42**
	59	55	**
13	62	50	48**
	48	50	**
14	50	43	69**
15	37	18	94**
16	77	79	52**
17	55	47	59**
18	170	166	35**
19	26	30	130**
****	2 K	8	******
0	198	200	40**
	196	193	**
	176	181	**
1	32	40	100**
	41	39	**
	35	30	**
2	89	88	41**
	88	89	**
	79	81	**
3	189	189	39**
	192	186	**
	166	176	**
4	94	95	42**
	89	94	**
	82	82	**
5	115	104	37**
	111	102	**
	98	98	**
6	32	45	106**
	47	46	**
	39	39	**
7	130	127	39**
	135	127	**
	112	121	**
8	214	218	42**
	212	215	**
	188	201	**
9	215	212	43**
	216	209	**
10	77	77	41**
	86	75	**
11	76	70	40**
	71	69	**
12	35	54	86**
	51	48	**
13	44	48	69**
	43	51	**
14	64	65	58**
15	23	37	-71**
16	14	5	-72**
17	115	114	34**
18	33	34	100**
19	76	75	47**
****	3 K	8	******
0	54	62	60**
	61	60	**
	52	55	**
1	55	53	60**
	56	49	**
	46	44	**
2	108	108	38**
	106	104	**
	94	97	**
3	33	36	98**
	31	32	**
	24	26	**
4	59	61	59**
	64	66	**
	57	53	**
5	102	104	43**
	106	102	**
	94	90	**
6	57	49	61**
	62	57	**
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	131	128	**
9	100	99	35**
	108	94	**
10	44	58	66**
	59	49	**
11	114	114	35**
	109	104	**
12	32	36	90**
	38	37	**
13	39	29	83**
14	67	66	53**
15	31	18	110**
16	28	39	133**
17	28	39	112**
18	19	19	-65**
19	22	19	-68**
****	4 K	8	******
0	50	58	73**
	61	56	**
	53	58	**
1	47	25	67**
	35	28	**
	24	28	**
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	116	108	**
	98	107	**
3	0	4	-64**
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	70	7	**
4	93	89	44**
	85	89	**
	78	79	**
5	170	171	39**
	183	166	**
	152	158	**
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	64	58	**
	58	54	**
7	49	33	71**
	40	33	**

K	FO	FC	SIG**
			**
	32	28	**
8	106	112	43**
	114	106	**
9	73	72	43**
	77	71	**
10	99	101	36**
	97	89	**
11	105	102	35**
	94	97	**
12	46	34	62**
	33	39	**
13	92	87	43**
14	101	97	42**
15	93	88	45**
16	41	44	77**
17	51	45	62**
18	28	38	117**
****	5 K	8	******
0	190	191	40**
	186	189	**
	171	176	**
1	36	42	93**
	40	38	**
	37	37	**
2	78	72	46**
	78	76	**
	70	72	**
3	115	114	40**
	122	118	**
	106	111	**
4	92	91	44**
	94	87	**
	85	81	**
5	94	85	43**
	86	79	**
	76	73	**
6	0	7	-66**
	0	2	**
7	176	175	34**
	177	177	**
8	30	33	96**
	37	35	**
9	100	101	35**
	93	95	**
10	166	162	35**
	161	160	**
11	95	99	38**
	84	94	**
12	72	68	51**
13	59	66	64**
14	62	60	62**
15	56	41	66**
16	45	28	70**
17	69	66	50**
18	35	52	98**
****	6 K	8	******
0	51	48	72**
	60	54	**
	51	51	**
1	127	126	39**
	129	123	**
	113	114	**
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	86	88	**
	77	82	**
3	111	112	41**
	110	111	**
	105	103	**
4	76	74	51**
	80	69	**
5	41	39	66**
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6	62	66	48**
	65	62	**
7	65	66	47**
	68	64	**
8	65	62	46**
	62	55	**
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	48	40	**
10	29	26	104**
	27	26	**
11	0	25	-69**
12	56	54	64**
13	33	49	114**
14	101	97	43**
15	81	85	42**
16	107	115	37**
17	77	77	47**
****	7 K	8	******
0	38	16	69**
	29	15	**
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	65	61	**
2	44	43	64**
	48	45	**
3	64	68	47**
	72	63	**
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	55	42	**
5	67	69	46**
	65	63	**
6	85	82	39**
	81	75	**
7	40	37	75**
	46	43	**
8	28	31	105**
	40	37	**
9	91	93	40**
10	121	116	37**
11	0	7	-70**
12	73	70	53**
13	52	53	75**
14	95	91	38**
15	60	57	56**
16	41	40	81**
****	8 K	8	******
0	114	101	34**
	104	100	**
1	87	80	40**
	79	79	**
2	36	34	88**
	38	27	**
3	125	120	35**
	113	114	**
4	141	131	35**
	129	126	**
5	52	49	60**
	47	48	**
6	25	26	121**
	29	22	**
7	59	62	56**
8	40	34	87**
9	46	41	77**
10	44	46	84**
11	36	35	104**
12	145	136	39**
13	96	89	40**
14	88	84	41**
15	22	24	-68**
****	9 K	8	******
0	78	74	43**
	69	65	**
1	80	74	42**
	68	73	**
2	131	129	35**
	103	116	**
3	81	78	44**
4	185	177	38**
5	43	49	86**
6	36	19	97**
7	48	48	75**
8	69	62	56**
9	45	57	87**
10	75	81	54**
11	58	39	55**
12	0	19	-64**
13	53	44	64**
14	76	77	47**
****	10 K	8	******
0	0	5	-70**
1	72	66	52**
2	58	54	64**
3	96	99	44**
4	52	43	72**
5	49	33	75**
6	108	102	41**
7	85	89	51**
8	19	44	-77**
9	39	40	81**
10	49	49	65**
11	80	78	44**
12	77	80	47**
****	11 K	8	******
0	126	114	39**
1	105	94	42**

Table 4 (*cont.*)

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  K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**   K   FO   FC  SIG**
                  **                   **                   **                   **                   **                   **                   **                   **                   **                   **                   **                   **                   **
****11 K    8 ******       49   50     **   6   79   78   41**   8  148  145   34**  13   77   73   43**       29   22     **   9   95   96   45**  11   68   64   52**   1    0   19  -68**   4    9   22  -69**   8   24    6  -62**   2   24   31  -63**   5   60   62   58**
  2   66   70   61**   4   33   17   81**       78   76     **      140  136     **  14   75   81   46**   2   37    2   71**  10   49   51   78**  12   85   90   44**   2   56   54   64**   5   73   76   54**   9   58   51   56**   3   55   51   58**   6   84   81   44**
  3   89   91   49**       27   16     **   7   60   60   51**   9   27   37  110**  15   23   16  -64**       84   10     **  11   29   15  107**  **** 9 K    9 ******   3   72   63   53**   6   23   42  -76**  10   45   39   71**   4   41   20   76**   7   78   65   45**
  4  141  141   40**   5  150  151   34**       55   56     **  10   40   46   88**  16   97   95   39**   3   32   30   88**  12   58   59   61**   0   60   52   67**   4   25   27  -70**   7   33   34  115**  11   73   70   47**   5   28   31  112**  **** 2 K   11 ******
  5   35   22   90**      156  152     **   8  167  170   35**  11   32   28  114**  **** 4 K    9 ******       37   32     **  13   48   44   66**   1   63   69   65**   5  102   97   43**   8   80   75   53**  12   44   46   76**   6   37   28   85**   0    0   17  -63**
  6   58   56   56**   6   85   87   40**      163  165     **  12   84   84   48**   0   73   73   41**   4   45   43   65**  14   24   25  -66**   2   56   47   69**   6   53   56   76**   9  114  106   35**  **** 5 K   10 ******   7   78   76   47**   1  101   88   37**
  7   34   23   94**       84   83     **   9   60   54   52**  13   55   56   70**       76   75     **       47   41     **  **** 7 K    9 ******   3   39   43   97**   7  130  129   39**  10   63   75   54**   0   55   39   65**   8   65   64   54**   2  109  112   37**
  8    0   22  -63**   7   42   38   68**       46   54     **  14  125  121   34**   1   33   27   81**   5   15   34  -60**   0   65   62   56**   4   89   83   40**   8   17    6  -77**  11   55   47   59**   1    8   15  -69**  **** 8 K   10 ******   3   66   48   50**
  9   59   46   56**       40   38     **  10  121  116   39**  15   39   32   82**       29   37     **       37   31     **   1   70   66   52**   5   83   80   42**   9   17   26  -78**  12   71   64   49**   2    3   27  -68**   0   32   16   98**   4  161  160   34**
 10   31    7  107**   8   31   43   99**  11   87   96   46**  16   76   70   47**   2   22    6  -53**   6   83   76   41**   2   56   48   63**   6   76   68   45**  10   71   72   51**  13   55   54   61**   3    0   12  -72**   1   30   36  108**   5  133  132   35**
 11   40   36   86**       38   43     **  12   35   22  104**  **** 3 K    9 ******        0    5     **   7   67   60   53**   3   38   29   88**   7   46   48   76**  11  110  113   38**  **** 3 K   10 ******   4   38   38   95**   2   27   21  119**   6   10   11  -67**
****12 K    8 ******   9   53   42   58**  13   39   27   96**   0   73   73   41**   3   17   28  -55**   8   91   93   44**   4   74   68   49**   8   60   55   59**  12  102  101   38**   0   39   31   88**   5   44   46   85**   3    0   17  -66**   7   39   35   86**
  0  152  151   34**       46   50     **  14   72   73   46**       78   74     **       33   33     **   9   67   69   56**   5   69   63   54**   9   96   88   42**  13   64   62   55**   1   46   46   76**   6   52   59   63**   4   26   41  -67**  **** 3 K   11 ******
  1   69   64   49**  10  216  213   41**  15  102   99   37**   1    0   12  -54**   4   48   35   58**  10   55   53   69**   6   23   34  -74**  10    0   20  -69**  **** 1 K   10 ******   2   57   54   63**   7   33   39   96**   5   45   46   74**   0    0    5  -63**
  2   40   35   80**  11   48   44   76**  16   62   57   55**       19   16     **       43   39     **  11   70   68   56**   7  107   99   41**  ****10 K    9 ******   0   44   41   79**   3   54   55   67**   8   49   41   65**   6   29   23  114**   1   63   65   52**
  3  105  100   36**  12   35   11  101**  **** 2 K    9 ******   2   46   54   61**   5   41   31   67**  12   68   67   48**   8   60   60   64**   0   42   43   77**   1   25    5  -66**   4  110  103   40**   9   27   26  120**  **** 9 K   10 ******   2   12   26  -64**
  4   87   91   42**  13  105  102   43**   0  129  127   32**       59   57     **       35   31     **  13    0   15  -63**   9   29   19  125**   1   60   61   55**   2   67   58   54**   5   72   75   54**  10    0   15  -67**   0   80   90   46**   3   54   51   62**
  5  128  127   35**  14   82   85   43**      131  129     **   3   56   60   51**   6   78   75   41**  14   53   48   62**  10   25   39  -63**   2   49   53   68**   3  108  104   39**   6   34   11  103**  11   46   47   74**   1   30   20  112**   4   32   35  104**
  6   17   20  -66**  15    0    7  -64**   1  132  135   32**       62   60     **       66   67     **  15    0   22  -66**  11   35   39   91**   3   59   58   56**   4  110  105   40**   7   91   78   45**  **** 6 K   10 ******   2   98   91   39**   5   17   31  -67**
  7    0   29  -67**  16  115  110   37**      129  132     **   4   54   49   52**   7  101  101   36**  **** 6 K    9 ******  12   52   42   64**   4   85   82   42**   5   71   64   55**   8   35   16   87**   0    0   28  -73**  **** 0 K   11 ******   6   84   80   43**
  8   59   54   59**  **** 1 K    9 ******   2   87   86   36**       54   53     **       81   93     **   0   29    0   99**  13   46   46   74**   5   63   57   53**   6  131  133   40**   9   90   84   39**   1   21   27  -73**   1   67   65   51**  **** 4 K   11 ******
****13 K    8 ******   0   35   34   97**       84   82     **   5   94   88   36**   8   59   57   61**       11    4     **  **** 8 K    9 ******   6   51   41   65**   7  131  128   40**  10    0   34  -65**   2   22    3  -71**   2   55   55   61**   0   40   22   80**
  0   91   81   40**       33   29     **   3   71   65   41**       85   83     **   9   39   26   89**   1   23   35  -59**   0    0    0  -72**   7   64   67   56**   8  148  144   39**  11   50   49   64**   3    7   16  -61**   3   11    8  -67**   1   17   29  -65**
  1   32   36  105**   1   86   85   45**       67   61     **   6   46   45   65**  10   25   35  -72**       38   38     **   1   48   52   75**   8   41   37   84**   9  124  118   34**  12   79   77   46**   4   59   51   52**   4   90   90   41**   2   50   50   66**
  2   46   37   74**       84   80     **   4   25   14  105**       53   46     **  11   90   84   44**   2   68   56   46**   2   68   57   55**  ****11 K    9 ******  10    0   16  -63**  **** 4 K   10 ******   5   57   52   55**   5   35   39   96**   3   41   23   78**
  3    0   18  -68**   2   50   38   53**      106  108     **   7  130  125   34**  12   23   31  -74**       48   58     **   3  100  105   43**   0   13    4  -66**  11   25   34  -66**   0   37   31   94**   6   31   21  100**   6  136  135   36**   4   21   15  -65**
  4   30   28  112**       43   38     **       19   14     **      118  115     **  13   37   42   87**   3   65   71   49**   4  114  108   40**   1   16   38  -67**  12   28   36  -66**   1   29   33  118**   7   52   49   61**   7   67   64   53**   5    3   11  -66**
**** 0 K    9 ******   3   56   59   51**   5   69   71   44**   8   76   82   44**  14   70   70   48**       55   65     **   5   25   30  -75**   2   43   44   80**  13   29   22  115**   2    0   27  -70**   8   37   43   88**  **** 1 K   11 ******  **** 5 K   11 ******
  1   39   35   89**       62   54     **       79   75     **       66   79     **  15    0   18  -65**   4   74   76   49**   6  129  125   39**   3   43   32   77**  **** 2 K   10 ******   3    0   16  -70**   9   60   56   58**   0   61   48   53**   0   59   65   58**
      40   29     **   4   74   66   40**   6   28   14  101**   9   92   86   43**  **** 5 K    9 ******   5   49   47   72**   7   50   53   81**   4   66   70   53**   0   23   15  -69**   4   49   47   74**  10    0   13  -66**   1   68   60   49**   1    0   12  -66**
  2    0    1  -76**       74   66     **       22   15     **  10   54   50   66**   0   49   49   60**   6   63   70   60**   8  117  112   35**   5   68   68   52**   1    6   24  -69**   5   73   73   53**  **** 7 K   10 ******   2   28   38  114**   2   45   29   72**
      27    8     **   5   62   58   48**   7  145  145   34**  11   88   93   47**       52   49     **   7   48   58   76**   9   98   92   39**  **** 0 K   10 ******   2   33   24  102**   6   23   16  -72**   0   50   41   63**   3   62   60   54**   3   54   57   61**
  3   40   38   66**       64   57     **      141  137     **  12   62   61   62**   1   37   21   75**   8   77   76   51**  10   74   73   47**   0   95   96   43**   3   40   24   87**   7   65   65   49**   1   38   21   80**   4   39   19   82**                   **
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Discussion

It seems appropriate to describe the structure primarily on the basis of the weighted-average coordinates of Table 3. In view of the probability that the estimated standard deviations of the individual determinations are unrealistically low, as is often the case (Hamilton & Abrahams, 1970), the deviations of the individual coordinates from their average values are hardly to be regarded as significant. In fact, if we multiply the apparent individual standard deviations by a factor of two, as has been suggested (Hamilton, 1965) as a rule of thumb, the extreme ratio of coordinate difference to corresponding standard deviation is only 3·1; and this extreme ratio is for a hydrogen coordinate, the x coordinate of H(O′6). Thus, although the agreement between the three sets of coordinates is not ideal, it appears to be about as good as is usually obtained when the same crystalline substance is subjected to X-ray analysis in different laboratories (Hamilton & Abrahams, 1970).

Fig. 1(*a*) shows the individual lengths and the average length for each C–C and C–O bond and the average apparent lengths of the C–H and O–H bonds.* Since the differences among angle values have about the same magnitudes in relation to the standard errors as those of the bond lengths, we report for the valence angles and torsion angles (Klyne & Prelog, 1960) involving carbon and oxygen atoms only the values calculated from the averaged coordinates [see Fig. 1(*b*) and (*c*)]. The average angles C–O–H are also shown in Fig. 1(*b*). The average angles (not shown) involving the C–H bonds all lie in the range 106 to 114°. The shape of the molecule is shown in the stereoscopic drawing in Fig. 2, in which the carbon and oxygen atoms are represented by their thermal ellipsoids of 50% probability (Johnson, 1970).

For the average molecular parameters in Fig. 1, the standard errors, *including the arbitrary factor of two* (see above), are as follows: C–O and C–C bonds, 0·003 to 0·004 Å; C–H bonds, 0·03 to 0·04 Å; O–H bonds, 0·04 to 0·05 Å; C–C–C, C–C–O, C–O–C, and torsion angles, 0·2°; C–C–H and O–C–H angles, 2°; C–O–H angles, 3 to 4°.

The C–C bond lengths in Fig. 1(*a*) based on the average coordinates have a mean of 1·523 Å and a range of 0·017 Å; the C–O bond lengths excluding those involving O(1), O(5), and O′(5) have a mean of 1·422 Å and a range of 0·011 Å. These values are in excellent agreement with those reported previously (Strahs, 1970) for α-pyranosyl systems, namely, 1·524 Å (range 0·021) and 1·425 Å (range 0·016). According to Strahs, in α-pyranosyl systems the anomeric effect on bond lengths (Berman, Chu & Jeffrey, 1967) leads on the average to deviations from the mean C–O length 1·425 Å of −0·024, −0·004, and +0·015 Å for the C(1)–O(1), C(1)–O(5), and C(5)–O(5) bonds, respectively. In trehalose, the corresponding deviations are −0·010, −0·004, and +0·008 Å for the unprimed system and −0·003, −0·021, and +0·006 Å for the primed system. The only major difference in these C–O bonds between the two halves of the molecule is the more marked shortening of C′(1)–O′(5), which may be related to the fact that O′(5) does not take part in hydrogen bonding whereas O(5) does.

Both of the pyranosyl rings have the *C*1 conformation (Reeves, 1949), with the torsion angles defined by the six ring bonds ranging in magnitude from 48·1 to 62·5° for one ring (unprimed atoms) and from 49·3 to 59·6° for the other. These are normal variations, showing some flexibility of the ring structure.

The nearly identical angles, 114·0 and 114·2°, at the two ring oxygen atoms are in the normal range for such angles in pyranose rings (see, for example, Sundaralingam, 1968). That the angle of 115·8° at O(1) is similarly in the normal range for glycosidic oxygen atoms is a fact of some interest, since, as already noted, α,α-trehalose is the first carbohydrate oligomer to have its structure determined which has a bridging oxygen atom axial to two rings. It seems that the demands of the conformational 'anomeric effect' (de Hoog, Buys, Altona & Havinga, 1969; Angyal, 1968) and of hydrogen bonding (see discussion below) are satisfied through adoption by the molecule of conformations about the bonds C(1)–O(1) and C′(1)–O(1) which produce an

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* In Figs. 1 and 2 the atom labels have been abbreviated by dropping the parentheses used in Table 3 and in the text.

almost maximally extended structure with no interactions tending to increase the angle at O(1).

The torsion angles about C(1)–O(1) and C′(1)–O(1) which are specified in Fig. 1(*c*) clearly describe for each of the two glucopyranosyl-O(1) groups the *A*1 conformer (de Hoog, *et al.*, 1969; Eliel, 1969), which is favored by the anomeric effect and which has often been found (Eliel & Giza, 1968) in crystalline pyranosides. Specifically, the torsion angles 74·8 and 61·7° describe *gauche* or +*syn-clinal* (Klyne & Prelog, 1960) conformations, and the angles −165 and −177° describe *trans* or *anti-periplanar* conformations.

To specify the relative conformation of the two glucopyranosyl rings, it is better (Rohrer, 1972) to consider pseudotorsion angles about the line between C(1) and C′(1) (see Fig. 3) rather than the torsion angles about the two bonds of the glycosidic linkage. The difference of only 6·8° between the pseudotorsion angles (C2)–C(1)···C′(1)–O′(5) and C′(2)–C′(1)··· C(1)–O(5) and the general appearance of Fig. 2 show

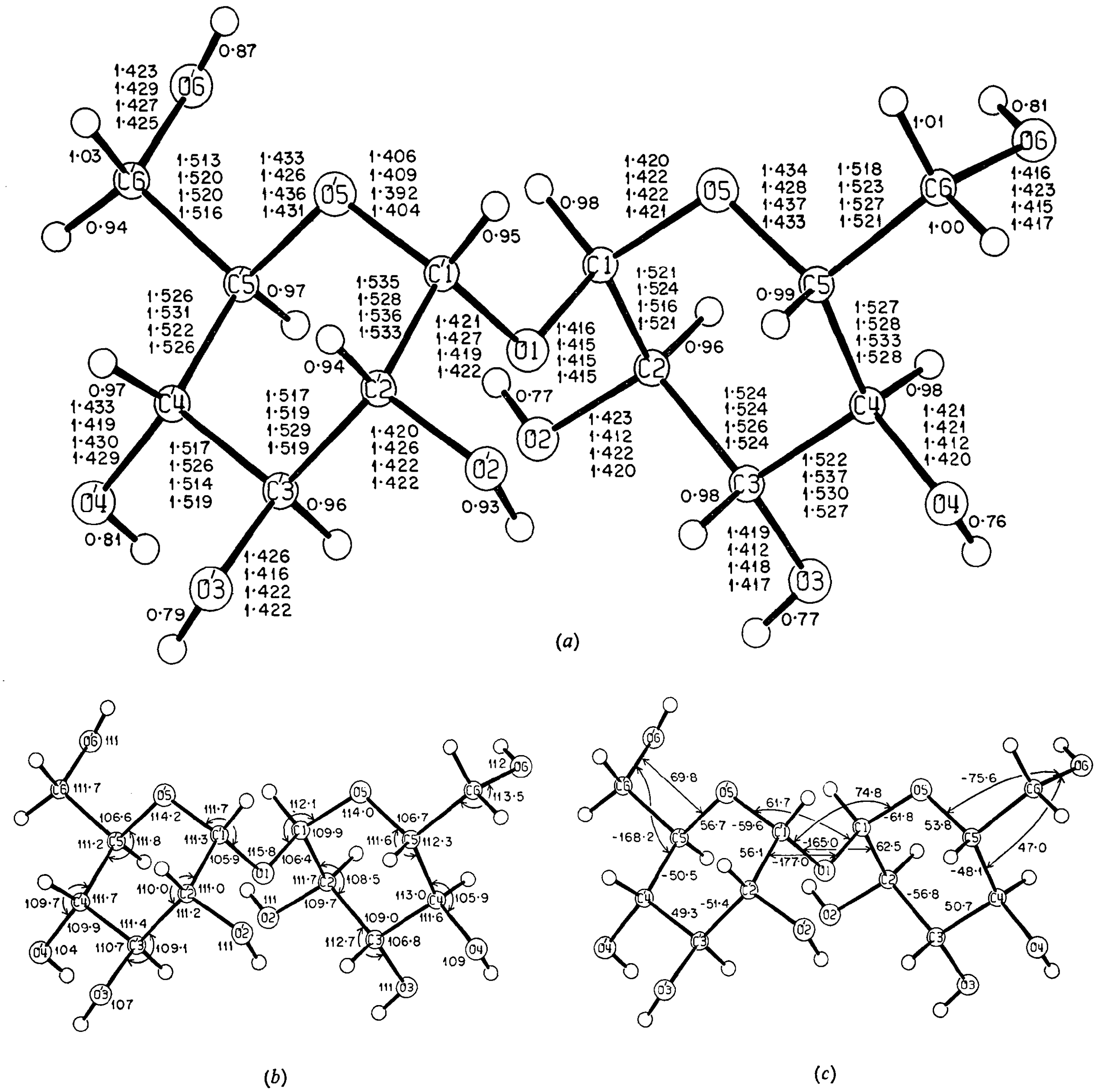

Fig. 1. Bond lengths, valence angles, and torsion angles in the molecule of α,α-trehalose. (*a*) For each C–C and C–O bond, the individual lengths from the three determinations and the average length (corresponding to the averaged coordinates) are shown. The order is, from top to bottom: Oak Ridge, Pittsburgh, Edinburgh, average. For the C–H and O–H bonds, only the average values are shown. (*b*) Average valence angles C–C–C, C–C–O, C–O–C, and C–O–H. (*c*) Average torsion angles. For each ring bond the torsion angle defined by the two adjacent ring bonds is written next to the bond. Torsion angles about other specific bonds are defined by double-headed arrows pointing in each case to two bonds attached at opposite ends of a central bond.

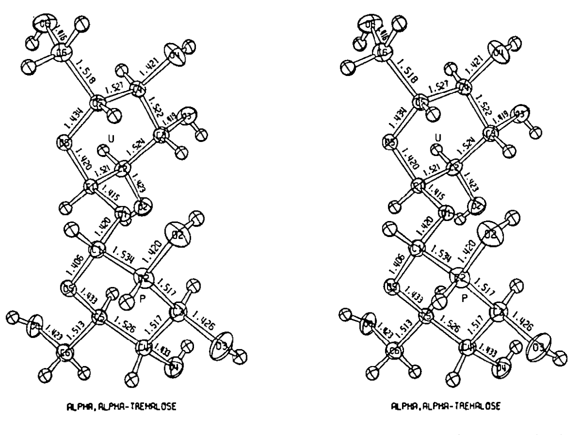

Fig. 2. Stereoscopic drawing of the molecule of α,α-trehalose based on the Oak Ridge parameters. Carbon and oxygen atoms are represented by their ellipsoids of 50 % probability and hydrogen atoms by spheres of an arbitrary radius. The unprimed and primed atoms are indicated by the letter *U* in one ring and the letter *P* in the other.

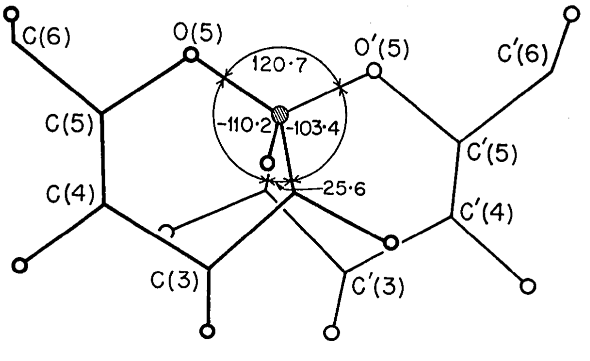

Fig. 3. View of the α,α-trehalose molecule along the line between C(1) and C′(1) and some pseudotorsion angles about this line'

that the departure of the molecule from the symmetry of point group C_2 is small.

The hydroxymethyl groups show the largest conformational difference between the two glucose moieties. The torsion angles about the C(5)–C(6) bond involving O(6) with O(5) and with C(4) are −75·6 and 47·0°, respectively, describing a *gauche–gauche* arrangement. The corresponding angles about the bond C′(5)–C′(6) are 69·8 and −168·2°, describing a *gauche–trans* conformation. Both of these conformations have been previously found in crystal structures containing α-D-glucosyl units (Fries, Rao & Sundaralingam, 1971). A third possible arrangement, *trans–gauche*, is thought to be forbidden because of interaction between O(6) and O(4).

The molecules of α,α-trehalose and water are held together in the crystal by a complex system of twelve crystallographically independent hydrogen bonds O–H···O (Table 5 and Figs. 4–6). Each hydroxyl group of the sugar molecule is both a donor and an acceptor in hydrogen-bond formation. The ring oxygen O(6) is an acceptor, but O′(5) and O(1) are not involved in hydrogen bonding. Each of the water molecules is a donor in the formation of two different hydrogen bonds. Molecule *W*(1) is an acceptor for two bonds and atom O(*W*1) is tetrahedrally coordinated, whereas molecule *W*(2) is an acceptor for only one hydrogen bond and atom O(*W*2) displays pyramidal coordination.

There is no direct intramolecular hydrogen bonding such as is found in sucrose (Brown & Levy, 1963), cellobiose (Chu & Jeffrey, 1968), methyl-β-cellobioside–methanol (Ham & Williams, 1970), β-maltose monohydrate (Quigley, Sarko & Marchessault, 1971), methyl-β-maltoside monohydrate (Chu & Jeffrey, 1967), and β-lactose monohydrate (Fries, Rao & Sundaralingam, 1971). However, water molecule *W*(1) is

Table 5. *Hydrogen bonds in the crystal structure of α,α-trehalose dihydrate*

The symmetry operations are those which generate the coordinates of the acceptor oxygen atoms. For each operation the first digit specifies one of the following: (1) x,y,z; (2) $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; (3) $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; (4) $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$. The last three digits specify a lattice translation.

Hydrogen bond O–H···O	Symmetry operation	Distances (Å) O–H	H···O	O···O	O–H···O	Angles (°) C–O–H or H–O–H	C–O···O or O···O ···O
O(2)——H(O2)····O(*W*2)	[1,000]	0·77	1·97	2·732	172	111	112·8
O(3)——H(O3)····O′(3)	[2,00$\bar{1}$]	0·77	2·01	2·750	159	111	125·7
O(4)——H(O4)····O(5)	[3,001]	0·76	2·23	2·882	144	109	122·1
O(6)——H(O6)····O′(4)	[4,000]	0·81	1·94	2·728	165	112	121·7
O′(2) —H(O′2) ···O(*W*1)	[2,000]	0·93	1·87	2·770	163	111	121·5
O′(3) —H(O′3) ···O(4)	[2,00$\bar{1}$]	0·79	2·12	2·906	176	107	108·2
O′(4) —H(O′4) ···O(*W*1)	[1,000]	0·81	2·09	2·882	169	104	99·9
O′(6) —H(O′6) ···O(6)	[3,$\bar{1}$01]	0·87	1·83	2·704	174	111	115·3
H(*W*1) ···O(2)	[1,000]	0·83	1·94	2·766	177		
O(*W*1)						106	108·6
H′(*W*1)···O′(2)	[1,00$\bar{1}$]	0·79	1·92	2·697	169		
H(*W*2) ···O(3)	[3,$\bar{1}$00]	0·76	2·05	2·803	170		
O(*W*2)						107	103·4
H′(*W*2)···O′(6)	[1,000]	0·82	1·96	2·764	168		
Standard errors		0·04 to 0·05	0·04 to 0·05	0·003 to 0·004	4 to 5	3 to 5	0·1 to 0·2

linked by hydrogen bonding both to O(2) and to O′(4), and molecule *W*(2) is linked both to O(2) and to O′(6), all within the same trehalose molecule. The same kind of indirect intramolecular hydrogen bonding through water molecules occurs in methyl-β-maltoside monohydrate, planteose dihydrate (Rohrer, 1972) and raffinose pentahydrate (Berman, 1970). Direct intramolecular hydrogen bonding is less likely in crystals of oligosaccharides as the number of water molecules per monosaccharide moiety increases.

A particularly interesting feature of the hydrogen bonding pattern is the bonding involving *W*(1) and O′(2)H. This bonding produces about the axis 2_1 at $\frac{1}{4},0,z$ the helix of hydrogen bonds shown schematically in Fig. 5 and also shown rather clearly between sugar molecules 6 and 7 in the stereoscopic drawing of Fig. 6. The helix around the 2_1 axis at $\frac{3}{4},\frac{1}{2},z$ is identical, but its vectors $O(W1) \rightarrow H'(W1)$ point in the opposite direction along the *c* axis. It is possible that because of these helices the crystal may show an abnormally high electric polarizability in the **c** direction and that in some temperature range it may show ferroelectric behavior. Thus, if in half the helices the hydroxyl O′(2)H were to reorient by rotating ~180° around bond C′(2)–O′(2) and if at the same time the water molecule *W*(1) were to rotate ~120° around the bond O(*W*1)–H(*W*1), possibly with some additional minor adjustments in the orientation of *W*(1), the result would be a highly polar structure of symmetry $P2_1$ with about the same stability as the $P2_12_12_1$ structure. From the X-ray analysis of Beevers & Hughes (1941) and the neutron analysis of Frazer (1962) (see also Hamilton & Ibers, 1968), a similar mechanism is thought to explain the ferroelectric behavior of Rochelle salt, $NaK(C_4H_4O_6).4H_2O$.

Another interesting feature of the hydrogen bonding is the spatial disposition of the bond O(4)–H(O4)··· O(5) relative to the C(1)–O(5)–C(5) group of atoms. In nearly every previously known case (Sundaralingam, 1968) the hydrogen bond to the ring oxygen of a pyranose system is equatorially oriented at the acceptor oxygen. In the present case, as can be seen in Fig. 6, the orientation is neither equatorial nor axial, but about halfway between; that is, the configuration of atoms C(1), O(5), C(5), and H(O4) is very nearly planar. The angles C(1)–O(5)–H(O4) and C(5)–O(5)–H(O4) are 104 (1) and 141 (1)°, and the sum of angles about O(5) is 359°.

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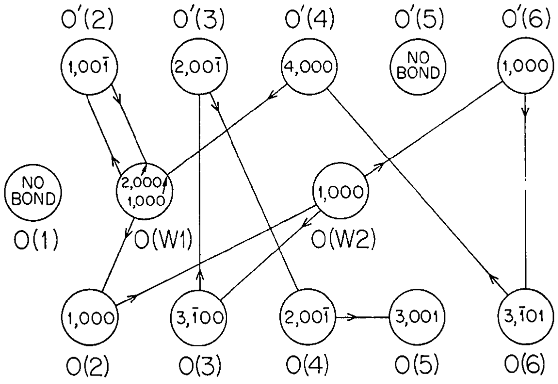

Fig. 4. Schematic diagram of hydrogen bonding in α,α-trehalose dihydrate. The large circles represent oxygen atoms; the arrows denote directions of donation of hydrogen atoms. Each oxygen atom functioning as a donor is to be understood to belong to the reference asymmetric unit (symmetry transformation [1,000] in the notation of Table 5). The symmetry transformation for each acceptor oxygen is indicated.

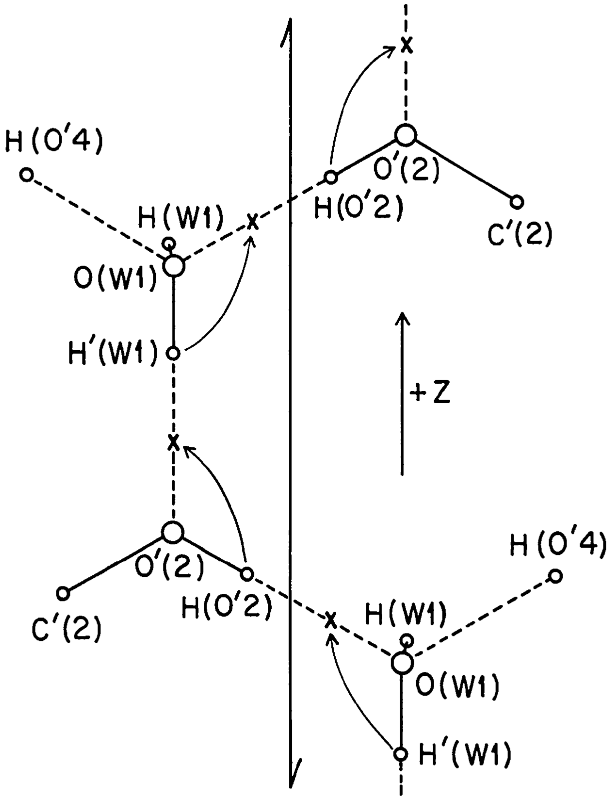

Fig. 5. Schematic drawing of helical arrangement of hydrogen bonds about axis $\frac{1}{4},0,z$.

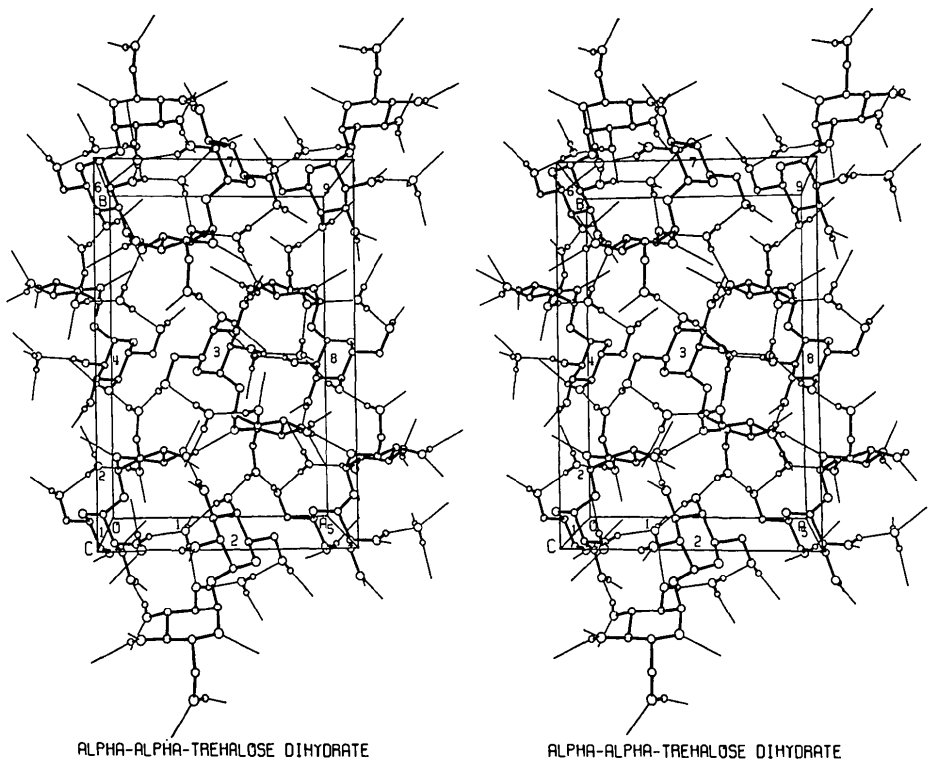

Fig. 6. Stereoscopic view of the packing of the sugar and water molecules in the crystal structure of α,α-trehalose dihydrate. Hydrogen atoms attached to carbon atoms are omitted. The thin lines connecting hydrogen atoms and oxygen atoms show the hydrogen bonding. Within the ring of primed atoms of each sugar molecule is a numerical label which identifies the symmetry operation generating that molecule according to the scheme used in Table 5: 1 = [1,000]; 2 = [2,000]; 3 = [3,001]; 4 = [4,000]; 5 = [1,100]; 6 = [1,010]; 7 = [2,010]; 8 = [4,100]; 9 = [1,110]. Two independent water molecules are labelled 1 and 2. Note, however, that by inadvertence water molecule 1 here is not the molecule $W(1)$ whose coordinates are given in Table 3 but rather the molecule $W(1)$ [2,000].

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Packing Analysis of Carbohydrates and Polysaccharides. I. Monosaccharides

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The minimum energy crystal structures of six monosaccharides: α- and β-D-glucose, β-lyxose, methyl-α-D-glucopyranoside, D-glucono-(1,5)-lactone, and β-arabinose, were calculated using a modified Williams procedure of minimization of nonbonded repulsion energy. In all cases but β-arabinose, the predicted structures were in close agreement with the real structures, and could easily serve as starting models for least-squares refinement procedures. The same potential energy parameter set was applicable in all cases. In the case of β-arabinose a structure was predicted which differed from the reported one by a shift of $-\frac{1}{4}a$. Subsequent refinement of the predicted structure with X-ray data revealed errors in the reported data and produced a corrected crystal structure and good agreement with the predicted one. Of all the nonbonded interactions present in these carbohydrates, those involving the hydrogens were the most important and those involving the carbons the least important. Little difficulty with predicted structures in false energy minima was encountered.

Introduction

The determination of polymer crystal structure is, in general, handicapped by a lack of observed diffraction data, necessitating reliance on information obtained from other sources. In principle, such information may be obtained from a computation of minimum potential energy structures which could serve as models for subsequent structure refinement with available diffraction data. This goal has not yet been achieved, but nevertheless, such calculations have been successful with low molecular weight hydrocarbons (Williams, 1969; Neuman, 1970; Warshel & Lifson, 1970) and, to some extent, with hydrocarbon polymers (Clark & Geering, 1970; Wobser & Blasenbrey, 1970). These calculations have been carried out in two different ways, either by minimization of the total potential energy or by the minimization of repulsive energy only (Williams, 1965, 1969). Calculations using the second approach have the advantage of being simpler and faster and appear to be sufficiently reliable.

The extension of the same techniques to the prediction of crystal structures of carbohydrates is somewhat more difficult owing to the presence of oxygens. First, at least three more nonbonded potential energy functions must be introduced. Second, hydrogen bonding must now be considered.

As part of work with biologically important polysaccharides, it was decided to investigate in detail the forces responsible for the conformation of these molecules and their packing into crystal structures. A suitable starting point seemed to be the attempt to predict the known crystal structures of carbohydrates of low molecular weight, in an effort to determine the best set of potential energy functions applicable to all such molecules. Calculations with the same potential parameter set for other, as yet undetermined carbohydrate structures might then provide reliable predictions of their crystal structures. In this communication we describe the calculation of the most probable crystal structures of α-D-glucose, β-D-glucose, β-lyxose, methyl-α-D-glucopyranose, D-glucono-(1,5)-lactone, and β-arabinose, using the method of minimization of repulsive nonbonded energies only.

Method of calculation

The method employed was that of Williams (1969) and consisted, basically, in moving a rigid molecule and its symmetry-related mates within the fixed unit cell until