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The Conformation of Non-Aromatic Ring Compounds. XXI*. The Crystal and Molecular Structure of 2-phenyl-1,3-dithiane.

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2-Phenyl-1,3-dithiane crystallizes in the orthorhombic system; the space group is $Pna2_1$, $a=22{\cdot}87$, $b=7{\cdot}774$, $c=5{\cdot}802$ Å, and $Z=4$. The structure was refined by means of three-dimensional data obtained with copper radiation at room temperature. The 1,3-dithiane ring has a somewhat flattened chair conformation. The phenyl group is in the equatorial position and has an orientation about perpendicular to the 'plane' of the dithiane ring.

Introduction

The present study is a part of investigations of the conformation of non-aromatic ring compounds carried out in this laboratory‡. The aim of this research was to determine the conformation and geometry of the 1,3-dithiane ring. To our knowledge no such compounds have been subjected to X-ray or electron diffraction studies. A few 1,3,5-trithianes have been studied by Hassel & Viervoll (1947); structure determinations of 1,4-dithiane (Marsh, 1955) and of *trans*-2,3-dichloro-1,4-dithiane (Kalff & Romers, 1965) were published in this journal, and a structure determination of 1,2-dithiane-3,6-dicarboxylic acid appeared elsewhere (Foss, Johnsen & Reistad, 1964).

Experimental

2-Phenyl-1,3-dithiane (Authenrieth & Wolff, 1899) crystallizes from ethanol in the orthorhombic system in the form of colourless needles. The density, determined by the flotation method, is $1{\cdot}24$ g.cm^{-3}.

Unit-cell dimensions were measured from zero layer Weissenberg photographs about [010] and [001], taken with unfiltered Cu $K\alpha$ radiation ($\lambda=1{\cdot}5418$ Å) at room temperature. The photographs were superposed with aluminum powder lines ($a=4{\cdot}9089$ Å at 20 °C) for calibration purposes. The cell dimensions are $a=22{\cdot}87\pm0{\cdot}02$, $b=7{\cdot}774\pm0{\cdot}004$, $c=5{\cdot}802\pm0{\cdot}004$ Å and it follows that the unit cell contains four molecules.

Systematic absences of reflexions $0kl$ with $k+l=$ odd and $h0l$ with $h=$ odd indicate the space groups $Pna2_1$ and $Pnam$. The former was accepted because the three-dimensional Patterson function (see below) could not be interpreted in terms of the centrosymmetric space group.

Three-dimensional diffraction data were collected with the equi-inclination Weissenberg method (Cu $K\alpha$ radiation at room temperature, multiple film technique) about [010] for the layers $k=0, 1, \ldots, 6$ and about [001] for the layers $l=0, 1, \ldots, 5$. The non-integrated intensities were estimated visually and reduced to structure factor moduli after multiplication with Lorentz, polarization and spot-shape factors. The linear absorption coefficient is 40 cm^{-1}. Since the cross-sections of the crystals in use were $0{\cdot}12\times0{\cdot}15$ mm in both cases no absorption corrections were applied.

The total number of indepent reflexions within the copper sphere is 1434, inclusive 129 reflexions that are forbidden by space group symmetry. The geometry of the applied Weissenberg technique allowed us to record all remaining 1305 reflexions, but 278 planes were too weak to be observable. However, 162 unobserved reflexions were included in the calculations with $\frac{1}{2}F_{\min}$ values ($F_{\min}$ is the lowest observable value on a film). The number of reflexions for which structure factors were calculated amounts to $1027+162=1189$.

The structure determination

The number of sulphur atoms per asymmetric unit is one for the space group $Pnam$, but two for the acentric group $Pna2_1$. A three-dimensional Patterson function settled this problem in favour of the latter. The heavy atom technique was applied in order to locate the carbon atoms in the electron density projection along [001]. The refinement of this projection (Fig. 1), in which the carbon atoms C(5), C(6), C(8), and C(9) show partial overlap (see Fig. 2 for the numbering of the atoms) was stopped after the R index had attained the value of 21·1%.

A close inspection of Fig. 1 made it clear that the dithiane ring has the chair form and that the phenyl group is attached to it in the equatorial position. A three-dimensional wire model of the molecule was constructed from which z parameters for all carbon atoms and improved x and y parameters for the atoms C(5), C(6), C(8), and C(9) were derived.

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‡ Consult parts XIV (Kalff & Romers, 1965) and XVI (Geise, Romers & Rutten, 1966) for other publications in this series.

Three-dimensional structure factors were now calculated with the contributions of sulphur (form factor of Dawson, 1960) and carbon (form factor according to Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal, 1955). The refinement was carried out by a least-squares method minimizing $\Sigma w(F_o-F_c)^2$. The weight factor was $w=(a+F_{\min})/(a+F_o+bF_o^2)$ with $a=5$, $b=0{\cdot}2$, and $F_{\min}=1$. After two cycles with isotropic temperature factors ($R=18{\cdot}2\%$) a difference Fourier synthesis was calculated which revealed a significant anisotropy in the thermal motion of the sulphur atoms. Three cycles were made with anisotropic temperature factors for the sulphur atoms alone ($R=15{\cdot}2\%$) and two more cycles with anisotropic vibrational parameters for all atoms, except hydrogen ($R=13{\cdot}3\%$).

Next, the hydrogen atoms were placed at calculated positions. The hydrogen atoms (scattering curve according to McWeeny, 1951) were kept in fixed positions throughout the last two cycles ($R=11{\cdot}7\%$) with isotropic temperature factors equal to those of the carbon atoms to which they are attached. At this stage it was discovered that the reduction program contained an error. The reduction of measured reflexion intensities to structure factor moduli was repeated and the parameters of the last cycle, with exception of those of the hydrogen atoms, were introduced ($R=15{\cdot}6\%$). After three further cycles (with $R=9{\cdot}12\%$, Table 1) the hydrogen atoms were placed at calculated positions once more and a last cycle was performed ($R=9{\cdot}09\%$). At this stage the shifts were not larger than 0·2 times the corresponding standard deviations.

The positional parameters and the thermal parameters U_{11}, U_{22}, *etc.* defined by the temperature factor

$$\exp\{-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}$$
$$+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23})\}$$

are listed in Table 2. The numbers in brackets refer to standard deviations of the corresponding parameters. The coordinates and the isotropic temperature parameters of the hydrogen atoms are also included in this table.

The standard deviations in the C–C and C–S bond lengths vary between 0·013 and 0·021 Å and between 0·011 and 0·015 Å respectively. These numbers are, however, deceptive, since no vibration corrections have been applied The rather high B values in the range of 5 to 9 Å^2 suggest vibration corrections that may amount to about 0·02 Å. We assume, therefore, in the following discussion of the structure (see below) standard deviations of 0·03 Å in the bond distances and of 1·5° in the bond angles.

Description of the structure

The conformation of the 1,3-dithiane ring (Fig. 2) is a chair form with the phenyl group in equatorial position. In view of the estimated errors the C–C and C–S distances seem quite normal in both rings and do not need comment. The same cannot be said of the bond angle in the dithiane ring. The C–S–C bond angles (mean value 100°) have the expected value for bivalent sulphur (Abrahams, 1956; Kalff & Romers 1965), but the carbon bond angles (mean value 116°) are significantly larger than both the theoretical tetrahedral value of 109·5° and the expected value of about 112° observed in paraffins, in cyclohexane and in 1,4-dioxane (Davis & Hassel, 1963) and in cyclohexane-1,4-dione (Mossel & Romers, 1964).

It has been pointed out by Bucourt & Hainaut (1965) that the valency angle C–C(X, Y)–C is equal to 109·5° if X and Y are carbon atoms, but tends to adopt a value of about 112° if X and Y are hydrogen atoms, because the repulsive H–C–H interactions are smaller than the corresponding C–C–C interactions. On the basis of calculations of valency angle strain and torsional strain these authors arrive at valency angles of 111·1° in cyclohexane. It is, however, not clear, whether valency angles of about 116° observed in 1,3-dithiane can be easily explained in such a way, because calculations have not been carried out so far. It is interesting to observe that abnormally large C–CH$_2$–C valency angles are also observed by Foss, Johnsen & Reistad (1964) in the 3,6-dicarboxylic acids of 1,2-dithiane (117°) and of 1,2-diselenane (126°).

The dihedral angles in the dithiane ring of 2-phenyl-1,3-dithiane are listed in Table 3. All atoms, with exception of C(2), C(4), S(1) and S(2), are coplanar. The equation of this plane was calculated with respect to coordinate system XYZ with directions **a**, **b** and **c** according to the method of Schomaker, Waser, Marsh & Bergman(1959). The equation is

$$0{\cdot}6115X-0{\cdot}6270Y+0{\cdot}4827Z-0{\cdot}1576=0\,.$$

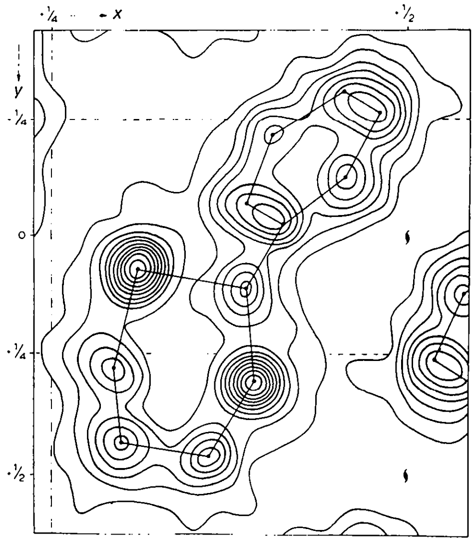

Fig. 1. Electron density projection along [001]. The contour lines are drawn on an arbitrary scale, those of the sulphur atoms at intervals 2·5 times as large as those for the carbon atoms.

Table 1. *Observed and calculated structure factors*

Non-observed reflexions, inserted as $\frac{1}{2}F_{\min}$, are indicated by *.

h	k	l	F_c	A_o	B_o	F_o
+2	+0	+0	+3.8	+3.3	−0.0	+3.3
+4			+78.9	−71.6	−0.0	+71.6
+6			+16.9	−14.1	+0.0	+14.1
+8			+4.2	+3.4	+0.0	+3.4
+10			+88.0	+87.9	−0.0	+87.9
+12			+46.5	−51.9	−0.0	+51.9
+14			+37.9	−45.5	−0.0	+45.5
+16			+6.9	+6.8	+0.0	+6.8
+18			+4.6	−4.1	−0.0	+4.1
+20			+15.3	+14.9	+0.0	+14.9
+22			+4.6	−5.6	+0.0	+5.6
+24			+9.5	−10.6	−0.0	+10.6
+26			+7.5	+7.9	−0.0	+7.9
+1	+1		+36.3	−41.9	−0.0	+41.9
+2			+46.5	+45.5	+0.0	+45.5
+3			+17.0	+14.9	+0.0	+14.9
+4			+78.6	−83.2	+0.0	+83.2
+5			+2.1	−2.4	+0.0	+2.4
+6			+28.7	−33.7	−0.0	+33.7
+7			+24.1	+24.3	+0.0	+24.3
+8			+58.6	−69.0	−0.0	+69.0
+9			+6.9	+6.7	+0.0	+6.7
+10			+4.3	+4.9	−0.0	+4.9
+11			+28.6	−32.3	−0.0	+32.3
+12			+23.6	+22.2	+0.0	+22.2
+13			+24.6	+29.5	−0.0	+29.5
+14			+21.3	−23.3	−0.0	+23.3
+15			+4.2	−3.6	−0.0	+3.6
+16			+6.9	−8.2	−0.0	+8.2
+17			+3.7	−2.7	−0.0	+2.7
+18			+1.9	−1.5	−0.0	+1.5
+19			+10.7	+10.5	+0.0	+10.5
+20			+7.7	+7.5	+0.0	+7.5
+21			+9.8	−10.9	−0.0	+10.9
+22			+7.7	+8.5	+0.0	+8.5
+23			+1.8	+1.5	−0.0	+1.5
+24			+6.8	−7.4	+0.0	+7.4
+25			+2.9	−1.7	−0.0	+1.7
+26			+4.1	−3.2	+0.0	+3.2
+27			+1.4	−1.4	−0.0	+1.4
+28 *			+1.5	+0.6	−0.0	+0.6
+29			+5.5	+4.5	−0.0	+4.5
+0	+2		+10.2	−10.3	−0.0	+10.3
+1			+14.7	+13.2	−0.0	+13.2
+2			+52.4	−55.4	+0.0	+55.4
+3			+51.6	+52.6	−0.0	+52.6
+4			+15.8	−18.1	−0.0	+18.1
+5			+8.0	+8.8	+0.0	+8.8
+6			+30.4	+32.5	+0.0	+32.5
+7			+45.0	−44.4	+0.0	+44.4
+8			+28.4	−33.5	+0.0	+33.5
+9			+13.0	+11.5	+0.0	+11.5
+10			+4.6	−3.4	+0.0	+3.4
+11			+9.1	+10.8	−0.0	+10.8
+12			+1.8	+2.4	−0.0	+2.4
+13			+5.6	+5.6	+0.0	+5.6
+14			+9.0	+9.3	+0.0	+9.3
+15			+4.5	+4.1	+0.0	+4.1
+16			+14.5	+15.1	+0.0	+15.1
+17			+22.6	−21.9	−0.0	+21.9
+18			+18.2	−18.4	−0.0	+18.4
+19			+4.3	+4.9	−0.0	+4.9
+20			+2.9	+1.8	−0.0	+1.8
+21			+5.2	+5.3	−0.0	+5.3
+22			+8.2	+8.3	−0.0	+8.3
+23 *			+2.0	−1.0	+0.0	+1.0
+24 *			+0.8	−1.0	−0.0	+1.0
+25			+3.0	+3.8	−0.0	+3.8
+26			+3.1	+2.4	+0.0	+2.4
+27			+4.8	−4.9	−0.0	+4.9
+28			+3.8	−3.2	−0.0	+3.2
+1	+3		+26.2	−26.7	−0.0	+26.7
+2			+16.6	+15.9	−0.0	+15.9
+3			+7.0	+5.0	−0.0	+5.0
+4			+38.5	−42.7	−0.0	+42.7
+5			+15.1	+14.6	−0.0	+14.6
+6			+34.6	+36.8	+0.0	+36.8
+7			+10.8	+11.5	−0.0	+11.5
+8			+9.7	+11.3	+0.0	+11.3
+9			+17.0	−19.2	−0.0	+19.2
+10			+13.9	−15.7	−0.0	+15.7
+11			+17.8	−19.5	+0.0	+19.5
+12			+15.6	+15.7	+0.0	+15.7
+13			+15.8	+16.5	−0.0	+16.5
+14			+14.0	−13.4	−0.0	+13.4
+15			+11.4	+10.3	+0.0	+10.3
+16			+18.0	+18.8	+0.0	+18.8
+17			+4.9	−4.7	−0.0	+4.7
+18			+9.4	+8.9	−0.0	+8.9
+19			+6.2	−5.4	−0.0	+5.4
+20			+10.7	−11.0	−0.0	+11.0
+21			+1.5	−1.7	−0.0	+1.7
+22			+8.0	+9.1	+0.0	+9.1
+23			+5.0	+4.9	−0.0	+4.9
+24			+4.1	−5.3	−0.0	+5.3
+25			+2.5	+2.3	−0.0	+2.3
+26 *			+1.0	+0.7	−0.0	+0.7
+27			+2.3	−1.9	−0.0	+1.9
+0	+4		+10.1	+9.3	−0.0	+9.3
+1			+27.7	−25.3	−0.0	+25.3
+2			+3.3	+2.8	−0.0	+2.8
+3			+1.3	−1.8	+0.0	+1.8
+4			+4.3	+4.9	−0.0	+4.9
+5			+15.0	+15.0	−0.0	+15.0
+6			+1.6	−2.7	−0.0	+2.7
+7			+9.7	+8.6	+0.0	+8.6
+8			+2.7	+2.4	+0.0	+2.4
+9			+27.6	+26.5	+0.0	+26.5
+10 *			+0.6	+0.9	−0.0	+0.9
+11			+23.9	−26.8	−0.0	+26.8
+12			+11.3	+11.7	+0.0	+11.7
+13			+14.1	−14.8	−0.0	+14.8
+14			+7.7	+6.6	−0.0	+6.6
+15			+16.8	+18.9	+0.0	+18.9
+16			+8.2	−7.5	−0.0	+7.5
+17			+2.2	−1.6	+0.0	+1.6
+18 *			+2.0	−1.1	−0.0	+1.1
+19 *			+0.5	+1.1	−0.0	+1.1
+20 *			+1.1	−1.0	−0.0	+1.0
+21			+7.4	−8.7	−0.0	+8.7
+22 *			+2.0	+0.9	−0.0	+0.9
+23			+3.8	−3.9	+0.0	+3.9
+24 *			+1.6	−0.8	−0.0	+0.8
+25			+8.7	+8.3	+0.0	+8.3
+26			+4.1	−3.9	−0.0	+3.9
+1			+33.1	+29.9	−0.0	+29.9
+2			+1.6	−1.1	−0.0	+1.1
+3			+17.7	−16.9	+0.0	+16.9
+4			+33.7	−33.4	−0.0	+33.4
+5			+6.7	−5.8	+0.0	+5.8
+6			+24.2	+24.7	+0.0	+24.7
+7 *			+0.9	−0.9	−0.0	+0.9
+8			+5.4	+5.8	+0.0	+5.8
+9			+12.4	+11.6	−0.0	+11.6
+10			+8.7	−9.2	−0.0	+9.2
+11 *			+0.5	−1.0	−0.0	+1.0
+12 *			+1.1	−1.1	−0.0	+1.1
+13			+25.6	−26.1	−0.0	+26.1
+14			+12.6	−12.8	−0.0	+12.8
+15 *			+1.6	−1.1	+0.0	+1.1
+16			+6.8	+6.5	−0.0	+6.5
+17			+6.3	+6.5	−0.0	+6.5
+18 *			+0.2	−1.0	−0.0	+1.0
+19			+4.8	+5.1	−0.0	+5.1
+20			+8.0	−8.5	−0.0	+8.5
+21 *			+1.7	+0.9	−0.0	+0.9
+22 *			+2.7	+0.8	+0.0	+0.8
+23			+6.7	6.5	0.0	+6.5
+0	+6		+12.9	−13.6	−0.0	+13.6
+1			+15.1	+14.1	−0.0	+14.1
+2			+12.0	+10.8	−0.0	+10.8
+3			+17.0	+19.5	−0.0	+19.5
+4			+15.7	−14.8	−0.0	+14.8
+5			+10.4	−10.4	−0.0	+10.4
+6			+12.9	−12.7	−0.0	+12.7
+7			+27.0	−27.1	−0.0	+27.1
+8			+16.8	+15.3	−0.0	+15.3
+9 *			+2.9	−1.1	−0.0	+1.1
+10			+5.5	−4.2	−0.0	+4.2
+11			+9.3	+9.8	−0.0	+9.8
+12			+5.0	+4.6	+0.0	+4.6
+13			+3.6	+3.2	−0.0	+3.4
+14			+4.6	−4.4	−0.0	+4.4
+15			+2.7	+1.8	+0.0	+1.8
+16			+7.5	−7.5	−0.0	+7.5
+17			+4.8	−4.8	−0.0	+4.8
+18			+8.4	+8.2	−0.0	+8.2
+19 *			+1.9	+0.9	−0.0	+0.9
+20 *			+0.3	−0.8	−0.0	+0.8
+21			+4.8	+4.7	−0.0	+4.7
+1	+7		+3.1	−2.8	−0.0	+2.8
+2			+10.8	+10.5	−0.0	+10.5
+3			+6.5	−6.1	−0.0	+6.1
+4			+4.4	+5.1	−0.0	+5.1
+5			+8.5	+8.3	+0.0	+8.3
+6			+7.1	−6.8	−0.0	+6.8
+7 *			+1.5	−1.1	+0.0	+1.1
+8 *			+1.2	+1.1	+0.0	+1.1
+9			+4.6	−5.1	−0.0	+5.1
+10			+4.5	+3.9	+0.0	+3.9
+11			+6.5	+7.0	−0.0	+7.0
+12			+5.7	+6.5	−0.0	+6.5
+13 *			+1.0	−1.0	+0.0	+1.0
+14 *			+0.7	−0.9	+0.0	+0.9
+15			+5.5	+5.8	−0.0	+5.8
+16			+4.6	−4.1	−0.0	+4.1
+17 *			+0.3	+0.8	−0.0	+0.8
+18 *			+1.0	+0.7	−0.0	+0.7
+19			+5.1	−6.5	−0.0	+6.5
+0	+8		+13.8	−15.5	−0.0	+15.5
+1			+2.9	+2.7	−0.0	+2.7
+2			+4.5	+4.6	−0.0	+4.6
+3 *			+0.7	+1.0	−0.0	+1.0
+4			+8.7	+9.1	−0.0	+9.1
+5 *			+1.2	−1.0	−0.0	+1.0
+6 *			+1.8	+1.0	−0.0	+1.0
+7 *			+2.2	+1.0	−0.0	+1.0
+8 *			+1.5	+0.9	−0.0	+0.9
+9 *			+0.7	−0.9	−0.0	+0.9
+10			+9.9	−10.5	−0.0	+10.5
+11 *			+0.3	+0.8	−0.0	+0.8
+12			+2.8	+2.2	−0.0	+2.2
+13 *			+0.2	−0.8	−0.0	+0.8
+14			+6.7	+7.7	−0.0	+7.7
+15 *			+0.1	+0.7	−0.0	+0.7
+16			+3.0	−2.2	−0.0	+2.2
+1 *	+9		+1.3	−0.8	−0.0	+0.8
+2			+6.6	−6.7	−0.0	+6.7
+3 *			+0.9	−0.8	−0.0	+0.8
+4 *			+0.2	+0.8	−0.0	+0.8
+5			+4.8	+5.8	−0.0	+5.8
+6 *			+0.1	−0.8	−0.0	+0.8
+7 *			+1.5	−0.7	−0.0	+0.7
+8			+5.6	+6.4	−0.0	+6.4
+9 *			+2.9	−0.7	−0.0	+0.7
+10 *			+0.2	+0.6	−0.0	+0.6
+11 *			+1.3	+0.6	−0.0	+0.6
+12			+7.4	−7.2	−0.0	+7.2
+2	+0	+1	+105.0	−11.6	−101.6	+102.3
+4			+111.8	−110.1	+9.0	+110.5
+6			+65.3	+67.3	+5.1	+67.5
+8			+16.7	−4.4	+15.9	+16.5
+10			+29.5	−21.9	−20.2	+29.8
+12			+37.7	−5.5	−37.6	+38.0
+14			+26.5	−24.2	+13.7	+27.8
+16			+23.7	+25.6	+5.1	+26.1
+18			+4.9	+3.8	+2.4	+4.5
+20			+12.7	−12.8	+1.7	+12.9
+22			+11.6	+3.9	−12.3	+12.9
+24			+4.9	−1.0	+5.0	+5.1
+26			+2.8	+1.7	+2.0	+2.6
+28			+3.3	+1.3	−2.1	+2.5
+0	+1		+90.5	−53.2	+45.1	+69.7
+1			+10.8	−3.0	+11.2	+11.6
+2			+17.6	+12.5	−14.7	+19.3
+3			+12.7	+11.3	+4.7	+12.2
+4			+75.6	−33.6	−65.6	+73.7
+5			+23.1	−4.8	+24.3	+24.8
+6			+36.6	−15.9	−33.6	+37.1
+7			+39.2	−29.6	+29.1	+41.5
+8			+27.8	+26.2	+11.2	+28.5
+9			+25.5	+16.5	−22.4	+27.8
+10			+31.2	−6.2	+32.9	+33.5
+11			+11.7	−7.3	+7.3	+10.3
+12			+12.8	+9.4	−8.5	+12.7
+13			+9.3	−8.3	+5.4	+9.9
+14			+18.1	−8.0	−17.5	+19.2
+15			+18.1	+15.8	−11.1	+19.3
+16			+5.2	−1.1	+4.2	+4.3
+17			+10.9	−7.5	+7.4	+10.6
+18			+14.5	+13.2	+7.7	+15.3
+19			+7.2	+2.9	−6.9	+7.5
+20			+6.4	+0.4	+6.4	+6.4
+21			+3.5	−0.4	−2.3	+2.3
+22			+4.6	−2.4	−3.9	+4.6
+23			+3.8	−2.6	+1.5	+3.0
+24			+4.9	−1.3	−4.6	+4.8
+25			+6.3	+6.1	−1.0	+6.2
+26			+3.5	+0.0	+2.1	+2.1
+27			+5.4	−2.7	+4.3	+5.1
+28			+3.2	+2.6	+1.3	+2.9
+1	+2		+34.1	+23.6	+16.3	+28.7
+2			+49.3	+38.7	−27.4	+47.4
+3			+46.7	−39.5	+23.7	+46.1
+4			+20.8	+0.9	+18.3	+18.3
+5			+31.3	−24.4	−17.6	+30.1
+6			+25.0	+10.9	−22.5	+25.0
+7			+3.6	−3.4	−2.0	+3.9
+8			+7.2	+4.6	+4.6	+6.5
+9			+20.8	+19.6	+1.0	+19.6
+10			+18.1	+1.5	+17.8	+17.9
+11			+23.1	+20.6	−11.6	+23.6
+12			+23.1	+22.6	+5.9	+23.3
+13			+21.0	−24.1	+3.8	+24.4
+14			+12.6	−8.9	+8.2	+12.1
+15			+14.4	−0.7	−15.1	+15.1
+16			+11.1	−1.8	−11.1	+11.2
+17			+9.1	+8.9	−1.8	+9.1
+18			+4.3	+2.7	+2.4	+3.6
+19			+9.5	−0.4	+9.4	+9.4
+20			+12.2	−3.8	+12.3	+12.9
+21			+3.6	+3.6	−0.6	+3.7
+22			+7.4	+7.6	−1.2	+7.7
+23			+7.3	−6.7	+2.4	+7.1
+24			+4.0	−3.4	−1.1	+3.6
+25			+2.3	+0.4	−1.3	+1.4
+26			+3.3	−1.8	−1.9	+2.6
+27			+3.3	+1.9	+0.1	+1.9
+0	+3		+41.1	−33.2	+18.3	+37.9
+1			+20.7	+15.3	+10.1	+18.3
+2			+41.7	+24.4	−32.0	+40.3
+3			+37.4	+30.7	+19.1	+36.1
+4			+35.7	+34.6	+14.5	+37.5
+5			+4.6	−1.7	−2.3	+2.8
+6			+32.3	−7.7	+35.3	+36.1
+7			+33.9	−20.0	−31.0	+36.9
+8			+7.1	+5.5	−5.1	+7.5
~~+9~~			+25.2	+9.3	−23.3	+25.1
+10			+29.2	−27.3	+15.3	+31.3
+11			+17.7	+13.9	+14.1	+19.8
+12			+11.9	+8.0	−7.8	+11.2
+13			+17.7	+2.7	+16.9	+17.1
+14			+13.0	+12.7	+5.0	+13.6
+15			+6.7	−5.3	−4.7	+7.1
+16			+19.7	−16.7	+13.7	+21.6
+17			+10.0	−7.4	−6.4	+9.8
+18			+11.4	+5.5	−10.6	+11.9
+19 *			+1.6	+1.1	+0.3	+1.1
+20			+5.8	−5.8	−0.6	+5.8
+21			+5.9	+3.4	+4.2	+5.4
+22			+3.3	+0.6	−3.2	+3.3
+23			+3.4	−1.2	+3.0	+3.2
+24			+5.4	+3.9	−2.4	+4.6
+25			+3.1	−1.3	−2.4	+2.7
+26			+5.8	−5.2	+2.6	+5.8
+27			+1.7	−0.7	−1.9	+2.0
+1	+4		+11.7	+1.4	−12.3	+12.4
+2			+9.3	−5.9	+7.6	+9.6
+3			+15.4	−3.4	+13.1	+13.5
+4			+7.9	−8.4	+0.3	+8.4
+5			+27.4	+26.8	+2.8	+26.9
+6			+8.9	−4.3	+7.2	+8.4
+7			+9.5	−10.3	+2.7	+10.7
+8			+3.5	−1.6	−2.9	+3.3
+9			+17.1	−13.4	−9.4	+16.4
+10			+2.7	+2.4	+1.0	+2.6
+11			+11.1	+4.1	−10.2	+11.0
+12			+7.0	−8.9	+0.0	+8.9
+13			+20.7	−6.7	+21.1	+22.1
+14			+10.8	−0.5	−10.7	+10.7
+15			+7.8	+7.5	+1.8	+7.7
+16			+4.3	−1.4	−3.7	+4.0
+17			+8.2	−2.0	−8.6	+8.8
+18 *			+1.5	−0.2	−1.0	+1.0
+19			+9.0	−9.8	−2.6	+10.1
+20 *			+1.6	+1.0	+0.0	+1.0
+21			+5.6	+5.0	−1.9	+5.4
+22 *			+2.6	−0.7	−0.5	+0.9
+23			+7.1	+0.5	+7.4	+7.4
+24			+2.8	+1.2	−2.7	+2.9
+0	+5		+32.7	−30.3	+1.9	+30.4
+1			+18.4	+1.3	−17.6	+17.7
+2			+15.2	+8.8	−11.1	+13.9
+3			+22.6	−16.6	−16.6	+23.5
+4			+6.5	+2.9	+4.2	+5.1
+5			+6.4	−1.9	+6.2	+6.5
+6			+11.2	−4.0	+9.6	+10.4
+7			+15.1	+12.5	+8.8	+15.3
+8			+15.7	+6.5	−14.0	+15.4
+9			+9.7	−8.7	+3.1	+9.2
+10			+14.3	−13.1	−4.3	+13.8
+11			+14.4	−4.8	−12.8	+13.7
+12			+6.2	+4.5	−2.8	+5.3
+13			+4.8	−2.3	−3.1	+3.9
+14			+4.4	+3.2	+2.3	+4.0
+15			+9.8	+4.1	+8.6	+9.5
+16			+6.7	−4.4	+5.2	+6.8
+17			+9.0	+8.3	+2.7	+8.7
+18			+7.6	+4.7	−7.1	+8.5
+19			+5.2	−4.7	+1.0	+4.8
+20			+2.5	−1.4	+1.1	+1.8
+21			+4.7	−2.3	−4.4	+5.0
+22			+2.5	−0.2	+2.5	+2.5
+23 *			+1.9	−0.7	−0.2	+0.7
+24			+2.9	+2.3	−0.7	+2.4
+25			+3.8	+0.5	+3.3	+3.3
+1	+6		+10.3	+4.4	+9.9	+10.8
+2			+12.7	−13.3	−4.6	+14.1
+3			+8.9	−7.0	−6.8	+9.8
+4			+15.0	+11.7	−11.1	+16.1
+5			+17.3	−7.5	−15.5	+17.2
+6			+17.6	−6.9	+15.9	+17.3
+7			+3.6	−1.0	+2.6	+2.8
+8			+10.4	+8.9	+6.6	+11.1
+9			+12.1	+5.3	+10.9	+12.1
+10			+3.1	+1.4	−2.9	+3.2
+11			+8.9	+9.8	+0.4	+9.8
+12			+9.2	−10.3	+1.3	+10.4
+13			+3.0	−2.8	−0.8	+2.9
+14			+8.4	+7.5	−5.1	+9.1
+15			+4.4	−2.3	−2.0	+3.0
+16			+5.9	+0.5	+6.5	+6.5
+17			+3.3	+2.6	+1.0	+2.8
+18			+3.1	+1.6	+2.2	+2.7
+19			+4.2	+0.2	+5.1	+5.1
+20			+3.3	+1.4	−3.3	+3.6
+21 *			+1.9	+0.5	−0.4	+0.7
+22			+3.5	−3.5	+1.3	+3.7
+23			+2.2	−1.7	−1.5	+2.3
+0	+7		+13.0	+8.2	+12.2	+14.7
+1			+5.0	+5.0	−0.8	+5.1
+2			+3.3	+0.7	+5.3	+5.3
+3			+7.8	+0.8	+8.0	+8.0
+4			+5.2	−3.8	−3.7	+5.5
+5 *			+0.6	−0.8	+0.6	+1.0
+6			+4.0	−3.6	+0.7	+3.7
+7			+11.2	+6.1	−11.5	+13.0
+8			+6.5	+5.5	+4.6	+7.2
+9			+4.5	−3.9	+3.4	+5.2
+10			+6.4	+8.9	+1.7	+9.1
+11			+3.4	+2.9	+2.2	+3.6
+12			+4.5	−3.4	−3.5	+4.9
+13			+3.6	+3.5	+3.3	+4.8
+14			+5.1	−2.7	−5.1	+5.8
+15			+4.9	−4.3	+1.1	+4.4
+16 *			+0.5	+0.2	−0.8	+0.8
+17			+5.0	+1.8	−5.5	+5.8
+18			+4.3	+3.0	+2.3	+3.8
+19			+2.6	−2.3	+2.0	+3.1
+1	+8		+2.6	−1.0	+3.4	+3.5
+2			+7.5	+4.0	+7.6	+8.6
+3			+5.3	+5.0	−6.3	+8.0
+4			+8.2	+7.6	−3.6	+8.4
+5 *			+1.5	+0.4	−0.8	+0.9
+6			+8.5	−8.3	−1.8	+8.5
+7 *			+1.1	−0.8	−0.4	+0.9
+8			+7.2	−3.0	−6.3	+7.0
+9 *			+2.4	−0.4	+0.7	+0.8
+10			+5.7	+5.9	−2.0	+6.2
+11			+2.7	−1.4	+2.6	+3.0
+12			+4.9	−0.3	+6.8	+6.8
+0	+		+9.6	−1.2	−8.8	+8.9
+1 *			+2.1	+0.8	+0.3	+0.8
+2			+2.8	−2.6	−1.1	+2.8
+3			+2.7	−0.5	+2.7	+2.7
+4			+4.3	+3.1	+2.0	+3.7
+5 *			+1.0	−0.6	+0.3	+0.7
+6			+3.9	+2.6	+2.2	+3.4
+7 *			+1.9	+0.1	−0.6	+0.6
+8			+4.6	−5.0	−0.3	+5.0
+9			+2.9	−2.2	+2.1	+3.0
+10			+6.3	0.7	−6.6	+6.6
+0	+0	+2	+35.1	+9.6	+34.8	+36.1
+2			+50.2	+30.0	−37.9	+48.4
+4			+20.0	−19.8	+11.3	+22.8
+6			+33.9	−11.0	+31.3	+33.2
+8			+47.2	+12.6	−49.6	+51.2
+10			+7.5	−5.7	−4.7	+7.4
+12			+15.9	+7.9	−12.5	+14.8
+14			+9.7	−3.1	+9.6	+10.1
+16			+21.0	−6.6	+21.0	+22.0
+18			+20.6	+3.2	−23.1	+23.3
+20			+4.8	+3.9	+2.4	+4.6
+22			+6.8	+1.2	+5.7	+5.8
+24 *			+0.3	+0.4	+0.9	+1.0
+26			+5.8	−1.3	+6.0	+6.1
+28			+4.4	−0.0	−3.7	+3.7
+1	+1		+17.7	−6.3	−15.4	+16.6
+2			+27.9	+2.3	−32.7	+32.8
+3			+29.8	−15.0	+26.1	+30.1
+4			+36.8	+9.5	−36.1	+37.5
+5			+10.2	+1.2	−10.8	+10.9
+6			+34.6	−22.8	+32.0	+39.3
+7			+12.8	+11.3	+6.0	+12.8
+8			+21.4	+2.0	+20.8	+20.9
+9			+7.0	+0.6	−5.3	+5.3
+10			+8.6	+4.5	−7.1	+8.3
+11			+17.6	+4.3	−18.9	+19.4
+12			+6.5	+4.5	−4.4	+6.3
+13			+26.0	+2.1	+27.2	+27.3
+14			+2.8	+1.2	−3.2	+3.4
+15			+4.3	+2.1	−3.5	+4.1
+16			+19.3	−6.4	+21.1	+22.0
+17			+9.8	+2.8	−9.5	+9.9
+18			+8.6	+0.3	+8.6	+8.6
+19			+3.9	−1.6	+3.1	+3.5
+20			+8.9	+1.5	−9.2	+9.3
+21			+3.7	+0.6	−2.4	+2.5
+22 *			+0.7	+1.0	+0.0	+1.0
+23			+8.5	−3.4	+10.6	+11.1
+24			+1.7	−2.1	+0.4	+2.1
+25			+2.9	−2.1	−1.7	+2.7
+26			+3.1	−1.2	+2.9	+3.2
+27			+4.5	+1.4	−3.9	+4.1
+0	+2		+56.3	−0.7	+56.1	+56.1
+1			+32.1	+0.9	−27.0	+27.0
+2			+22.7	−1.3	−20.0	+20.0
+3			+15.4	+5.5	−14.5	+15.5
+4			+11.4	+6.9	−6.0	+9.1
+5			+18.4	+17.6	+8.3	+19.4
+6			+21.8	−3.1	+24.2	+24.4
+7			+15.8	+17.2	+3.5	+17.6
+8			+5.5	−2.7	+5.0	+5.7
+9			+17.7	−2.0	+19.3	+19.4
+10			+26.5	−10.4	+24.8	+26.9
+11			+21.6	−4.7	−24.3	+24.7
+12			+16.1	−3.4	−18.9	+19.2
+13			+9.9	+5.9	−7.9	+9.9
+14			+11.8	+6.6	−9.8	+11.8
+15			+17.5	+0.7	+20.5	+20.5
+16			+12.0	−6.6	+10.2	+12.1
+17			+4.0	−3.5	−2.6	+4.4
+18			+2.4	−1.1	−3.6	+3.8
+19			+7.0	−6.5	+2.4	+6.9
+20			+3.6	−0.5	+4.4	+4.4
+21			+5.5	−2.4	−5.8	+6.3
+22			+5.8	+0.5	−5.1	+5.1
+23			+4.5	+3.5	−2.2	+4.1
+24			+7.1	+2.6	−6.5	+7.0
+25			+6.3	−0.4	+6.3	+6.3
+26			+3.6	−0.5	+3.0	+3.0
+27			+2.8	−0.4	−2.5	+2.5
+1	+3		+29.2	+5.8	+26.3	+26.9
+2			+44.8	+2.5	+44.2	+44.3
+3			+17.6	+1.0	−16.4	+16.4
+4			+24.1	−3.4	−23.2	+23.5
+5			+37.1	+7.9	−35.1	+36.0
+6			+19.3	−15.5	+11.5	+19.1
+7			+6.4	+4.4	+2.7	+5.2
+8			+25.2	−9.3	−25.6	+27.2
+9			+28.6	−5.4	+30.9	+31.4
+10			+14.2	+12.0	−9.9	+15.6
+11			+12.1	−10.5	+6.6	+12.4
+12			+19.2	−4.0	+19.2	+19.6
+13			+9.5	−4.0	−8.2	+9.1
+14			+18.2	+2.0	−19.7	+19.8
+15			+9.1	+2.1	−10.1	+10.3
+16 *			+2.4	+0.3	+1.0	+1.1
+17 *			+1.4	+0.5	+1.0	+1.1
+18			+4.0	+1.9	−2.6	+3.2
+19			+8.6	−1.9	+9.5	+9.7
+20			+9.0	+7.8	−6.3	+10.0
+21			+2.4	−1.1	−1.1	+1.6
+22			+7.8	−2.0	+7.0	+7.3
+23			+4.0	+0.7	−3.0	+3.1
+24			+3.9	−0.5	−3.4	+3.4
+0	+4		+16.6	−4.0	−13.8	+14.4
+1			+2.1	−0.5	+1.4	+1.5
+2 *			+1.3	−0.3	+0.8	+0.8
+3			+24.7	−10.8	+22.9	+25.3
+4			+6.0	−5.5	−3.1	+6.3
+5			+1.4	−0.5	−1.2	+1.3
+6			+1.5	+0.7	−1.1	+1.3
+7			+24.7	+7.1	−24.0	+25.0
+8 *			+1.9	+0.3	−1.0	+1.0
+9			+17.1	−4.2	+18.3	+18.8
+10			+13.1	+4.6	−14.3	+15.0
+11			+10.1	−8.8	+9.3	+12.8
+12			+9.7	+9.7	+5.3	+11.1
+13			+4.2	−4.0	−2.7	+4.8
+14			+4.1	+2.0	+3.3	+3.9
+15 *			+2.3	+0.7	−0.9	+1.1
+16 *			+0.4	+1.1	−0.3	+1.1
+17			+14.6	+3.9	−15.9	+16.4
+18 *			+3.1	−1.0	+0.4	+1.1
+19			+7.2	−0.6	+7.1	+7.1
+20 *			+1.6	+0.7	−0.7	+1.0
+21			+6.1	−2.1	+6.2	+6.6
+22			+2.9	+0.3	+2.5	+2.5
+23			+3.7	+0.8	−2.7	+2.8
+24			+1.7	−1.0	+0.5	+1.9
+1	+5		+4.0	−0.6	−3.6	+3.7
+2			+18.0	−4.9	+17.5	+18.2
+3			+1.3	+1.3	−0.4	+1.4
+4			+10.2	+2.3	−9.3	+9.6
+5			+17.7	−2.9	+18.3	+18.5
+6			+5.7	−2.2	+4.6	+5.1
+7			+3.2	+1.8	−3.5	+3.9
+8			+7.1	+6.9	−3.2	+7.6
+9			+13.1	−1.8	−12.8	+12.9
+10			+2.1	+1.5	−0.6	+1.6
+11			+3.3	−2.0	−2.2	+3.0
+12			+14.7	−5.0	+15.2	+16.0
+13 *			+0.5	+1.0	−0.5	+1.1
+14			+3.9	−0.5	−3.9	+3.9
+15			+8.7	−0.9	+9.2	+9.2
+16 *			+2.3	−0.4	+1.0	+1.1
+17 *			+2.6	+0.3	−1.0	+1.1
+18 *			+1.2	−0.6	+0.8	+1.0
+19			+6.6	+2.5	−7.2	+7.6
+20			+3.5	−0.2	−3.7	+3.7
+21			+4.1	+0.5	+3.4	+3.4
+22			+5.4	−1.0	+5.9	+6.0
+0	+6		+21.8	+9.3	−24.6	+26.3
+1			+8.7	+3.8	−8.6	+9.4
+2			+8.6	−4.8	+8.3	+9.6
+3			+8.9	+6.9	−8.3	+10.7
+4			+11.2	−5.3	+10.6	+11.8
+5 *			+2.3	−1.0	−0.5	+1.1
+6			+3.3	−1.3	+2.8	+3.1
+7			+4.8	−4.1	+2.4	+4.7
+8			+4.9	+0.4	+4.7	+4.7
+9			+7.0	−1.4	+7.6	+7.7
+10			+15.5	+6.9	−17.6	+18.9
+11			+6.4	+0.9	−5.5	+5.6
+12			+5.1	−1.1	+5.2	+5.3
+13			+7.0	+4.4	−6.1	+7.5
+14			+7.5	−2.0	+8.3	+8.5
+15			+6.3	+0.3	+4.9	+4.9
+16			+4.9	−0.1	−5.1	+5.1
+17			+3.0	−0.5	+3.4	+3.4
+18 *			+0.5	−0.2	+0.9	+0.9
+19 *			+0.7	−0.4	+0.7	+0.8

Table 1 (*cont.*)

h	k	l	F_c	A_o	B_o	F_o
+20			+4.5	+0.8	−5.8	+5.9
+1	+7		+6.4	−1.5	+6.9	+7.1
+2			+6.2	+1.2	−7.0	+7.1
+3			+9.1	+2.2	−9.9	+10.1
+4			+4.1	+0.5	−3.0	+3.0
+5 *			+2.2	+1.1	+0.3	+1.1
+6			+5.9	+3.6	+4.8	+6.0
+7			+3.0	−0.8	−2.7	+2.8
+8			+4.3	+2.0	+3.4	+3.9
+9			+3.8	−0.7	+2.6	+2.7
+10			+6.6	+2.0	−7.4	+7.7
+11			+7.7	−1.3	+7.4	+7.5
+12			+6.7	−0.8	−6.7	+6.7
+13			+6.7	+2.2	−7.1	+7.4
+14 *			+1.5	+0.1	+0.8	+0.8
+15 *			+0.7	+0.7	+0.5	+0.8
+16			+4.2	−0.2	+5.1	+5.1
+0	+8		+3.1	+3.7	−0.4	+3.7
+1			+2.8	+1.6	+2.0	+2.6
+2			+4.6	+1.1	+5.7	+5.8
+3			+2.2	+1.3	−2.3	+2.6
+4			+8.4	+0.8	−9.6	+9.6
+5 *			+1.9	−0.8	−0.6	+1.0
+6			+8.0	+3.1	−9.4	+9.9
+7			+4.1	−2.3	+2.5	+3.4
+8			+8.3	−0.8	+10.8	+10.8
+9 *			+0.6	−0.8	+0.5	+0.8
+10 *			+1.3	−0.7	+0.4	+0.8
+11 *			+1.3	+0.5	+0.7	+0.8
+12			+2.1	−2.0	+0.2	+2.0
+13			+2.5	+0.2	−2.3	+2.3
+14			+2.6	−1.2	−2.5	+2.8
+1	+9		+2.2	−2.4	+1.2	+2.7
+2			+5.6	−1.2	+5.7	+5.8
+3 *			+1.5	+0.2	−0.7	+0.7
+4			+6.8	−3.0	+7.8	+8.4
+5 *			+0.8	+0.1	+0.6	+0.6
+6			+6.6	+0.2	−7.5	+7.5
+2	+0	+3	+17.7	−12.6	+15.3	+19.8
+4			+42.6	−30.0	−33.0	+44.6
+6			+12.5	+12.2	+6.5	+13.8
+8			+25.0	+21.2	−10.2	+23.5
+10			+5.9	+0.4	−5.8	+5.8
+12			+24.8	−8.8	+22.2	+23.9
+14			+20.9	−17.9	−10.9	+20.9
+16			+10.0	+8.4	+4.0	+9.3
+18			+9.7	+6.9	+7.9	+10.5
+20			+7.0	−7.1	−3.0	+7.7
+22			+8.0	−2.5	+8.2	+8.6
+24			+6.2	−4.4	−4.8	+6.5
+26			+3.8	+2.1	−2.1	+3.0
+0	+1		+28.7	+3.9	−29.2	+29.5
+1			+13.3	−12.1	−5.3	+13.2
+2			+3.5	−0.6	−3.2	+3.2
+3			+17.6	+0.2	+17.8	+17.8
+4			+14.9	−12.5	+10.4	+16.2
+5			+6.3	+4.4	+4.5	+6.3
+6			+11.1	−10.2	+1.1	+10.3
+7			+17.5	+0.8	−17.1	+17.1
+8			+11.5	+10.8	+6.5	+12.6
+9			+14.1	+5.6	+13.9	+15.0
+10			+8.2	+5.0	−6.1	+7.9
+11			+14.8	−16.3	+2.0	+16.4
+12			+9.4	−5.0	+8.1	+9.5
+13			+3.7	+0.7	−3.7	+3.8
+14			+13.3	−8.8	+9.6	+13.0
+15			+13.2	+13.4	+3.3	+13.8
+16			+7.9	−6.0	−6.3	+8.7
+17			+9.1	−2.0	−9.1	+9.3
+18			+8.8	+9.2	−0.9	+9.2
+19			+5.6	−2.9	+5.9	+6.6
+20			+3.9	+1.5	−2.6	+3.0
+21			+4.2	−3.6	+0.9	+3.7
+22			+1.9	−1.3	−0.3	+1.3
+23			+4.9	+1.1	−3.8	+4.0
+24			+2.2	−1.1	+0.8	+1.4
+25			+5.1	+4.0	+3.5	+5.3
+26			+3.8	+0.1	−2.7	+2.7
+1	+2		+17.1	+16.0	+2.8	+16.2
+2			+25.2	+24.6	+3.2	+24.8
+3			+13.9	−11.8	−4.1	+12.5
+4			+17.8	−2.7	−16.7	+16.9
+5			+19.2	−10.0	+16.5	+19.3
+6			+23.0	−3.9	+23.1	+23.4
+7			+10.0	−5.8	−8.5	+10.3
+8			+9.1	−9.7	−1.3	+9.8
+9			+16.9	+13.8	−10.4	+17.3
+10			+12.4	+8.5	−9.6	+12.8
+11			+12.6	+12.3	+8.0	+14.7
+12			+9.7	+10.4	+4.5	+11.3
+13			+13.3	−13.7	−5.1	+14.6
+14			+9.5	−5.1	−10.0	+11.2
+15			+5.1	−3.2	+3.8	+5.0
+16			+6.4	−1.1	+5.8	+5.9
+17			+2.7	+1.0	−2.3	+2.5
+18			+0.6	−0.7	−0.7	+1.0
+19			+6.1	+2.7	−5.4	+6.0
+20			+7.5	+3.8	−5.9	+7.0
+21			+6.7	+1.7	+6.5	+6.7
+22			+5.0	+5.1	+2.8	+5.8
+23			+4.4	−4.6	−0.8	+4.7
+0	+3		+29.0	−15.9	−23.4	+28.3
+1			+15.3	+11.2	−6.3	+12.9
+2			+20.5	+11.4	+14.6	+18.5
+3			+19.2	+17.1	−6.8	+18.4
+4			+9.5	+5.1	−6.1	+7.9
+5			+7.7	−5.5	+4.3	+7.0
+6			+12.3	+1.0	−11.8	+11.8
+7			+18.8	−18.6	+5.1	+19.3
+8			+18.4	+2.9	+18.1	+18.3
+9 *			+1.7	−0.8	−0.3	+0.9
+10			+15.5	−10.7	−12.2	+16.2
+11			+11.3	+9.8	−8.1	+12.7
+12			+9.8	+7.2	+8.1	+10.8
+13			+5.2	+2.9	−3.1	+4.2
+14			+2.6	+1.3	+0.9	+1.6
+15			+6.9	−3.3	+7.0	+7.7
+16			+6.7	−0.3	−6.9	+6.9
+17			+7.0	−6.9	+1.3	+7.0
+18			+9.6	+1.3	+9.5	+9.6
+19			+3.0	+0.6	−2.1	+2.2
+20			+4.9	−4.1	−3.4	+5.3
+21			+4.6	+3.5	−1.2	+3.7
+22 *			+1.3	+0.4	−0.7	+0.8
+23			+0.9	+2.3	+0.0	+2.3
+24 *			+2.2	+0.3	+0.5	+0.6
+25			+2.9	−0.7	+2.1	+2.2
+1	+4		+18.5	−11.9	+12.2	+17.0
+2			+10.0	−8.0	+0.6	+8.0
+3			+12.0	+2.9	−10.6	+11.0
+4			+8.7	−4.3	+7.8	+8.9
+5			+17.9	+17.2	+0.1	+17.2
+6			+4.9	−1.4	−4.9	+5.1
+7			+6.2	−5.7	−2.8	+6.3
+8			+8.4	+7.7	+4.5	+8.9
+9			+13.4	−12.6	+1.0	+12.6
+10			+5.6	−3.6	+5.1	+6.3
+11			+5.8	+2.5	+5.2	+5.8
+12			+5.4	−5.8	+1.2	+5.9
+13			+15.6	+3.8	−13.5	+14.0
+14 *			+1.4	−0.7	+0.7	+1.0
+15			+8.5	+9.2	+0.2	+9.2
+16			+4.8	−0.0	−5.3	+5.3
+17			+6.3	−2.3	+5.6	+6.0
+18 *			+1.1	+0.5	+0.9	+0.9
+19			+6.4	−6.5	−1.5	+6.7
+20			+1.7	−1.5	+0.5	+1.6
+21			+4.2	+2.3	+2.4	+3.3
+22 *			+1.0	−0.0	−0.6	+0.6
+23			+3.3	+0.8	−2.1	+2.3
+0	+5		+15.6	−12.2	−7.4	+14.3
+1			+5.8	+1.3	+4.7	+4.9
+2			+7.8	−1.6	+7.0	+7.2
+3			+2.3	−1.3	−0.7	+1.5
+4			+5.5	+3.0	+2.2	+3.7
+5			+6.1	−0.3	−7.3	+7.3
+6			+4.2	+0.2	−4.3	+4.3
+7			+7.1	+5.4	−2.5	+6.0
+8			+8.3	+2.3	+7.9	+8.2
+9			+5.9	+0.5	−5.5	+5.5
+10			+8.7	−5.5	−5.3	+7.6
+11			+5.0	−1.0	+4.7	+4.8
+12 *			+1.8	−1.0	+0.0	+1.0
+13			+3.9	−1.9	+3.6	+4.1
+14			+2.3	+2.4	+1.6	+2.9
+15 *			+2.7	+0.3	−0.9	+1.0
+16			+6.1	+0.8	−6.4	+6.4
+17			+6.2	+5.5	+4.5	+7.0
+18			+4.9	+3.7	+4.5	+5.8
+19			+2.8	−1.9	+0.4	+1.9
+20			+3.0	−2.4	−0.8	+2.5
+21			+2.7	−3.0	+1.6	+3.4
+22			+1.8	−0.2	−1.3	+1.3
+1	+6		+8.2	+8.5	−4.4	+9.6
+2			+10.3	−10.1	−1.0	+10.1
+3			+3.5	−1.9	−3.2	+3.7
+4			+8.8	+0.4	+9.0	+9.0
+5			+7.0	−4.6	+4.4	+6.4
+6			+10.5	+4.8	−8.5	+9.8
+7			+5.1	−5.0	−0.6	+5.0
+8			+8.1	+7.8	−1.3	+7.9
+9			+5.6	+4.6	−1.7	+4.9
+10			+4.6	−1.1	+4.8	+4.9
+11			+8.3	+8.1	+5.1	+9.6
+12			+8.3	−8.3	−4.2	+9.3
+13			+4.1	−2.1	+1.6	+2.6
+14			+4.5	+2.9	+1.7	+3.4
+15			+5.4	−5.6	+2.6	+6.2
+16			+5.7	+3.7	−4.3	+5.7
+17 *			+1.5	−0.7	−0.4	+0.8
+18 *			+2.0	+0.7	−0.2	+0.7
+19			+3.4	+1.6	−2.7	+3.2
+20			+4.1	−0.5	+2.3	+2.4
+0	+7		+5.8	+4.8	−3.7	+6.0
+1			+5.5	+5.1	+3.2	+6.0
+2			+2.7	+3.4	+0.1	+3.4
+3			+3.3	+0.6	−2.3	+2.4
+4			+3.8	−2.3	+2.5	+3.4
+5 *			+1.5	−0.8	+0.4	+0.9
+6 *			+1.7	−0.8	+0.2	+0.8
+7			+6.9	−0.5	+6.4	+6.4
+8			+4.4	+3.6	−2.4	+4.3
+9			+4.3	−2.4	−2.7	+3.6
+10			+4.4	+4.6	−2.6	+5.3
+11			+3.2	+3.3	+0.4	+3.3
+12			+2.2	−2.5	+1.2	+2.8
+13 *			+0.2	+0.6	−0.4	+0.7
+14			+4.1	−3.9	+1.9	+4.3
+15			+3.1	−1.5	−1.6	+2.2
+16 *			+0.9	+0.4	−0.5	+0.6
+17			+2.4	+0.0	+1.5	+1.5
+1 *	+8		+0.6	+0.2	−0.8	+0.8
+2			+6.9	+3.8	−6.1	+7.2
+3 *			+1.9	+0.5	+0.6	+0.8
+4			+4.8	+4.3	+3.9	+5.8
+5			+2.5	−2.1	−1.7	+2.7
+6			+6.2	−7.4	−0.8	+7.4
+7 *			+0.7	−0.3	+0.6	+0.7
+8			+4.3	−3.8	+2.5	+4.6
+9 *			+0.5	+0.0	−0.6	+0.6
+10 *			+1.3	+0.6	+0.0	+0.6
+11 *			+1.0	+0.4	−0.4	+0.6
+12			+4.3	+2.2	−4.4	+4.9
+0	+9		+7.1	−4.6	+4.9	+6.7
+1 *			+1.1	+0.3	+0.3	+0.4
+2			+2.9	−2.7	−1.1	+2.9
+3 *			+0.5	+0.4	−0.0	+0.4
+4			+4.2	+4.1	−1.5	+4.4
+0	+0	+4	+34.2	−43.3	−19.2	+47.4
+2			+8.5	+9.0	−1.4	+9.1
+4			+12.9	+16.1	+2.1	+16.2
+6 *			+0.8	−0.2	+0.8	+0.8
+8			+8.7	+5.4	+7.7	+9.4
+10			+24.9	−24.2	−11.8	+26.9
+12			+5.4	+4.4	−4.0	+6.0
+14			+12.1	+8.5	+8.2	+11.8
+16			+6.9	−7.9	−0.3	+7.9
+18			+3.9	+3.4	+2.5	+4.2
+20			+6.9	−7.0	−4.2	+8.2
+22			+4.1	+2.9	−3.2	+4.3
+24			+6.1	+5.1	+3.1	+6.0
+1	+1		+4.2	−3.4	+3.1	+4.6
+2			+15.4	−15.7	−2.3	+15.9
+3			+9.5	−8.7	−5.7	+10.4
+4			+3.3	+3.0	−0.1	+3.0
+5			+15.0	+17.4	+2.5	+17.6
+6			+5.6	+6.0	+0.7	+6.0
+7			+6.3	−7.6	−0.2	+7.6
+8			+7.3	+5.8	+4.7	+7.5
+9			+5.6	−5.0	−3.0	+5.8
+10			+7.6	−5.1	+7.5	+9.1
+11			+10.7	+10.0	+4.5	+11.0
+12			+12.7	−11.3	−4.8	+12.3
+13			+2.8	−2.5	+1.4	+2.9
+14			+8.5	+8.0	−2.4	+8.4
+15			+4.7	+5.3	+1.2	+5.4
+16			+5.3	+5.4	+1.4	+5.6
+17			+2.4	−2.6	−1.1	+2.8
+18			+1.8	+0.9	+1.2	+1.5
+19			+5.9	−5.1	−3.6	+6.2
+20			+2.2	−0.6	+1.3	+1.4
+21			+5.3	+5.1	+2.8	+5.8
+22			+4.6	−3.4	−3.8	+5.1
+23			+2.2	−3.1	+0.7	+3.2
+24			+3.8	+2.9	−0.3	+2.9
+0	+2		+6.5	+2.5	−6.1	+6.6
+1			+4.2	+3.1	−2.7	+4.1
+2			+14.6	+13.7	+6.9	+15.3
+3			+12.8	−9.7	−8.5	+12.9
+4			+9.4	−9.3	+0.8	+9.3
+5			+3.6	+2.8	+1.8	+3.3
+6			+10.5	−12.1	+1.1	+12.1
+7			+20.9	+18.9	+13.4	+23.2
+8			+13.1	+12.5	+6.5	+14.1
+9			+4.7	−4.4	−0.6	+4.4
+10			+6.6	−0.9	−5.8	+5.9
+11			+5.3	−1.6	−5.5	+5.7
+12			+1.1	+1.9	−0.0	+1.9
+13			+4.1	−5.3	−2.5	+5.8
+14			+4.4	−5.0	−0.2	+5.0
+15			+2.7	−2.7	−0.1	+2.7
+16			+3.5	−2.5	−2.0	+3.2
+17			+7.2	+6.7	+3.2	+7.4
+18			+7.5	+7.8	+3.1	+8.4
+19			+4.9	−4.7	−2.2	+5.2
+20			+1.2	−1.0	+1.7	+2.0
+21			+3.1	−2.1	−2.7	+3.4
+22			+2.8	−2.2	−0.4	+2.2
+1	+3		+14.9	+10.4	+10.9	+15.1
+2			+10.3	−11.0	+3.7	+11.6
+3			+6.6	−4.2	−3.2	+5.3
+4			+14.5	+10.6	+10.1	+14.6
+5			+12.2	−8.0	−9.5	+12.4
+6			+20.9	−16.3	−14.3	+21.7
+7 *			+0.8	−0.6	−0.9	+1.1
+8			+4.0	−0.2	−4.5	+4.5
+9			+7.4	+5.5	+3.8	+6.7
+10			+5.7	+2.6	+3.4	+4.3
+11			+4.7	+3.9	+3.7	+5.4
+12			+4.0	−3.5	−1.4	+3.8
+13			+8.6	−9.2	−2.8	+9.6
+14			+8.7	+8.7	+5.0	+10.0
+15			+6.5	−4.0	−4.7	+6.2
+16			+6.2	−6.4	−3.1	+7.1
+17			+4.5	+4.1	−0.5	+4.1
+18 *			+1.6	−0.6	−0.7	+0.9
+19			+3.7	+1.9	+0.9	+2.1
+20			+4.4	+3.5	+1.7	+3.9
+21			+2.3	+0.7	+2.0	+2.1
+22			+2.1	−1.3	−0.6	+1.4
+23			+2.7	−2.6	+0.0	+2.6
+0	+4		+4.7	−4.4	−0.6	+4.4
+1			+15.6	+12.5	+1.1	+12.6
+2			+8.2	−5.8	−3.4	+6.7
+3			+7.2	+6.6	−1.7	+6.8
+4			+2.3	+1.5	+0.9	+1.8
+5			+5.7	−5.0	−2.7	+5.7
+6 *			+2.5	+0.9	+0.6	+1.1
+7			+3.8	−3.4	+1.9	+3.9
+8			+2.9	−1.0	−1.5	+1.8
+9			+7.2	−6.5	−1.6	+6.7
+10			+1.9	+2.0	+0.1	+2.0
+11			+10.8	+10.7	−0.4	+10.7
+12			+0.9	−0.9	−2.0	+2.2
+13			+5.5	+5.0	+2.9	+5.8
+14			+3.3	+1.8	+1.3	+2.2
+15			+9.0	−8.8	−1.5	+8.9
+16 *			+1.1	+1.0	+0.0	+1.0
+17 *			+1.1	+0.9	+0.4	+1.0
+18 *			+1.1	−0.5	−0.7	+0.9
+19 *			+0.5	−0.8	−0.1	+0.8
+20 *			+0.7	−0.0	+0.7	+0.7
+21			+2.7	+2.7	+0.6	+2.8
+1	+5		+5.0	−3.9	−2.2	+4.5
+2			+2.0	−1.1	+1.4	+1.8
+3			+6.8	+6.3	+0.5	+6.3
+4			+10.3	+9.4	+4.2	+10.3
+5			+2.5	+1.7	+1.2	+2.1
+6			+4.9	−4.3	−3.4	+5.5
+7			+1.8	+0.7	+2.6	+2.7
+8			+2.1	+0.2	−2.7	+2.7
+9			+4.5	−5.1	−0.5	+5.1
+10			+4.3	+4.0	+2.3	+4.6
+11			+4.8	−4.0	−2.9	+4.9
+12 *			+1.9	−1.0	−0.5	+1.1
+13			+6.3	+5.3	+2.0	+5.7
+14			+6.0	+4.6	+3.0	+5.5
+15			+2.7	−0.8	+2.0	+2.2
+16			+2.9	−2.5	+0.3	+2.5
+17			+2.4	−1.3	−0.3	+1.3
+18			+2.9	−1.2	−2.2	+2.5
+19			+1.0	−1.5	−0.9	+1.8
+0	+6		+1.6	+2.2	+1.0	+2.4
+1			+2.5	−2.8	+1.6	+3.2
+2			+4.6	−4.2	−2.6	+4.9
+3			+6.9	−7.5	−1.0	+7.6
+4			+6.0	+6.6	+1.2	+6.7
+5 *			+1.6	+0.1	−1.1	+1.1
+6			+6.9	+6.0	+4.5	+7.5
+7			+6.4	+6.2	+2.0	+6.5
+8			+7.5	−7.1	−1.4	+7.[illegible]
+9			+2.5	−1.2	+1.7	+2.1
+10			+1.5	+1.8	+0.1	+1.[illegible]
+11			+3.3	−4.3	+0.4	+4.[illegible]
+12			+0.6	+0.3	−1.9	+1.9
+13			+2.6	−1.5	−1.8	+2.3
+14			+2.0	+2.1	+0.5	+2.2
+15			+1.9	+0.5	−1.9	+2.0
+16			+3.5	+1.6	+3.0	+3.4
+17 *			+3.3	+0.3	+0.1	+0.5
+18			+5.3	−1.9	−0.6	+2.0
+1 *	+7		+0.6	+1.0	+0.0	+1.0
+2			+4.2	−4.0	−1.7	+4.4
+3			+2.5	+1.8	+1.8	+2.5
+4 *			+0.8	−0.9	−0.1	+0.9
+5			+3.5	−5.6	−1.6	+5.8
+6			+3.6	+2.9	+1.7	+3.4
+7			+2.3	+2.2	−0.8	+2.3
+8			+2.6	+1.9	+2.5	+3.2
+9			+2.1	+2.2	−0.1	+2.2
+10			+2.5	−1.7	−1.1	+2.0
+11			+2.0	−1.9	−0.4	+1.9
+12			+3.4	−3.1	−2.8	+4.2
+13			+1.7	+1.3	+1.6	+2.1
+0	+8		+7.4	+6.3	+4.0	+7.5
+1			+1.8	−1.6	−0.7	+1.8
+2 *			+1.7	−0.7	−0.2	+0.7
+3 *			+0.6	−0.0	−0.7	+0.7
+4			+3.3	−3.6	−1.9	+4.1
+2	+0	+5	+13.4	−4.1	+15.3	+15.8
+4			+10.6	+12.9	−0.6	+12.9
+6			+12.5	−14.0	−8.9	+16.6
+8			+9.3	+4.4	−10.6	+11.5
+10			+10.8	+10.4	+8.1	+13.2
+12			+11.3	−8.5	+9.8	+13.0
+14			+2.9	+1.4	−1.0	+1.7
+16			+6.1	−5.8	−1.9	+6.1
+18			+2.5	+0.2	−2.4	+2.4
+20			+6.2	+5.1	+2.7	+5.8
+0	+1		+11.4	+0.1	−12.4	+12.4
+1			+7.7	+8.2	−2.0	+8.4
+2			+3.1	−2.5	−0.1	+2.5
+3			+2.7	−0.9	+3.1	+3.2
+4			+8.9	+6.4	+8.1	+10.3
+5			+2.9	−2.4	+1.3	+2.7
+6			+7.0	+4.1	+7.1	+8.2
+7			+4.2	+3.6	−0.2	+3.6
+8			+9.3	−10.1	−1.7	+10.2
+9			+7.1	−6.4	+3.7	+7.4
+10			+6.6	+0.1	−6.7	+6.7
+11			+2.4	+2.2	−1.6	+2.7
+12			+2.6	+1.3	+3.5	+3.7
+13			+2.0	+2.2	+0.2	+2.2
+14			+3.0	+0.7	+3.0	+3.1
+15			+2.8	−2.6	−0.1	+2.6
+16			+1.3	+0.7	+1.2	+1.4
+17			+4.3	+4.0	−2.9	+4.9
+18			+4.8	−4.0	−2.5	+4.7
+19			+2.4	−2.6	+1.0	+2.8
+20			+3.6	+2.3	−2.5	+3.4
+1	+2		+2.6	−0.3	−2.8	+2.8
+2			+7.8	−7.9	−0.8	+7.9
+3			+4.9	+3.7	+2.9	+4.7
+4			+3.9	+3.4	−0.9	+3.5
+5			+10.9	−7.2	+8.5	+11.2
+6			+3.5	−3.3	+0.1	+3.3
+7			+2.7	+1.5	−2.0	+2.5
+8			+3.4	+3.1	+0.1	+3.1
+9			+6.5	+2.6	−6.2	+6.7
+10			+3.1	+0.7	−3.0	+3.1
+11			+3.7	−2.7	−2.3	+3.5
+12			+5.4	−5.0	−2.5	+5.6
+13			+3.6	+3.9	+0.2	+3.9
+14			+4.1	+3.7	−0.2	+3.7
+15			+3.6	−2.0	+3.0	+3.6
+16			+2.9	+0.2	+3.0	+3.0
+17			+2.0	−0.5	−1.9	+2.0
+18			+1.5	−1.2	+0.6	+1.3
+19			+3.0	+1.6	−1.8	+2.4
+20			+2.6	+1.0	−1.9	+2.2
+0	+3		+7.3	+5.8	+2.2	+6.2
+1			+6.1	+1.1	−5.7	+5.8
+2			+7.5	−6.7	+0.2	+6.7
+3			+7.9	+0.0	−7.5	+7.5
+4			+6.3	+2.4	−5.0	+5.6
+5 *			+0.7	−0.4	−1.0	+1.1
+6			+7.2	+4.9	−5.0	+7.0
+7			+5.5	+1.2	+4.9	+5.0
+8			+7.1	−7.0	+2.5	+7.4
+9			+3.5	−1.9	+2.8	+3.4
+10			+6.9	+5.6	+3.9	+6.8
+11			+5.8	−1.2	−6.2	+6.3
+12			+3.2	−1.8	+1.6	+2.4
+13			+4.5	+1.8	−4.0	+4.4
+14 *			+2.1	−0.6	−0.7	+0.9
+15			+2.7	+0.9	+1.9	+2.1
+16			+3.7	+3.2	−1.2	+3.4
+17			+4.0	+0.9	+3.5	+3.6
+18			+3.4	−2.4	+2.1	+3.2
+19			+2.0	−1.3	+0.9	+1.6
+1	+4		+2.7	−0.0	+2.1	+2.1
+2 *			+0.4	+0.0	+1.0	+1.0
+3			+4.0	+2.3	−3.2	+3.9
+4 *			+2.3	−1.0	+0.3	+1.0
+5			+6.7	−7.0	−1.0	+7.1
+6			+3.4	+2.9	+2.6	+3.9
+7			+3.1	+3.2	−2.2	+3.9
+8 *			+1.3	+0.2	+0.9	+0.9
+9			+5.8	+4.8	+3.6	+6.0
+10 *			+1.0	−0.1	+0.9	+0.9
+11			+4.1	−3.7	+2.4	+4.4
+12 *			+0.4	−0.6	+0.7	+0.9
+13			+4.4	+2.1	−4.6	+5.1
+14 *			+0.9	−0.5	+0.6	+0.8
+15			+1.5	−1.7	−0.0	+1.7
+16			+0.7	+1.5	+0.1	+1.5
+0	+5		+5.1	+4.7	+1.9	+5.1
+1			+5.1	+0.2	+4.2	+4.2
+2			+4.1	−2.6	+2.1	+3.4
+3			+6.0	+3.0	+4.1	+5.1
+4			+2.1	+0.2	−2.3	+2.3
+5			+2.0	+0.3	−2.2	+2.2
+6			+3.3	+2.9	−1.3	+3.2
+7			+6.3	−3.5	−4.4	+5.6
+8			+4.0	−2.8	+2.4	+3.7
+9			+3.2	+2.6	−1.5	+3.0
+10			+2.9	+1.9	+0.8	+2.1
+11			+5.1	+0.8	+5.1	+5.2
+12			+2.4	−2.2	+0.3	+2.2
+13 *			+1.6	−0.3	+0.7	+0.7
+14			+3.3	−1.5	−2.2	+2.7
+15 *			+1.7	−0.1	−0.6	+0.6
+16			+3.2	+1.8	−0.3	+1.8
+1	+6		+3.1	−0.7	−2.9	+3.0
+2			+3.3	+2.5	+1.6	+3.0
+3			+3.1	+2.7	+1.2	+3.0
+4			+5.1	−3.9	+2.2	+4.5
+5			+3.3	−0.1	+3.0	+3.0
+6			+2.8	+1.8	−2.3	+2.9
+7 *			+1.2	−0.7	−0.1	+0.7
+8 *			+1.2	−0.4	−0.6	+0.7
+9			+2.6	−1.1	−2.3	+2.6
+0	+7		+2.2	−0.3	−0.5	+0.6
+1			+2.9	−3.3	−0.2	+3.3
+2 *			+0.5	−0.5	−0.3	+0.6
+3 *			+1.5	−0.1	−0.6	+0.6
+4			+2.5	+0.5	+2.6	+2.7
+2	+0	+6	+6.6	−4.0	+5.6	+6.9
+4			+6.6	+6.8	−7.2	+9.9
+6			+7.2	+6.0	−3.2	+6.8
+8			+11.1	−7.5	+9.9	+12.4
+10			+2.7	−1.7	−0.8	+1.9
+12			+2.7	−2.2	−1.3	+2.5
+14			+4.3	+0.3	−4.7	+4.7
+16			+3.8	+3.0	−0.7	+3.1
+1	+1		+1.2	−0.7	+1.8	+1.9
+2			+2.6	−1.0	+3.0	+3.2
+3			+3.0	+0.9	−2.5	+2.7
+4			+4.9	−3.0	+3.8	+4.8
+5			+4.4	−3.0	+3.2	+4.4
+6			+6.1	+1.9	−6.0	+6.3
+7			+2.2	+0.1	−1.8	+1.8
+8			+1.9	+0.3	−1.8	+1.8
+9			+2.3	+1.6	−0.6	+1.7
+10 *			+2.1	−0.6	+0.4	+0.7
+11			+3.1	−0.6	+2.6	+2.7
+12 *			+0.9	+0.3	+0.6	+0.7
+13			+2.3	+1.2	−1.6	+2.0
+14 *			+0.7	−0.5	+0.3	+0.6
+15 *			+1.2	−0.1	+0.6	+0.6
+16			+3.7	+2.1	−2.4	+3.2
+0	+2		+5.2	+3.0	−4.4	+5.3
+1			+4.7	−2.8	+4.5	+5.3
+2 *			+1.6	−0.8	+0.6	+1.0
+3			+1.4	−1.8	+1.3	+2.2
+4 *			+1.4	−0.0	+0.9	+0.9
+5			+1.9	+1.3	−1.6	+2.1
+6 *			+0.7	+0.6	−0.7	+0.9
+7 *			+1.0	+0.9	+0.1	+0.9
+8			+1.5	−2.7	+0.5	+2.8
+9			+3.8	+3.2	−2.3	+3.9
+10			+4.0	+3.0	−3.5	+4.6
+11			+3.2	−0.8	+3.5	+3.6
+12 *			+1.4	+0.2	+0.8	+0.8
+13			+2.5	−2.2	+0.4	+2.2
+14			+2.7	−1.3	+2.1	+2.5
+15			+2.8	+0.5	−2.6	+2.6
+16			+1.3	+0.7	−1.3	+1.5
+1	+3		+2.2	+1.4	−1.2	+1.9
+2			+4.7	+1.5	−3.5	+3.8
+3			+0.4	+0.6	+0.5	+0.8
+4 *			+3.6	−2.2	+1.6	+2.7
+5			+3.5	−2.3	+2.9	+3.7
+6			+2.2	+1.6	−0.8	+1.8
+7			+1.6	−1.4	−1.1	+1.8
+8			+2.6	−1.1	+1.4	+1.8
+9 *			+3.0	+0.4	−0.6	+0.7
+10 *			+1.9	−0.7	+0.2	+0.7
+11 *			+1.5	+0.7	+0.2	+0.7
+12			+3.8	+2.2	−2.7	+3.5
+13 *			+1.4	−0.1	+0.6	+0.6
+14			+2.8	−0.7	+2.7	+2.8
+0	+4		+2.1	−1.5	−1.1	+1.9
+1 *			+1.2	−0.1	+0.8	+0.8
+2 *			+0.8	−0.4	−0.7	+0.8
+3			+3.7	+2.2	−3.1	+3.8
+4 *			+1.3	−0.3	+0.8	+0.8
+5 *			+1.3	+0.8	+0.1	+0.8
+6 *			+1.3	+0.2	+0.8	+0.8
+7			+5.1	−2.5	+4.2	+4.9
+1	+5		+2.6	+0.2	+2.3	+2.3
+2			+3.8	+3.1	−2.6	+4.0
+3 *			+0.5	+0.6	−0.3	+0.7
+4			+2.1	−0.4	+2.2	+2.2
+5			+4.6	+1.7	−4.5	+4.8
+6 *			+0.7	+0.5	−0.4	+0.6
+7			+1.6	−0.9	+1.7	+1.9
+8			+1.7	−1.1	+0.7	+1.3
+9			+3.1	−1.1	+1.5	+1.[illegible]
+2	+0	+7	+4.1	+3.8	−2.4	+4.5
+4			+5.6	+1.6	+3.8	+4.1
+6			+3.5	−2.3	−3.1	+3.8
+8			+1.8	−2.4	+0.1	+2.4
+0	+1		+1.9	−1.2	+0.4	+1.3
+1			+1.7	+0.4	+1.2	+1.3
+2			+1.7	−0.1	−1.3	+1.3
+3 *			+1.1	−0.1	−0.6	+0.6
+4			+2.0	+1.7	+0.6	+1.8
+5 *			+0.5	−0.0	−0.6	+0.6
+6 *			+1.2	+0.3	+0.4	+0.5
+7			+2.4	−0.2	+2.1	+2.1
+1 *	+2		+1.5	−0.5	+0.3	+0.6
+2			+1.7	−1.4	−0.1	+1.4
+3 *			+1.0	+0.4	+0.5	+0.6
+4			+2.0	−0.5	+1.2	+1.3
+5			+2.5	+0.9	−2.3	+2.5

The atoms C(2), C(4), S(1) and S(2) are at distances of 1·25, 1·27, 1·53 and 1·51 Å respectively from this plane, indicating that the molecule, at least approximately, has a mirror plane. This is also clear from a Newman projection along the bond C(1)–C(5). The dihedral angles S(1)–C(1)–C(5)–C(10) and S(2)–C(1)–C(5)–C(10) have values of 59·7° and 66·0°. The difference of 6° is not significant, since the standard deviation in the dihedral angles is about 2·5°.

The packing of the molecules is illustrated in a projection of the structure (Fig. 4) along [001]. All intermolecular distances less than 4·5 Å have been calculated and no exceptionally small distances were found. The molecule I at *x*, *y*, *z* has contacts with molecules

Table 2. *Final atomic coordinates (fractions of cell edges) and thermal parameters* (Å^2)

Standard deviations of the parameters (Å and Å^2 respectively) are given in brackets.

Atom	x	y	z	B_{iso}	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{23}$	$2U_{13}$
S(1)	0·1914	0·5716	0·6414	—	0·0564	0·0686	0·0772	0·0182	0·0001	−0·0190
	(0·002)	(0·002)	(0·004)	—	(0·001)	(0·001)	(0·001)	(0·002)	(0·003)	(0·002)
S(2)	0·1082	0·8114	0·3901	—	0·0692	0·0528	0·0827	0·0025	0·0077	−0·0357
	(0·002)	(0·002)	(0·004)	—	(0·001)	(0·001)	(0·001)	(0·002)	(0·002)	(0·002)
C(1)	0·1175	0·6193	0·5606	—	0·0643	0·0731	0·0714	0·0086	−0·0161	0·0102
	(0·008)	(0·009)	(0·010)	—	(0·004)	(0·005)	(0·005)	(0·007)	(0·009)	(0·008)
C(2)	0·1417	0·9673	0·5855	—	0·0907	0·0645	0·1333	0·0072	− 0·0279	−0·0656
	(0·009)	(0·009)	(0·015)	—	(0·006)	(0·005)	(0·011)	(0·009)	(0·013)	(0·014)
C(3)	0·2016	0·9311	0·6558	—	0·0782	0·0761	0·0858	− 0·0199	0·0011	−0·0424
	(0·008)	(0·008)	(0·014)	—	(0·005)	(0·005)	(0·006)	(0·008)	(0·011)	(0·013)
C(4)	0·2114	0·7674	0·7912	—	0·0871	0· 0866	0·1100	−0·0291	−0·0098	−0·0714
	(0·010)	(0·010)	(0·014)	—	(0·006)	(0·006)	(0·009)	(0·010)	(0·013)	(0·013)
C(5)	0·0928	0·4693	0·4229	—	0·0662	0·0539	0·0710	0·0152	0·0017	−0·0336
	(0·007)	(0·007)	(0·010)	—	(0·004)	(0·003)	(0·005)	(0·006)	(0·008)	(0·009)
C(6)	0·1156	0·4180	0·2147	—	0·0952	0·0714	0·0768	0·0280	0·0096	0·0087
	(0·010)	(0·009)	(0·012)	—	(0·006)	(0·005)	(0·006)	(0·009)	(0·010)	(0·010)
C(7)	0·0925	0·2875	0·0953	—	0·1429	0·0929	0·0816	0·0901	−0·0337	−0·0440
	(0·013)	(0·011)	(0·014)	—	(0·009)	(0·007)	(0·008)	(0·013)	(0·013)	(0·014)
C(8)	0·0428	0·2025	0·1789	—	0·1206	0·0630	0·1483	0·0410	−0·0480	−0·1508
	(0·011)	(0·009)	(0·016)	—	(0·008)	(0·005)	(0·012)	(0·010)	(0·014)	(0·019)
C(9)	0·0189	0·2488	0·3933	—	0·0747	0·0639	0·1439	−0·0143	0·0387	−0·0550
	(0·009)	(0·008)	(0·017)	—	(0·005)	(0·004)	(0·010)	(0·008)	(0·016)	(0·015)
C(10)	0·0431	0·3850	0·5083	—	0·0752	0·0743	0·0857	0·0328	0·0108	−0·0019
	(0·008)	(0·009)	(0·012)	—	(0·005)	(0·005)	(0·006)	(0·009)	(0·011)	(0·011)
H(1)	0·092	0·633	0·716	5·3	—	—	—	—	—	—
H(2)	0·114	0·985	0·735	7·7	—	—	—	—	—	—
H(3)	0·139	0·095	0·512	7·7	—	—	—	—	—	—
H(4)	0·219	0·040	0·749	6·4	—	—	—	—	—	—
H(5)	0·230	0·934	0·508	6·4	—	—	—	—	—	—
H(6)	0·189	0·774	0·954	7·7	—	—	—	—	—	—
H(7)	0·256	0·760	0·847	7·7	—	—	—	—	—	—
H(8)	0·151	0·482	0·149	6·5	—	—	—	—	—	—
H(9)	0·112	0·249	−0·061	8·4	—	—	—	—	—	—
H(10)	0·023	0·105	0·081	8·8	—	—	—	—	—	—
H(11)	—0·015	0·182	0·463	7·5	—	—	—	—	—	—
H(12)	0·025	0·427	0·660	6·3	—	—	—	—	—	—

Table 3. *Dihedral angles in the dithiane ring of* 2-*phenyl*-1,3-*dithiane*

Central bond	S(1)–C(1)	C(1)–S(2)	S(2)–C(2)	C(2)–C(3)	C(3)–C(4)	C(4)–S(1)
Dihedral angle	57°	56·9°	56·1°	62·5°	60·7°	53·6°

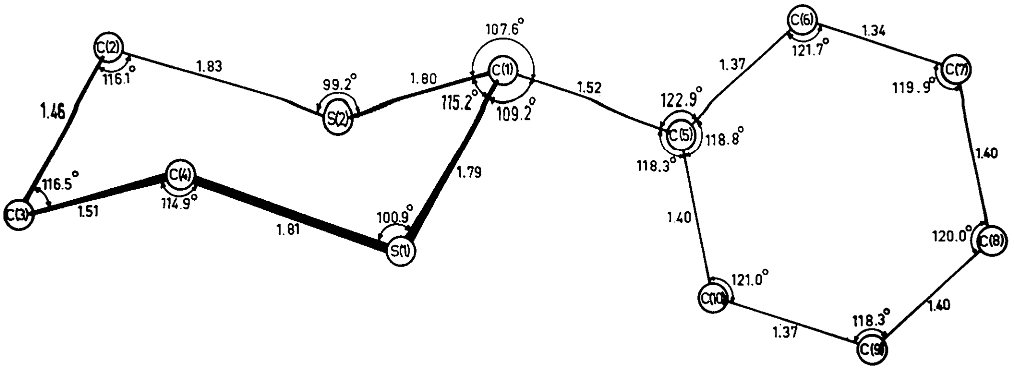

Fig. 2. Bond distances (Å) and bond angles (°) in 2-phenyl-1,3-dithiane.

II at $\bar{x}, \bar{y}, \frac{1}{2}+z$ and at $\bar{x}, \bar{y}, -\frac{1}{2}+z$;
III at $\bar{x}, 1-y, \frac{1}{2}+z$ and at $\bar{x}, 1-y, -\frac{1}{2}+z$;
IV at $x, 1+y, z$ and at $x, 1+y, 1+z$
V at $x, -1+y, z$ and at $x, -1-y, -1+z$
VI at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$ and at $\frac{1}{2}-x, \frac{1}{2}+y, -\frac{1}{2}+z$
VIIat $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}+z$ and at $\frac{1}{2}-x, -\frac{1}{2}+y, -\frac{1}{2}+z$
I at $x, y, 1+z$ and at $x, y, -1+z$.

In this way each molecule is surrounded by 14 neighbours and a close packing (Kitaigorodskii, 1960) is attained.

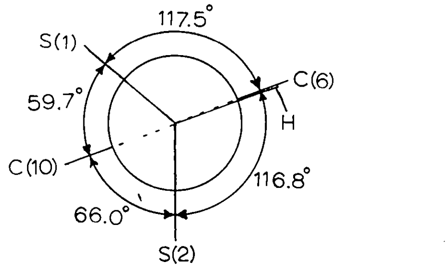

Fig. 3. Newman projection along the bond C(1)–C(5).

It is interesting to note that the phenyl rings in their clustering about the screw axes at $0,\frac{1}{2},z$ exhibit a herring-bone type of packing. The molecule does not use its mirror plane to accommodate itself to the special position 4(*c*) of the centrosymmetric space group *Pnam* (no. 62). A similar phenomenon has been encountered in the crystal structure of *trans*-2,3-dichloro-1,4-dithiane (Kalff & Romers, 1965). This molecule with symmetry *C*2 crystallizes in the space group *Pn*, but could have occupied the special position 2(*f*) or 2(*e*) (twofold axis) in the space group *P*2/*n* (no. 13). Nowacki (1942, 1943) and Kitaigorodskii (1960) have shown that mirror planes and twofold axes in crystals are unfavorable symmetry elements to accomplish a close packing of molecules.

All calculations mentioned in this paper were carried out on the X1 computer of the University of Leiden.

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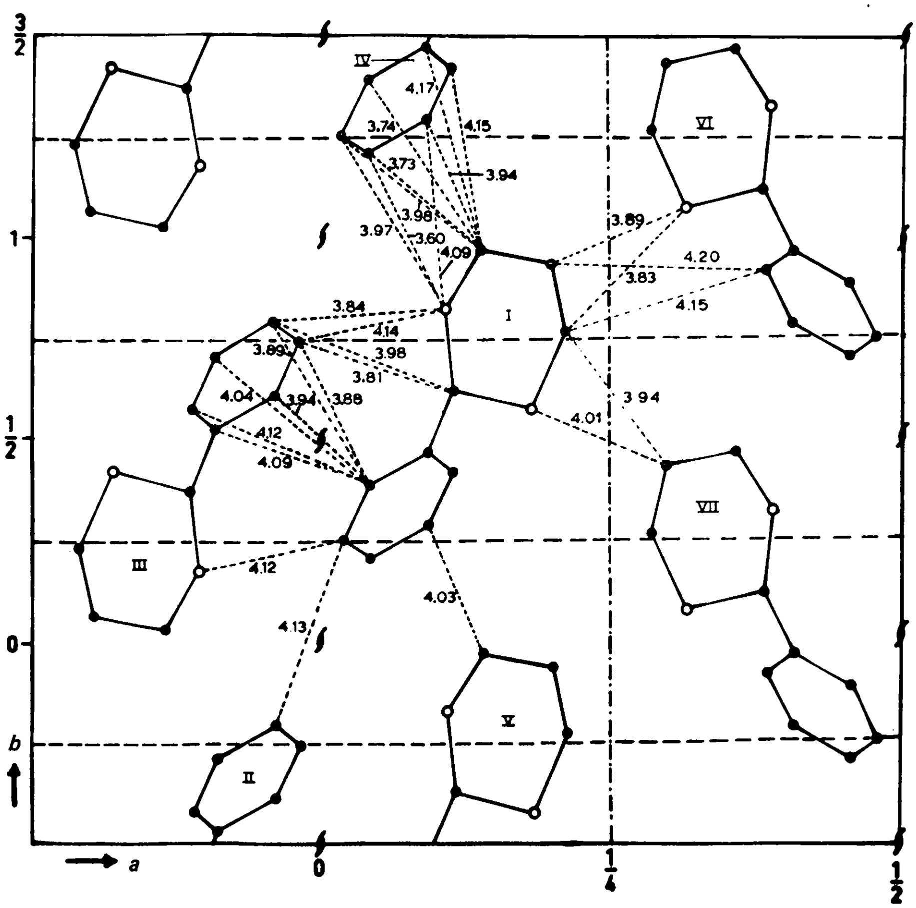

Fig. 4. A view of the structure along [001]. Only half the distances are given. Not shown are distances of molecules with parameters *xyz* and *xyz*+1: [S(1)–C(6) 3,94; S(1)–C(7) 4·11; C(1)–C(6) 4·11; C(1)–C(7) 4·07; C(5)–C(7) 4·15; C(10)–C(7) 3·67; C(10–C(8) 4·14 Å]. For the parameters of the molecules see text. Solid circles: carbon atoms; open circles: sulphur atoms.

References

ABRAHAMS, S. C. (1956). *Quart. Rev. Chem. Soc. Lond.* **10**, 414.

AUTHENRIETH, W. & WOLFF, K. (1899). *Ber. dtsch chem. Ges.* **32**, 1375.

BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.

BUCOURT, R. & HAINAUT, D. (1965). *Bull. Soc. chim. Fr.* p. 1366.

DAVIS, M. & HASSEL, O. (1963). *Acta Chem. Scand.* **17**, 1181.

DAWSON, B. (1960). *Acta Cryst.* **14**, 753.

FOSS, O., JOHNSEN, K. & REISTAD, T. (1964). *Acta Chem. Scand.* **18**, 2345.

GEISE, H. J., ROMERS, C. & RUTTEN, E. W. M. (1966). *Acta Cryst.* **20**, 249.

HASSEL, O. & VIERVOLL, H. (1947). *Acta Chem. Scand.* **1**, 149.

KALFF, H. T. & HAVINGA, E. (1966). *Rec. Trav. chim. Pays-Bas.* In the press.

KALFF, H. T. & ROMERS, C. (1965). *Acta Cryst.* **18**, 164.

KITAIGORODSKII, A. J. (1960). *X-ray Crystallography of Organic Compounds.* New York: Consultants Bureau.

MARSH, R. E. (1955). *Acta Cryst.* **8**, 91.

MCWEENY, R. (1951). *Acta Cryst.* **4**, 513.

MOSSEL, A. & ROMERS, C. (1964). *Acta Cryst.* **17**, 1217.

NOWACKI, W. (1942). *Helv. Chim. Acta*, **25**, 863.

NOWACKI, W. (1943). *Helv. Chim. Acta*, **26**, 459.

SCHOMAKER, V., WASER, J., MARSH, R. & BERGMAN, G. (1959). *Acta Cryst.* **12**, 600.

Acta Cryst. (1966). **20**, 496

A General X-ray Method for Orienting a Crystal

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A method for ascertaining the orientation of a randomly set crystal and adjusting it to a preferred orientation is described. Normal-beam, flat-film rotation photographs yield data from which are calculated (ϱ) angles that define the directions of reciprocal lattice vectors with reference to the rotation axis and the planes of the goniometer arcs. The method of plotting the vectors reveals the principal zones and their orientation. The use of monochromatic radiation provides a quantitative estimate of the relative 'importance' of each zone.

The method has several advantages. It is systematic and thereby eliminates the customary search through a series of trial and error photographs for a useful expression of the crystal's structure. It circumvents the complex problem, encountered in cylindrical-film methods, of dealing with the movement of reciprocal points on a curved surface. The magnitude of arc movements required to adjust a zone axis to a desired setting can be evaluated by inspection with a Wulff net. The method is particularly effective for low-symmetry crystals.

Introduction

The Laue, oscillation and precession methods all include systematic techniques for detecting and correcting errors in the orientation of a crystal. However the techniques are limited to the evaluation of small misalignments and are therefore not satisfactory for orienting unknown crystals, or even known crystals with no diagnostic morphological traits.

Most practical X-ray methods for determining the orientation of a randomly-set crystal are based on a preliminary trial and error approach involving a search through a number of photographs of the crystal in different arbitrary orientations, for some sign of a symmetry plane or prominent zone or axis. They are best suited to crystals of high symmetry.

The method described here is a systematic method for ascertaining the orientation of a randomly set known crystal and adjusting it to within about 1° of a preferred orientation. The final adjustment is made with one of the techniques especially suited to correcting small misalignments. The data are plotted in such a manner that the principal zones in the crystal become apparent and thus the method can be applied in the general case to locate a principal zone axis in an unknown, randomly oriented crystal and set it for rotation or precession in one of the standard single-crystal methods of analysis. In contrast to orientation procedures that use Laue photographs, application of this method is simplified by a decrease in crystal symmetry.

An expression for the orientation of a randomly set reflecting plane

The locus of a reciprocal point Q, representing a randomly oriented direct-lattice plane (hkl), is confined to the surface of a sphere, centered at the origin P and having a radius of $PQ=\lambda/d_{hkl}$. This may be called the