X-Ray Crystallographic Studies of a 4-Demethoxythiodaunomycinone Derivative and 1,2,4-Triazole

by

Nola Hua Li

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NOLA HUA LI

A thesis submitted to the Faculty of Graduate Studies of the University of Manitoba in partial fulfillment of the requirements of the degree of

MASTER OF SCIENCE

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ABSTRACT

Two molecular structures have been studied. The first molecule, 7,8,9,10-tetrahydrobenzo[b]-6,11-dimethoxy-7,9-*cis*-dihydroxy-9-acetylthioxanthen-12-one-α-5-oxide, $C_{21}H_{20}O_7S$, is a thio derivative of daunomycinone. The crystal is triclinic, space group $P\bar{1}$ with unit cell parameters *a* = 9.5708(18), *b* = 11.1965(16), *c* = 11.3634(20)Å, α = 75.982(13), β = 83.323(15), γ = 74.629(19)°, and *Z* = 2. Refinement of 342 parameters using 3198 data led to an R value of 0.065. The multiple ring system of this molecule is bent so that the two flat portions intersect along the sulfur...carbonyl carbon line in ring B with a dihedral angle of 40.1°. The crystal structure exhibits an intermolecular hydrogen bond between the sulfoxide oxygen and the 9-hydroxy group in an adjacent molecule, and an intramolecular hydrogen bond between the 7- and 9-hydroxy groups. The structure includes a solvent molecule with some orientational disorder.

The second compound, 1,2,4-triazole, $C_2H_3N_3$, crystallizes in orthorhombic, space group *Pcab*. The unit cell has dimensions *a* = 7.1892(13), *b* = 9.3600(13), *c* = 9.7590(11) Å, and *Z* = 8. The structure was refined to R = 0.043 for 449 observed reflections. The present structure was studied at

room temperature. It has been shown in this study that 1,2,4-triazole has the same molecular structure at both room and low (-160°) temperatures. Initially, this crystal was studied with the intent of determining the crystal and molecular structures of O^4-n-butyl-thymidine, but it turned out to be the redetermination of the crystal and molecular structure for 1,2,4-triazole.

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Chapter I

GENERAL INTRODUCTION

1.1 CRYSTALLOGRAPHIC INTRODUCTION

Since the earliest experiments on the scattering of x-rays by a crystal performed by Friedrich and Knipping in 1912, x-ray crystallography has been greatly developed and improved through the years in both the theoretical and experimental fields. Today with the aid of modern computers, x-ray diffraction methods have become much more powerful and applicable not only in solving complicated structures, but also in routinely providing answers to structural problems arising in many related fields.

The underlying principle in single crystal x-ray diffraction methods is that the regularly repeating arrays in the crystal will diffract the incident x-rays at specific angles. Diffraction takes place when the following condition is satisfied:

$$n\lambda = 2d\sin\theta$$

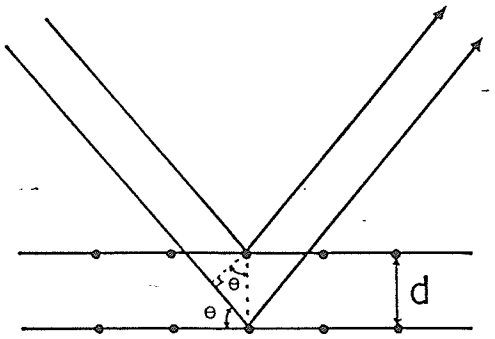


Figure 1: Diffraction of x-rays according to Bragg's law.

where n is an integer, λ is the incident wavelength, θ is the incident and the reflection angle, d is the separation distance between planes. This is known as Bragg's law which outlines the condition for observing diffracted x-rays from a crystal. The repeating arrays in the crystal which diffract x-rays can be considered as three dimensional planes. Once the crystallographic axes are chosen, these planes can be described in terms of Miller indices (h,k,l). Bragg's law can be rearranged to:

$$\sin\theta = \frac{n\lambda}{2} \frac{1}{d(hkl)}$$

where d(hkl) is the perpendicular distance between planes of the set (h,k,l). Since $\sin\theta$ values are directly proportional to 1/d(hkl), crystallographers find it is more convenient to use this reciprocal quantity, 1/d(hkl), in describing the 3-d arrays or lattice. The reciprocal lattice is constructed by considering normals to every set of planes from some direct lattice point taken as the origin, then, terminating each normal at a distance equal to the reciprocal of the interplanar spacing. Therefore, with the known wavelength and diffraction angles, it is possible to search where atoms are located in the unit cell.

1.2 DATA COLLECTION

The preliminary step in x-ray diffraction analyses is the selection and preparation of the sample. The sample should be a single crystal (i.e. with uniform internal structure) of proper size (ideally 0.3 x 0.3 x 0.3 mm^3). The crystal can be mounted on the goniometer using a variety of techniques depending on the crystal nature, i.e. whether it is heat or moisture sensitive, etc.. The crystals studied in this thesis were stable at room temperature and pressure, and were mounted on a glass fiber directly on the goniometer in a random orientation for data collection on a Nicolet R3m automated diffractometer.

Since the crystal is mounted in an arbitrary orientation in relation to the instrument coordinate system (x,y,z), an orientation matrix relating the unit cell coordinates to the x, y, z of the diffractometer system must be determined before systematic data collection may begin. This is achieved by, first, taking a diffraction photograph of the crystal rotating 360° about the Ø-axis on the diffractometer. Usually twenty-five strong reflections with a wide range of angles are chosen from the resultant photo. Each of these reflections undergoes a process of automatic centering whereby their exact positions are found by accurately setting the four angles (ω,Ø,X,2θ) of the instrument. From this set of reflections, the orientation matrix A for the crystal, which describes the reciprocal vectors a*, b*, and c* in terms of their components in the instrument coordinate system, is calculated.

$$A = \begin{pmatrix} a^*_x & a^*_y & a^*_z \\ b^*_x & b^*_y & b^*_z \\ c^*_x & c^*_y & c^*_z \end{pmatrix}$$

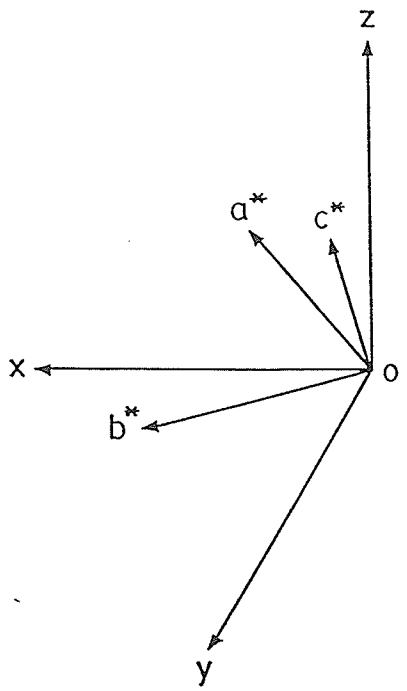


Figure 2: Crystal axes in diffractometer coordinates where x, y, z are the diffractometer coordinates, and a*, b*, c* are the crystal coordinates.

With the orientation matrix A known, the x, y, z components of any reciprocal vector can be found by the following relationship:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = A \cdot \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

where, h, k, l are the Miller indices of a reflection. The Miller indices of the twenty five reflections from the photograph (each with known values of x, y and z) are calculated according to the relationship shown below:

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = A^{-1} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

where, A^{-1} is the inverse of the orientation matrix.

One of the available scan techniques of the instrument is the ω-2θ scan in which the crystal is rotated in ω to bring the lattice points into the reflection sphere, while the detector moves by the 2θ circle at an angular rate twice that of the crystal's. The other two circles, Ø and X, will adjust the crystal orientation relative to the diffractometer coordinate system to bring the desired reciprocal lattice points into contact with the reflection sphere in the plane defined by the radiation source, the crystal and the detector. The desired maximum and minimum scan speeds are set before starting the data collection. For each reflection, the instrument will scan through the peak with a fast preliminary 2s scan. If the intensity is too strong, the attenuator will automatically be inserted to remeasure the peak and the reported intensity will be scaled by the attenuation factor. For weaker intensities the instrument will automatically select an appropriate scan speed within the set range to re-collect the actual peak intensity. The scan width for each individual peak is given by:

$$\text{Scan Width} = \text{RNG 1} + \text{RNG 2} + (2\theta K\alpha_2 - 2\theta K\alpha_1)$$

where RNG 1 and RNG 2 are background to scan ratios. They are both 1 for the ω-2θ scan type.

Normally, three check reflections are periodically measured during the whole data collection time to ensure the crystal orientation and stability of the system. If any of these check reflections falls below a certain percentage of the minimum intensity, the collection process will be automatically terminated. The intensity of the collected data is calculated by:

$$I = [\text{total scan count} - (\text{sum of BG counts})/(\text{BG to scan ratio})] \times \text{scan rate}$$

and the associated standard deviation is:

$$\sigma = [\text{total scan count} + (\text{sum of BG counts})/(\text{BG to scan ratio})^2]^{1/2} \times \text{scan rate}$$

where, BG = background of the reflection peak.

All of the collected data undergo a processing step and are stored on disk for later use in structure determination. During the data processing stage, each intensity peak is checked for background inbalance, and the peak profile is examined for peak centering and symmetry. Systematically absent reflections (if there are any) will be deleted from the data list, and an empirical absorption correction is applied to the data if necessary (i.e. depending on the magnitude of the absorption coefficient of the sample). Equivalent reflections related by crystal system symmetry will be flagged so the processed data file contains unique data only. Intensity data will then undergo Lorentz and polarization corrections. The former is a correction for the relative time spent by a reciprocal lattice point in the dif-

fracting condition. This depends on the location of the lattice point in reciprocal space and the direction in which it approaches the reflection sphere. The latter is a geometrical correction for the partial polarization of the x-ray beams diffracted from the graphite monochromator and the sample crystal. Intensity data are also classified as "observed" and "unobserved" during the process. The intensity data obtained from the two crystals studied in this thesis were classified as observed if $I \geq 2.5\ \sigma(I)$, where $\sigma(I) = SR[SC + BL + BR]^{1/2}$, SR = scan rate, SC = total scan count, BL and BR are left and right backgrounds.

1.3 STRUCTURE SOLUTION

The available information from an x-ray diffraction experiment is the observed intensities, I(hkl), which result from coherent scattering of the radiation by electrons in the molecules. From these intensities the amplitude of the combined scattered waves, |F(hkl)|, can be calculated according to the following equation:

$$I(hkl) = k^2 C(hkl) |F(hkl)|^2$$

where |F(hkl)| is the structure factor amplitude for the set of planes (h,k,l), C(hkl) combines several geometric and physical factors which depends upon both the (h,k,l) and the experimental conditions, such as the Lorentz, polarization and absorption corrections. The factor k is the scale factor

associated with |F(hkl)|. However, knowing only the intensity or the amplitude of the structure factor is not enough to determine the structure, because the corresponding phase of the scattered x-ray wave, Ø(hkl), is not directly measurable. Determination of the structure amounts to determination of the phase. This is generally referred to as the "phase problem".

To obtain the correct phase angle, there are two different types of methods, namely, the Patterson method (or the heavy atom method), and direct methods. The Patterson method was first used more than five decades ago and is well explained in crystallographic texts (1,2). The method works best when the structure contains a few heavy atoms. Then the resultant Fourier (Patterson) map will show outstanding peaks related to the interatomic vectors between the heavy atoms. However, in the case where the structure has no heavy atoms or has too many of them, the Patterson map will be overcrowded so that individual peaks can not all be recognized.

For a structure which contains no heavy atoms, direct methods are a better choice for solving the phase problem. This class of methods attempts to derive the phases of the structure factors directly from the intensity information by means of mathematical derivations, such as taking into account the probability distributions of the intensity data and to correlate them to molecules in the unit cell. Detailed explanations of these methods are also contained in several x-ray texts (1-3) and the references therein.

An important fact in the application of direct methods is that these methods consider structure factors corresponding to point atoms which have no thermal motion. Therefore, instead of the structure factor amplitudes ($|F(hkl)|$), normalized structure factor amplitudes ($|E(hkl)|$) are used in the phase determination process. The normalized structure factor amplitude is calculated by:

$$|E(hkl)|^2 = k^2|F(hkl)|^2/(\epsilon \Sigma f_j{}^2)$$

where f is the scattering factor of the j atom, and k is the scaling factor which is used to bring the F(hkl) to an absolute level. The ϵ-factor is an integer which depends upon the crystal class. Generally it is 1, but may assume other values for special sets of reflections in certain space groups. The expectation value for $E(hkl)^2$ is:

$$<|E(hkl)|^2> = <|F(hkl)|^2>/\Sigma f_j{}^2 = 1.000$$

The advantage of using the $|E(hkl)|$ values instead of the $|F(hkl)|$'s is that they are structure dependent but scattering angle independent. This is due to the fact that the scattering factor for the point atom is the same for every reflection in the unit cell and there is no tendency for the resultant scatering amplitudes to systematically decrease with increasing scattering angle.

The next approach to the problem is to find a way to obtain the exact phase for the structure factors. In the case of centrosymmetric crystals, the origin of the x, y and

z coordinates of the structure is taken on one of the eight centers of symmetry in the unit cell. Instead of the phase $\emptyset(hkl)$, one can use the sign, S(hkl) of the structure factor, where $\emptyset(hkl) = 0$ corresponds to $S(hkl) = +1$ and $\emptyset(hkl) = \pi$ corresponds to $S(hkl) = -1$. For primitive, centrosymmetric space groups, the first step is to allocate arbitrary signs to three of the reflections in order to specify the origin at one of the centers of symmetry. The following step is to obtain a sign list of reflection triples for a given set of data using the Σ_2-relationship. For centrosymmetric space group, this is simplified to the triple product sign relationship:

$$S(hkl) \approx S(h'k'l')S(h-h',k-k',l-l')$$

where the sign $\approx$ means "is probably equal to". The probability for S(hkl) to be +ve depends on the magnitude of E as shown in the following expression:

$$P_+ = 0.5 + 0.5\tanh\{1/N\ |E(hkl),E(h'k'l'),E(h-h',k-k',l-l')|\}$$

where N is the number of equal atoms in the crystal. The probability for S(hkl) to be -ve is simply:

$$P_- = 1 - P_+$$

The starting set in the structure solving process is comprised of reflections (usually three or less) which have both large $|E(hkl)|$ values and show maximum entrance to the Σ_2-combination relationship. The sign of the starting set is assumed to be reliable enough to use for sign propagation

process. Therefore, if a highly probable correct sign is obtained from this basic set, a "snowballing" technique will allow more and more reflections to be included as the analysis proceeds.

As many phases as possible are determined from the starting set via the Σ_2-relationship, the resultant sets of phases are then tested by different criteria to find the three figures of merit (FOM) to rank the solutions in order of plausibility. The first figure of merit is the 'absolute figure of merit' (ABSFOM) which measures the internal consistency among the Σ_2-relationships. The next figure of merit is the zero check (PSI(ZERO)). This figure of merit tests the phases of the weak reflections, and if the weak reflections are correctly phased the probability for the strong reflections to be correct is high. For a correct set of phases, PSI(ZERO) should be small. The third figure of merit is the residual-type function (RESID). This is a combined figure of merit between a PSI(ZERO) figure of merit and a weighted residual on α (a parameter which gives a measure of the reliability of the phase being tested). This measures how well the Σ_2-relationships have followed the statistical expectations. Generally, the set of phases which have the highest combined figure of merit (CFOM) will give the correct solution of the structure. Detailed explanation and calculations for different types of figure of merits can be obtained in the text (3). Once this set of phases is found, the remaining task is to calculate a Fouri-

er synthesis by using |E(hkl)| values as the coefficients, with the resultant E-map hopefully showing the correct structure of the molecule.

Today, MULTAN (the multiple-tangent-formula method) (4) is one of the most popular computer programs used in direct methods to obtain structure solutions. In summary, the steps in MULTAN are:

a) Convert the experimentally obtained |F(hkl)| to the corresponding |E(hkl)| values.

b) Choose a set of large E's (a set with sufficient number of E's to solve the structure) and find their Σ_2-relationships.

c) Select the origin and the starting set from the set of large |E|'s using the convergence process.

d) Assign values to the unknown phases in the starting set.

e) All permutations of phases for starting set reflections are used as initial values for tangent formula phase extension and refinement.

f) Calculate all FOM's and rank the phase sets in a order of decreasing plausibility.

g) Calculate the E-map using the phase which has the highest CFOM.

1.4 STRUCTURE REFINEMENT

The correct trial structure is usually refined by the full matrix least-squares method. This process is applied to adjust the positional and temperature parameters of the atoms in the unit cell so as to obtain the best agreement between the experimental |Fo| values and the calculated |Fc| quantities. The function minimized in the least-squares process is:

$$\Sigma w(|Fo| - k|Fc|)^2$$

where Fo and Fc are the observed (experimental) and calculated structure factors, respectively, k is the scale factor, and w is a weighting factor which varies inversely with the square of the error in |Fo|; if properly chosen, the weight can give significant improvement in the results of a given set of data.

Agreement between the observed and calculated data is indicated by the residual index (R factor) which is defined as:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo|$$

and the weighted residual is given by:

$$wR = [\Sigma w(|Fo| - k|F|)^2/\Sigma w|Fo|^2]^{1/2}$$

Both R and wR are percentage values for different cycles of refinement. The lower the values of R and wR the better the agreement between the refined and calculated structures.

Usually, after least-squares refinement, a difference-Fourier synthesis is calculated. Extra electron density peaks may appear and could represent atoms not included in the model, such as hydrogen atoms and sometimes, unexpected solvent molecules in the crystal. For an ideal fit of the model to the structure, the net result of the difference-Fourier synthesis should be zero. Typically, residual electron density values are in the range of +1.0 to -1.0 e $Å^{-3}$.

Chapter II

7,8,9,10-TETRAHYDROBENZO[B]-6,11-DIMETHOXY-7,9-CIS-DIHYDROXY-9-ACETYLTHIOXANTHEN-12-ONE-α-5-OXIDE

2.1 INTRODUCTION

DNA, the genetic material in a living cell, can interact with certain classes of drugs, carcinogens, mutagens, and dyes in a suitable environment. These interactions may change the biological replication and protein biosynthesis of the living system and may also alter cell metabolism, diminishing, and in some cases terminating, cell growth. One such example is daunomycin (Fig.3) (5), one of the most active and effective anticancer chemotherapeutic agents, which interacts with DNA by intercalation of its planar aromatic portion between adjacent base pairs in the oligonucleotide. The antitumour properties, in many cases, correlate with the ability of the chromophore of the drug to intercalate to the DNA template. The first model of a DNA-daunomycin complex was built by Pigram, Fuller and Hamilton (6) in the early 1970's. In the model, they showed that the amino sugar of the daunomycin is located in the large groove of the DNA, and is close to a sugar-phosphate chain. This enables the ionized amino groups to interact strongly with the second DNA phosphate away from the intercalation site. A hydrogen bond is postulated between the first phosphate and the hydroxyl attached to the saturated ring on the daunomycin chromophore. Other studies (7, and references therein) have also suggested that planar, aromatic 3.4 Å-thick drug molecules will slip between base-pairs without disturbing the overall base stacking pattern, but the sugar-phosphate backbone is distorted and the regular helical structure is altered locally.

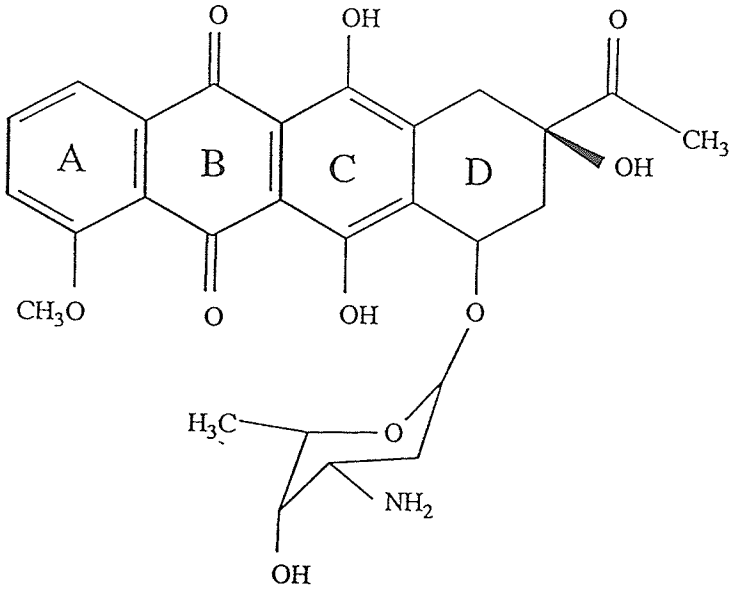
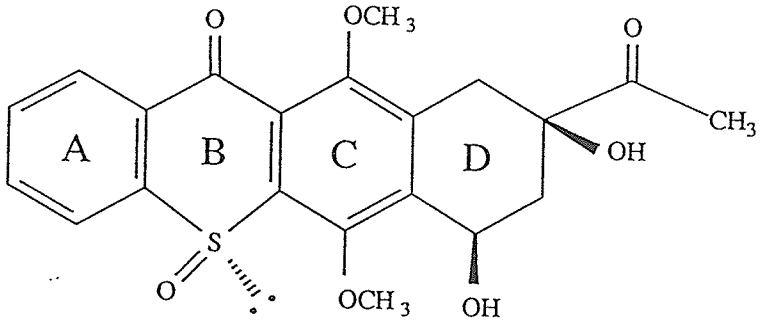


Figure 3: Molecular structure of daunomycin.



I

Figure 4: Molecular structure of the 4-demethoxythiodaunomycinone derivative.

Although daunomycin is a very powerful anticancer drug, its clinical use is limited primarily by a dose-dependent cardiomyopathy. Studies (8-10) have shown the quinone moiety of the molecule may be enzymatically reduced and may subsequently autoxidize, resulting in the generation of hydrogen peroxide, superoxide anion, and hydrogen radicals. These free radicals may, in turn, react with endogenous lipid and cause membrane damage, especially to heart cells which have relatively low levels of superoxide dismutase. Analogues of daunomycin are being sought which have reduced toxicity yet an improved therapeutic index. The title compound (I) investigated by this study (Fig.4) was synthesized and crystallized by Professor C. M. Wong and his group. It is a thio derivative of daunomycinone (11-13), a precursor in the synthesis of daunomycin. The sulfoxide portion of the ring system is expected to confer on the molecule a different oxidation-reduction potential compared to daunomycinone and it is thought that this will alter the free radical formation process in the living cell with a concomitant decrease in the toxicity of the drug. Because the synthesis affords both α and β isomers (epimeric at S), the present study was undertaken to identify the isomer as α or β and to provide structural details of a compound representative of a series of possibly significantly improved anticancer drugs.

2.2 EXPERIMENTAL

Yellow transparent pinacoidal crystals were grown from a solution of ether and methylene chloride by slow evaporation. A crystal of dimensions 0.28 x 0.36 x 0.48 mm^3 was selected for structure determination by x-ray diffraction analysis. Since the sample was stable at room temperature and pressure, it was glued directly onto a thin glass rod along the longest dimension and then fixed on the goniometer head for data collection. Data were collected on a Nicolet R3m automated diffractometer which was equipped with a molybdenum x-ray tube operated at 50 Kv and 40 mA under the control of Nicolet softeware, viz. P3 computer programs. The radiation source was monochromatized by a graphite crystal yielding a MoKα x-ray beam of weighted mean wavelength of 0.70169 Å incident on the sample.

Crystal Data: $C_{21}H_{20}O_7S.CH_2Cl_2$; Mr = 501.382, triclinic, $P\bar{1}$, a = 9.5708(18), b = 11.1965(16), c = 11.3634(20) Å, α = 75.982(13), β = 83.323(15), γ = 74.629(19)°. V = 1137.39(33) $Å^3$, Z = 2, Dm = 1.45 Mg m^{-3}, Dx = 1.46 Mg m^{-3} (floatation), λ(Mo Kα) = 0.71069 Å, μ = 1.60 cm^{-1}. T = 294 K, F(000) = 520 electrons.

Reflection data ±h, ±k, +l (±12, ±14, +14) were collected with an ω-2θ scan type in the range of $2° \leq 2\theta \leq 50°$. The scan speeds ranged from 4.0 to 29.30 deg. $min.^{-1}$, and scan widths were given by $2.00° + (2\theta K\alpha_2 - 2\theta K\alpha_1)°$. Each scan was extended on both sides of the peak to allow for background

measurement. Three strong reflections (020,115,322) which were well distributed in reciprocal space were remeasured every 45 data to ensure the stability of the system and sample orientation. It was found that these standard intensities changed very little (mean and final intensity changes were 0.01% and 0.45%, respectively) during the data collection time. Hence, no intensity correction was required.

A total of 4524 reflections were collected. Among them, 285 were standards, 6 were collected with the attenuator applied and only 1 was rejected because of the unbalanced backgrounds. Reflections were considered to have bad backgrounds if $|BL - BR| > 20.0[(BL + BR) + 0.45(Net - BL - BR)]^{1/2}$, where BL and BR are left and right backgrounds, Net represents the net number of counts detected. In the remaining 4238 reflections, 222 equivalent data were averaged during the data reduction process. There were 4016 independent reflections, of which 3198 were classified as observed having intensity $I \geq 2.5\sigma(I)$. Since the sample contains mainly carbon, nitrogen, oxygen and hydrogen atoms which do not absorb MoKα radiation significantly (absorption coefficient of the molecule $\mu = 1.6\ cm^{-1}$), an absorption correction for the data was not necessary. All reflections were corrected by Lorentz and polarization factors during the data processing step. From a density calculation suggesting two molecules in the unit cell and the E-statistics (vide infra), the space group $P\bar{1}$ was assigned.

2.3 STRUCTURE SOLUTION AND REFINEMENT

The structure was solved by direct methods using MULTAN80(14) computer programs. Since the normalized structure factors account only for stationary point atoms, which are independent of both scattering angles and thermal motions, scale factor (k) and overall temperature factor (B) are required in order to bring all the structure factors to an absolute comparison level. These factors can be obtained from a Wilson plot, where the slope and intercept of the curve will yield the temperature and scale factors, respectively. Assuming a random distribution of atoms in the unit cell, the Wilson plot should theoretically give a straight line of slope -2B and intercept ln C, and the scale factor is inversely proportional to the square root of C (1). Experimentally, the slope and intercept are obtained from the least-squares line drawn through the observed data. In some cases, such as the present one, there are significant deviations from the least-squares line indicating a less than random distribution of atomic positions (Fig.5). The Debye curve, on the other hand, has fewer humps and fits the least squares line better, because molecules, rather than atoms, are more randomly distributed in the unit cell. Hence, the values from the slope and intercept of this curve were considered to be more reliable in solving this structure. This Debye curve is derived by using the molecular scattering factors calculated based upon a known structure which has a fragment similar to the molecule under investigation.

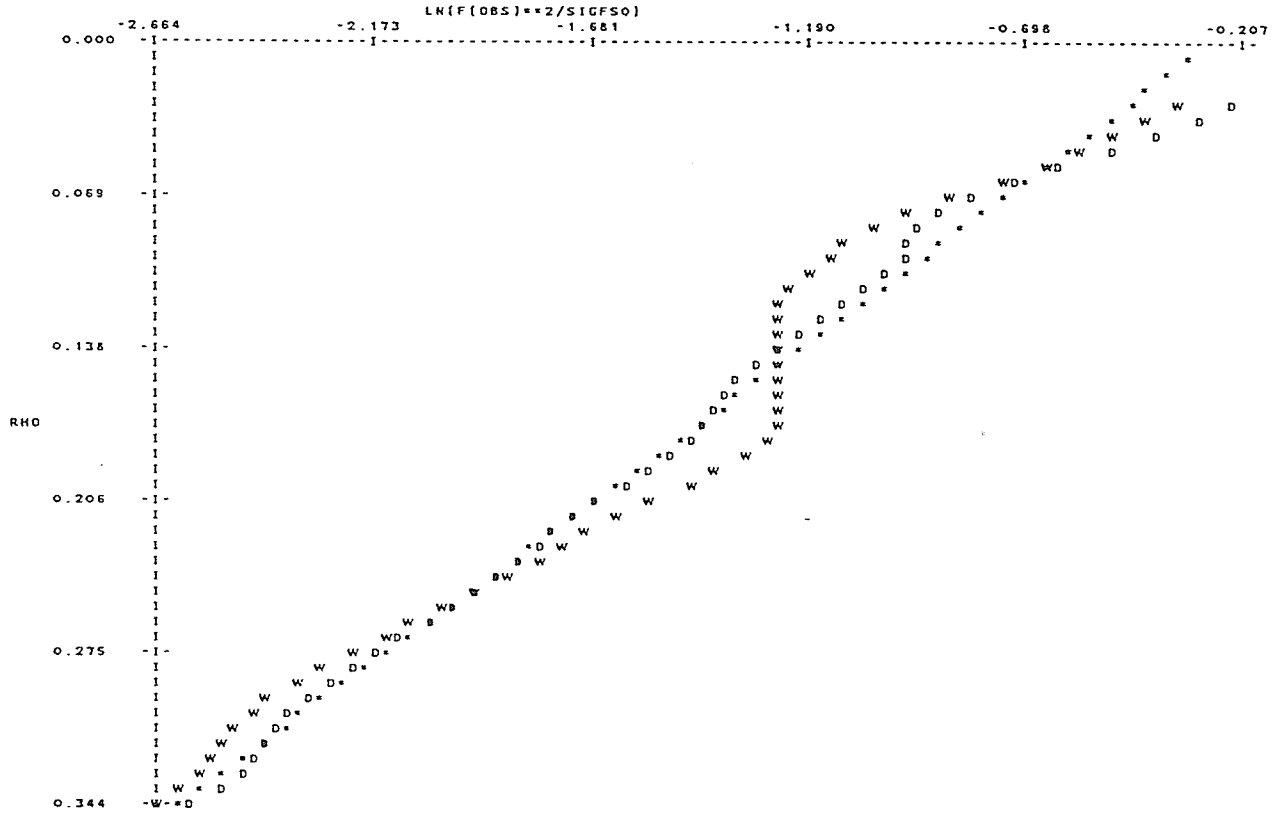


Figure 5: Plot of Wilson and Debye curves and least squares straight line.

* is the least squares straight line.
W is the Wilson's curve.
D is the Debye's curve.

Statistical analysis shows that the experimental data have a centeric distribution of intensities, which provides evidence for the space group $P\bar{1}$. To solve the structure, 450 of the largest E-values were used in the phase determination process, and there were 32 possible phase solutions generated by the program. The set of phase angles which had the highest combined figure of merit (CFOM) gave the correct solution for the structure. The resulting Fourier map (Fig.6) revealed 33 individual electron density peaks giving the basic structure of the molecule.

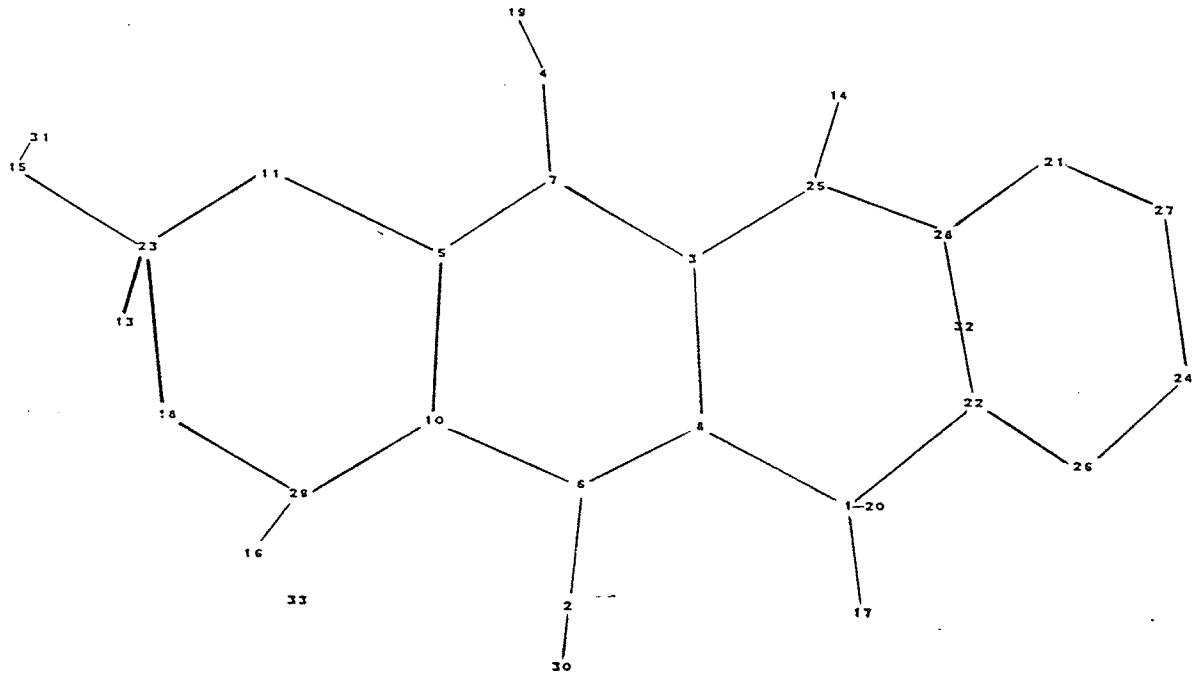


Figure 6: E-map, projection onto the least-squares plane through the peaks.
Numbers correspond to electron density peaks, which are inversely proportional to peak height.

Twenty-nine non-hydrogen atoms of the molecule were located on the Fourier map, and after three cycles of full-matrix least-squares refinement of positional parameters and isotropic temperature factors the R factor was 0.360. A subsequent difference Fourier synthesis was calculated which showed three relatively large electron density peaks that were away from the major fragment of the molecule under study but near the border of the c axis of the unit cell. The electron density and the distances between the central peak and the other two peaks (1.7614 and 1.7224 Å) were similar to the C-Cl bond length in a methylene chloride molecule. Since the crystal was grown from a methylene chloride solution, it was possible for the solvent molecules to be trapped in the crystal. Therefore, it was reasonable to assume that there was a methylene chloride molecule in the unit cell.

After the solvent molecule was located, 32 non-hydrogen atoms were refined anisotropically. The R factor from this refinement was reduced to 0.170. Eleven of the twenty-four hydrogen atoms were located by different Fourier maps and were refined isotropically, but the rest of the hydrogens were not found. Therefore, they were placed in calculated positions according to theoretical bond angles and lengths. Only four of the hydrogens in calculated positions were refined isotropically; the others were not refined because attempts to refine their positional parameters and temperature factors did not improve the structure.

During the latter stages of refinement, the position and temperature parameters of the solvent molecule showed large variations which could not be settled by further cycles of refinement. Difference Fourier maps revealed some unreasonablely large electron density peaks near the solvent region. Large positional parameter shifts associated with the solvent atoms were oscillating and their temperature factors were too large in comparison to the normal atomic vibrations in the crystalline state. The model at this point yielded an R of 0.10. To account for the excess electron density, the methylene chloride molecule was considered to be disordered with two orientations such that the carbon and one of the chlorine atoms had 55% occupancy in one orientation and 45% in the other. Only the pivotal chlorine, i.e. the 100% occupancy Cl, was refined anisotropically; the other chlorine and the carbon atom were refined isotropically. In the case of the carbon atom, only the temperature factor was refined since the positional and temperature parameters were highly correlated. In fact, there was only one broad carbon peak found for the solvent, but for structural soundness, it was necessary to have the carbon atom split into two locations with the same occupancies as the disordered chlorine atom so that each disordered molecule had chemically reasonable geometry.

The maximum and minimum electron residuals from the final difference map were 1.306 and -1.291 e $Å^{-3}$ with the maximum located between Cl(1) and C(17'), while the minimum lies

near the Cl(2") atom. The extinction correction for reflection data was minor with a final g-value of 0.51×10^4. Final R = 0.065, wR = 0.088 for 3198 observed reflections, R = 0.078, wR = 0.088 for 4016 data; $w = (15.0/|Fo|)^2$ for $|Fo| \geq 15.0$, and $w = 1.0$ for $|Fo| < 15.0$; unobserved data were assigned w = 0. The mean and maximum parameter shifts in the final cycle were 0.158 and 0.974 (for methyl H(15c)), respectively, and the GOF for the structure was 0.921 calculated by $\{[\Sigma w(|Fo| - k|Fc|)^2]/(NO - NV)\}^{1/2}$, where NO is the number of observed reflections and NV is the number of variables. Atomic scattering factors were obtained from references 15 and 16. The non-hydrogen and hydrogen atom positional parameters are given in Tables 1 and 2, respectively. Table 3 shows the anisotropic thermal parameters for non-hydrogen atoms. Structure factor data are given in Appendix A.

TABLE 1

Final positional parameters (fractional x 10^4) and isotropic thermal parameters ($Å^2$ X 10^3) with estimated standard deviations in parentheses

'designates 55% occupancy, " designates 45% occupancy

Atom	x	y	z	Ueq†/Uiso
C(1)	1035(6)	2028(5)	9230(5)	48
C(2)	1164(7)	3101(6)	9583(5)	58
C(3)	1045(8)	4230(6)	8734(5)	59
C(4)	835(6)	4308(5)	7531(5)	47
C(4a)	741(5)	3231(4)	7180(4)	37
S	400(1)	3395(1)	5632(1)	35
C(5a)	1378(5)	1841(4)	5469(4)	34
C(6)	2001(5)	1724(4)	4330(4)	37
C(6a)	2753(5)	543(4)	4112(4)	37
C(7)	3495(6)	437(5)	2864(4)	45
C(8)	4622(6)	-819(5)	2888(5)	50
C(9)	4038(5)	-1944(5)	3591(5)	42
C(10)	3642(7)	-1835(5)	4899(5)	42
C(10a)	2812(5)	-536(4)	5056(4)	35
C(11)	2112(5)	-417(4)	6190(4)	33
C(11a)	1402(5)	763(4)	6427(4)	34
C(12)	777(5)	916(4)	7662(4)	38
C(12a)	840(5)	2087(4)	8029(4)	39
C(13)	2806(7)	3534(6)	3135(6)	61
C(14)	5187(6)	-3193(5)	3590(5)	47
C(15)	4881(14)	-4158(9)	3044(14)	103
C(16)	1153(8)	-2167(6)	7193(6)	52

O(1)	-1178(4)	3443(3)	5599(4)	51
O(2)	283(5)	102(3)	8375(3)	55
O(3)	2273(4)	-1499(3)	7107(3)	41
O(4)	6308(5)	-3380(5)	4053(5)	80
O(5)	2769(4)	-1895(4)	2999(3)	48
O(6)	2452(5)	684(4)	1991(3)	60
O(7)	1756(4)	2781(3)	3385(3)	43
C(17')*	2670	-2070	119	78(4)
C(17")*	3011	-2254	38	73(5)
Cl(1)	3148(4)	-3772(3)	53(3)	133
Cl(2')	4148(5)	-1422(5)	-348(4)	94(1)
Cl(2")	4796(7)	-1983(6)	-170(5)	101(2)

† Ueq is equal to one third the trace of the diagonalized temperature factor matrix.

* atoms in calculated positions.

TABLE 2

Final hydrogen positional parameters (fractional x 10^3) and isotropic thermal parameters ($Å^2$ x 10^3) with estimated standard deviations in parentheses

' designates 55% occupancy, " designates 45% occupancy

Atom	x	y	z	Uiso
H(1)*	106	119	993	82
H(2)*	140	306	1057	93
H(3)	122(6)	495(6)	901(5)	60(17)
H(4)	76(6)	504(6)	701(5)	59(17)
H(O5)	226(7)	-236(6)	354(6)	62(18)
H(O6)	219(9)	2(8)	209(7)	90(27)
H(7)	421(4)	105(4)	266(3)	18(9)
H(8a)	547(7)	-84(6)	343(6)	66(18)
H(8b)	496(6)	-95(5)	209(5)	54(16)
H(10a)	304(7)	-242(6)	528(5)	60(17)
H(10b)	444(7)	-207(6)	529(5)	55(17)
H(13a)*	373	294	284	104
H(13b)*	265	375	385	126
H(13c)*	253	418	235	130
H(15a)	550(10)	-474(9)	320(7)	89(28)
H(15b)*	394(12)	-412(9)	316(9)	113(36)
H(15c)*	466(11)	-379(9)	223(9)	137(36)
H(16a)	41(9)	-179(8)	744(7)	77(26)
H(16b)*	108(7)	-238(6)	641(7)	70(19)
H(16c)*	136(9)	-285(9)	783(8)	111(28)

H(17a')*	186	-160	-42	79
H(17b')*	235	-199	97	79
H(17a")*	241	-170	-64	75
H(17b")*	254	-206	83	75

* atoms in calculated positions.

TABLE 3

Final anisotropic thermal parameters

(U_{ij} x 10^3 Å^2, for S, x 10^4 Å^2)*
and their estimated standard deviations

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	62(3)	40(3)	38(3)	-10(2)	-3(2)	-6(2)
C(2)	84(4)	53(3)	43(3)	-21(3)	-5(3)	-16(3)
C(3)	87(5)	43(3)	53(3)	-22(3)	-2(3)	-19(3)
C(4)	64(4)	31(3)	47(3)	-12(2)	-4(3)	-8(2)
C(4a)	40(3)	32(2)	39(2)	-9(2)	0(2)	-8(2)
C(5)	46(3)	30(2)	34(2)	-16(2)	-9(2)	3(2)
C(5a)	43(3)	26(2)	34(2)	-13(2)	-7(2)	-2(2)
S	441(7)	241(6)	354(6)	-108(5)	-63(5)	12(4)
C(6a)	44(3)	35(2)	34(2)	-16(2)	-5(2)	-3(2)
C(7)	59(3)	42(3)	37(3)	-22(2)	2(2)	-5(2)
C(8)	54(3)	52(3)	46(3)	-21(3)	10(3)	-12(3)
C(9)	41(3)	42(3)	45(3)	-11(2)	-1(2)	-10(2)
C(10)	50(3)	33(3)	40(3)	-6(2)	-5(2)	-5(2)
C(10a)	41(3)	29(2)	36(2)	-11(2)	-7(2)	-3(2)
C(11)	41(3)	28(2)	30(2)	-13(2)	-8(2)	1(2)
C(11a)	42(3)	28(2)	32(2)	-13(2)	-6(2)	-2(2)
C(12)	47(3)	33(2)	33(2)	-14(2)	-2(2)	0(2)
C(12a)	45(3)	33(2)	37(2)	-10(2)	2(2)	-8(2)
C(13)	69(4)	46(3)	64(4)	-31(3)	0(3)	11(3)
C(14)	45(3)	47(3)	48(3)	-10(2)	2(2)	-11(2)
C(15)	92(7)	56(5)	170(12)	8(5)	-50(7)	-51(6)
C(16)	72(4)	39(3)	49(3)	-29(3)	0(3)	-1(3)
O(1)	47(2)	42(2)	63(2)	-12(2)	-12(2)	-4(2)

O(2)	84(3)	42(2)	41(2)	-30(2)	9(2)	-3(2)
O(3)	57(2)	29(2)	35(2)	-14(1)	-10(1)	3(1)
O(4)	48(3)	90(4)	100(4)	7(2)	-16(2)	-40(3)
O(5)	47(2)	49(2)	50(2)	-17(2)	-9(2)	-4(2)
O(6)	85(3)	53(3)	39(2)	-15(2)	-12(2)	-3(2)
O(7)	57(2)	33(2)	36(2)	-19(2)	-10(2)	7(1)
Cl(1)	181(3)	85(2)	141(2)	-38(2)	-80(2)	0(1)

* The anisotropic thermal parameters employed in the refinement are $\underline{U}_{ij}$ in the expression:

$$\underline{f} = \underline{f}^{\circ} \exp(-2\pi^2 \Sigma\Sigma \underline{U}_{ij} \underline{h}_i \underline{h}_j \underline{a}^*_i \underline{a}^*_j)$$

2.4 DISCUSSION

The bulk of the molecule is formed by four six membered rings of which two are aromatic, one is a heterocyclic sulfoxide and the fourth is a mostly saturated ring containing acetyl and hydroxyl substituents. Unlike the daunomycinone moiety of daunomycin (Fig.7) (11) and the other similar compounds such as carminomycin I hydrochloride monohydrate (17)

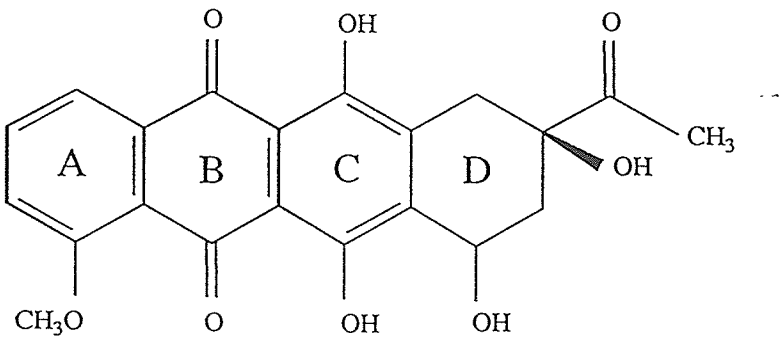


Figure 7: Molecular structure of daunomycinone.

which exhibit overall planarity of three aromatic rings, A, B and C, the present compound has a significantly altered geometry (bond lengths and angles, Tables 4-7) due to the introduction of sulfur into the B ring (Fig.8). The replacement of an sp^2 hybridized carbon by an sp^3 sulfur atom means that ring B can no longer keep its aromaticity. The longer S-C bonds (average length of 1.788 Å) in place of the C-C bonds increase the ring strain which is relieved somewhat by the bent conformation (Fig.9).

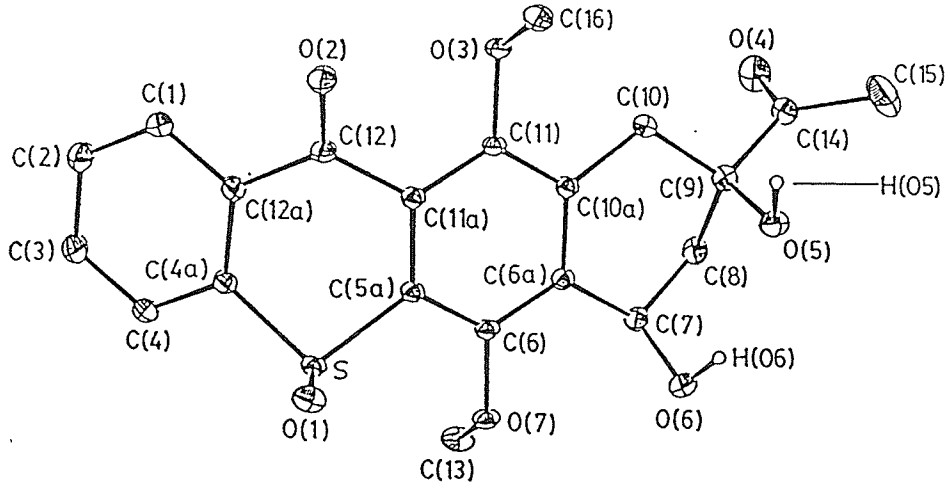


Figure 8: ORTEP view, with non-hydrogen atom thermal ellipsoids drawn at the 50% probability level.

Ring B adopts a boat-like conformation with S and C(12) atoms deviating from the mean plane through C(4a), C(5a), C(11a) and C(12a) by 0.5940 and 0.3557 Å, respectively. The folding along the S...C line in the molecule is common to similar multiple ring compounds containing a sulfur heterocyclic ring (18-20). The torsion angles (Table 8) of

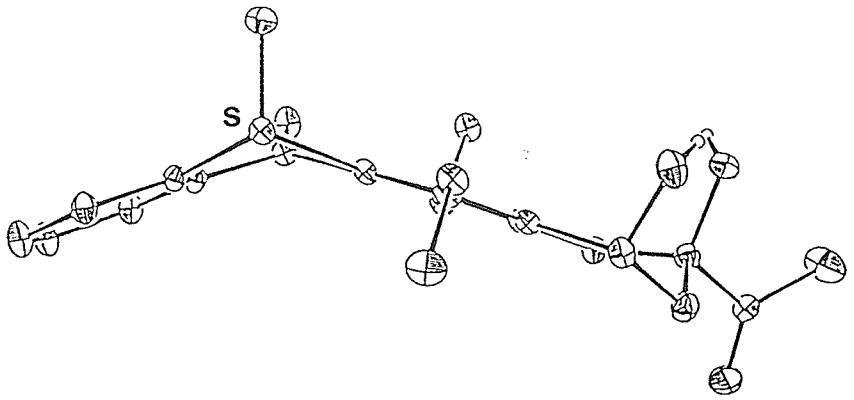


Figure 9: Side view of the ORTEP diagram with the S atom in front of the ring. Non-hydrogen atom thermal ellipsoids at 50% probability level.

4.7(8)° for S-C(4a)-C(12a)-C(12) and -8.5(6)° for S-C(5a)-C(11a)-C(12) indicate that the two essentially flat portions of the molecule comprised of rings A and C and their immediate bonded atoms are not strictly planar. However, the individual rings A and C more closely approximate planes with average deviations from their respective least-squares planes of 0.0060 and 0.0132 Å.

The overall planarity of the first three rings (A, B and C) is believed to be one of the most critical criteria in determining whether this molecule is a suitable one for further drug synthesis because the anticancer ability of the drug mainly depends on the intercalation and different hydrogen bonding abilities of the drug to duplex DNA. The lack of overall planarity in the present molecule imparted by the sulfur in the B-ring may hinder the intercalative binding of the molecule to DNA. Relative to the intercalating portion of daunomycin, the tetracyclic fragment of the

TABLE 4

Bond lengths (Å) for non-hydrogen atoms with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1)-C(2)	1.394(8)	C(9)-C(10)	1.517(7)
C(1)-C(12a)	1.383(7)	C(9)-C(14)	1.543(7)
C(2)-C(3)	1.379(8)	C(9)-O(5)	1.458(6)
C(3)-C(4)	1.384(8)	C(10)-C(10a)	1.506(7)
C(4)-C(4a)	1.387(7)	C(10a)-C(11)	1.406(7)
C(4a)-S	1.785(5)	C(11)-C(11a)	1.393(6)
C(4a)-C(12a)	1.392(7)	C(11)-O(3)	1.379(5)
S -C(5a)	1.791(5)	C(11a)-C(12)	1.494(7)
S -O(1)	1.531(4)	C(12)-C(12a)	1.487(7)
C(5a)-C(6)	1.384(7)	C(12)-O(2)	1.226(6)
C(5a)-C(11a)	1.414(6)	C(13)-O(7)	1.454(6)
C(6)-C(6a)	1.396(7)	C(14)-C(15)	1.477(10)
C(6)-O(7)	1.380(5)	C(14)-O(4)	1.214(7)
C(6a)-C(7)	1.532(7)	C(16)-O(3)	1.462(7)
C(6a)-C(10a)	1.401(6)	C(17')-Cl(1)	1.856(3)
C(7)-C(8)	1.534(8)	C(17')-Cl(2')	1.753(5)
C(7)-O(6)	1.430(7)	C(17")-Cl(1)	1.665(3)
C(8)-C(9)	1.528(7)	C(17")-Cl(2")	1.824(6)

present molecule is approximately 3 Å thicker. This is calculated by taking the best plane which passes through C(2), C(3), C(7) and C(10) atoms and the deviation distances of

TABLE 5

Bond angles (deg) involving non-hydrogen atoms with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2)-C(1)-C(12a)	120.2(5)	C(10)-C(9)-O(5)	109.7(4)
C(1)-C(2)-C(3)	119.5(5)	C(14)-C(9)-O(5)	112.1(4)
C(2)-C(3)-C(4)	121.0(5)	C(9)-C(10)-C(10a)	114.9(4)
C(3)-C(4)-C(4a)	119.2(5)	C(6a)-C(10a)-C(10)	121.6(4)
C(4)-C(4a)-S	117.5(4)	C(6a)-C(10a)-C(11)	119.9(4)
C(4)-C(4a)-C(12a)	120.5(5)	C(10)-C(10a)-C(11)	118.5(4)
S -C(4a)-C(12a)	122.0(4)	C(10a)-C(11)-C(11a)	121.7(4)
C(4a)-S -C(5a)	97.8(2)	C(10a)-C(11)-O(3)	117.5(4)
C(4a)-S -O(1)	107.0(2)	C(11a)-C(11)-O(3)	120.5(4)
C(5a)-S -O(1)	106.7(2)	C(5a)-C(11a)-C(11)	117.4(4)
S -C(5a)-C(6)	117.1(3)	C(5a)-C(11a)-C(12)	120.3(4)
S -C(5a)-C(11a)	121.2(4)	C(11)-C(11a)-C(12)	122.2(4)
C(6)-C(5a)-C(11a)	121.2(4)	C(11a)-C(12)-C(12a)	116.9(4)
C(5a)-C(6)-C(6a)	121.0(4)	C(11a)-C(12)-O(2)	122.7(4)
C(5a)-C(6)-O(7)	118.5(4)	C(12a)-C(12)-O(2)	120.3(4)
C(6a)-C(6)-O(7)	120.3(4)	C(1)-C(12a)-C(4a)	119.6(4)
C(6)-C(6a)-C(7)	120.4(4)	C(1)-C(12a)-C(12)	119.3(4)
C(6)-C(6a)-C(10a)	118.7(4)	C(4a)-C(12a)-C(12)	121.1(4)
C(7)-C(6a)-C(10a)	120.9(4)	C(9)-C(14)-C(15)	118.8(6)
C(6a)-C(7)-C(8)	113.1(4)	C(9)-C(14)-O(4)	120.1(5)
C(6a)-C(7)-O(6)	109.8(4)	C(15)-C(14)-O(4)	121.1(7)
C(8)-C(7)-O(6)	113.2(4)	C(11)-O(3)-C(16)	113.6(4)
C(7)-C(8)-C(9)	110.8(4)	C(10)-C(9)-C(14)	108.3(4)

C(8)-C(9)-C(10)	110.1(4)	C(6)-O(7)-C(13)	116.9(4)
C(8)-C(9)-C(14)	109.7(4)	Cl(1)-C(17')-Cl(2')	110.1(2)
C(8)-C(9)-O(5)	106.9(4)	Cl(1)-C(17")-Cl(2")	108.5(2)

TABLE 6

Bond lengths* (Å) involving hydrogen atoms with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1)-H(1)	1.07	C(13)-H(13b)	0.89
C(2)-H(2)	1.17	C(13)-H(13c)	1.01
C(3)-H(3)	0.99(6)	C(15)-H(15a)	0.77(9)
C(4)-H(4)	0.87(6)	C(15)-H(15b)	0.91(10)
C(7)-H(7)	1.07(4)	C(15)-H(15c)	0.95(10)
C(8)-H(8a)	1.08(6)	C(16)-H(16a)	0.79(8)
C(8)-H(8b)	0.96(6)	C(16)-H(16b)	0.99(7)
C(10)-H(10a)	0.99(7)	C(16)-H(16c)	0.91(9)
C(10)-H(10b)	0.88(6)	O(5)-H(O5)	0.90(6)
C(13)-H(13a)	1.04	O(6)-H(O6)	0.82(8)

* Bond lengths without standard deviation include H's in calculated but not refined positions.

TABLE 7

Bond angles* (deg) involving hydrogen atoms with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2)-C(1)-H(1)	117.2	O(7)-C(13)-H(13a)	104.8
C(12a)-C(1)-H(1)	122.6	O(7)-C(13)-H(13b)	94.6
C(1)-C(2)-H(2)	121.7	O(7)-C(13)-H(13c)	105.6
C(3)-C(2)-H(2)	118.8	H(13a)-C(13)-H(13b)	126.2
C(2)-C(3)-H(3)	116(3)	H(13a)-C(13)-H(13c)	100.8
C(4)-C(3)-H(3)	122(3)	H(13b)-C(13)-H(13c)	121.6
C(3)-C(4)-H(4)	119(4)	C(14)-C(15)-H(15a)	105(7)
C(4a)-C(4)-H(4)	121(4)	C(14)-C(15)-H(15b)	109(6)
C(6a)-C(7)-H(7)	108(2)	C(14)-C(15)-H(15c)	109(6)
C(8)-C(7)-H(7)	97(2)	H(15a)-C(15)-H(15b)	128(9)
O(6)-C(7)-H(7)	115(2)	H(15a)-C(15)-H(15c)	120(9)
C(7)-C(8)-H(8a)	108(3)	H(15b)-C(15)-H(15c)	84(8)
C(7)-C(8)-H(8b)	113(3)	O(3)-C(16)-H(16a)	113(6)
C(9)-C(8)-H(8a)	103(3)	O(3)-C(16)-H(16b)	111(4)
C(9)-C(8)-H(8b)	109(3)	O(3)-C(16)-H(16c)	106(6)
H(8a)-C(8)-H(8b)	112(5)	H(16a)-C(16)-H(16b)	112(7)
C(9)-C(10)-H(10a)	109(4)	H(16a)-C(16)-H(16c)	100(7)
C(9)-C(10)-H(10b)	108(4)	H(16b)-C(16)-H(16c)	115(7)
C(10a)-C(10)-H(10a)	106(4)	C(9)-O(5)-H(O5)	107(4)
C(10a)-C(10)-H(10b)	110(4)	C(7)-O(6)-H(O6)	106(6)
H(10a)-C(10)-H(10b)	108(5)		

* Bond angles without standard deviation include H's in calculated but not refined positions.

TABLE 8

Torsion angles* (deg) with estimated standard deviations in parentheses

Atoms	Value(deg)
C(12a)-C(1)-C(2)-C(3)	2.3(10)
C(2)-C(1)-C(12a)-C(4a)	-1.5(8)
C(2)-C(1)-C(12a)-C(12)	177.0(5)
C(1)-C(2)-C(3)-C(4)	-1.6(10)
C(2)-C(3)-C(4)-C(4a)	0.0(10)
C(3)-C(4)-C(4a)-S	177.6(5)
C(3)-C(4)-C(4a)-C(12a)	0.8(8)
C(4)-C(4a)-S -C(5a)	147.9(4)
C(4)-C(4a)-S -O(1)	-102.0(4)
C(12a)-C(4a)-S -C(5a)	-35.4(4)
C(12a)-C(4a)-S -O(1)	74.8(4)
C(4)-C(4a)-C(12a)-C(1)	0.1(8)
C(4)-C(4a)-C(12a)-C(12)	-178.5(5)
S -C(4a)-C(12a)-C(1)	-176.8(4)
S -C(4a)-C(12a)-C(12)	4.8(7)
C(4a)-S -C(5a)-C(6)	-148.7(4)
C(4a)-S -C(5a)-C(11a)	37.1(4)
O(1)-S -C(5a)-C(6)	100.9(4)
O(1)-S -C(5a)-C(11a)	-73.4(4)
S -C(5a)-C(6)-C(6a)	-178.4(4)
S -C(5a)-C(6)-O(7)	-4.1(6)
C(11a)-C(5a)-C(6)-C(6a)	-4.1(7)
C(11a)-C(5a)-C(6)-O(7)	170.2(4)
S -C(5a)-C(11a)-C(11)	175.8(3)

S -C(5a)-C(11a)-C(12)	-8.5(6)
C(6)-C(5a)-C(11a)-C(11)	1.8(7)
C(6)-C(5a)-C(11a)-C(12)	177.5(4)
C(5a)-C(6)-C(6a)-C(7)	-177.1(4)
C(5a)-C(6)-C(6a)-C(10a)	2.9(7)
O(7)-C(6)-C(6a)-C(7)	8.7(7)
O(7)-C(6)-C(6a)-C(10a)	-171.3(4)
C(5a)-C(6)-O(7)-C(13)	94.3(6)
C(6a)-C(6)-O(7)-C(13)	-91.5(6)
C(6)-C(6a)-C(7)-C(8)	162.4(5)
C(6)-C(6a)-C(7)-O(6)	-70.1(6)
C(10a)-C(6a)-C(7)-C(8)	-17.6(7)
C(10a)-C(6a)-C(7)-O(6)	109.9(5)
C(6)-C(6a)-C(10a)-C(10)	-178.0(5)
C(6)-C(6a)-C(10a)-C(11)	0.5(7)
C(7)-C(6a)-C(10a)-C(10)	2.1(7)
C(7)-C(6a)-C(10a)-C(11)	-179.5(4)
C(6a)-C(7)-C(8)-C(9)	47.0(6)
O(6)-C(7)-C(8)-C(9)	-78.7(6)
C(7)-C(8)-C(9)-C(10)	-61.5(6)
C(7)-C(8)-C(9)-C(14)	179.5(4)
C(7)-C(8)-C(9)-O(5)	57.7(6)
C(8)-C(9)-C(10)-C(10a)	45.7(7)
C(14)-C(9)-C(10)-C(10a)	165.6(5)
O(5)-C(9)-C(10)-C(10a)	-71.7(6)
C(8)-C(9)-C(14)-C(15)	-119.8(9)
C(8)-C(9)-C(14)-O(4)	61.5(7)
C(10)-C(9)-C(14)-C(15)	120.0(9)

C(10)-C(9)-C(14)-O(4)	-58.7(7)
O(5)-C(9)-C(14)-C(15)	-1.2(9)
O(5)-C(9)-C(14)-O(4)	-179.8(5)
C(9)-C(10)-C(10a)-C(6a)	-16.5(7)
C(9)-C(10)-C(10a)-C(11)	165.0(4)
C(6a)-C(10a)-C(11)-C(11a)	-2.8(7)
C(6a)-C(10a)-C(11)-O(3)	-176.4(4)
C(10)-C(10a)-C(11)-C(11a)	175.7(5)
C(10)-C(10a)-C(11)-O(3)	2.2(7)
C(10a)-C(11)-C(11a)-C(5a)	1.6(7)
C(10a)-C(11)-C(11a)-C(12)	-173.9(4)
O(3)-C(11)-C(11a)-C(5a)	175.0(4)
O(3)-C(11)-C(11a)-C(12)	0.6(7)
C(10a)-C(11)-O(3)-C(16)	-92.9(6)
C(11a)-C(11)-O(3)-C(16)	93.4(5)
C(5a)-C(11a)-C(12)-C(12a)	-31.1(6)
C(5a)-C(11a)-C(12)-O(2)	152.0(5)
C(11)-C(11a)-C(12)-C(12a)	144.4(5)
C(11)-C(11a)-C(12)-O(2)	-32.6(8)
C(11a)-C(12)-C(12a)-C(1)	-145.1(5)
C(11a)-C(12)-C(12a)-C(4a)	33.3(7)
O(2)-C(12)-C(12a)-C(1)	31.9(8)
O(2)-C(12)-C(12a)-C(4a)	-149.6(5)
Cl(2')-C(17')-Cl(1)-C(17")	2.5(2)
Cl(2")-C(17")-Cl(1)-C(17')	170.7(2)
C(12a)-C(1)-C(2)-H(2)	-176.1
H(1)-C(1)-C(2)-C(3)	-175.8
H(1)-C(1)-C(2)-H(2)	5.8

H(1)-C(1)-C(12a)-C(4a)	176.5
H(1)-C(1)-C(12a)-C(12)	-5.0
C(1)-C(2)-C(3)-H(3)	-175(4)
H(2)-C(2)-C(3)-C(4)	176.9
H(2)-C(2)-C(3)-H(3)	3
C(2)-C(3)-C(4)-H(4)	179(5)
H(3)-C(3)-C(4)-C(4a)	174(4)
H(3)-C(3)-C(4)-H(4)	-7(6)
H(4)-C(4)-C(4a)-S	-2(5)
H(4)-C(4)-C(4a)-C(12a)	-179(5)
C(6)-C(6a)-C(7)-H(7)	56(2)
C(10a)-C(6a)-C(7)-H(7)	-124(2)
C(6a)-C(7)-C(8)-H(8a)	-65(3)
C(6a)-C(7)-C(8)-H(8b)	169(4)
O(6)-C(7)-C(8)-H(8a)	169(3)
O(6)-C(7)-C(8)-H(8b)	44(4)
H(7)-C(7)-C(8)-C(9)	160(2)
H(7)-C(7)-C(8)-H(8a)	47(4)
H(7)-C(7)-C(8)-H(8b)	-78(4)
C(6a)-C(7)-O(6)-H(O6)	-80(6)
C(8)-C(7)-O(6)-H(O6)	48(6)
H(7)-C(7)-O(6)-H(O6)	158(6)
H(8a)-C(8)-C(9)-C(10)	54(3)
H(8a)-C(8)-C(9)-C(14)	-65(3)
H(8a)-C(8)-C(9)-O(5)	173(3)
H(8b)-C(8)-C(9)-C(10)	174(4)
H(8b)-C(8)-C(9)-C(14)	55(4)
H(8b)-C(8)-C(9)-O(5)	-67(4)
C(8)-C(9)-C(10)-H(10a)	165(4)

C(8)-C(9)-C(10)-H(10b)	-77(4)
C(14)-C(9)-C(10)-H(10a)	-75(4)
C(14)-C(9)-C(10)-H(10b)	43(4)
O(5)-C(9)-C(10)-H(10a)	48(4)
O(5)-C(9)-C(10)-H(10b)	165(4)
C(8)-C(9)-O(5)-H(O5)	-160(4)
C(10)-C(9)-O(5)-H(O5)	-41(4)
C(14)-C(9)-O(5)-H(O5)	79(4)
H(10a)-C(10)-C(10a)-C(6a)	-137(4)
H(10a)-C(10)-C(10a)-C(11)	44(4)
H(10b)-C(10)-C(10a)-C(6a)	105(4)
H(10b)-C(10)-C(10a)-C(11)	-73(4)
H(13a)-C(13)-O(7)-C(6)	65.9
H(13b)-C(13)-O(7)-C(6)	-63.5
H(13c)-C(13)-O(7)-C(6)	171.8
C(9)-C(14)-C(15)-H(15a)	-172(7)
C(9)-C(14)-C(15)-H(15b)	-33(7)
C(9)-C(14)-C(15)-H(15c)	57(7)
O(4)-C(14)-C(15)-H(15a)	6(7)
O(4)-C(14)-C(15)-H(15b)	146(7)
O(4)-C(14)-C(15)-H(15c)	-124(7)
H(16a)-C(16)-O(3)-C(11)	-70(6)
H(16b)-C(16)-O(3)-C(11)	56(4)
H(16c)-C(16)-O(3)-C(11)	-179(6)

* Torsion angles without standard deviation include H's in calculated but not refined positions.

the two equatorial oxygens in ring B from this plane. The thickness of the plane suggests that, if this modified fragment used in a daunomycin-like drug is to intercalate, considerably more unwinding of the the DNA helix would be required to accommodate the drug.

The ketone and sulfoxide oxygens lie on the same side of the bent B ring and extend upward from the S and C(12) apices. This "boat equatorial" conformation of the S=O group in ring B is also found in the similar molecule, thioxanthenone 10-oxide (18). The least-squares plane through S, C(12), O(1) and O(2) shows an average deviation of 0.0095 Å and makes identical dihedral angles of 70.4° with rings A and C. The methoxy substituents on ring C lie in a plane which is essentially perpendicular to the ring plane (dihedral angle, 90.09°). These methoxy groups serve only as the protecting groups at this stage of the synthesis and are removed later by a demethylation reaction, since the ultimate substituents on ring C are to be two hydroxyl groups. The comparison of bond lengths and angles (Table 9) indicates the non-planar ring D has a very similar structure as in daunomycin (5). Both of the D rings adopt a half-chair conformation. In the present study, C(8) deviates from the other five atom plane (average deviation 0.0769 Å) by 0.631 Å, whereas in daunomycin, the same deviation is 0.58 Å.

O(5) is <u>cis</u> to the O(6) hydroxyl group with an interatomic distance of 2.785(6) Å and an O(5)...H(O6)-O(6) angle of

TABLE 9

Comparison of Bond Lengths and Angles in Ring D

Bond	Angstrom*	Angstrom**
C(6a)-C(7)	1.516(8)	1.58
C(7)-C(8)	1.528(10)	1.49
C(8)-C(9)	1.522(9)	1.51
C(9)-C(10)	1.511(9)	1.58
C(10)-C(10a)	1.502(8)	1.44
C(10a)-C(6a)	1.400(8)	1.39
C(9)-O(5)	1.442(7)	1.45
C(9)-C(14)	1.535(9)	1.53
C(14)-C(15)	1.482(11)	1.53
C(14)-O(4)	1.201(8)	1.22
Angle	**Degree***	**Degree****
C(6a)-C(7)-C(8)	113.0(5)	112
C(7)-C(8)-C(9)	111.5(5)	114
C(8)-C(9)-C(10)	110.5(5)	111
C(9)-C(10)-C(10a)	114.7(5)	111
C(10)-C(10a)-C(6a)	121.5(5)	129
C(10a)-C(6a)-C(7)	121.4(5)	117
C(8)-C(9)-O(5)	106.3(5)	112
O(5)-C(9)-C(14)	111.1(5)	106
C(10)-C(9)-C(14)	108.4(5)	108

* values from present molecule.
** values from daunomycin.

140(8)°. This intramolecular hydrogen bond which helps to stabilize the half-chair conformation in the ring D is also found in the daunomycin structure where the bond length is 2.12 Å and the angle is 142°.

All bonds and intra-annular angles of rings A, C and D are not significantly different from those in daunomycin and the daunomycin-butanol complex (5,21). In ring B, the mean

value of the two C-S bond lengths is 1.788 Å, and the C(4a)-S-C(5a) bond angle is 97.8(2)°. The S-O bond length is 1.531(4) Å, and the mean value of the two C-S-O bond angles is 106.9°. Except for the C-S-O bond angles, these values are very similar to the ones found in thioxanthenone 10-oxide (18) where the mean value for the C-S-O angle is 108.2°. The smaller bond angle in the present molecule may be due, in part, to packing effects such as the intermolecular hydrogen bond formed between the O(1)(x,y,z) and O(5)(-x,-y,1-z) atoms (vide infra). Although the S atom is considered sp^3 hybridized, all the angles involving S are smaller than the normal tetrahedral value (109.5°).

Molecules in the crystal (Fig.10) are infinitely stacked back-to-back in H-bonded dimers along the a axis. The molecules in dimers are related to each other by a center of inversion, so that the two oxygens in ring B (x,y,z) and the equatorial hydroxyl groups in ring D (-x,-y,1-z) are facing each other. Each dimer is internally linked by two intermolecular hydrogen bonds between the O(1)(x,y,z) and O(5)(-x,-y,1-z) atoms, where the O(1)...O(5) distance is 2.731(5) Å and the O(1)...H(O5)-O(5) angle is 169(6)° (Fig.11).

The methylene chloride solvent molecule is located in the vicinity of ring A(x,y,z) (Fig.11). Figure 12 shows the disordered nature of the solvent molecule. The structure analysis revealed that the molecule is disordered with Cl(1) in

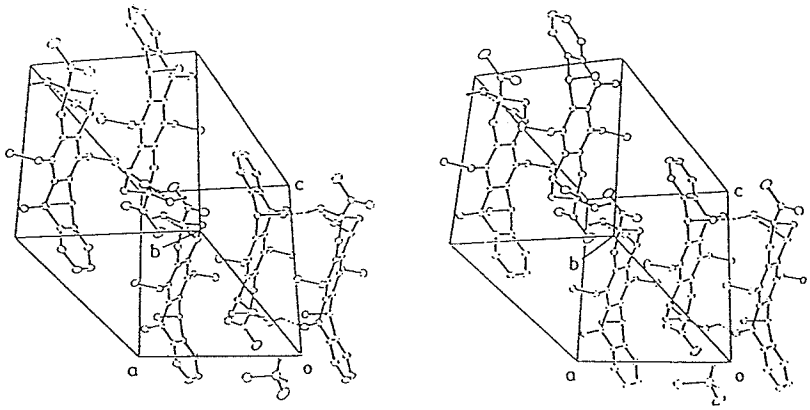


Figure 10: Stereo diagram of the molecular packing in the unit cell.

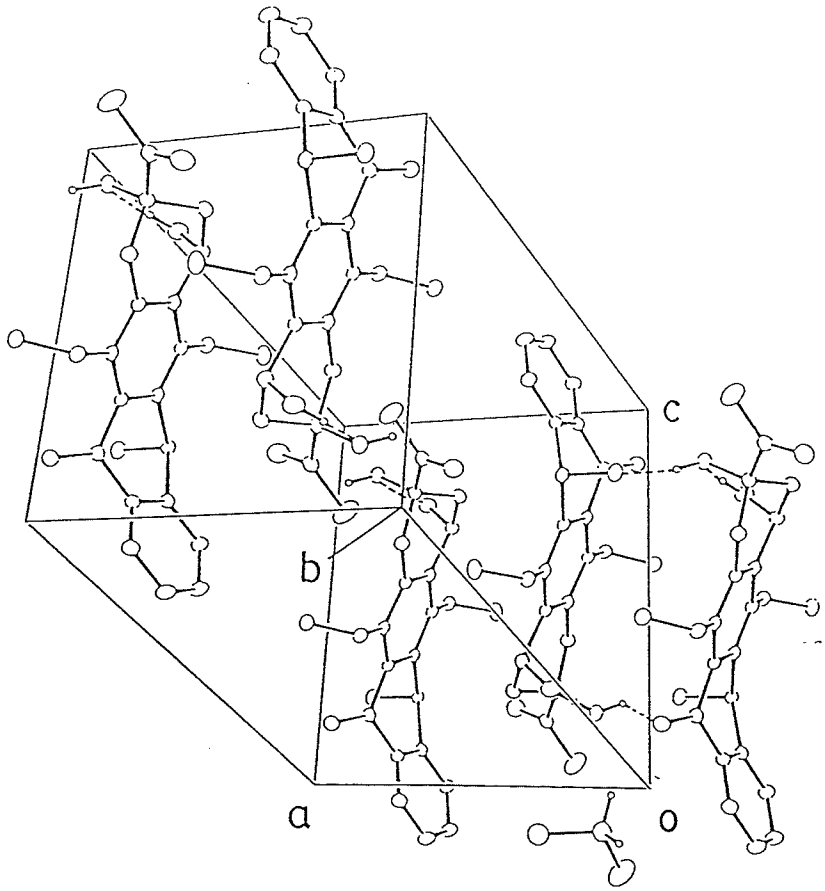


Figure 11: H-bonding dimers in the unit cell.

a fixed position and Cl(2) occupying two other positions resulting in two orientations of the molecule with 55% and 45% occupancies. The separation between Cl(2') and Cl(2") is 0.718(7) Å and the angle for C(17')-Cl(1)-C(17") is 9.83(3)°. Although the difference map indicated only one carbon peak, C(17) had to be assigned two positions with the same occupancy as the Cl(2) in order to satisfy the CH_2Cl_2 molecular geometry. The separation distance between C(17') and C(17") is 0.357 Å. For the two orientations, the angles for Cl(1)-C(17')-Cl(2') and Cl(1)-C(17")-Cl(2") are 110.1(2)° and 108.5(2)° respectively. The positions for the four hydrogen atoms are calculated based on the bond lengths and angles of a tetrahedral model. The present geometry assignment for the solvent molecule is assumed to be the best one since it consumes the maximum extra electron density in that region of the cell while yielding a reasonable

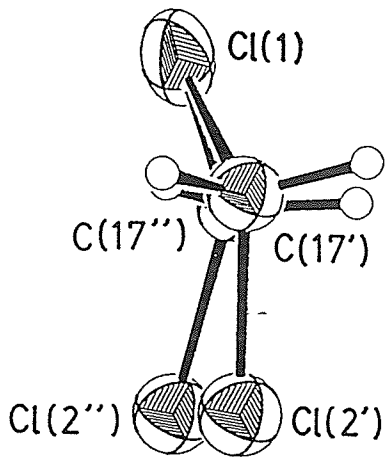


Figure 12: ORTEP view of the solvent molecule with non-hydrogenatom thermal ellipsoids at 50% probability level.

description of the disorder.

2.5 SUMMARY

The major structural difference between the present molecule and daunomycinone is the bending of the B ring in the conjugated ring system. This bending causes the molecule to be approximately 3 Å thicker than those planar, aromatic drug molecules which are able to slip between DNA base pairs without disturbing the overall stacking pattern. If the present molecule is used for further drug synthesis, it is reasonable to expect that the drug would cause a large geometry alteration in the base pairs because of the increased thickness of the molecule. However, whether or not this molecule could be part of a successful anticancer drug is best answered by clinical trials.

Chapter III

1,2,4-TRIAZOLE

3.1 INTRODUCTION

Many alkylating agents are known to be carcinogens which may have varying degrees of structural and mutagenic effects in their reactions with different nucleophilic sites of DNA (22,23). Detailed molecular structures of the base-modified nucleosides may provide useful information in the understanding of the basic mechanism of these carcinogen-modification reactions. The crystal investigated in this study was synthesized by Mr. Gary Buchko (under the supervision of Professor F. E. Hruska), and was originally assumed to be the O^4-n-butyl-thymidine which was synthesized at room temperature by the following steps:

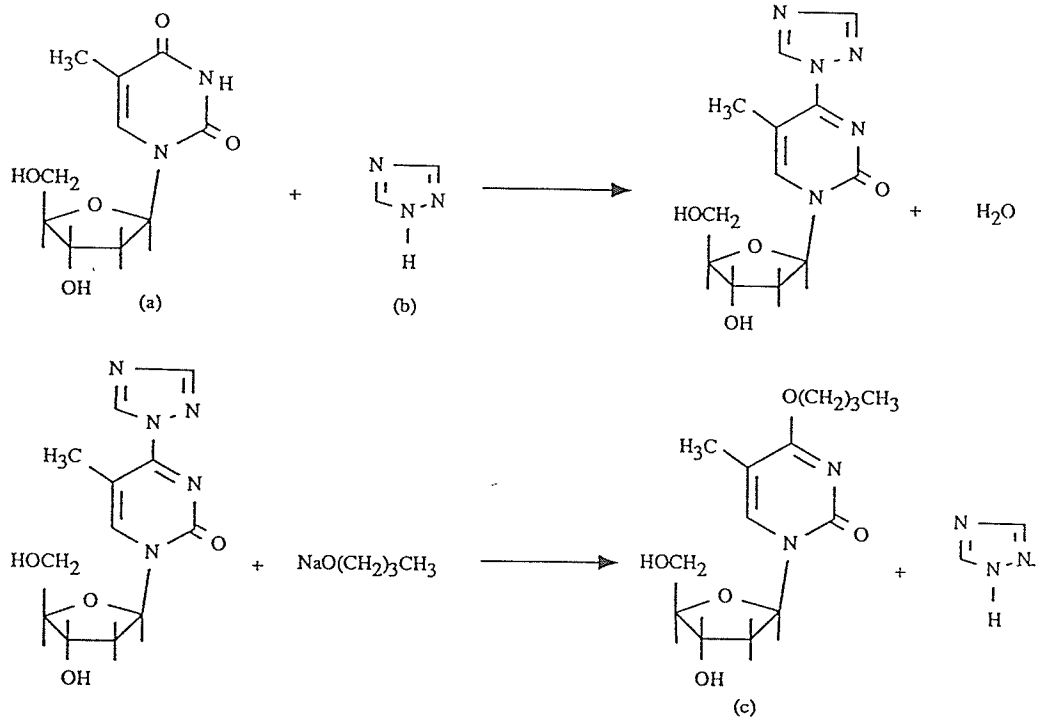


Figure 13: Synthesis scheme for O^4-n-butyl-thymidine.

where (a) is thymidine, (b) is 1,2,4-triazole and (c) is O^4-n-butyl-thymidine. The final products were separated by passing the solution through a Sep-Pak which is a miniature reverse phase separation column. It was hoped that the Sep-Pak would separate the O^4-n-butyl-thymidine from the 1,2,4-triazole on the basis of different polarities. The separated solution which was thought to contain the desired product was later characterized by ^1H NMR spectroscopy. The resultant spectrum showed not only the corresponding peaks for the O^4-n-butyl-thymidine but also showed an unknown peak at 8.347 ppm which at that time was considered to be a minor impurity in the solution.

Crystals suitable for x-ray analysis were grown from the same solution used in the NMR study. Evidence from the X-ray study clearly indicated the crystal was not the O^4-n-butyl-thymidine, but rather, a smaller organic molecule. The structure solution showed that the crystal used for this study was 1,2,4-triazole, a reagent which was regenerated in the reaction shown above.

The crystal and molecular structures for 1,2,4-triazole have been studied at both room and low temperatures (-160°) by Deuschl (24) and Goldstein (25), respectively, but a structure search using the Cambridge Crystallographic Database did not reveal these studies. The present study turned out to be a redetermination of the crystal and molecular structure of 1,2,4-triazole at room temperature.

3.2 EXPERIMENTAL

Colourless prismatic crystals grew from a CH_2Cl_2 solution. One of these crystals measuring 0.35 x 0.35 x 0.28 mm^3 was mounted on a glass rod and used for data collection on a Nicolet R3m automated diffractometer.

Twenty-five strong reflections were chosen from the rotation photo in order to determine the orientation matrix and unit cell parameters. The unit cell constants revealed the crystal class as orthorhombic.

Final crystal data: $C_2H_3N_3$, Mr = 69.0658, orthorhombic, space group Pcab, a = 7.1892(13), b = 9.3600(13), c = 9.7590(11) Å, V = 656.34(13) $Å^3$. Z = 8, Dm = 1.40 g cm^{-3}, $\lambda(M_oK\alpha)$ = 0.71069 Å, μ = 0.9 cm^{-1}, F(000) = 288 electrons.

Reflections were collected using the ω-2θ technique within the range $2° \leq 2\theta \leq 50°$. Scan speeds were selected between 4.0 and 29.30 deg. $min.^{-1}$. Since the unit cell is orthorhombic, only an octant of data was collected in the +h, +k, +l region of reciprocal space. During data collection, the three standard reflections (112, 332, 140) were employed to check crystal orientations after every 45 reflections. The mean and final intensity changes for these standards were 3% and 6% respectively. Since the standard intensities did not change significantly throughout the data collection process, no intensity corrections were required. Lorentz and polarization correction factors were applied to all data in the usual manner but no absorption corrections

were done. The orthorhombic unit cell and the absence conditions hk0, k odd, 0kl, l odd and h0l, h odd in the collected data, uniquely determined the space group of the present molecule as Pcab.

Of the 764 reflections collected on the diffractometer 48 were standards, 2 were rejected because of unbalanced backgrounds and 140 were systematically absent. Among the remaining 574 reflections, 456 were considered unique, observed reflections with intensities $I \geq 2.5\ \sigma(I)$. During structure refinement, 7 observed reflections which were collected with the attenuator in place showed poor agreement with the model and could not be improved by using different weighting schemes or by applying extinction corrections. They were therefore deleted from the latter stages of the refinement to eliminate the systematic error.

3.3 STRUCTURE SOLUTION AND REFINEMENT

Assuming the molecule contained no heavy atoms, direct methods were applied to solve the structure. Structure factor amplitudes, |F(hkl)|, were converted to the corresponding normalized structure factor amplitudes, |E(hkl)|, by the MULTAN80 computer programs (14) and later used for phase determination. Since the O^4-n-butyl-thymidine molecule has neither a center of inversion nor a pseudo-inversion center, the space group symmetry dictates that there would have to be at least 8 individual molecules in the symmetry related

positions in the unit cell. Furthermore, if indeed the molecule was the one expected, the unit cell density would be approximately three times beyond the normal range (1.2-1.6 g cm^{-3}) for organic molecules, or in other words, the unit cell volume is too small to contain eight O^4-n-butyl-thymidine molecules. Taking these factors into account, the unit cell was considered to have only 48 carbon atoms assuming a cell density of about 1.4 g cm^{-3} and giving only 6 atoms in the 8 symmetry related positions.

In the first attempt to solve the structure, 72 largest E-values were used in the phase determination step. Results of data analysis showed that the reflections had a centric distribution of intensities, which corroborated the assigned centrosymmetric space group. Unfortunately, these 72 E-values did not give rise to an acceptable phase at this time (the highest probability for the accepted phase was 0.830 for the reflection 2,0,0). Since there were no acceptable starting phases found for the "unknown" structure (i.e. the sample was an unknown compound), the probability of obtaining a correct set of phases for solving the structure was low. Therefore, phase determination did not continue for this attempt. A Patterson synthesis was also used in trying to solve the structure, but most of the resultant interatomic vectors in the Patterson map had undesirable lengths and showed irregularity in their orientations. The Patterson method, although a suitable one for solving this structure was not straightforward and therefore was not pursued.

Finally, 141 of the largest E-values were selected from the total of 2068 reflections and applied in the phase determination process. The outcome of this process showed three individual reflections correctly phased (all probabilities ≥ 0.986), where the probability for reflection (0,10,0) to have Ø = 360° was 0.998. The electron density map (Fig.14) generated from these E-values showed only 8 relatively strong peaks and among them, only the first 6 were connected in the given range of bonding lengths and angles (max./min. bonding distance is 1.10 and 1.95 Å, max./min. bonding angle is 85.0 and 145.0°). Joining the five highest peaks in the electron density map, a five membered ring clearly emerged. From the ratio of the peak heights in the E-map, peaks 1 to 3 were identified as nitrogens, while 4 and 5 were identified as carbon atoms.

To reaffirm the information obtained from the NMR study, crystals were redissolved in D_2O and characterized by ^1H NMR. The resultant spectrum was found to be identical to the one obtained from pure 1,2,4-triazole.

All positional parameters and anisotropic temperature factors of the non-hydrogen atoms were refined by full matrix least-squares methods. After 5 cycles of refinement (R = 0.120), 2 hydrogen atoms were located on a difference-Fourier map and later were refined isotropically. However, the hydrogen which was expected to be near the N(1) atom was unable to be located. Therefore, it was placed in the calculated position. No parameters were refined for this hydro-

TABLE 10

Electron density peaks in the Fourier-map

Peak	Height	x	y	z
1	1937	0.7958	0.0922	0.5091
2	1022	0.8007	0.0722	0.2890
3	1775	0.9045	0.1993	0.4642
4	1676	0.9036	0.1953	0.3385
5	1309	0.7455	-0.0027	0.3981
6	562	0.7809	0.1016	0.7025
7	438	0.8866	-0.0382	0.3253
8	411	0.7964	0.1455	0.3912

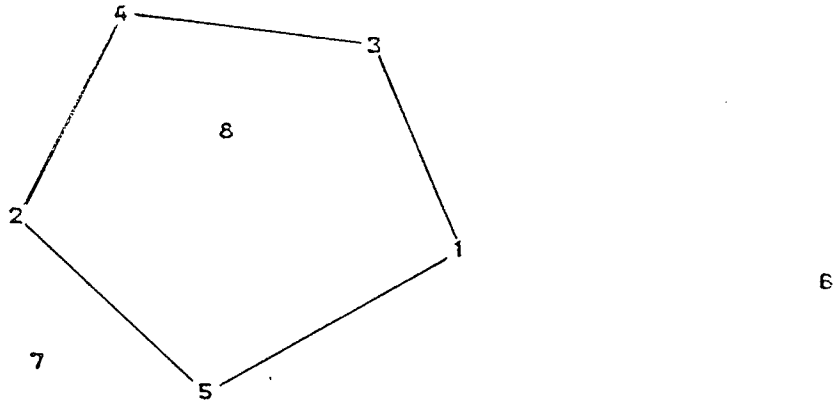


Figure 14: E-map, projection onto least-squares planes through electron density peaks.

gen because attempts at refinement gave poor R-values and tended to increase the error index for the structure. During the final stages of refinement, all reflections were assigned unit weight, since other weighting schemes did not improve the refinement or the structure. The present structural model has a final residual index R = 0.043 and wR =

0.046 for 449 observed reflections, for 574 recorded data, R = 0.053 and wR = 0.046, w = 1 for observed data, for unobserved reflections w = 0. The maximum and minimum electron density residuals in the final difference synthesis were 0.166 and -0.253 e $Å^{-3}$; G.O.F. for the final refinement was 0.6431 and the mean and maximum parameter shifts were 0.936 and 4.837σ (for N(2)). Final positional and corresponding isotropic temperature factors for all atoms are shown in Tables 11 and 12; Table 13 shows the anisotropic temperature factors for the non-hydrogen atoms. Atomic scattering factors are from references 15 and 16. The structure factor table is shown in Appendix B.

TABLE 11

Final positional parameters (fractional x 10^4) and isotropic thermal parameters (Å x 10^3) with estimated standard deviations in parentheses

Atom	x	y	z	Ueq†/Uiso
N(1)	7893(3)	864(2)	5048(2)	44
N(2)	8902(3)	2036(2)	4726(2)	53
C(3)	9028(4)	1928(3)	3384(3)	52
N(4)	8175(3)	771(2)	2843(2)	48
C(5)	7476(4)	137(3)	3931(2)	45

† Ueq is equal to one third the trace of the diagonalized temperature factor matrix.

TABLE 12

Final hydrogen positional parameters (fractional x 10^3) and isotropic thermal parameters ($Å^2$ x 10^3) with estimated standard deviations in parentheses

Atom	x	y	z	Uiso
H(1)*	754	62	595	63
H(3)	969(4)	263(3)	278(3)	78(9)
H(5)	678(4)	-74(3)	390(3)	66(8)

* atom in calculated position.

TABLE 13

Final anisotropic thermal parameters (U_{ij}x 10^4 $Å^2$)* and their estimated standard deviations

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	51(1)	51(1)	30(1)	4(1)	1(1)	0(1)
N(2)	58(1)	49(1)	53(1)	-4(1)	-1(1)	-11(1)
C(3)	56(2)	50(2)	49(1)	-2(1)	6(1)	7(1)
N(4)	62(1)	53(1)	30(1)	-2(1)	0(1)	0(1)
C(5)	58(2)	42(1)	36(1)	-4(1)	-3(1)	-1(1)

*The anisotropic thermal parameters employed in the refinement are U_{ij} in the expression:

$$f = f^{\circ}\exp(-2\pi^2 \sum_{i}\sum_{j} U_{ij} h_i h_j a^*_i a^*_j)$$

3.4 DISCUSSION

1,2,4-triazole (Fig.15) is a five membered heterocyclic compound with N(1) and N(2) adjacent to each other but the third nitrogen atom, N(4), is separated from these two by two carbons (C(3) and C(5)). There are two possible tautomeric forms, (I) and (II) (Fig.16), for the molecule (25), the first one having perfect two fold and mirror symmetry and the second one has a pseudo two fold symmetry generated by a C_2 axis along the N(4) atom bisecting the N(1)-N(2) bond.

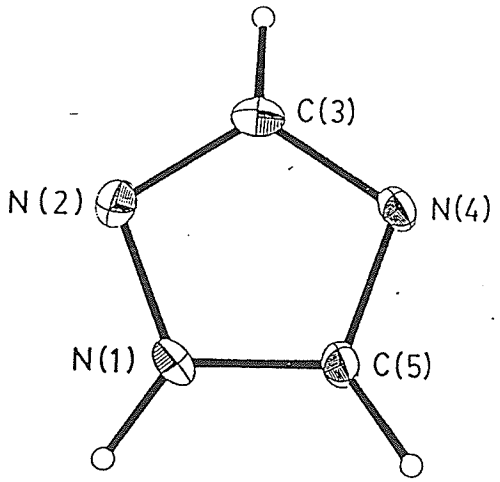


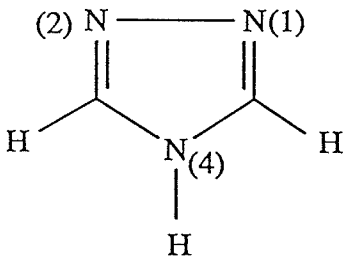
Figure 15: ORTEP view for the 1,2,4-triazole molecule. Non-hydrogen atoms are represented by thermal ellipsoids at the 50% probability level.

Since all atoms in the ring are sp^2 hybridized, the molecule is expected to be flat. Calculations show that the average deviation for ring atoms from the least-squares plane is 0.0011 Å which leads to a χ^2 value of 1.2889 sug-

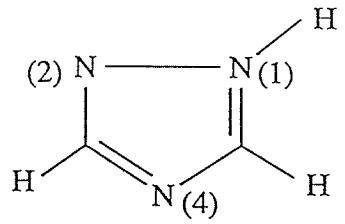
gesting that the probability of the molecule being planar is greater than 50%. H(1) and H(4) atoms are slightly below the ring plane (-0.0049 and -0.0062 Å respectively), while H(5) deviates from the plane on the opposite side by 0.0088 Å. The least-squares plane calculated by Hamilton's method (26) is given by the following equation:

$$6.0599x - 4.9477y + 0.97953z = 4.8497$$

Where x, y, z are the orthogonal coordinates, and 4.8497 is the perpendicular distance from the origin to the plane. Table 14 compares the deviation distance for each atom from the corresponding plane in different studies.



(I)



(II)

Figure 16: Tautomeric forms of 1,2,4-triazole.

Bond distances between non-hydrogen atoms in the present structure (Table 15) are not significantly different from those in the other two studies. These distances are in

TABLE 14

Comparison of deviation distance for atoms

Atom	Room T+	Low T++	Room T*
N(1)	0.0006(20)	-0.001	0.013
N(2)	0.0002(24)	0.001	-0.015
C(3)	-0.0015(29)	-0.000	-0.004
N(4)	0.0012(21)	-0.000	-0.011
C(5)	-0.0019(27)	0.000	-0.015
H(1)	-0.0049	-0.002	
H(3)	-0.0062	-0.018	
H(5)	0.0088	-0.038	

+ Present structure.
++ Structure studied at -160° by Goldstein.
* Room temperature structure studied by Deuschl.

agreement with the theoretical bond lengths calculated based upon the five possible resonance forms (Fig.17) of the molecule in its ground state (25). The C-H bond lengths in the present structure are similar to those found by Goldstein but the N-H bond distance is different (where the difference is 0.09 Å). However, since the H(1) atom is placed in a calculated position with an arbitrary length in the current study, the comparison of the N-H length is not meaningful.

The comparison of bond angles in Table 16 shows that the corresponding angles in the present structure do not differ by lowering the temperature. However, the structure studied by Deuschl at the room temperature shows poor agreement with the present study and that of Goldstein's. Bond angles involving hydrogen atoms in the present and low temperature

TABLE 15

Comparison of bond lengths (Å) at room, low temperatures and calculated values

Bond	Room T+	Room T++	Low T*	Cal.**
N(1)-N(2)	1.353(3)	1.354(14)	1.359(3)	1.359
N(2)-C(3)	1.317(3)	1.330(14)	1.323(3)	1.325
C(3)-N(4)	1.352(3)	1.353(14)	1.359(3)	1.359
N(4)-C(5)	1.351(3)	1.352(14)	1.324(3)	1.325
N(1)-C(5)	1.319(3)	1.344(14)	1.331(3)	1.332
N(1)-H(1)	0.941(2)		1.03(2)	
C(3)-H(3)	1.01(3)		0.93(2)	
C(5)-H(5)	0.96(3)		0.93(2)	

+ Present study.
++ Based on Deuschl's results.
* Based on Goldstein's results.
** Calculated bond lengths.

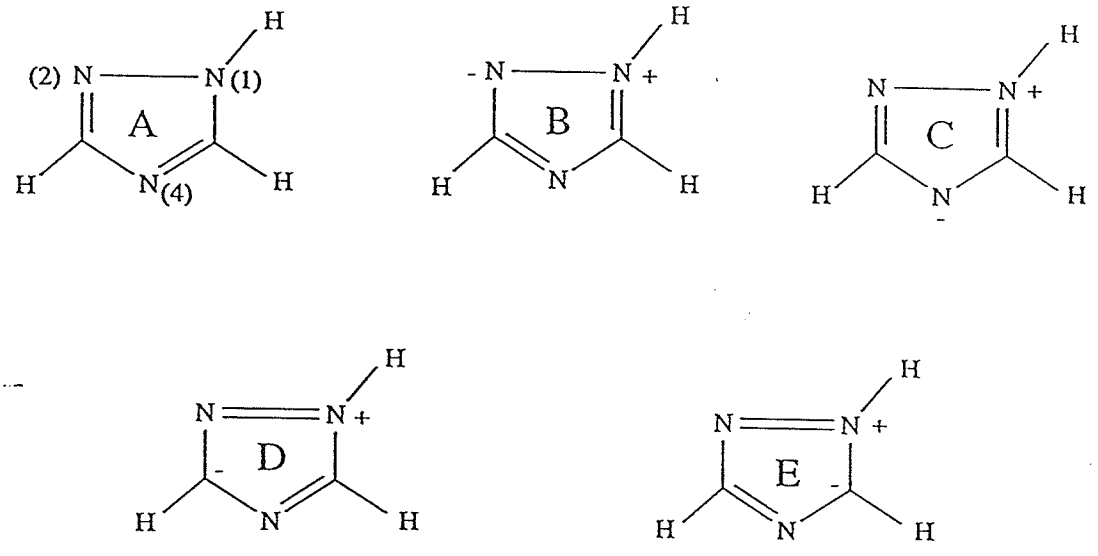


Figure 17: Resonance forms of 1,2,4-triazole.

studies are basically the same except for the N(2)-C(3)-H(3) angle where the value found in the present study is 7° larger. The angle obtained in the current study is closer to the theoretical sp^2 bond angle 120°. However, the comparison of bond lengths and angles shows that the molecule studied in the present case has the identical structure to the one studied at low temperature.

TABLE 16

Comparison of bond angles (deg) at different temperatures

Angle	Room T+	Room T++	Low T*
N(1)-N(2)-C(3)	101.8(2)	101.8(9)	102.1(2)
N(2)-C(3)-N(4)	114.7(2)	114.5(9)	114.6(2)
C(3)-N(4)-C(5)	102.7(2)	104.3(9)	103.0(2)
N(4)-C(5)-N(1)	110.3(2)	107.1(9)	110.1(2)
C(5)-N(1)-N(2)	110.4(2)	112.2(9)	110.2(2)
N(2)-N(1)-H(1)	124.0(2)		124.0(14)
C(5)-N(1)-H(1)	125.6(2)		126.0(14)
N(2)-C(3)-H(3)	121.0(2)		114.0(14)
N(4)-C(3)-H(3)	125(2)		132.0(14)
N(1)-C(5)-H(5)	126.0(15)		123.0(14)
N(4)-C(5)-H(5)	123.7(15)		127.0(14)

+ Present study.
++ Based on Deuschl's results.
* Based on Goldstein's results.

The negative charge on N(2) and N(4) in resonance forms B and C suggest they should be stabilized by hydrogen bonds. In the present study, a N-H...N intermolecular hydrogen bond is found between the N(1) and N(4) atoms

(x,y,z,1.5-x,y,0.5+z) with a distance of 2.836(3) Å between the nitrogen atoms and the angle, N(1)-H(1)...N(4), is 161.6(1)°. These values are slightly larger than those reported by Goldstein (2.821 Å and 160.5° respectively). In 1959, W. Fuller did a survey of the hydrogen bond lengths and angles observed in crystals (27). Compared to the shortest distance between the donor and the acceptor in an N-H...N hydrogen bond reported by Fuller (2.88 Å), the distance between the N(1) and N(4) in the present study is even shorter by 0.04 Å. This short distance in the present structure indicates a large residual positive charge on N(1) (resonance forms B to E in Fig.17), which makes this atom a better hydrogen donor. The strength of this hydrogen bond is considered to be a major factor contributing to the observed molecular packing in the crystal.

There is a strong van der Waals interaction between atom H(5) and N(2) (x,y,z,1.5-x,-0.5+y,1-z) since their separation (2.014(24) Å) is 0.736 Å shorter than the van der Waals radii sum of a hydrogen and nitrogen atom (2.75 Å) (28). The distance between the C(5) and N(2) atoms in the present structure is 3.335(3) Å. Goldstein had classified this as a weak hydrogen bond but C-H...N hydrogen bonding is very rare, for a carbon atom is not a good hydrogen donor, even though nitrogen acts as a good acceptor. The earliest C-H...N hydrogen bond was reported in 1951 by Dulmage and Lipscomb (29) in the study of hydrogen cyanide crystal structure where they found the separation between the donor

and acceptor is 3.18 Å at both -80 ° and -120°. This distance is noticeably smaller than the van der Waals radii sum of a carbon and nitrogen atom (3.40 Å). Considering the C-H...N interaction in both hydrogen cyanide and triazole crystals, they should be quite different because in the first case the triple bonded nitrogen which is more electronegative than the carbon attracts the electron cloud. Therefore, the nitrogen atom becomes slightly more negative and leaves the carbon atom more positive, hence, a better hydrogen donor:

$$H-C^{+\delta} \equiv N^{-\delta}$$

In the second case, C(5) is a poor hydrogen donor since the adjacent nitrogen, N(1), has a greater chance of being positively charged (as shown in the resonance forms). Therefore, this carbon will not easily participate in a hydrogen bonding interaction. Although the interaction between the N(2) and C(5) can not be considered a classical hydrogen bond, the close contact nevertheless, does suggest a stronger than normal van der Waals attraction, thus contributing to the overall packing energy.

Viewing the unit cell from the a direction (Fig.18), molecules are seen lined up in infinite chains in the direction [011] approximately diagonal to the cell. Careful examination of each chain shows that each individual molecule is related to the adjacent one by screw axes parallel to c but the relationship to the one in the next chain is by a c

glide operation. The intermolecular N-H...N hydrogen bond can be best visualized from this view (Fig.19) where the strong hydrogen bond connects the c glide symmetry related molecules to form extensive undulating chains. Crystal packing is even more striking looking from the c direction (Fig.20), where only the edge of the five membered ring is observed. Molecules in the chain are in a zig-zag arrangement with a dihedral angle between ring planes of 65.10°. The wavy pattern also arises from the large tilt (dihedral angle of 63.82°) between adjacent molecules which are joined by the strong van der Waals interaction and related by the b screw axes (Fig.21). These wave-like chains extend along the b and c axes forming a 3-d network throughout the entire crystal.

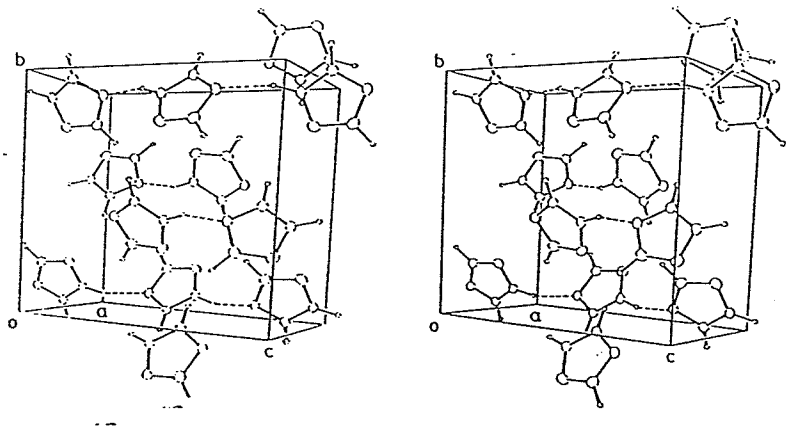


Figure 18: Stereo diagram of the molecular packing of the unit cell viewed approximately down a.

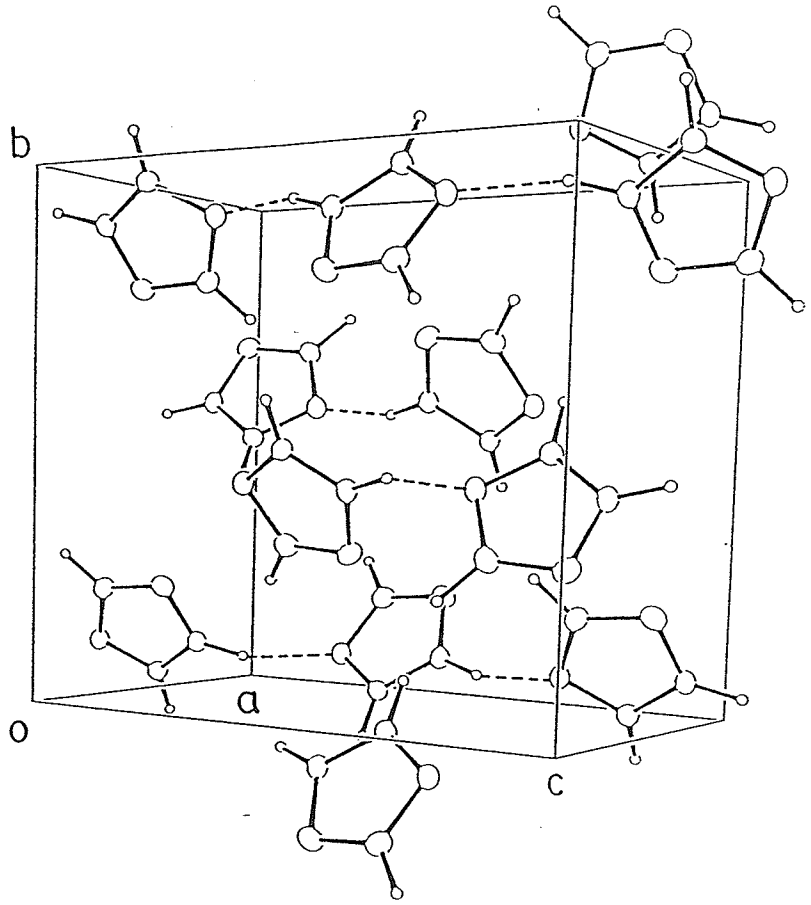


Figure 19: H-bonding molecules in the unit cell viewed approximately down a.

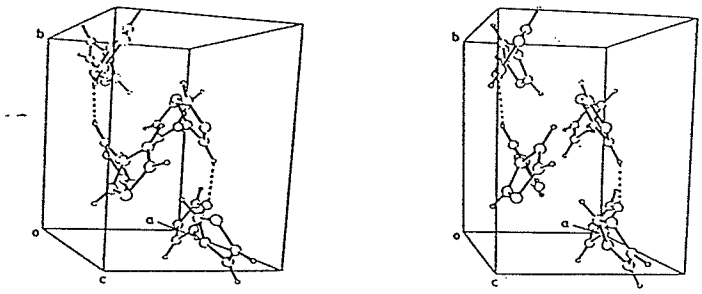


Figure 20: Stereo diagram of the molecular packing of the unit cell viewed approximately down c.

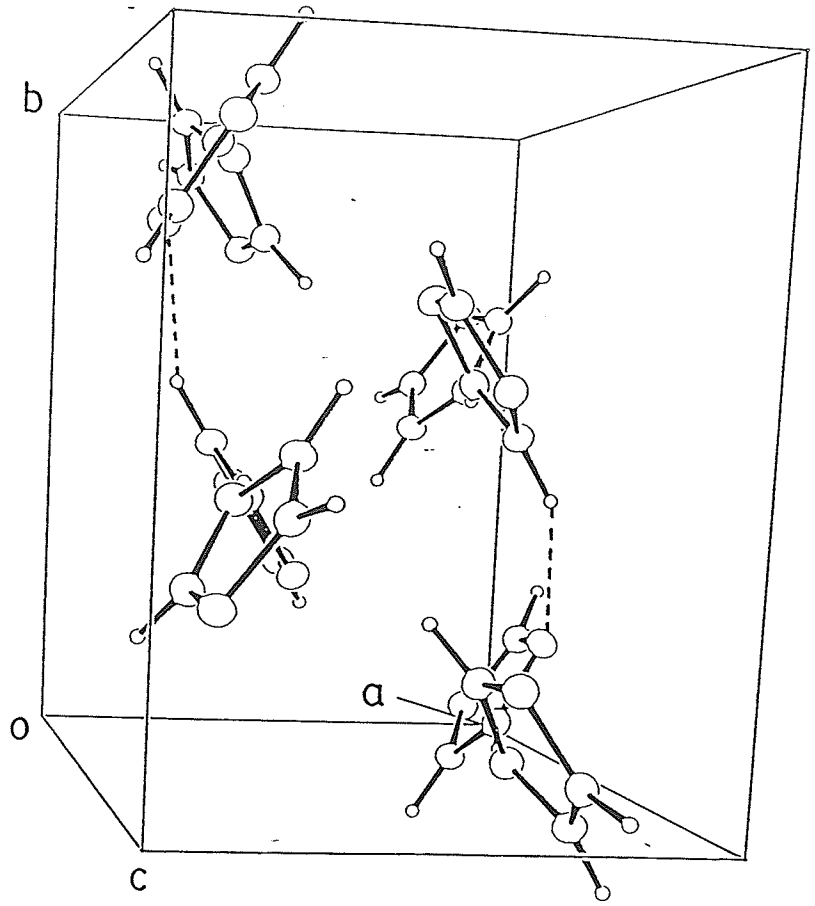


Figure 21: Van der Waals interaction between molecules in the unit cell viewed approximately down c.

3.5 SUMMARY

Unlike the information provided by the ^1H NMR study which was misleading, the structural study by x-ray diffraction methods showed conclusively that the crystal sample was none other than the regenerated reagent, 1,2,4-triazole, from the synthesis of O^4-n-butyl-thymidine. The redetermination of the crystal and molecular structures for 1,2,4-triazole at room temperature revealed that the molecule has the same conformation at both room and low temperatures (-160°). The

crystal packing is dominated by the intermolecular hydrogen bonding along the c direction in the unit cell.

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Appendix A

STRUCTURE FACTORS FOR THE 4-DEMETHOXYTHIODAUNOMYCINONE DERIVATIVE

* denotes weak reflection.

H	K	L	FO	FC
1-12	0		10.69	11.24
1-11	0		5.07	4.31
2-11	0		0.80*	1.23
3-11	0		3.26	3.11
1-10	0		2.84	4.10
2-10	0		0.77*	1.29
3-10	0		3.36	2.87
4-10	0		3.07	4.04
1 -9	0		7.77	7.32
2 -9	0		8.38	9.48
3 -9	0		4.49	3.13
4 -9	0		2.04*	1.11
5 -9	0		2.38*	2.62
1 -8	0		9.63	10.02
2 -8	0		2.05*	1.63
3 -8	0		1.84*	1.42
4 -8	0		6.18	6.71
5 -8	0		5.95	3.96
6 -8	0		4.53	5.34
1 -7	0		2.97	2.04
2 -7	0		6.19	7.29
3 -7	0		2.16*	0.29
4 -7	0		11.52	9.74
5 -7	0		11.35	13.21
6 -7	0		6.94	6.29
7 -7	0		2.96	3.25
1 -6	0		0.98*	0.77
2 -6	0		14.91	14.26
3 -6	0		14.61	16.26
4 -6	0		3.70	2.12
5 -6	0		12.64	12.68
6 -6	0		3.71	4.54
7 -6	0		2.33*	4.04
8 -6	0		0.80*	1.31
1 -5	0		14.64	12.88
2 -5	0		10.58	10.61
3 -5	0		4.52	5.64
4 -5	0		6.70	6.70
5 -5	0		13.60	14.90
6 -5	0		11.23	9.87
7 -5	0		8.72	10.26
8 -5	0		2.11*	0.81
9 -5	0		2.21*	0.95
1 -4	0		61.80	61.08
2 -4	0		32.72	31.61
3 -4	0		4.04	4.01
4 -4	0		8.70	8.94
5 -4	0		15.45	13.93
6 -4	0		12.69	14.56
7 -4	0		7.07	6.64
8 -4	0		6.84	7.55
9 -4	0		8.19	8.64
1 -3	0		44.71	45.81
2 -3	0		22.85	19.03
3 -3	0		33.50	34.40
4 -3	0		24.99	24.54
5 -3	0		1.25*	1.00
6 -3	0		10.55	10.99
7 -3	0		10.23	9.88
8 -3	0		2.40*	1.85
9 -3	0		3.31	2.01
10 -3	0		4.16	4.36
1 -2	0		30.22	28.63
2 -2	0		16.34	14.87
3 -2	0		1.51*	4.42
4 -2	0		21.33	22.61
5 -2	0		24.15	22.71
6 -2	0		15.10	15.84
7 -2	0		4.82	4.05
8 -2	0		5.48	6.56
9 -2	0		0.78*	0.39
10 -2	0		2.38*	1.30
1 -1	0		13.62	13.56
2 -1	0		46.44	49.97
3 -1	0		30.68	24.34
4 -1	0		36.75	37.33
5 -1	0		15.74	14.83
6 -1	0		10.11	9.45
7 -1	0		15.56	15.52
8 -1	0		3.36	2.85
9 -1	0		4.55	3.99
10 -1	0		1.79*	2.17
1 0	0		33.84	36.80
2 0	0		8.33	7.12
3 0	0		4.84	5.16
4 0	0		3.33	1.60
5 0	0		30.68	30.61
6 0	0		16.97	16.09
7 0	0		5.12	5.13
8 0	0		5.14	5.49
9 0	0		6.55	6.47
10 0	0		0.80*	0.16
0 1	0		27.79	49.25
1 1	0		11.27	14.55
2 1	0		134.49	131.04
3 1	0		51.69	47.67
4 1	0		5.84	4.54
5 1	0		18.27	19.68
6 1	0		26.36	28.86
7 1	0		6.70	6.13
8 1	0		0.74*	1.31
9 1	0		0.77*	0.12
10 1	0		3.08	3.34
11 1	0		3.71	3.31
0 2	0		69.30	61.92
1 2	0		18.05	13.71
2 2	0		30.65	29.94
3 2	0		45.05	44.94
4 2	0		22.92	21.54
5 2	0		41.68	41.07
6 2	0		20.77	19.18
7 2	0		7.11	6.46
8 2	0		6.01	6.52
9 2	0		8.54	8.19
10 2	0		5.09	4.91
11 2	0		4.21	4.47
0 3	0		38.18	34.97
1 3	0		24.08	25.35
2 3	0		5.02	1.63
3 3	0		37.27	35.85
4 3	0		13.36	11.77
5 3	0		16.61	14.99
6 3	0		19.23	19.67
7 3	0		8.69	8.22
8 3	0		6.59	6.82
9 3	0		10.24	9.62
10 3	0		5.96	6.06
11 3	0		0.82*	0.19
0 4	0		47.37	45.87
1 4	0		36.33	34.38
2 4	0		38.23	36.35
3 4	0		20.20	19.01
4 4	0		13.07	13.78
5 4	0		13.11	12.85
6 4	0		3.79	4.04
7 4	0		4.79	3.55
8 4	0		12.45	13.49
9 4	0		9.75	10.33
10 4	0		6.57	6.68
11 4	0		5.31	5.66
0 5	0		30.48	31.43
1 5	0		29.37	31.18
2 5	0		7.58	5.00
3 5	0		22.89	22.15
4 5	0		9.67	8.79
5 5	0		1.97*	3.10
6 5	0		9.99	9.27
7 5	0		19.63	19.15
8 5	0		10.36	11.33
9 5	0		6.04	5.72
10 5	0		5.99	5.68
11 5	0		6.07	6.57
0 6	0		35.02	33.59
1 6	0		37.01	34.29
2 6	0		10.42	11.29
3 6	0		19.99	18.59
4 6	0		4.09	4.77
5 6	0		10.38	8.87
6 6	0		10.82	10.60
7 6	0		2.31*	1.00
8 6	0		0.74*	0.11
9 6	0		8.18	8.20
10 6	0		5.68	5.36
11 6	0		2.14*	2.73
0 7	0		35.88	34.85
1 7	0		10.86	10.60
2 7	0		1.38*	0.35
3 7	0		30.58	29.65
4 7	0		17.93	17.51
5 7	0		23.65	22.46
6 7	0		0.74*	1.73
7 7	0		18.13	19.30
8 7	0		5.13	5.14
9 7	0		0.78*	1.39
10 7	0		1.71*	1.15
0 8	0		35.23	34.23
1 8	0		1.55*	0.50
2 8	0		1.79*	0.87
3 8	0		16.44	17.48
4 8	0		16.99	17.15
5 8	0		34.00	33.79
6 8	0		22.91	23.82
7 8	0		6.85	5.31
8 8	0		0.78*	1.29
9 8	0		4.60	4.95
10 8	0		1.96*	1.40
0 9	0		3.75	4.31
1 9	0		33.56	33.10
2 9	0		57.10	57.49
3 9	0		14.53	13.69
4 9	0		5.95	5.39
5 9	0		13.85	14.62
6 9	0		11.22	12.03
7 9	0		15.35	13.67
8 9	0		8.68	10.52
9 9	0		7.71	6.44
0 10	0		6.29	5.49
1 10	0		3.19	2.55
2 10	0		17.21	17.40
3 10	0		20.88	21.38
4 10	0		31.66	31.12
5 10	0		18.40	18.72
6 10	0		3.76	3.65
7 10	0		4.67	4.13
8 10	0		3.07	2.88
9 10	0		0.83*	1.11
0 11	0		2.24*	0.68
1 11	0		8.72	8.30
2 11	0		0.75*	0.52
3 11	0		0.77*	1.88
4 11	0		6.72	6.33
5 11	0		9.95	10.63
6 11	0		10.84	11.02
7 11	0		9.87	10.11
8 11	0		5.71	6.01
0 12	0		7.36	7.29
1 12	0		5.29	5.48
2 12	0		4.70	5.24
3 12	0		1.48*	1.33
4 12	0		1.61*	1.87
5 12	0		1.81*	1.14
6 12	0		3.16	3.96
-5-12	1		3.13	1.87
-4-12	1		6.87	6.60
-3-12	1		12.23	11.76
-2-12	1		1.72*	2.65
-1-12	1		10.31	10.26
0-12	1		15.74	15.20
-7-11	1		8.97	8.93
-6-11	1		7.27	7.94
-5-11	1		8.55	8.44
-4-11	1		6.64	6.25
-3-11	1		7.68	7.00
-2-11	1		5.94	5.69
-1-11	1		7.37	8.13
0-11	1		1.38*	0.15
1-11	1		1.43*	1.22
2-11	1		8.05	8.03
3-11	1		9.62	8.62
-8-10	1		7.38	7.59
-7-10	1		8.53	9.17
-6-10	1		13.60	12.80
-5-10	1		7.21	7.48
-4-10	1		1.71*	0.45
-3-10	1		2.91	2.81
-2-10	1		14.25	13.86
-1-10	1		0.74*	1.84
0-10	1		7.62	7.92
1-10	1		10.92	10.02
2-10	1		6.18	7.11
3-10	1		4.80	3.75
4-10	1		0.80*	1.22
-9 -9	1		3.23	2.17
-8 -9	1		3.92	2.90
-7 -9	1		7.14	6.14
-6 -9	1		9.42	9.08
-5 -9	1		9.63	10.10
-4 -9	1		5.40	4.73
-3 -9	1		19.78	20.22
-2 -9	1		31.93	32.17
-1 -9	1		9.61	10.01
0 -9	1		18.55	19.20
1 -9	1		0.73*	0.37
2 -9	1		2.33*	0.76
3 -9	1		7.70	8.82
4 -9	1		0.78*	0.93
5 -9	1		4.00	3.96
-10 -8	1		4.73	6.10
-9 -8	1		15.69	14.36
-8 -8	1		15.90	16.33
-7 -8	1		13.54	14.46
-6 -8	1		10.89	10.72
-5 -8	1		8.23	8.65
-4 -8	1		8.38	8.06
-3 -8	1		18.89	19.50
-2 -8	1		8.35	7.35
-1 -8	1		2.85	1.47
0 -8	1		44.55	43.53
1 -8	1		6.04	5.28
2 -8	1		17.73	17.23
3 -8	1		3.53	3.06
4 -8	1		4.99	4.06
5 -8	1		12.04	13.63
6 -8	1		9.42	7.53
-10 -7	1		1.94*	2.64
-9 -7	1		6.21	4.90
-8 -7	1		3.55	5.31
-7 -7	1		18.56	17.13
-6 -7	1		5.38	5.70
-5 -7	1		1.45*	1.48

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-4	-7	1	6.15	5.59	-4	-4	1	23.13	22.18	-10	-1	1	6.12	5.40	7	1	1	13.07	14.68	1	4	1	37.65	36.83
-3	-7	1	24.16	24.94	-3	-4	1	23.02	22.84	-9	-1	1	10.00	9.80	8	1	1	12.24	12.18	2	4	1	56.92	55.86
-2	-7	1	26.10	25.39	-2	-4	1	19.97	20.52	-8	-1	1	6.79	7.11	9	1	1	3.50	3.72	3	4	1	12.73	11.77
-1	-7	1	11.22	12.09	-1	-4	1	26.78	27.76	-7	-1	1	18.04	18.97	10	1	1	1.30*	0.99	4	4	1	35.26	32.30
0	-7	1	11.01	10.40	0	-4	1	21.57	18.85	-6	-1	1	18.04	16.19	11	1	1	1.86*	1.31	5	4	1	10.16	11.57
1	-7	1	17.93	18.11	1	-4	1	8.16	8.66	-5	-1	1	46.96	46.36	-10	2	1	4.48	4.52	6	4	1	11.79	11.90
2	-7	1	13.93	14.41	2	-4	1	1.85*	0.38	-4	-1	1	22.48	21.11	-9	2	1	2.58	3.36	7	4	1	7.85	7.35
3	-7	1	13.30	11.88	3	-4	1	12.88	12.05	-3	-1	1	12.09	11.69	-8	2	1	4.63	5.66	8	4	1	9.16	9.45
4	-7	1	1.22*	1.75	4	-4	1	7.38	5.79	-2	-1	1	54.53	50.56	-7	2	1	14.44	15.44	9	4	1	7.56	6.75
5	-7	1	0.75*	3.47	5	-4	1	3.35	5.20	-1	-1	1	43.33	39.87	-6	2	1	23.22	22.62	10	4	1	9.94	8.79
6	-7	1	6.44	6.34	6	-4	1	23.66	22.15	0	-1	1	57.36	57.34	-5	2	1	23.95	23.79	11	4	1	3.63	4.44
7	-7	1	7.17	6.93	7	-4	1	3.07	3.73	1	-1	1	33.99	31.67	-4	2	1	18.61	20.42	-9	5	1	3.51	2.72
-10	-6	1	1.50*	1.54	8	-4	1	1.92*	1.01	2	-1	1	49.76	52.71	-3	2	1	12.38	9.87	-8	5	1	3.67	4.08
-9	-6	1	2.84	2.52	9	-4	1	7.21	6.45	3	-1	1	6.43	10.22	-2	2	1	33.41	33.14	-7	5	1	7.22	6.86
-8	-6	1	3.07	3.59	-11	-3	1	2.58*	2.39	4	-1	1	4.23	5.29	-1	2	1	38.41	41.49	-6	5	1	10.15	10.96
-7	-6	1	0.74*	2.23	-10	-3	1	6.11	5.17	5	-1	1	17.05	16.19	0	2	1	34.06	28.95	-5	5	1	6.29	4.72
-6	-6	1	19.01	17.44	-9	-3	1	2.92	3.50	6	-1	1	4.84	5.05	1	2	1	6.99	10.33	-4	5	1	18.06	19.52
-5	-6	1	27.70	26.53	-8	-3	1	0.74*	0.05	7	-1	1	20.16	19.66	2	2	1	58.00	53.97	-3	5	1	2.83	2.54
-4	-6	1	22.68	22.08	-7	-3	1	10.11	11.27	8	-1	1	8.21	8.96	3	2	1	15.16	17.43	-2	5	1	8.40	8.04
-3	-6	1	13.61	14.65	-6	-3	1	16.58	15.18	9	-1	1	2.75	3.07	4	2	1	67.11	65.89	-1	5	1	24.43	21.96
-2	-6	1	5.94	4.11	-5	-3	1	1.08*	0.39	10	-1	1	2.33*	1.32	5	2	1	6.26	5.86	0	5	1	8.74	10.76
-1	-6	1	19.13	19.68	-4	-3	1	16.14	14.61	-10	0	1	1.28*	1.59	6	2	1	8.64	8.87	1	5	1	18.65	20.82
0	-6	1	31.30	28.59	-3	-3	1	33.68	30.82	-9	0	1	8.39	8.11	7	2	1	1.91*	2.22	2	5	1	51.27	50.36
1	-6	1	15.39	15.28	-2	-3	1	81.31	82.85	-8	0	1	5.89	6.43	8	2	1	1.70*	2.11	3	5	1	1.82*	2.22
2	-6	1	6.19	6.06	-1	-3	1	2.36	3.18	-7	0	1	4.74	4.25	9	2	1	13.76	14.27	4	5	1	4.14	3.38
3	-6	1	3.40	1.94	0	-3	1	48.33	48.93	-6	0	1	20.17	19.66	10	2	1	0.79*	0.37	5	5	1	38.72	38.42
4	-6	1	7.08	7.49	1	-3	1	48.02	42.98	-5	0	1	22.98	23.15	11	2	1	2.06*	0.24	6	5	1	13.17	13.67
5	-6	1	1.55*	1.78	2	-3	1	56.96	61.11	-4	0	1	27.03	28.65	-9	3	1	0.79*	1.82	7	5	1	10.82	10.97
6	-6	1	8.15	8.70	3	-3	1	17.82	19.82	-3	0	1	66.07	65.78	-8	3	1	7.67	7.94	8	5	1	15.59	14.98
7	-6	1	4.39	4.31	4	-3	1	1.66*	2.41	-2	0	1	69.50	68.02	-7	3	1	2.52	1.97	9	5	1	1.50*	1.31
8	-6	1	2.52*	2.11	5	-3	1	23.33	23.03	-1	0	1	20.95	17.94	-6	3	1	2.60	1.59	10	5	1	1.47*	1.62
-11	-5	1	3.01	3.51	6	-3	1	6.53	5.20	1	0	1	25.96	26.20	-5	3	1	4.77	5.54	11	5	1	1.74*	1.78
-10	-5	1	8.28	7.80	7	-3	1	9.64	11.00	2	0	1	97.78	99.52	-4	3	1	34.54	33.44	-8	6	1	2.29*	1.37
-9	-5	1	6.65	6.63	8	-3	1	5.84	5.12	3	0	1	81.00	79.20	-3	3	1	45.63	41.12	-7	6	1	0.79*	0.80
-8	-5	1	4.07	3.15	9	-3	1	4.18	5.41	4	0	1	26.88	25.88	-2	3	1	43.48	37.10	-6	6	1	5.43	5.90
-7	-5	1	16.49	16.28	-11	-2	1	7.48	6.95	5	0	1	8.53	9.71	-1	3	1	13.03	16.77	-5	6	1	6.89	6.82
-6	-5	1	1.60*	1.99	-10	-2	1	1.45*	0.86	6	0	1	7.50	7.99	0	3	1	20.64	20.97	-4	6	1	2.84	3.34
-5	-5	1	29.18	27.03	-9	-2	1	2.38*	2.15	7	0	1	1.43*	0.94	1	3	1	2.31	5.76	-3	6	1	5.67	4.12
-4	-5	1	2.73	1.14	-8	-2	1	9.77	9.54	8	0	1	12.26	12.41	2	3	1	23.10	25.86	-2	6	1	4.43	4.68
-3	-5	1	0.59*	1.36	-7	-2	1	33.15	32.77	9	0	1	7.36	7.35	3	3	1	3.27	4.48	-1	6	1	15.93	17.47
-2	-5	1	3.32	2.75	-6	-2	1	21.40	22.17	10	0	1	6.85	7.46	4	3	1	7.51	5.08	0	6	1	23.71	21.34
-1	-5	1	12.21	13.06	-5	-2	1	12.78	13.56	-10	1	1	5.31	4.71	5	3	1	0.62*	1.04	1	6	1	1.48*	2.36
0	-5	1	31.93	32.58	-4	-2	1	32.97	31.54	-9	1	1	8.02	8.39	6	3	1	28.41	29.52	2	6	1	14.18	12.79
1	-5	1	26.38	24.17	-3	-2	1	29.11	28.39	-8	1	1	9.14	9.59	7	3	1	10.78	8.89	3	6	1	24.48	24.29
2	-5	1	11.85	11.68	-2	-2	1	45.38	43.19	-7	1	1	24.76	25.62	8	3	1	9.40	9.87	4	6	1	10.52	10.70
3	-5	1	21.22	21.78	-1	-2	1	6.84	1.67	-6	1	1	21.18	20.37	9	3	1	7.86	7.86	5	6	1	21.73	20.29
4	-5	1	8.57	9.50	0	-2	1	51.77	54.83	-5	1	1	17.56	17.41	10	3	1	2.52	1.40	6	6	1	6.84	7.82
5	-5	1	5.61	4.30	1	-2	1	52.63	52.54	-4	1	1	0.59*	3.12	11	3	1	3.33	3.02	7	6	1	33.04	32.63
6	-5	1	12.84	14.08	2	-2	1	8.70	8.15	-3	1	1	25.37	21.55	-9	4	1	2.57*	3.22	8	6	1	2.30*	1.88
7	-5	1	6.55	5.20	3	-2	1	9.56	11.37	-2	1	1	114.23	115.42	-8	4	1	1.21*	0.93	9	6	1	11.06	11.16
8	-5	1	2.08*	0.08	4	-2	1	19.95	21.33	-1	1	1	0.47*	1.33	-7	4	1	6.25	7.78	10	6	1	5.63	5.17
-11	-4	1	1.95*	1.93	5	-2	1	26.98	27.32	0	1	1	28.45	27.45	-6	4	1	0.74*	2.22	11	6	1	2.49*	1.81
-10	-4	1	3.30	2.78	6	-2	1	24.67	22.42	1	1	1	41.95	35.85	-5	4	1	2.19*	2.87	-7	7	1	2.41*	2.43
-9	-4	1	1.09*	0.66	7	-2	1	5.82	3.52	2	1	1	120.43	118.56	-4	4	1	15.02	14.18	-6	7	1	3.97	5.95
-8	-4	1	10.72	10.55	8	-2	1	13.41	12.13	3	1	1	2.88	1.21	-3	4	1	25.54	23.00	-5	7	1	11.91	10.88
-7	-4	1	5.52	6.83	9	-2	1	1.25*	0.51	4	1	1	13.84	14.28	-2	4	1	62.13	55.88	-4	7	1	4.94	6.16
-6	-4	1	20.17	19.79	10	-2	1	4.75	4.67	5	1	1	8.98	6.91	-1	4	1	44.22	42.10	-3	7	1	16.10	16.64
-5	-4	1	5.14	3.70	-11	-1	1	3.27	2.96	6	1	1	1.94*	2.09	0	4	1	7.81	8.87	-2	7	1	22.36	21.60

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-1	7	1	18.36	17.63	8	10	1	2.60	3.08	-4	-9	2	3.89	2.97	4	-6	2	20.29	21.27	4	-3	2	19.89	19.28
0	7	1	27.07	26.95	9	10	1	1.89*	1.72	-3	-9	2	2.55	2.03	5	-6	2	0.74*	0.22	5	-3	2	15.73	15.83
1	7	1	21.12	21.30	-3	11	1	8.85	8.33	-2	-9	2	3.09	2.95	6	-6	2	2.10*	1.73	6	-3	2	9.56	10.04
2	7	1	19.75	18.45	-2	11	1	0.80*	0.46	-1	-9	2	16.76	16.24	7	-6	2	5.29	5.94	7	-3	2	4.33	5.84
3	7	1	4.34	5.65	-1	11	1	0.79*	2.68	0	-9	2	8.98	8.57	8	-6	2	3.65	4.07	8	-3	2	1.50*	1.66
4	7	1	9.69	10.07	0	11	1	3.06	3.33	1	-9	2	6.24	5.69	-10	-5	2	1.67*	1.25	9	-3	2	0.79*	1.18
5	7	1	25.81	25.59	1	11	1	15.25	14.10	2	-9	2	13.37	13.88	-9	-5	2	6.01	5.86	-10	-2	2	5.08	4.32
6	7	1	4.68	4.71	2	11	1	16.78	16.74	3	-9	2	3.45	2.66	-8	-5	2	1.80*	0.45	-9	-2	2	6.73	7.25
7	7	1	17.59	17.53	3	11	1	3.24	2.00	4	-9	2	0.78*	0.20	-7	-5	2	3.89	4.45	-8	-2	2	2.44	3.14
8	7	1	5.90	6.78	4	11	1	16.68	17.31	5	-9	2	4.85	4.30	-6	-5	2	18.99	16.99	-7	-2	2	20.38	18.90
9	7	1	0.78*	1.82	5	11	1	11.96	12.18	-9	-8	2	1.43*	2.78	-5	-5	2	5.85	4.00	-6	-2	2	5.06	4.29
10	7	1	2.75	2.63	6	11	1	13.08	13.30	-8	-8	2	2.24*	1.71	-4	-5	2	2.79	2.32	-5	-2	2	4.97	4.73
-6	8	1	9.58	8.94	7	11	1	5.52	5.57	-7	-8	2	3.46	2.85	-3	-5	2	40.95	38.64	-4	-2	2	30.55	28.16
-5	8	1	4.48	4.30	8	11	1	5.03	4.81	-6	-8	2	7.91	7.46	-2	-5	2	6.44	6.09	-3	-2	2	5.32	2.99
-4	8	1	12.45	12.75	-1	12	1	5.58	5.14	-5	-8	2	16.49	16.49	-1	-5	2	28.29	29.13	-2	-2	2	54.55	53.11
-3	8	1	18.74	18.24	0	12	1	2.62	2.72	-4	-8	2	1.69*	1.71	0	-5	2	19.63	17.71	-1	-2	2	13.52	14.65
-2	8	1	7.41	7.85	1	12	1	2.67	1.99	-3	-8	2	14.73	15.90	1	-5	2	30.09	30.13	0	-2	2	68.42	64.60
-1	8	1	14.11	13.22	2	12	1	2.30*	0.05	-2	-8	2	10.52	11.30	2	-5	2	35.81	35.18	1	-2	2	6.75	6.78
0	8	1	0.70*	0.73	3	12	1	3.66	3.31	-1	-8	2	17.19	16.78	3	-5	2	4.73	3.60	2	-2	2	42.04	39.99
1	8	1	11.61	10.57	4	12	1	8.65	7.85	0	-8	2	20.22	21.11	4	-5	2	4.79	6.04	3	-2	2	18.17	19.23
2	8	1	20.83	20.95	5	12	1	3.26	3.86	1	-8	2	13.37	13.21	5	-5	2	1.90*	3.25	4	-2	2	16.53	17.18
3	8	1	1.79*	2.46	6	12	1	1.16*	2.09	2	-8	2	6.50	6.94	6	-5	2	6.00	4.44	5	-2	2	5.95	5.30
4	8	1	14.64	14.06	7	12	1	7.46	7.84	3	-8	2	3.02	2.74	7	-5	2	4.28	5.15	6	-2	2	17.74	19.49
5	8	1	11.43	11.59	2	13	1	5.47	5.34	4	-8	2	5.56	6.73	8	-5	2	2.64	2.49	7	-2	2	18.44	19.93
6	8	1	2.54	2.37	3	13	1	7.12	6.31	5	-8	2	10.45	9.48	-10	-4	2	2.55*	2.29	8	-2	2	5.11	6.28
7	8	1	4.35	4.81	4	13	1	3.45	3.35	6	-8	2	6.73	7.23	-9	-4	2	4.53	4.65	9	-2	2	0.78*	0.11
8	8	1	2.75	2.81	-4	12	2	0.82*	0.45	-10	-7	2	8.92	8.17	-8	-4	2	2.80	3.22	10	-2	2	3.21	2.67
9	8	1	9.40	8.46	-3	12	2	10.43	9.95	-9	-7	2	6.15	7.32	-7	-4	2	31.49	29.21	-10	-1	2	2.83	3.00
10	8	1	1.89*	0.22	-2	12	2	6.01	5.94	-8	-7	2	12.83	11.57	-6	-4	2	26.59	27.66	-9	-1	2	16.51	17.27
-6	9	1	2.84	1.86	-1	12	2	7.33	7.87	-7	-7	2	6.09	7.91	-5	-4	2	27.27	24.67	-8	-1	2	6.07	6.74
-5	9	1	1.45*	1.30	-7	11	2	0.82*	0.23	-6	-7	2	19.30	18.90	-4	-4	2	4.05	2.41	-7	-1	2	4.29	3.77
-4	9	1	12.50	11.46	-6	11	2	5.26	5.52	-5	-7	2	6.20	7.24	-3	-4	2	53.67	52.45	-6	-1	2	17.60	18.10
-3	9	1	15.56	16.19	-5	11	2	2.26*	2.09	-4	-7	2	14.38	13.83	-2	-4	2	25.02	23.84	-5	-1	2	16.82	16.01
-2	9	1	13.55	12.95	-4	11	2	0.78*	0.76	-3	-7	2	8.52	8.27	-1	-4	2	34.77	33.67	-4	-1	2	9.74	10.22
-1	9	1	15.46	16.07	-3	11	2	1.92*	1.16	-2	-7	2	7.21	7.63	0	-4	2	7.12	8.91	-3	-1	2	13.27	12.71
0	9	1	22.23	21.92	-2	11	2	12.16	12.25	-1	-7	2	21.31	21.65	1	-4	2	3.85	2.87	-2	-1	2	35.77	37.58
1	9	1	14.20	14.21	-1	11	2	14.96	14.41	0	-7	2	6.64	6.68	2	-4	2	5.14	3.76	-1	-1	2	16.99	19.57
2	9	1	14.53	14.08	0	11	2	8.01	8.21	1	-7	2	7.24	7.69	3	-4	2	6.93	6.14	0	-1	2	11.75	10.67
3	9	1	15.06	15.02	1	11	2	5.81	5.59	2	-7	2	25.07	23.79	4	-4	2	15.50	16.57	1	-1	2	80.79	80.43
4	9	1	23.30	23.08	2	11	2	4.13	4.23	3	-7	2	2.79	3.93	5	-4	2	2.11*	2.49	2	-1	2	45.63	49.84
5	9	1	20.21	19.72	-8	10	2	4.67	5.15	4	-7	2	3.30	5.06	6	-4	2	9.52	10.38	3	-1	2	12.04	9.37
6	9	1	13.05	13.35	-7	10	2	12.93	11.77	5	-7	2	0.77*	1.28	7	-4	2	3.37	3.10	4	-1	2	3.81	5.67
7	9	1	6.73	7.37	-6	10	2	6.68	7.02	6	-7	2	4.38	4.32	8	-4	2	6.50	6.45	5	-1	2	15.63	15.51
8	9	1	5.73	4.12	-5	10	2	2.41*	1.37	7	-7	2	8.49	8.95	9	-4	2	6.41	7.57	6	-1	2	15.01	15.65
9	9	1	0.80*	0.83	-4	10	2	3.52	3.63	-10	-6	2	9.16	8.03	-10	-3	2	3.48	3.15	7	-1	2	14.95	14.82
10	9	1	0.83*	2.45	-3	10	2	7.95	7.85	-9	-6	2	5.37	4.25	-9	-3	2	3.17	3.30	8	-1	2	14.66	15.12
-4	10	1	2.35*	1.67	-2	10	2	8.93	9.40	-8	-6	2	5.50	5.58	-8	-3	2	1.62*	1.50	9	-1	2	0.78*	1.44
-3	10	1	0.79*	1.69	-1	10	2	13.78	14.29	-7	-6	2	9.46	8.81	-7	-3	2	1.47*	2.22	10	-1	2	0.82*	1.77
-2	10	1	8.58	8.90	0	10	2	5.84	5.74	-6	-6	2	9.38	10.70	-6	-3	2	4.84	6.28	-10	0	2	2.98	3.04
-1	10	1	22.64	22.41	1	10	2	0.75*	0.20	-5	-6	2	13.13	12.14	-5	-3	2	1.55*	0.77	-9	0	2	7.11	7.00
0	10	1	25.00	25.41	2	10	2	2.36*	1.96	-4	-6	2	4.01	4.46	-4	-3	2	15.30	15.77	-8	0	2	1.18*	1.92
1	10	1	13.65	13.39	3	10	2	1.28*	1.16	-3	-6	2	23.47	22.45	-3	-3	2	18.16	17.19	-7	0	2	18.38	18.51
2	10	1	0.73*	1.51	4	10	2	4.69	5.14	-2	-6	2	4.99	5.14	-2	-3	2	10.26	10.30	-6	0	2	25.86	27.31
3	10	1	15.56	15.42	-9	-9	2	4.49	4.72	-1	-6	2	24.37	22.64	-1	-3	2	82.22	82.03	-5	0	2	6.40	6.43
4	10	1	25.58	25.88	-8	-9	2	7.52	6.77	0	-6	2	28.08	27.97	0	-3	2	22.95	20.88	-4	0	2	16.95	17.49
5	10	1	1.56*	0.72	-7	-9	2	3.32	3.66	1	-6	2	0.67*	0.91	1	-3	2	10.64	8.59	-3	0	2	6.36	8.38
6	10	1	0.78*	1.58	-6	-9	2	3.82	3.48	2	-6	2	27.17	27.34	2	-3	2	7.17	5.66	-2	0	2	8.49	7.93
7	10	1	8.02	7.60	-5	-9	2	3.03	1.72	3	-6	2	6.93	5.24	3	-3	2	17.14	15.87	-1	0	2	52.13	49.43

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	0	2	16.13	10.93	-6	3	2	6.24	6.22	11	5	2	1.35*	2.29	-4	9	2	12.74	13.47	-4	-11	3	9.33	8.96
1	0	2	0.75*	0.63	-5	3	2	6.20	5.94	-8	6	2	1.72*	1.98	-3	9	2	3.36	1.24	-3	-11	3	6.87	6.80
2	0	2	5.76	5.21	-4	3	2	0.64*	0.18	-7	6	2	1.69*	0.09	-2	9	2	1.60*	0.12	-2	-11	3	3.37	3.25
3	0	2	38.77	38.87	-3	3	2	40.09	41.23	-6	6	2	7.06	6.61	-1	9	2	6.38	6.59	-1	-11	3	7.09	7.65
4	0	2	18.85	19.33	-2	3	2	36.46	40.48	-5	6	2	2.52	3.24	0	9	2	5.01	5.63	0	-11	3	4.35	4.28
5	0	2	3.99	2.72	-1	3	2	1.42*	3.21	-4	6	2	2.87	4.30	1	9	2	5.08	5.20	1	-11	3	2.40*	2.97
6	0	2	3.63	2.99	0	3	2	4.24	3.67	-3	6	2	12.86	13.97	2	9	2	5.84	5.49	-7	-10	3	12.05	12.37
7	0	2	4.74	3.99	1	3	2	55.94	56.32	-2	6	2	30.06	29.91	3	9	2	6.00	7.26	-6	-10	3	12.72	12.51
8	0	2	1.81*	3.12	2	3	2	1.80	0.98	-1	6	2	6.83	8.10	4	9	2	10.04	10.76	-5	-10	3	2.21*	1.64
9	0	2	11.27	12.03	3	3	2	28.58	25.92	0	6	2	36.11	35.22	5	9	2	1.90*	1.82	-4	-10	3	2.68	3.07
10	0	2	6.38	5.42	4	3	2	40.78	41.64	1	6	2	28.64	25.59	6	9	2	11.98	12.70	-3	-10	3	6.80	6.68
-10	1	2	15.83	15.23	5	3	2	34.58	33.68	2	6	2	8.46	9.10	7	9	2	8.92	7.97	-2	-10	3	3.67	3.48
-9	1	2	5.67	6.25	6	3	2	39.33	37.00	3	6	2	35.89	35.53	8	9	2	5.16	3.48	-1	-10	3	3.38	3.59
-8	1	2	5.11	5.19	7	3	2	12.34	13.60	4	6	2	2.52	1.47	9	9	2	3.65	3.00	0	-10	3	4.73	4.44
-7	1	2	3.71	2.84	8	3	2	0.73*	1.67	5	6	2	18.02	17.30	10	9	2	0.83*	0.37	1	-10	3	3.19	4.00
-6	1	2	6.41	6.33	9	3	2	3.90	3.33	6	6	2	16.33	15.18	-4	10	2	7.38	6.72	2	-10	3	5.09	4.16
-5	1	2	13.81	14.57	10	3	2	5.67	5.25	7	6	2	15.60	16.30	-3	10	2	8.78	10.06	3	-10	3	8.92	9.09
-4	1	2	26.75	25.58	11	3	2	5.72	5.26	8	6	2	4.29	4.44	-2	10	2	15.93	15.20	-8	-9	3	1.82*	0.44
-3	1	2	52.16	55.01	-9	4	2	1.70*	1.60	9	6	2	2.46	2.78	-1	10	2	7.08	7.33	-7	-9	3	1.36*	2.31
-2	1	2	27.95	33.42	-8	4	2	4.15	3.58	10	6	2	0.80*	1.65	0	10	2	8.82	8.80	-6	-9	3	4.04	3.47
-1	1	2	3.22	3.18	-7	4	2	6.84	6.40	11	6	2	0.82*	0.66	1	10	2	3.35	3.29	-5	-9	3	14.20	15.54
0	1	2	53.88	55.37	-6	4	2	5.11	4.36	-7	7	2	2.53*	2.66	2	10	2	5.33	4.97	-4	-9	3	11.74	10.95
1	1	2	30.17	26.81	-5	4	2	0.70*	0.50	-6	7	2	6.39	6.93	3	10	2	1.96*	1.31	-3	-9	3	2.87	4.00
2	1	2	114.76	110.41	-4	4	2	12.82	13.40	-5	7	2	1.36*	4.63	4	10	2	11.27	11.32	-2	-9	3	4.07	3.19
3	1	2	14.05	11.86	-3	4	2	4.00	4.60	-4	7	2	1.60*	0.46	5	10	2	8.33	8.46	-1	-9	3	12.48	12.85
4	1	2	33.02	27.01	-2	4	2	45.49	45.16	-3	7	2	16.80	15.78	6	10	2	9.32	9.20	0	-9	3	13.84	13.71
5	1	2	2.98	5.06	-1	4	2	73.19	69.58	-2	7	2	11.50	11.48	7	10	2	2.43*	2.45	1	-9	3	8.87	9.37
6	1	2	1.38*	1.32	0	4	2	45.19	45.71	-1	7	2	4.85	3.93	8	10	2	7.60	7.83	2	-9	3	8.01	7.40
7	1	2	8.38	9.24	1	4	2	4.73	2.16	0	7	2	24.55	26.29	9	10	2	8.28	7.37	3	-9	3	6.40	6.57
8	1	2	6.69	6.60	2	4	2	2.91	2.09	1	7	2	14.25	13.64	-3	11	2	0.80*	0.08	4	-9	3	1.75*	1.47
9	1	2	4.24	4.46	3	4	2	37.26	38.28	2	7	2	7.41	8.53	-2	11	2	8.90	8.05	5	-9	3	4.39	4.83
10	1	2	0.79*	0.80	4	4	2	37.96	37.07	3	7	2	1.70*	3.04	-1	11	2	3.92	4.41	-9	-8	3	3.86	3.90
11	1	2	4.99	4.28	5	4	2	3.90	2.12	4	7	2	13.11	13.61	0	11	2	12.52	11.77	-8	-8	3	2.57*	2.76
-10	2	2	2.87	2.16	6	4	2	1.77*	0.54	5	7	2	2.14*	2.17	1	11	2	14.63	14.93	-7	-8	3	0.77*	0.52
-9	2	2	12.16	11.67	7	4	2	5.46	5.15	6	7	2	2.10*	0.91	2	11	2	7.11	7.48	-6	-8	3	8.38	6.71
-8	2	2	8.69	9.59	8	4	2	6.26	5.73	7	7	2	7.42	7.18	3	11	2	1.66*	2.19	-5	-8	3	0.74*	0.83
-7	2	2	18.43	17.72	9	4	2	2.19*	2.61	8	7	2	3.11	3.00	4	11	2	8.16	8.45	-4	-8	3	6.09	6.55
-6	2	2	17.54	18.19	10	4	2	4.05	3.91	9	7	2	14.83	14.69	5	11	2	11.80	12.08	-3	-8	3	2.75	2.58
-5	2	2	12.55	11.65	11	4	2	4.35	3.09	10	7	2	4.74	4.25	6	11	2	23.18	23.43	-2	-8	3	5.36	5.94
-4	2	2	8.75	8.19	-8	5	2	4.13	3.61	-6	8	2	5.38	6.55	7	11	2	7.03	6.93	-1	-8	3	13.65	14.10
-3	2	2	22.84	26.54	-7	5	2	7.09	7.78	-5	8	2	1.47*	2.78	8	11	2	2.78	2.92	0	-8	3	18.08	18.61
-2	2	2	22.77	23.00	-6	5	2	9.80	9.23	-4	8	2	1.57*	0.52	-2	12	2	3.01	2.12	1	-8	3	6.70	5.77
-1	2	2	68.57	70.05	-5	5	2	13.47	14.21	-3	8	2	2.99	4.25	-1	12	2	6.43	6.02	2	-8	3	6.55	6.49
0	2	2	28.41	26.06	-4	5	2	20.45	20.96	-2	8	2	0.73*	1.91	0	12	2	2.48*	1.46	3	-8	3	10.89	11.05
1	2	2	23.66	26.14	-3	5	2	1.33*	0.33	-1	8	2	10.87	10.17	1	12	2	2.85	3.07	4	-8	3	5.67	4.38
2	2	2	42.43	41.66	-2	5	2	6.67	4.62	0	8	2	30.66	29.33	2	12	2	4.16	4.04	5	-8	3	3.33	4.87
3	2	2	55.87	59.49	-1	5	2	30.16	29.79	1	8	2	1.91*	2.69	3	12	2	6.14	5.54	6	-8	3	4.43	3.94
4	2	2	36.05	31.13	0	5	2	57.41	54.22	2	8	2	1.85*	3.30	4	12	2	9.75	9.77	-9	-7	3	6.14	4.30
5	2	2	18.20	19.81	1	5	2	30.70	27.39	3	8	2	18.85	19.35	5	12	2	2.98	2.53	-8	-7	3	0.78*	1.57
6	2	2	19.23	17.91	2	5	2	25.91	25.92	4	8	2	5.47	4.41	6	12	2	3.66	3.99	-7	-7	3	7.90	6.19
7	2	2	0.72*	0.67	3	5	2	8.58	8.57	5	8	2	2.49	3.34	7	12	2	7.61	8.09	-6	-7	3	8.07	9.00
8	2	2	3.24	4.00	4	5	2	8.58	8.10	6	8	2	12.28	12.27	1	13	2	15.12	14.75	-5	-7	3	24.02	23.77
9	2	2	8.48	9.11	5	5	2	25.23	24.76	7	8	2	9.63	9.52	2	13	2	3.38	4.21	-4	-7	3	1.74*	0.14
10	2	2	3.63	3.26	6	5	2	33.00	32.50	8	8	2	2.91	3.27	3	13	2	4.53	3.89	-3	-7	3	21.08	20.01
11	2	2	1.74*	0.85	7	5	2	3.72	3.54	9	8	2	9.63	10.41	4	13	2	0.82*	0.61	-2	-7	3	4.55	5.74
-9	3	2	0.79*	0.47	8	5	2	1.97*	0.53	10	8	2	2.41*	2.90	5	13	2	5.29	4.99	-1	-7	3	2.69	3.08
-8	3	2	0.77*	0.91	9	5	2	3.33	3.13	-6	9	2	12.82	13.50	-6	-11	3	1.80*	1.21	0	-7	3	11.71	12.00
-7	3	2	10.83	10.70	10	5	2	2.19*	1.67	-5	9	2	11.87	11.66	-5	-11	3	2.18*	2.87	1	-7	3	6.34	6.35

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	-7	3	22.56	24.76	5	-4	3	5.61	6.61	2	-1	3	15.87	18.30	-4	2	3	9.99	10.76	-8	5	3	4.04	5.71
3	-7	3	6.78	4.83	6	-4	3	20.96	20.23	3	-1	3	18.88	23.56	-3	2	3	2.45	2.58	-7	5	3	9.89	9.19
4	-7	3	10.64	9.87	7	-4	3	6.87	7.50	4	-1	3	17.26	15.96	-2	2	3	22.29	22.67	-6	5	3	3.40	3.95
5	-7	3	5.28	4.83	8	-4	3	4.74	5.06	5	-1	3	18.02	18.20	-1	2	3	40.19	39.18	-5	5	3	1.28*	1.00
6	-7	3	13.75	13.57	9	-4	3	3.11	2.95	6	-1	3	15.24	16.06	0	2	3	93.55	94.39	-4	5	3	0.69*	0.13
7	-7	3	7.36	7.43	-10	-3	3	0.80*	0.04	7	-1	3	3.57	3.37	1	2	3	24.01	23.18	-3	5	3	2.41	2.98
-10	-6	3	5.07	6.13	-9	-3	3	4.07	3.26	8	-1	3	16.18	15.94	2	2	3	19.91	18.36	-2	5	3	35.11	33.74
-9	-6	3	5.85	6.95	-8	-3	3	6.68	7.01	9	-1	3	3.08	1.63	3	2	3	22.72	21.25	-1	5	3	23.25	25.62
-8	-6	3	11.09	10.42	-7	-3	3	14.27	14.20	10	-1	3	0.82*	1.07	4	2	3	69.50	71.15	0	5	3	44.77	36.89
-7	-6	3	4.31	4.66	-6	-3	3	13.28	12.03	-10	0	3	1.71*	1.45	5	2	3	17.11	17.74	1	5	3	60.08	58.70
-6	-6	3	19.86	19.03	-5	-3	3	21.95	22.83	-9	0	3	13.36	12.92	6	2	3	8.18	6.22	2	5	3	10.06	8.90
-5	-6	3	10.72	11.48	-4	-3	3	38.26	36.77	-8	0	3	6.83	7.42	7	2	3	21.58	21.52	3	5	3	11.53	10.49
-4	-6	3	3.89	3.86	-3	-3	3	13.63	15.83	-7	0	3	8.09	7.96	8	2	3	9.16	9.16	4	5	3	17.95	17.29
-3	-6	3	14.85	15.29	-2	-3	3	2.16	1.15	-6	0	3	1.69*	0.77	9	2	3	4.18	4.24	5	5	3	6.05	6.14
-2	-6	3	14.77	15.05	-1	-3	3	10.47	10.08	-5	0	3	8.11	9.17	10	2	3	2.19*	2.90	6	5	3	12.52	13.34
-1	-6	3	4.41	5.20	0	-3	3	8.49	4.92	-4	0	3	5.14	4.13	11	2	3	2.70	1.74	7	5	3	6.38	5.78
0	-6	3	11.25	11.68	1	-3	3	5.19	4.73	-3	0	3	41.01	38.42	-9	3	3	2.79	2.23	8	5	3	12.64	12.69
1	-6	3	31.99	31.71	2	-3	3	4.06	3.94	-2	0	3	7.38	7.73	-8	3	3	5.19	5.04	9	5	3	0.75*	0.85
2	-6	3	23.38	24.38	3	-3	3	9.33	7.79	-1	0	3	82.71	81.55	-7	3	3	17.48	18.14	10	5	3	2.06*	1.15
3	-6	3	5.89	6.77	4	-3	3	9.89	9.89	0	0	3	83.63	82.23	-6	3	3	17.58	16.89	11	5	3	0.82*	0.89
4	-6	3	26.82	27.92	5	-3	3	4.74	4.13	1	0	3	55.74	55.72	-5	3	3	11.60	11.90	-8	6	3	4.63	4.04
5	-6	3	2.98	2.54	6	-3	3	22.52	22.00	2	0	3	54.48	54.02	-4	3	3	12.14	11.64	-7	6	3	5.94	6.00
6	-6	3	3.18	2.45	7	-3	3	3.79	3.01	3	0	3	5.62	6.23	-3	3	3	4.39	1.92	-6	6	3	13.41	13.67
7	-6	3	1.65*	0.74	8	-3	3	4.26	2.95	4	0	3	0.59*	0.49	-2	3	3	19.33	23.88	-5	6	3	12.77	12.36
-10	-5	3	0.82*	0.22	9	-3	3	3.55	5.18	5	0	3	4.73	5.25	-1	3	3	32.14	30.08	-4	6	3	19.43	20.18
-9	-5	3	3.32	3.53	-10	-2	3	7.41	7.34	6	0	3	12.73	12.44	0	3	3	20.06	21.80	-3	6	3	10.06	8.99
-8	-5	3	6.36	6.15	-9	-2	3	0.77*	0.07	7	0	3	14.96	14.20	1	3	3	25.94	27.35	-2	6	3	10.19	9.48
-7	-5	3	2.31*	1.30	-8	-2	3	1.57*	0.10	8	0	3	6.40	7.36	2	3	3	43.55	45.17	-1	6	3	17.98	20.09
-6	-5	3	4.98	7.93	-7	-2	3	10.14	10.25	9	0	3	12.15	11.66	3	3	3	5.27	5.20	0	6	3	6.78	8.20
-5	-5	3	6.14	3.44	-6	-2	3	5.40	5.63	10	0	3	5.76	6.88	4	3	3	28.88	27.12	1	6	3	17.37	15.79
-4	-5	3	22.59	19.26	-5	-2	3	23.81	23.35	-10	1	3	8.43	7.96	5	3	3	10.55	9.72	2	6	3	7.18	5.34
-3	-5	3	25.87	24.47	-4	-2	3	18.02	17.10	-9	1	3	6.31	6.89	6	3	3	63.25	64.02	3	6	3	26.99	23.62
-2	-5	3	8.25	6.74	-3	-2	3	20.17	17.89	-8	1	3	10.58	10.56	7	3	3	11.32	11.12	4	6	3	12.76	13.42
-1	-5	3	13.56	12.21	-2	-2	3	27.39	31.18	-7	1	3	7.06	7.23	8	3	3	7.96	8.57	5	6	3	0.68*	0.60
0	-5	3	23.16	25.60	-1	-2	3	14.63	12.50	-6	1	3	7.86	8.14	9	3	3	4.74	6.25	6	6	3	14.83	14.23
1	-5	3	5.94	5.96	0	-2	3	4.75	2.50	-5	1	3	6.53	7.41	10	3	3	0.79*	0.19	7	6	3	13.42	12.95
2	-5	3	5.07	5.51	1	-2	3	8.85	9.51	-4	1	3	23.30	22.67	11	3	3	4.05	4.55	8	6	3	13.51	13.52
3	-5	3	10.70	10.04	2	-2	3	12.54	14.35	-3	1	3	12.45	11.76	-9	4	3	0.82*	0.83	9	6	3	1.85*	2.57
4	-5	3	18.08	19.90	3	-2	3	7.90	7.22	-2	1	3	22.63	25.30	-8	4	3	6.23	7.23	10	6	3	0.79*	0.80
5	-5	3	5.90	7.62	4	-2	3	4.16	3.81	-1	1	3	3.81	4.65	-7	4	3	2.94	4.60	11	6	3	2.52*	2.05
6	-5	3	7.96	7.12	5	-2	3	16.15	15.38	0	1	3	24.85	23.18	-6	4	3	3.80	3.20	-7	7	3	2.19*	0.10
7	-5	3	0.80*	1.03	6	-2	3	9.18	8.58	1	1	3	64.37	64.47	-5	4	3	6.23	5.31	-6	7	3	5.35	3.53
8	-5	3	4.89	5.55	7	-2	3	2.21*	0.45	2	1	3	2.48	1.47	-4	4	3	0.68*	1.37	-5	7	3	3.21	3.51
-10	-4	3	6.67	6.48	8	-2	3	5.36	6.35	3	1	3	20.69	18.80	-3	4	3	17.57	18.29	-4	7	3	4.13	2.81
-9	-4	3	9.01	8.83	9	-2	3	1.58*	0.09	4	1	3	34.93	36.87	-2	4	3	8.19	6.74	-3	7	3	2.23*	1.16
-8	-4	3	6.53	5.56	10	-2	3	1.27*	0.40	5	1	3	24.80	27.76	-1	4	3	49.75	47.07	-2	7	3	5.18	5.59
-7	-4	3	8.97	10.54	-10	-1	3	4.85	4.74	6	1	3	13.46	13.70	0	4	3	0.57*	1.05	-1	7	3	16.32	16.58
-6	-4	3	18.66	17.35	-9	-1	3	0.78*	1.34	7	1	3	3.14	2.76	1	4	3	32.15	29.81	0	7	3	16.71	14.99
-5	-4	3	7.42	8.11	-8	-1	3	0.75*	2.11	8	1	3	7.89	8.79	2	4	3	13.41	14.62	1	7	3	2.29	0.94
-4	-4	3	9.26	9.12	-7	-1	3	2.49	1.86	9	1	3	3.67	2.36	3	4	3	42.29	39.86	2	7	3	30.14	28.50
-3	-4	3	25.46	23.89	-6	-1	3	3.74	3.08	10	1	3	0.80*	0.33	4	4	3	6.83	6.86	3	7	3	4.58	4.33
-2	-4	3	31.21	28.42	-5	-1	3	33.87	31.83	11	1	3	8.60	8.97	5	4	3	8.24	8.09	4	7	3	22.79	22.87
-1	-4	3	31.89	28.37	-4	-1	3	18.55	18.36	-10	2	3	1.61*	1.63	6	4	3	27.56	28.60	5	7	3	8.63	8.02
0	-4	3	32.26	34.23	-3	-1	3	30.12	28.88	-9	2	3	11.66	12.53	7	4	3	7.17	6.95	6	7	3	6.59	6.33
1	-4	3	45.95	46.76	-2	-1	3	8.69	9.04	-8	2	3	11.19	10.03	8	4	3	12.42	12.91	7	7	3	16.82	16.99
2	-4	3	11.36	9.70	-1	-1	3	13.70	12.52	-7	2	3	1.97*	2.04	9	4	3	7.11	7.34	8	7	3	8.59	8.74
3	-4	3	24.88	26.69	0	-1	3	59.56	57.88	-6	2	3	5.43	4.81	10	4	3	0.79*	0.95	9	7	3	7.91	7.61
4	-4	3	14.37	13.22	1	-1	3	46.77	48.61	-5	2	3	4.55	4.57	11	4	3	3.09	3.51	10	7	3	4.18	4.17

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-6	8	3	3.14	3.45	8	11	3	2.40*	2.79	-7	-7	4	3.21	4.53	-2	-4	4	9.74	8.79	-3	-1	4	10.84	10.96
-5	8	3	2.64	2.38	-2	12	3	1.41*	1.89	-6	-7	4	7.52	6.83	-1	-4	4	9.56	9.06	-2	-1	4	7.38	7.06
-4	8	3	0.75*	0.17	-1	12	3	0.80*	0.95	-5	-7	4	3.33	2.28	0	-4	4	15.49	13.93	-1	-1	4	20.92	22.48
-3	8	3	3.04	3.26	0	12	3	3.50	3.39	-4	-7	4	8.24	7.47	1	-4	4	0.64*	4.66	0	-1	4	37.17	36.20
-2	8	3	12.49	12.32	1	12	3	2.88	3.19	-3	-7	4	3.72	2.23	2	-4	4	8.33	8.77	1	-1	4	12.11	12.31
-1	8	3	2.88	2.15	2	12	3	8.23	8.15	-2	-7	4	17.06	16.62	3	-4	4	13.84	13.14	2	-1	4	36.59	38.06
0	8	3	16.51	16.97	3	12	3	7.84	8.14	-1	-7	4	1.97*	1.33	4	-4	4	12.03	13.99	3	-1	4	5.61	8.50
1	8	3	16.39	15.52	4	12	3	8.21	7.94	0	-7	4	0.72*	2.08	5	-4	4	11.95	10.47	4	-1	4	17.92	16.38
2	8	3	24.88	27.30	5	12	3	3.94	4.70	1	-7	4	10.31	10.35	6	-4	4	10.86	12.18	5	-1	4	23.52	22.46
3	8	3	5.18	5.70	6	12	3	3.95	4.30	2	-7	4	8.58	8.02	7	-4	4	2.59	2.85	6	-1	4	14.15	14.37
4	8	3	9.17	9.03	7	12	3	10.06	10.31	3	-7	4	4.75	6.19	8	-4	4	0.80*	2.87	7	-1	4	7.40	7.11
5	8	3	3.75	3.24	1	13	3	1.69*	1.66	4	-7	4	1.18*	0.37	-10	-3	4	7.42	7.03	8	-1	4	6.92	7.55
6	8	3	0.73*	0.36	2	13	3	1.74*	3.15	5	-7	4	10.69	11.25	-9	-3	4	6.60	6.89	9	-1	4	4.28	5.16
7	8	3	9.51	10.40	3	13	3	0.80*	0.20	6	-7	4	8.28	8.62	-8	-3	4	6.96	6.86	10	-1	4	3.82	2.88
8	8	3	5.24	5.70	4	13	3	6.87	6.95	-9	-6	4	13.01	11.86	-7	-3	4	14.23	13.59	-10	0	4	3.41	3.47
9	8	3	4.10	4.03	5	13	3	7.08	7.36	-8	-6	4	21.38	21.68	-6	-3	4	8.74	10.60	-9	0	4	6.10	5.19
10	8	3	0.82*	0.22	-4	-11	4	3.02	2.72	-7	-6	4	3.89	3.38	-5	-3	4	9.38	7.75	-8	0	4	9.35	9.12
-5	9	3	6.77	7.39	-3	-11	4	5.41	5.16	-6	-6	4	0.74*	0.78	-4	-3	4	12.42	11.47	-7	0	4	14.25	14.23
-4	9	3	3.33	3.93	-2	-11	4	1.75*	1.01	-5	-6	4	6.57	6.67	-3	-3	4	29.60	28.65	-6	0	4	3.12	2.62
-3	9	3	3.19	3.63	-1	-11	4	4.21	4.28	-4	-6	4	20.51	20.39	-2	-3	4	16.24	15.67	-5	0	4	11.07	11.38
-2	9	3	2.67	2.88	0	-11	4	5.03	5.60	-3	-6	4	1.35*	1.64	-1	-3	4	22.11	21.94	-4	0	4	25.18	24.50
-1	9	3	5.22	6.20	-6	-10	4	6.85	7.42	-2	-6	4	4.07	4.30	0	-3	4	31.81	33.06	-3	0	4	23.75	24.75
0	9	3	2.30*	1.99	-5	-10	4	1.46*	0.86	-1	-6	4	17.98	18.44	1	-3	4	10.87	9.00	-2	0	4	19.96	20.83
1	9	3	5.43	6.42	-4	-10	4	1.70*	1.88	0	-6	4	2.31	1.86	2	-3	4	18.23	16.29	-1	0	4	17.20	15.45
2	9	3	3.28	2.90	-3	-10	4	1.60*	0.13	1	-6	4	1.75*	2.20	3	-3	4	20.32	19.64	0	0	4	50.26	48.57
3	9	3	2.23*	0.38	-2	-10	4	2.98	2.77	2	-6	4	12.35	11.67	4	-3	4	14.49	15.56	1	0	4	15.06	15.51
4	9	3	11.38	11.70	-1	-10	4	3.56	2.63	3	-6	4	2.18*	1.99	5	-3	4	11.94	11.84	2	0	4	8.52	8.82
5	9	3	2.74	3.29	0	-10	4	8.59	8.57	4	-6	4	35.50	35.78	6	-3	4	17.88	19.74	3	0	4	12.72	12.13
6	9	3	13.01	12.97	1	-10	4	8.00	7.70	5	-6	4	8.63	9.04	7	-3	4	9.55	8.27	4	0	4	21.63	21.49
7	9	3	9.46	10.09	2	-10	4	0.79*	2.34	6	-6	4	4.01	4.99	8	-3	4	12.01	12.99	5	0	4	34.30	32.24
8	9	3	8.43	8.06	-7	-9	4	3.82	4.35	7	-6	4	2.59*	3.31	9	-3	4	3.99	3.59	6	0	4	20.27	20.64
9	9	3	2.08*	1.90	-6	-9	4	8.89	8.94	-10	-5	4	2.23*	0.44	-10	-2	4	4.28	3.89	7	0	4	20.20	21.82
10	9	3	4.84	4.99	-5	-9	4	19.87	18.96	-9	-5	4	2.49*	2.26	-9	-2	4	3.28	3.10	8	0	4	18.03	17.28
-4	10	3	6.46	7.55	-4	-9	4	14.19	15.03	-8	-5	4	12.19	11.71	-8	-2	4	10.07	9.57	9	0	4	4.20	4.89
-3	10	3	4.06	3.93	-3	-9	4	2.74	3.39	-7	-5	4	11.50	10.29	-7	-2	4	8.58	9.95	10	0	4	1.77*	1.87
-2	10	3	0.75*	0.96	-2	-9	4	0.74*	0.27	-6	-5	4	0.74*	0.29	-6	-2	4	7.06	6.19	-10	1	4	3.77	3.14
-1	10	3	0.74*	1.12	-1	-9	4	12.47	12.40	-5	-5	4	7.71	5.33	-5	-2	4	7.09	6.15	-9	1	4	5.61	5.78
0	10	3	9.89	8.99	0	-9	4	14.17	14.79	-4	-5	4	2.10*	0.79	-4	-2	4	21.59	20.04	-8	1	4	2.49	2.67
1	10	3	2.82	2.95	1	-9	4	3.63	3.97	-3	-5	4	11.03	10.92	-3	-2	4	8.26	5.22	-7	1	4	3.60	2.76
2	10	3	16.04	16.44	2	-9	4	0.78*	0.11	-2	-5	4	1.41*	2.68	-2	-2	4	15.95	16.61	-6	1	4	5.13	5.47
3	10	3	0.73*	1.72	3	-9	4	5.17	5.91	-1	-5	4	15.92	17.28	-1	-2	4	41.93	44.14	-5	1	4	16.86	16.69
4	10	3	3.96	3.12	4	-9	4	5.70	5.50	0	-5	4	18.89	17.55	0	-2	4	42.67	39.80	-4	1	4	17.77	17.75
5	10	3	12.08	12.10	-8	-8	4	2.84	3.55	1	-5	4	15.49	15.94	1	-2	4	15.11	13.61	-3	1	4	17.31	14.00
6	10	3	5.55	6.08	-7	-8	4	2.44*	1.19	2	-5	4	20.63	20.14	2	-2	4	1.71*	1.23	-2	1	4	8.01	8.77
7	10	3	2.59	1.96	-6	-8	4	5.31	7.43	3	-5	4	4.70	4.78	3	-2	4	22.44	24.28	-1	1	4	95.11	95.60
8	10	3	0.79*	0.79	-5	-8	4	13.69	13.16	4	-5	4	14.29	13.10	4	-2	4	0.67*	1.58	0	1	4	24.51	24.18
9	10	3	2.39*	3.31	-4	-8	4	1.99*	1.10	5	-5	4	4.62	6.91	5	-2	4	2.74	3.05	1	1	4	16.24	16.83
-3	11	3	2.18*	2.27	-3	-8	4	13.84	14.26	6	-5	4	24.06	25.98	6	-2	4	7.56	5.76	2	1	4	43.75	44.06
-2	11	3	5.75	6.35	-2	-8	4	8.16	8.08	7	-5	4	4.74	3.10	7	-2	4	2.06*	0.92	3	1	4	40.60	38.49
-1	11	3	8.97	8.13	-1	-8	4	13.33	13.05	8	-5	4	7.72	7.12	8	-2	4	6.36	6.11	4	1	4	10.39	8.64
0	11	3	9.60	10.06	0	-8	4	9.09	8.90	-10	-4	4	2.46*	1.78	9	-2	4	2.70	2.11	5	1	4	7.28	4.47
1	11	3	5.70	5.49	1	-8	4	18.80	19.48	-9	-4	4	6.34	5.51	-10	-1	4	8.14	7.56	6	1	4	5.66	7.66
2	11	3	9.45	10.13	2	-8	4	14.86	15.20	-8	-4	4	4.94	3.50	-9	-1	4	3.27	2.26	7	1	4	7.24	7.57
3	11	3	6.96	6.45	3	-8	4	6.24	5.72	-7	-4	4	1.71*	0.93	-8	-1	4	4.85	4.19	8	1	4	8.94	8.32
4	11	3	2.02*	2.76	4	-8	4	2.23*	3.73	-6	-4	4	7.37	4.33	-7	-1	4	1.69*	0.62	9	1	4	7.19	7.37
5	11	3	9.08	8.41	5	-8	4	0.80*	1.54	-5	-4	4	6.26	5.58	-6	-1	4	11.59	12.74	10	1	4	2.01*	2.68
6	11	3	15.25	15.72	-9	-7	4	4.67	3.60	-4	-4	4	18.61	19.96	-5	-1	4	6.64	5.95	-9	2	4	8.04	7.05
7	11	3	3.71	4.23	-8	-7	4	0.79*	2.56	-3	-4	4	10.11	11.19	-4	-1	4	11.95	11.90	-8	2	4	11.80	12.43

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-7	2	4	2.75	3.02	9	4	4	11.77	11.30	8	7	4	4.23	4.73	5	11	4	4.24	4.50	0	-7	5	13.84	15.06
-6	2	4	4.11	4.28	10	4	4	6.04	5.53	9	7	4	3.33	3.32	6	11	4	4.99	4.71	1	-7	5	4.98	4.03
-5	2	4	5.57	6.01	11	4	4	4.00	3.16	10	7	4	1.71*	2.02	7	11	4	1.35*	1.90	2	-7	5	4.78	6.36
-4	2	4	5.65	6.32	-8	5	4	1.17*	1.65	-6	8	4	0.80*	1.02	8	11	4	6.83	5.93	3	-7	5	12.25	11.15
-3	2	4	29.68	28.51	-7	5	4	1.46*	2.21	-5	8	4	1.58*	1.86	-1	12	4	4.59	4.14	4	-7	5	2.68	3.63
-2	2	4	13.51	13.95	-6	5	4	7.47	7.61	-4	8	4	0.75*	0.09	0	12	4	9.13	9.12	5	-7	5	5.50	5.63
-1	2	4	8.83	6.46	-5	5	4	1.16*	0.29	-3	8	4	1.22*	0.45	1	12	4	5.86	6.24	6	-7	5	3.35	3.12
0	2	4	9.50	9.75	-4	5	4	10.18	10.10	-2	8	4	9.56	9.53	2	12	4	3.82	4.41	-9	-6	5	4.57	5.09
1	2	4	17.27	17.20	-3	5	4	2.80	2.58	-1	8	4	5.75	6.43	3	12	4	10.28	9.90	-8	-6	5	16.57	15.98
2	2	4	6.06	6.28	-2	5	4	16.78	17.22	0	8	4	9.07	8.16	4	12	4	3.42	3.75	-7	-6	5	2.36*	1.06
3	2	4	3.91	1.56	-1	5	4	7.04	6.60	1	8	4	4.28	5.37	5	12	4	1.97*	2.07	-6	-6	5	10.58	9.98
4	2	4	3.13	0.95	0	5	4	47.91	50.42	2	8	4	3.62	3.31	6	12	4	4.39	4.83	-5	-6	5	4.52	4.31
5	2	4	24.85	24.24	1	5	4	34.50	36.43	3	8	4	10.93	11.57	7	12	4	9.51	9.50	-4	-6	5	11.96	13.28
6	2	4	3.47	2.55	2	5	4	8.18	8.93	4	8	4	0.73*	0.00	1	13	4	0.82*	1.21	-3	-6	5	14.06	13.68
7	2	4	1.82*	1.15	3	5	4	6.35	8.03	5	8	4	1.70*	1.43	2	13	4	3.18	3.25	-2	-6	5	12.34	11.61
8	2	4	11.21	12.27	4	5	4	5.01	4.76	6	8	4	4.83	4.35	3	13	4	4.63	4.17	-1	-6	5	0.72*	0.02
9	2	4	5.58	5.16	5	5	4	15.80	16.32	7	8	4	0.74*	0.17	4	13	4	0.82*	1.25	0	-6	5	2.65	1.07
10	2	4	5.47	5.51	6	5	4	2.99	2.47	8	8	4	4.20	4.02	5	13	4	4.80	4.65	1	-6	5	3.55	3.80
11	2	4	2.58*	0.60	7	5	4	14.29	14.98	9	8	4	5.63	5.18	-5	-10	5	6.36	6.43	2	-6	5	18.12	18.35
-9	3	4	0.82*	1.31	8	5	4	13.78	15.28	10	8	4	1.57*	1.34	-4	-10	5	2.11*	2.55	3	-6	5	4.28	5.24
-8	3	4	4.29	4.20	9	5	4	4.92	4.68	-5	9	4	5.61	4.66	-3	-10	5	4.90	4.48	4	-6	5	2.28*	3.00
-7	3	4	16.73	16.46	10	5	4	9.55	9.76	-4	9	4	2.74	2.29	-2	-10	5	7.70	7.43	5	-6	5	10.70	10.12
-6	3	4	24.37	24.60	11	5	4	3.92	4.03	-3	9	4	6.15	7.10	-1	-10	5	5.66	6.42	6	-6	5	5.80	6.26
-5	3	4	3.17	3.33	-8	6	4	6.74	7.54	-2	9	4	0.74*	1.22	0	-10	5	4.00	3.78	7	-6	5	2.01*	1.59
-4	3	4	0.67*	0.24	-7	6	4	8.25	8.77	-1	9	4	9.57	10.27	1	-10	5	7.76	8.25	-9	-5	5	0.82*	2.14
-3	3	4	4.04	1.90	-6	6	4	9.21	9.03	0	9	4	22.54	22.01	-7	-9	5	5.58	5.25	-8	-5	5	4.43	5.43
-2	3	4	7.07	9.01	-5	6	4	8.97	8.75	1	9	4	6.44	6.37	-6	-9	5	9.26	9.14	-7	-5	5	12.38	13.69
-1	3	4	10.40	11.64	-4	6	4	3.01	2.12	2	9	4	0.72*	0.31	-5	-9	5	6.41	7.71	-6	-5	5	33.60	31.72
0	3	4	19.03	19.46	-3	6	4	10.33	9.29	3	9	4	8.24	8.69	-4	-9	5	9.94	9.22	-5	-5	5	5.63	3.45
1	3	4	6.69	7.46	-2	6	4	25.19	24.15	4	9	4	12.69	12.26	-3	-9	5	0.77*	0.89	-4	-5	5	6.72	5.23
2	3	4	17.64	18.86	-1	6	4	9.66	10.81	5	9	4	13.13	13.83	-2	-9	5	1.70*	1.59	-3	-5	5	11.14	11.24
3	3	4	15.26	15.89	0	6	4	1.42*	0.87	6	9	4	12.72	12.72	-1	-9	5	6.87	6.44	-2	-5	5	23.03	23.61
4	3	4	1.76*	3.82	1	6	4	6.63	5.48	7	9	4	12.63	11.95	0	-9	5	2.59	2.53	-1	-5	5	17.59	16.51
5	3	4	28.40	29.81	2	6	4	33.72	33.23	8	9	4	7.45	8.44	1	-9	5	1.77*	0.20	0	-5	5	11.25	11.39
6	3	4	41.57	39.24	3	6	4	10.31	10.50	9	9	4	8.58	8.04	2	-9	5	8.91	9.89	1	-5	5	11.82	11.82
7	3	4	10.30	12.16	4	6	4	8.43	8.17	10	9	4	1.77*	0.76	3	-9	5	8.98	8.75	2	-5	5	2.85	2.41
8	3	4	2.73	1.30	5	6	4	3.37	2.57	-4	10	4	6.99	6.53	-8	-8	5	2.25*	1.54	3	-5	5	11.23	10.70
9	3	4	3.11	2.27	6	6	4	29.57	30.63	-3	10	4	10.31	10.52	-7	-8	5	3.14	1.04	4	-5	5	1.67*	0.85
10	3	4	1.19*	2.28	7	6	4	3.61	3.56	-2	10	4	1.70*	0.45	-6	-8	5	1.99*	1.93	5	-5	5	5.28	6.47
11	3	4	0.82*	1.16	8	6	4	15.81	16.51	-1	10	4	3.56	4.36	-5	-8	5	2.96	2.73	6	-5	5	19.26	18.16
-9	4	4	1.75*	2.22	9	6	4	10.87	10.34	0	10	4	8.14	8.43	-4	-8	5	9.96	9.23	7	-5	5	4.10	4.24
-8	4	4	5.07	3.67	10	6	4	4.94	6.20	1	10	4	13.32	14.63	-3	-8	5	36.28	37.74	-9	-4	5	0.79*	0.74
-7	4	4	0.78*	2.87	11	6	4	0.84*	0.79	2	10	4	1.19*	0.70	-2	-8	5	19.43	20.18	-8	-4	5	6.21	5.10
-6	4	4	0.75*	1.82	-7	7	4	3.70	2.52	3	10	4	1.75*	2.26	-1	-8	5	7.84	8.25	-7	-4	5	4.35	6.19
-5	4	4	13.23	13.64	-6	7	4	10.18	10.91	4	10	4	0.73*	0.21	0	-8	5	15.54	15.31	-6	-4	5	21.42	20.88
-4	4	4	10.08	9.93	-5	7	4	7.90	6.83	5	10	4	3.51	4.23	1	-8	5	6.64	6.79	-5	-4	5	1.91*	1.75
-3	4	4	21.35	19.97	-4	7	4	8.45	9.50	6	10	4	10.06	9.79	2	-8	5	2.26*	2.26	-4	-4	5	18.25	19.64
-2	4	4	4.89	3.58	-3	7	4	9.56	9.87	7	10	4	1.51*	0.07	3	-8	5	0.79*	1.05	-3	-4	5	1.89*	2.32
-1	4	4	7.37	6.82	-2	7	4	0.70*	1.02	8	10	4	2.74	2.92	4	-8	5	4.99	6.35	-2	-4	5	7.80	9.34
0	4	4	34.87	34.88	-1	7	4	5.45	6.60	9	10	4	6.02	4.81	5	-8	5	6.25	5.74	-1	-4	5	10.11	9.99
1	4	4	28.19	28.75	0	7	4	14.42	15.34	-3	11	4	5.01	4.58	-8	-7	5	4.73	3.14	0	-4	5	29.34	29.46
2	4	4	15.45	13.15	1	7	4	7.84	6.60	-2	11	4	6.59	5.76	-7	-7	5	7.36	6.52	1	-4	5	12.70	11.97
3	4	4	23.52	23.63	2	7	4	30.00	30.27	-1	11	4	8.57	10.18	-6	-7	5	10.09	10.28	2	-4	5	6.73	6.36
4	4	4	4.31	4.92	3	7	4	13.64	12.10	0	11	4	7.01	5.72	-5	-7	5	6.05	5.83	3	-4	5	11.16	11.82
5	4	4	8.97	10.50	4	7	4	4.02	3.25	1	11	4	3.51	3.70	-4	-7	5	6.43	7.54	4	-4	5	1.60*	0.88
6	4	4	16.87	16.16	5	7	4	30.00	30.19	2	11	4	0.77*	1.64	-3	-7	5	10.10	11.20	5	-4	5	10.49	11.17
7	4	4	12.53	11.96	6	7	4	4.14	4.76	3	11	4	5.62	5.74	-2	-7	5	4.78	4.55	6	-4	5	13.25	13.00
8	4	4	25.62	26.59	7	7	4	4.24	3.79	4	11	4	7.36	7.31	-1	-7	5	28.12	28.86	7	-4	5	0.80*	0.23

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	-4	5	8.30	8.41	9	-1	5	3.82	3.65	7	2	5	0.72*	0.74	7	5	5	11.66	11.48	-4	9	5	4.88	4.08
-9	-3	5	0.79*	0.44	10	-1	5	4.40	4.12	8	2	5	1.56*	0.94	8	5	5	21.62	22.05	-3	9	5	0.77*	0.04
-8	-3	5	0.78*	1.03	-9	0	5	0.78*	0.96	9	2	5	3.68	4.17	9	5	5	11.07	10.95	-2	9	5	5.29	5.23
-7	-3	5	4.74	4.72	-8	0	5	8.63	8.40	10	2	5	2.33*	1.32	10	5	5	12.96	13.38	-1	9	5	9.79	10.75
-6	-3	5	4.50	2.76	-7	0	5	3.37	3.07	-9	3	5	2.00*	1.82	-7	6	5	3.37	2.57	0	9	5	6.11	6.51
-5	-3	5	7.06	8.88	-6	0	5	7.48	7.81	-8	3	5	1.77*	1.98	-6	6	5	1.36*	1.17	1	9	5	9.90	9.46
-4	-3	5	9.58	8.42	-5	0	5	2.69	2.03	-7	3	5	11.90	12.31	-5	6	5	1.67*	2.30	2	9	5	3.18	3.20
-3	-3	5	17.64	16.47	-4	0	5	0.65*	1.81	-6	3	5	17.48	16.83	-4	6	5	2.98	1.73	3	9	5	5.60	5.87
-2	-3	5	27.42	25.86	-3	0	5	20.24	17.37	-5	3	5	6.18	6.15	-3	6	5	8.04	7.42	4	9	5	15.54	16.50
-1	-3	5	13.86	12.69	-2	0	5	0.60*	3.54	-4	3	5	5.56	5.93	-2	6	5	19.24	19.31	5	9	5	12.20	12.30
0	-3	5	29.44	28.90	-1	0	5	10.82	9.41	-3	3	5	10.91	11.87	-1	6	5	7.92	8.82	6	9	5	9.94	9.48
1	-3	5	6.78	6.93	0	0	5	16.47	16.07	-2	3	5	2.39	4.83	0	6	5	2.28	3.05	7	9	5	2.52	3.69
2	-3	5	8.62	7.81	1	0	5	14.82	15.44	-1	3	5	15.65	17.70	1	6	5	3.77	3.55	8	9	5	1.57*	1.42
3	-3	5	7.28	6.88	2	0	5	16.17	15.58	0	3	5	24.41	25.41	2	6	5	17.40	16.42	9	9	5	5.33	5.07
4	-3	5	1.74*	0.73	3	0	5	38.41	37.63	1	3	5	8.58	8.18	3	6	5	2.96	3.17	-4	10	5	2.91	4.22
5	-3	5	18.86	20.44	4	0	5	11.51	12.05	2	3	5	2.39	3.02	4	6	5	1.04*	2.29	-3	10	5	5.67	5.01
6	-3	5	18.22	15.82	5	0	5	17.38	17.64	3	3	5	21.65	20.77	5	6	5	1.42*	2.49	-2	10	5	2.49*	1.61
7	-3	5	11.96	13.28	6	0	5	11.72	12.38	4	3	5	33.64	34.76	6	6	5	11.38	11.06	-1	10	5	1.35*	0.95
8	-3	5	14.14	13.58	7	0	5	1.76*	0.87	5	3	5	11.20	12.99	7	6	5	7.79	8.04	0	10	5	0.75*	0.38
9	-3	5	3.37	3.26	8	0	5	3.77	5.85	6	3	5	13.62	14.16	8	6	5	3.68	2.90	1	10	5	11.04	12.48
-10	-2	5	6.40	6.36	9	0	5	0.78*	1.58	7	3	5	5.17	3.98	9	6	5	8.96	9.22	2	10	5	1.66*	2.36
-9	-2	5	3.06	2.39	10	0	5	0.82*	0.39	8	3	5	5.35	5.84	10	6	5	9.48	10.50	3	10	5	1.35*	1.48
-8	-2	5	6.70	7.35	-9	1	5	3.72	4.57	9	3	5	1.53*	0.28	-7	7	5	6.40	6.52	4	10	5	6.24	6.21
-7	-2	5	14.82	13.37	-8	1	5	1.72*	0.77	10	3	5	1.57*	1.02	-6	7	5	6.62	6.19	5	10	5	6.98	7.26
-6	-2	5	3.23	4.68	-7	1	5	6.26	5.99	-8	4	5	2.98	2.22	-5	7	5	2.96	4.33	6	10	5	12.28	12.55
-5	-2	5	6.04	4.52	-6	1	5	9.09	9.53	-7	4	5	2.11*	0.30	-4	7	5	5.41	4.62	7	10	5	17.48	17.35
-4	-2	5	7.50	5.27	-5	1	5	4.90	5.18	-6	4	5	3.28	3.23	-3	7	5	2.23*	2.43	8	10	5	11.38	11.52
-3	-2	5	38.48	36.18	-4	1	5	10.79	11.58	-5	4	5	23.91	23.43	-2	7	5	1.62*	0.39	9	10	5	4.41	4.14
-2	-2	5	7.56	5.76	-3	1	5	9.71	9.98	-4	4	5	21.46	21.17	-1	7	5	16.33	16.69	-3	11	5	3.36	3.36
-1	-2	5	17.02	15.89	-2	1	5	13.51	14.04	-3	4	5	3.46	3.68	0	7	5	8.23	9.43	-2	11	5	3.37	4.13
0	-2	5	47.16	46.84	-1	1	5	79.53	75.70	-2	4	5	2.99	3.83	1	7	5	5.72	7.36	-1	11	5	9.01	8.46
1	-2	5	42.57	42.25	0	1	5	20.93	19.89	-1	4	5	11.42	11.16	2	7	5	18.75	17.91	0	11	5	4.69	4.43
2	-2	5	23.51	22.55	1	1	5	44.28	43.30	0	4	5	15.90	17.22	3	7	5	6.49	6.90	1	11	5	3.30	3.82
3	-2	5	26.30	26.02	2	1	5	3.97	5.40	1	4	5	16.46	15.97	4	7	5	39.66	39.83	2	11	5	11.91	11.95
4	-2	5	15.70	15.42	3	1	5	11.04	10.10	2	4	5	22.74	23.97	5	7	5	16.61	16.15	3	11	5	13.76	15.00
5	-2	5	12.92	13.20	4	1	5	5.06	7.42	3	4	5	28.61	29.51	6	7	5	11.81	11.65	4	11	5	7.67	8.36
6	-2	5	19.10	20.59	5	1	5	22.92	21.41	4	4	5	4.36	4.28	7	7	5	3.58	3.86	5	11	5	2.24*	2.18
7	-2	5	4.54	3.72	6	1	5	28.88	28.12	5	4	5	12.13	12.79	8	7	5	9.35	9.85	6	11	5	5.43	4.68
8	-2	5	7.65	8.68	7	1	5	7.48	7.59	6	4	5	21.52	21.25	9	7	5	3.37	2.99	7	11	5	2.75	3.24
9	-2	5	7.19	6.86	8	1	5	5.42	5.57	7	4	5	13.64	14.20	10	7	5	4.00	3.21	8	11	5	1.58*	2.68
-9	-1	5	1.66*	0.44	9	1	5	11.72	12.08	8	4	5	16.48	17.51	-6	8	5	0.80*	0.46	-1	12	5	4.90	4.50
-8	-1	5	4.45	4.76	10	1	5	1.27*	0.60	9	4	5	7.02	7.54	-5	8	5	1.69*	0.37	0	12	5	6.73	7.18
-7	-1	5	10.04	10.13	-9	2	5	3.13	2.94	10	4	5	0.80*	1.96	-4	8	5	2.21*	2.52	1	12	5	9.96	10.20
-6	-1	5	3.35	3.30	-8	2	5	7.03	6.37	-8	5	5	3.17	3.23	-3	8	5	4.10	4.84	2	12	5	3.18	2.72
-5	-1	5	6.57	6.36	-7	2	5	3.30	2.97	-7	5	5	3.23	3.44	-2	8	5	3.35	3.12	3	12	5	3.09	3.17
-4	-1	5	16.88	16.09	-6	2	5	4.90	5.08	-6	5	5	3.86	4.47	-1	8	5	14.28	13.90	4	12	5	1.12*	1.69
-3	-1	5	15.41	13.83	-5	2	5	4.15	4.28	-5	5	5	15.34	15.34	0	8	5	9.11	10.00	5	12	5	9.30	9.10
-2	-1	5	4.33	3.30	-4	2	5	10.94	11.58	-4	5	5	16.85	16.62	1	8	5	14.96	13.86	6	12	5	5.11	4.92
-1	-1	5	33.39	32.43	-3	2	5	10.67	11.48	-3	5	5	16.95	17.21	2	8	5	14.61	15.14	7	12	5	3.14	3.27
0	-1	5	18.72	18.70	-2	2	5	3.84	4.15	-2	5	5	1.81*	2.52	3	8	5	1.76*	0.64	2	13	5	0.82*	0.12
1	-1	5	24.23	25.31	-1	2	5	60.75	58.62	-1	5	5	16.66	17.95	4	8	5	19.76	19.32	3	13	5	1.57*	1.02
2	-1	5	4.99	2.48	0	2	5	42.90	42.55	0	5	5	17.84	16.93	5	8	5	13.88	14.09	4	13	5	5.19	5.06
3	-1	5	25.48	26.92	1	2	5	66.93	65.85	1	5	5	31.86	32.64	6	8	5	15.60	16.20	-3	-10	6	8.20	7.52
4	-1	5	9.90	10.12	2	2	5	53.94	52.67	2	5	5	12.54	12.01	7	8	5	11.65	11.51	-2	-10	6	7.96	8.63
5	-1	5	14.30	14.13	3	2	5	0.59*	2.18	3	5	5	6.88	7.23	8	8	5	4.99	4.72	-1	-10	6	8.06	7.55
6	-1	5	9.56	9.68	4	2	5	3.65	5.09	4	5	5	11.61	11.15	9	8	5	2.25*	1.79	-5	-9	6	4.98	4.43
7	-1	5	11.82	12.15	5	2	5	11.58	11.12	5	5	5	3.37	2.66	10	8	5	1.97*	1.24	-4	-9	6	0.79*	2.01
8	-1	5	0.77*	1.53	6	2	5	9.01	8.69	6	5	5	10.94	10.82	-5	9	5	0.82*	2.00	-3	-9	6	0.79*	0.24

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	-9	6	4.13	3.52	5	-5	6	8.49	7.83	-9	-1	6	2.69	2.83	10	1	6	0.82*	1.07	10	4	6	1.84*	1.22
-1	-9	6	4.09	4.46	6	-5	6	12.87	14.06	-8	-1	6	2.65	3.34	-9	2	6	2.78	3.00	-7	5	6	4.65	3.76
0	-9	6	9.52	9.32	7	-5	6	4.38	3.60	-7	-1	6	1.09*	0.31	-8	2	6	2.16*	1.35	-6	5	6	3.68	2.98
1	-9	6	0.80*	0.04	-9	-4	6	1.72*	1.26	-6	-1	6	4.11	4.47	-7	2	6	2.23*	2.64	-5	5	6	8.04	7.98
2	-9	6	0.80*	1.89	-8	-4	6	2.00*	3.14	-5	-1	6	9.99	9.84	-6	2	6	1.58*	0.76	-4	5	6	14.97	14.79
-7	-8	6	0.83*	2.09	-7	-4	6	10.64	9.51	-4	-1	6	16.27	15.78	-5	2	6	7.92	7.40	-3	5	6	41.14	40.69
-6	-8	6	13.23	12.04	-6	-4	6	9.95	11.31	-3	-1	6	5.58	6.24	-4	2	6	5.60	6.11	-2	5	6	24.46	25.78
-5	-8	6	9.56	10.12	-5	-4	6	18.11	18.63	-2	-1	6	11.56	10.18	-3	2	6	11.55	11.84	-1	5	6	11.32	10.98
-4	-8	6	9.72	10.37	-4	-4	6	20.12	21.35	-1	-1	6	26.47	29.24	-2	2	6	18.48	19.13	0	5	6	16.84	18.66
-3	-8	6	11.02	11.20	-3	-4	6	7.60	6.66	0	-1	6	19.25	19.21	-1	2	6	44.21	44.22	1	5	6	0.65*	1.23
-2	-8	6	7.46	7.80	-2	-4	6	5.22	5.75	1	-1	6	6.73	6.06	0	2	6	7.62	7.60	2	5	6	26.50	25.50
-1	-8	6	6.44	6.70	-1	-4	6	18.47	19.12	2	-1	6	39.95	40.78	1	2	6	58.58	54.53	3	5	6	11.25	11.96
0	-8	6	1.99*	3.01	0	-4	6	20.17	19.14	3	-1	6	16.64	14.51	2	2	6	25.69	26.28	4	5	6	1.51*	0.95
1	-8	6	1.46*	2.41	1	-4	6	39.25	39.14	4	-1	6	9.33	8.76	3	2	6	6.28	7.39	5	5	6	3.96	3.90
2	-8	6	3.01	3.02	2	-4	6	16.31	17.37	5	-1	6	2.26*	1.96	4	2	6	27.52	27.54	6	5	6	5.89	6.61
3	-8	6	4.25	4.67	3	-4	6	4.54	5.20	6	-1	6	3.52	3.76	5	2	6	2.92	1.69	7	5	6	3.40	2.27
4	-8	6	0.82*	0.21	4	-4	6	1.75*	3.61	7	-1	6	8.19	9.21	6	2	6	4.09	4.14	8	5	6	5.46	5.53
-7	-7	6	2.39*	0.38	5	-4	6	12.44	11.99	8	-1	6	1.28*	0.75	7	2	6	10.11	10.23	9	5	6	12.65	12.85
-6	-7	6	1.67*	0.53	6	-4	6	3.85	4.44	9	-1	6	7.33	8.08	8	2	6	0.75*	0.79	10	5	6	12.97	13.92
-5	-7	6	2.26*	3.14	7	-4	6	8.43	7.67	-9	0	6	0.80*	0.91	9	2	6	2.10*	0.58	-7	6	6	3.89	3.42
-4	-7	6	2.10*	1.62	8	-4	6	9.86	11.22	-8	0	6	10.40	10.07	10	2	6	2.65	2.54	-6	6	6	2.29*	1.50
-3	-7	6	0.75*	1.75	-9	-3	6	0.80*	0.08	-7	0	6	7.41	7.32	-8	3	6	3.16	2.81	-5	6	6	0.77*	2.29
-2	-7	6	15.25	15.37	-8	-3	6	5.46	5.80	-6	0	6	17.12	17.28	-7	3	6	7.58	7.66	-4	6	6	4.46	5.00
-1	-7	6	31.01	32.15	-7	-3	6	10.78	9.90	-5	0	6	7.45	9.04	-6	3	6	12.30	12.95	-3	6	6	16.27	17.02
0	-7	6	12.69	12.60	-6	-3	6	3.82	6.24	-4	0	6	18.24	16.81	-5	3	6	8.63	8.25	-2	6	6	19.88	20.10
1	-7	6	10.41	10.57	-5	-3	6	17.65	14.81	-3	0	6	10.60	9.04	-4	3	6	7.29	7.09	-1	6	6	26.33	27.07
2	-7	6	6.41	5.22	-4	-3	6	20.10	22.47	-2	0	6	3.70	2.31	-3	3	6	1.66*	0.76	0	6	6	11.84	11.26
3	-7	6	0.77*	2.58	-3	-3	6	6.19	7.56	-1	0	6	33.10	31.85	-2	3	6	17.05	18.86	1	6	6	8.87	9.57
4	-7	6	2.19*	1.84	-2	-3	6	5.70	5.15	0	0	6	11.52	11.27	-1	3	6	6.36	5.35	2	6	6	7.41	8.16
5	-7	6	2.98	3.09	-1	-3	6	7.47	6.65	1	0	6	27.06	27.42	0	3	6	20.60	21.58	3	6	6	6.20	6.23
-8	-6	6	8.89	8.67	0	-3	6	6.18	6.18	2	0	6	30.52	31.63	1	3	6	24.97	24.04	4	6	6	12.31	11.11
-7	-6	6	6.79	7.47	1	-3	6	3.40	1.81	3	0	6	12.11	12.98	2	3	6	17.20	15.34	5	6	6	16.86	16.08
-6	-6	6	4.63	4.40	2	-3	6	4.30	5.18	4	0	6	2.08*	0.59	3	3	6	4.77	4.02	6	6	6	21.38	21.81
-5	-6	6	1.76*	2.99	3	-3	6	17.83	16.95	5	0	6	14.37	14.22	4	3	6	3.95	2.15	7	6	6	1.69*	2.15
-4	-6	6	15.26	14.39	4	-3	6	13.22	13.93	6	0	6	0.73*	0.20	5	3	6	21.31	23.59	8	6	6	1.57*	1.34
-3	-6	6	3.23	3.91	5	-3	6	17.21	16.16	7	0	6	7.87	7.22	6	3	6	3.92	5.13	9	6	6	3.26	3.44
-2	-6	6	1.06*	0.49	6	-3	6	5.65	7.15	8	0	6	7.96	7.60	7	3	6	2.21*	0.93	10	6	6	0.82*	2.02
-1	-6	6	3.51	3.23	7	-3	6	10.69	9.38	9	0	6	4.30	4.86	8	3	6	12.26	12.45	-6	7	6	2.79	2.87
0	-6	6	4.16	4.41	8	-3	6	7.12	7.98	10	0	6	3.56	3.01	9	3	6	0.78*	0.27	-5	7	6	1.19*	0.17
1	-6	6	15.46	15.75	-9	-2	6	2.78	2.64	-9	1	6	1.33*	0.83	10	3	6	1.96*	1.26	-4	7	6	5.06	5.51
2	-6	6	3.27	3.49	-8	-2	6	0.77*	2.11	-8	1	6	2.33*	2.62	-8	4	6	0.80*	0.40	-3	7	6	4.35	4.47
3	-6	6	6.05	5.96	-7	-2	6	1.51*	0.77	-7	1	6	8.59	7.77	-7	4	6	2.21*	1.09	-2	7	6	13.32	13.66
4	-6	6	1.76*	0.77	-6	-2	6	13.71	12.24	-6	1	6	11.50	11.67	-6	4	6	2.94	2.12	-1	7	6	6.62	6.73
5	-6	6	3.50	5.58	-5	-2	6	2.13*	0.72	-5	1	6	7.75	7.54	-5	4	6	13.88	13.76	0	7	6	0.72*	0.23
6	-6	6	6.54	5.73	-4	-2	6	0.70*	3.01	-4	1	6	20.79	20.22	-4	4	6	22.23	22.93	1	7	6	2.04*	3.85
-8	-5	6	0.79*	1.51	-3	-2	6	6.20	8.33	-3	1	6	20.94	20.80	-3	4	6	7.74	7.98	2	7	6	7.90	7.33
-7	-5	6	16.13	13.99	-2	-2	6	6.06	4.78	-2	1	6	15.55	16.01	-2	4	6	8.30	7.83	3	7	6	1.36*	0.20
-6	-5	6	23.07	24.91	-1	-2	6	5.62	6.80	-1	1	6	13.27	12.06	-1	4	6	8.78	8.25	4	7	6	5.55	5.71
-5	-5	6	5.41	2.75	0	-2	6	10.62	9.22	0	1	6	6.05	6.33	0	4	6	10.89	11.29	5	7	6	18.02	18.53
-4	-5	6	15.42	13.75	1	-2	6	15.20	15.14	1	1	6	34.56	33.88	1	4	6	11.61	11.79	6	7	6	17.26	17.32
-3	-5	6	7.11	7.40	2	-2	6	2.38	1.53	2	1	6	10.35	11.95	2	4	6	16.46	17.43	7	7	6	1.65*	2.05
-2	-5	6	10.60	10.48	3	-2	6	15.90	16.55	3	1	6	28.18	28.59	3	4	6	15.45	15.14	8	7	6	16.56	16.54
-1	-5	6	15.53	16.15	4	-2	6	14.78	14.18	4	1	6	20.07	17.49	4	4	6	18.17	17.99	9	7	6	5.67	5.68
0	-5	6	4.48	5.32	5	-2	6	0.74*	0.11	5	1	6	14.54	15.84	5	4	6	12.59	11.50	10	7	6	0.82*	0.75
1	-5	6	7.12	7.65	6	-2	6	17.64	16.23	6	1	6	7.51	7.59	6	4	6	26.59	27.58	-6	8	6	4.83	4.42
2	-5	6	9.22	8.74	7	-2	6	18.30	18.67	7	1	6	7.62	6.75	7	4	6	11.52	11.45	-5	8	6	5.03	4.10
3	-5	6	5.62	4.55	8	-2	6	6.60	6.32	8	1	6	7.19	6.94	8	4	6	11.86	11.49	-4	8	6	6.62	7.38
4	-5	6	15.50	16.51	9	-2	6	5.57	5.83	9	1	6	2.18*	1.19	9	4	6	3.28	3.41	-3	8	6	10.40	9.64

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	8	6	4.41	4.63	4	12	6	5.43	5.74	-8	-4	7	0.82*	0.85	0	-1	7	12.06	12.74	4	2	7	6.40	6.47
-1	8	6	16.37	17.41	5	12	6	0.82*	0.90	-7	-4	7	0.80*	3.67	1	-1	7	29.81	30.23	5	2	7	18.70	18.95
0	8	6	7.66	6.58	6	12	6	5.76	5.96	-6	-4	7	2.50*	1.65	2	-1	7	10.72	10.65	6	2	7	14.20	14.89
1	8	6	10.62	11.24	3	13	6	12.09	11.91	-5	-4	7	17.77	18.05	3	-1	7	6.39	5.74	7	2	7	0.75*	0.48
2	8	6	1.70*	1.63	-4	-9	7	3.57	2.81	-4	-4	7	32.21	31.40	4	-1	7	11.14	11.72	8	2	7	9.61	9.54
3	8	6	10.86	11.15	-3	-9	7	0.80*	1.02	-3	-4	7	4.62	3.74	5	-1	7	13.95	13.42	9	2	7	4.74	5.48
4	8	6	5.22	5.20	-2	-9	7	1.46*	1.45	-2	-4	7	6.85	6.23	6	-1	7	15.01	14.59	10	2	7	0.82*	0.31
5	8	6	1.90*	1.66	-1	-9	7	2.79	2.86	-1	-4	7	13.25	14.04	7	-1	7	1.94*	0.32	-8	3	7	3.65	3.18
6	8	6	7.60	7.39	0	-9	7	6.97	6.73	0	-4	7	18.16	18.01	8	-1	7	6.70	7.53	-7	3	7	3.24	4.10
7	8	6	16.18	16.39	-5	-8	7	6.01	5.58	1	-4	7	4.24	4.02	9	-1	7	3.53	2.84	-6	3	7	1.31*	0.21
8	8	6	5.58	5.51	-4	-8	7	2.39*	1.95	2	-4	7	5.01	4.59	-8	0	7	6.98	7.23	-5	3	7	2.30*	2.01
9	8	6	0.79*	0.95	-3	-8	7	2.83	2.78	3	-4	7	1.67*	2.08	-7	0	7	3.76	3.62	-4	3	7	8.06	7.44
10	8	6	2.82	2.90	-2	-8	7	3.07	2.01	4	-4	7	18.53	18.79	-6	0	7	2.55	1.30	-3	3	7	17.83	18.14
-5	9	6	0.82*	0.47	-1	-8	7	3.35	2.76	5	-4	7	9.48	9.13	-5	0	7	6.06	5.22	-2	3	7	18.64	18.49
-4	9	6	9.92	10.16	0	-8	7	5.61	5.86	6	-4	7	0.80*	1.84	-4	0	7	12.15	10.93	-1	3	7	17.07	16.75
-3	9	6	2.40*	2.64	1	-8	7	3.86	4.01	7	-4	7	2.40*	3.40	-3	0	7	1.58*	4.17	0	3	7	5.84	5.80
-2	9	6	6.06	5.50	2	-8	7	0.78*	0.46	-8	-3	7	5.47	5.26	-2	0	7	11.41	10.06	1	3	7	3.77	3.00
-1	9	6	7.67	7.91	3	-8	7	0.82*	0.77	-7	-3	7	5.91	6.16	-1	0	7	20.54	23.57	2	3	7	22.87	24.63
0	9	6	11.13	10.71	-7	-7	7	4.59	4.83	-6	-3	7	12.57	11.03	0	0	7	30.69	30.25	3	3	7	26.76	26.06
1	9	6	14.29	15.90	-6	-7	7	11.51	11.01	-5	-3	7	7.18	9.37	1	0	7	4.30	4.14	4	3	7	1.02*	0.63
2	9	6	14.30	14.18	-5	-7	7	1.85*	1.79	-4	-3	7	31.86	29.69	2	0	7	1.74*	1.08	5	3	7	10.63	9.92
3	9	6	12.74	13.68	-4	-7	7	6.29	6.06	-3	-3	7	27.87	26.34	3	0	7	29.03	29.81	6	3	7	12.05	13.25
4	9	6	10.43	10.77	-3	-7	7	5.94	5.99	-2	-3	7	16.09	16.78	4	0	7	10.83	10.77	7	3	7	2.97	1.79
5	9	6	7.03	7.23	-2	-7	7	0.77*	1.92	-1	-3	7	21.52	21.16	5	0	7	2.10*	0.70	8	3	7	3.11	3.46
6	9	6	7.27	7.25	-1	-7	7	19.83	19.63	0	-3	7	15.01	15.67	6	0	7	3.04	2.55	9	3	7	0.79*	0.12
7	9	6	0.78*	1.78	0	-7	7	10.86	11.86	1	-3	7	13.75	14.53	7	0	7	3.22	1.91	10	3	7	0.80*	0.84
8	9	6	4.74	5.02	1	-7	7	2.96	3.62	2	-3	7	26.98	27.71	8	0	7	2.43*	3.74	-7	4	7	4.70	4.03
9	9	6	4.19	3.62	2	-7	7	7.40	8.12	3	-3	7	25.18	25.65	9	0	7	3.58	3.21	-6	4	7	5.57	6.31
-4	10	6	4.68	4.03	3	-7	7	3.26	2.36	4	-3	7	0.75*	1.35	-8	1	7	6.46	6.07	-5	4	7	6.98	7.77
-3	10	6	0.80*	1.01	4	-7	7	4.77	3.66	5	-3	7	2.30*	0.86	-7	1	7	7.09	7.55	-4	4	7	11.38	11.46
-2	10	6	5.90	5.92	-7	-6	7	7.34	6.48	6	-3	7	5.04	6.00	-6	1	7	23.05	23.42	-3	4	7	5.26	4.72
-1	10	6	4.65	4.79	-6	-6	7	10.36	11.63	7	-3	7	0.79*	0.01	-5	1	7	0.74*	0.80	-2	4	7	9.17	9.43
0	10	6	7.63	7.35	-5	-6	7	3.24	2.88	8	-3	7	3.82	3.25	-4	1	7	8.30	9.13	-1	4	7	4.63	3.81
1	10	6	3.16	2.89	-4	-6	7	10.13	9.26	-8	-2	7	4.39	3.53	-3	1	7	1.07*	0.41	0	4	7	18.21	18.09
2	10	6	10.16	10.86	-3	-6	7	2.25*	0.56	-7	-2	7	0.78*	2.17	-2	1	7	7.33	6.54	1	4	7	5.29	5.45
3	10	6	5.62	4.96	-2	-6	7	2.29*	3.31	-6	-2	7	3.76	5.42	-1	1	7	15.66	15.58	2	4	7	19.44	19.22
4	10	6	7.65	8.38	-1	-6	7	8.65	7.75	-5	-2	7	23.46	22.36	0	1	7	14.23	13.43	3	4	7	2.21	0.78
5	10	6	13.35	13.88	0	-6	7	9.53	10.02	-4	-2	7	0.73*	2.38	1	1	7	16.97	17.73	4	4	7	15.20	14.99
6	10	6	8.43	8.57	1	-6	7	19.20	20.08	-3	-2	7	16.15	14.82	2	1	7	7.80	6.26	5	4	7	15.07	15.60
7	10	6	6.06	5.67	2	-6	7	6.28	6.59	-2	-2	7	34.54	36.41	3	1	7	4.79	4.15	6	4	7	13.03	12.71
8	10	6	8.31	9.00	3	-6	7	7.80	6.94	-1	-2	7	6.15	5.14	4	1	7	7.42	5.46	7	4	7	3.53	3.72
9	10	6	3.67	3.50	4	-6	7	2.06*	2.52	0	-2	7	4.52	5.08	5	1	7	8.16	6.54	8	4	7	4.44	5.05
-2	11	6	6.28	5.79	5	-6	7	6.33	6.08	1	-2	7	9.60	9.71	6	1	7	23.19	23.74	9	4	7	4.55	4.01
-1	11	6	5.37	6.48	-8	-5	7	7.67	6.52	2	-2	7	4.92	5.70	7	1	7	3.55	3.72	10	4	7	1.89*	1.17
0	11	6	11.81	11.71	-7	-5	7	5.75	6.54	3	-2	7	14.13	13.48	8	1	7	1.75*	2.11	-7	5	7	2.98	3.00
1	11	6	7.50	7.33	-6	-5	7	13.42	11.87	4	-2	7	10.57	11.21	9	1	7	1.37*	1.38	-6	5	7	3.07	2.75
2	11	6	5.81	6.64	-5	-5	7	3.87	1.79	5	-2	7	16.92	16.36	-8	2	7	0.82*	2.02	-5	5	7	3.50	2.88
3	11	6	1.87*	1.84	-4	-5	7	4.94	3.99	6	-2	7	4.80	5.95	-7	2	7	5.72	5.22	-4	5	7	5.97	5.64
4	11	6	3.86	4.01	-3	-5	7	2.44	2.43	7	-2	7	2.11*	1.69	-6	2	7	1.66*	0.63	-3	5	7	18.87	19.25
5	11	6	3.91	4.07	-2	-5	7	0.73*	0.90	8	-2	7	2.69	0.53	-5	2	7	11.38	12.02	-2	5	7	21.08	20.89
6	11	6	11.87	12.43	-1	-5	7	9.56	8.89	-8	-1	7	10.45	10.49	-4	2	7	20.30	19.56	-1	5	7	9.52	9.88
7	11	6	5.79	6.05	0	-5	7	11.07	11.78	-7	-1	7	5.97	5.17	-3	2	7	2.39	1.38	0	5	7	9.19	9.56
8	11	6	3.85	3.59	1	-5	7	10.58	10.37	-6	-1	7	6.51	6.17	-2	2	7	6.55	5.77	1	5	7	18.51	19.65
-1	12	6	5.08	5.23	2	-5	7	11.01	10.99	-5	-1	7	5.18	5.30	-1	2	7	10.82	11.74	2	5	7	2.05*	0.47
0	12	6	11.86	11.24	3	-5	7	13.27	14.84	-4	-1	7	0.73*	2.29	0	2	7	7.71	8.03	3	5	7	11.72	12.67
1	12	6	9.47	10.30	4	-5	7	4.49	3.28	-3	-1	7	21.90	20.44	1	2	7	3.72	3.88	4	5	7	7.56	7.39
2	12	6	3.40	3.55	5	-5	7	9.94	11.17	-2	-1	7	10.24	8.34	2	2	7	12.26	12.21	5	5	7	2.74	2.36
3	12	6	2.64	3.04	6	-5	7	2.11*	1.75	-1	-1	7	17.46	15.56	3	2	7	3.33	3.26	6	5	7	24.00	24.28

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	5	7	15.17	15.45	0	9	7	8.74	9.11	-2	-6	8	3.47	4.15	0	-2	8	35.18	35.02	6	1	8	18.65	19.17
8	5	7	8.31	8.07	1	9	7	14.53	14.32	-1	-6	8	6.05	6.43	1	-2	8	11.80	12.06	7	1	8	9.47	9.55
9	5	7	4.13	4.13	2	9	7	7.60	8.07	0	-6	8	10.99	11.09	2	-2	8	5.67	6.20	8	1	8	1.46*	0.14
10	5	7	1.35*	2.38	3	9	7	0.74*	0.90	1	-6	8	20.16	20.53	3	-2	8	7.67	7.89	9	1	8	6.67	6.24
-7	6	7	0.83*	0.57	4	9	7	2.18*	1.88	2	-6	8	3.19	4.04	4	-2	8	1.46*	2.65	-8	2	8	1.41*	2.29
-6	6	7	1.99*	0.39	5	9	7	0.75*	0.47	3	-6	8	2.19*	2.08	5	-2	8	7.92	8.57	-7	2	8	6.48	6.72
-5	6	7	0.77*	0.64	6	9	7	9.19	8.71	4	-6	8	8.67	8.12	6	-2	8	1.85*	0.89	-6	2	8	3.28	3.54
-4	6	7	1.62*	1.89	7	9	7	1.75*	0.21	-7	-5	8	9.60	8.32	7	-2	8	6.49	6.65	-5	2	8	2.10*	2.20
-3	6	7	6.40	6.41	8	9	7	0.79*	2.35	-6	-5	8	4.13	5.93	8	-2	8	4.53	4.53	-4	2	8	8.86	10.42
-2	6	7	19.44	19.25	9	9	7	6.16	6.66	-5	-5	8	9.68	8.18	-8	-1	8	4.09	4.69	-3	2	8	4.57	3.96
-1	6	7	28.28	27.79	-3	10	7	2.25*	1.67	-4	-5	8	8.48	10.16	-7	-1	8	4.11	3.78	-2	2	8	5.89	4.31
0	6	7	35.45	36.59	-2	10	7	1.82*	2.13	-3	-5	8	5.56	6.02	-6	-1	8	1.14*	0.29	-1	2	8	20.40	19.35
1	6	7	32.45	33.72	-1	10	7	0.79*	0.98	-2	-5	8	1.61*	1.43	-5	-1	8	2.14*	1.53	0	2	8	9.74	9.91
2	6	7	13.45	12.67	0	10	7	7.29	8.08	-1	-5	8	4.79	4.33	-4	-1	8	7.53	6.56	1	2	8	11.69	10.98
3	6	7	20.13	20.44	1	10	7	5.89	6.19	0	-5	8	0.75*	0.74	-3	-1	8	4.92	6.83	2	2	8	5.52	4.87
4	6	7	15.92	16.54	2	10	7	4.06	4.00	1	-5	8	5.36	5.40	-2	-1	8	13.86	12.75	3	2	8	8.94	8.15
5	6	7	12.44	12.69	3	10	7	7.12	7.37	2	-5	8	0.77*	1.37	-1	-1	8	16.31	17.48	4	2	8	1.84*	1.52
6	6	7	15.29	16.38	4	10	7	0.77*	0.71	3	-5	8	23.99	23.15	0	-1	8	9.97	9.05	5	2	8	7.02	6.99
7	6	7	0.75*	1.05	5	10	7	8.04	7.65	4	-5	8	2.46*	3.61	1	-1	8	15.41	15.72	6	2	8	6.73	5.70
8	6	7	8.84	9.15	6	10	7	0.78*	0.84	5	-5	8	1.87*	1.74	2	-1	8	7.28	7.65	7	2	8	7.43	7.65
9	6	7	6.74	6.21	7	10	7	4.16	4.46	-7	-4	8	0.80*	1.33	3	-1	8	12.16	12.58	8	2	8	11.87	12.57
10	6	7	0.83*	0.12	8	10	7	8.34	8.50	-6	-4	8	7.79	7.74	4	-1	8	15.39	15.05	9	2	8	3.08	2.55
-6	7	7	2.48*	2.40	-2	11	7	6.00	6.75	-5	-4	8	12.08	11.40	5	-1	8	4.13	3.77	-7	3	8	2.96	3.18
-5	7	7	0.79*	2.03	-1	11	7	0.80*	1.29	-4	-4	8	18.71	20.06	6	-1	8	5.99	5.74	-6	3	8	4.14	3.58
-4	7	7	3.85	3.41	0	11	7	1.97*	0.50	-3	-4	8	2.35*	3.43	7	-1	8	6.26	6.67	-5	3	8	4.90	5.51
-3	7	7	3.19	3.66	1	11	7	1.25*	0.32	-2	-4	8	8.78	8.64	8	-1	8	3.22	2.18	-4	3	8	3.37	2.82
-2	7	7	2.31*	1.34	2	11	7	2.58	2.18	-1	-4	8	3.41	3.95	-8	0	8	1.67*	0.12	-3	3	8	0.73*	0.21
-1	7	7	17.77	17.85	3	11	7	3.33	3.69	0	-4	8	5.55	5.48	-7	0	8	0.79*	0.10	-2	3	8	9.57	9.99
0	7	7	8.99	7.97	4	11	7	13.45	13.59	1	-4	8	5.79	5.99	-6	0	8	7.70	9.32	-1	3	8	12.73	14.13
1	7	7	2.16*	3.25	5	11	7	2.02*	1.11	2	-4	8	3.11	3.14	-5	0	8	4.67	3.10	0	3	8	12.10	12.85
2	7	7	9.96	10.95	6	11	7	0.82*	2.43	3	-4	8	12.98	12.94	-4	0	8	2.53	0.62	1	3	8	11.43	12.18
3	7	7	16.82	17.42	7	11	7	9.19	9.01	4	-4	8	0.79*	1.61	-3	0	8	8.15	6.67	2	3	8	10.28	9.12
4	7	7	12.09	12.79	0	12	7	7.42	8.43	5	-4	8	11.35	11.09	-2	0	8	4.80	5.62	3	3	8	27.09	26.37
5	7	7	3.18	3.19	1	12	7	0.83*	3.26	6	-4	8	5.04	4.70	-1	0	8	25.04	23.92	4	3	8	13.91	15.14
6	7	7	22.41	22.15	2	12	7	6.83	6.48	-8	-3	8	0.82*	0.46	0	0	8	14.20	14.64	5	3	8	3.65	4.99
7	7	7	14.62	15.23	3	12	7	4.14	4.14	-7	-3	8	1.42*	0.34	1	0	8	15.80	15.63	6	3	8	3.62	3.75
8	7	7	1.92*	0.79	4	12	7	6.51	5.90	-6	-3	8	1.42*	2.09	2	0	8	2.52	1.67	7	3	8	4.26	3.49
9	7	7	4.59	3.97	5	12	7	5.97	6.05	-5	-3	8	4.69	2.83	3	0	8	5.84	5.71	8	3	8	5.55	5.65
10	7	7	4.04	4.28	6	12	7	3.77	3.07	-4	-3	8	9.87	8.11	4	0	8	17.45	17.70	9	3	8	6.15	6.18
-5	8	7	4.19	4.64	-4	-8	8	2.59*	3.67	-3	-3	8	28.17	29.50	5	0	8	3.76	3.54	-7	4	8	5.63	6.00
-4	8	7	1.43*	2.29	-3	-8	8	1.14*	0.64	-2	-3	8	43.52	42.63	6	0	8	16.07	16.60	-6	4	8	5.57	5.48
-3	8	7	1.67*	0.38	-2	-8	8	6.72	7.04	-1	-3	8	5.41	6.50	7	0	8	3.08	3.23	-5	4	8	3.17	3.88
-2	8	7	0.75*	0.03	-1	-8	8	5.85	5.85	0	-3	8	3.27	2.50	8	0	8	2.83	2.09	-4	4	8	7.03	6.95
-1	8	7	3.84	3.55	0	-8	8	1.52*	0.37	1	-3	8	5.91	5.92	9	0	8	0.83*	0.27	-3	4	8	3.04	2.87
0	8	7	2.63	1.70	1	-8	8	1.48*	0.76	2	-3	8	1.47*	1.47	-8	1	8	7.29	7.58	-2	4	8	4.62	4.28
1	8	7	10.67	10.74	-5	-7	8	2.00*	0.92	3	-3	8	6.91	8.16	-7	1	8	1.33*	1.54	-1	4	8	2.65	3.31
2	8	7	10.45	10.46	-4	-7	8	2.54*	3.74	4	-3	8	2.77	0.74	-6	1	8	8.02	9.15	0	4	8	21.82	23.06
3	8	7	4.78	4.10	-3	-7	8	5.70	5.77	5	-3	8	6.28	4.92	-5	1	8	5.82	5.06	1	4	8	11.80	12.23
4	8	7	2.97	2.48	-2	-7	8	4.57	4.38	6	-3	8	1.45*	0.23	-4	1	8	2.10*	1.90	2	4	8	17.30	17.92
5	8	7	11.03	11.39	-1	-7	8	3.04	3.08	7	-3	8	1.57*	1.47	-3	1	8	5.31	5.31	3	4	8	19.29	18.59
6	8	7	22.08	22.87	0	-7	8	10.40	10.00	-8	-2	8	9.45	8.55	-2	1	8	2.98	2.40	4	4	8	12.91	12.49
7	8	7	6.18	6.45	1	-7	8	4.25	4.00	-7	-2	8	8.36	9.57	-1	1	8	1.87*	0.33	5	4	8	26.12	25.31
8	8	7	10.01	9.66	2	-7	8	1.35*	1.57	-6	-2	8	13.70	12.57	0	1	8	7.42	6.26	6	4	8	2.96	2.85
9	8	7	2.97	2.61	3	-7	8	4.82	3.68	-5	-2	8	11.89	13.63	1	1	8	18.87	18.31	7	4	8	5.96	5.63
-4	9	7	5.75	5.09	-6	-6	8	4.54	3.63	-4	-2	8	22.92	22.38	2	1	8	1.07*	0.15	8	4	8	9.86	10.18
-3	9	7	7.07	7.01	-5	-6	8	2.60	0.16	-3	-2	8	0.75*	1.65	3	1	8	5.32	5.29	9	4	8	2.88	1.77
-2	9	7	7.41	7.90	-4	-6	8	7.92	8.70	-2	-2	8	4.63	3.71	4	1	8	7.72	7.26	-6	5	8	4.93	4.94
-1	9	7	16.23	16.30	-3	-6	8	12.62	11.83	-1	-2	8	32.80	33.26	5	1	8	12.00	12.63	-5	5	8	7.03	7.13

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-4	5	8	12.04	12.77	8	8	8	4.55	3.92	-3	-5	9	1.86*	2.11	2	-1	9	14.56	15.78	-4	3	9	1.53*	1.95
-3	5	8	6.14	5.88	9	8	8	0.80*	0.58	-2	-5	9	9.58	8.49	3	-1	9	7.33	7.66	-3	3	9	4.67	4.42
-2	5	8	10.40	11.44	-4	9	8	10.04	8.71	-1	-5	9	7.33	8.46	4	-1	9	8.10	7.01	-2	3	9	1.36*	0.78
-1	5	8	4.21	4.10	-3	9	8	7.19	6.86	0	-5	9	8.26	8.31	5	-1	9	6.82	6.99	-1	3	9	11.65	11.44
0	5	8	6.01	5.99	-2	9	8	2.74	2.51	1	-5	9	11.52	11.25	6	-1	9	6.83	6.56	0	3	9	15.12	15.63
1	5	8	10.98	10.97	-1	9	8	5.48	6.14	2	-5	9	5.50	4.93	7	-1	9	6.11	6.18	1	3	9	16.12	16.29
2	5	8	8.83	10.29	0	9	8	6.00	5.57	3	-5	9	11.28	12.10	-7	0	9	1.61*	1.25	2	3	9	6.31	5.71
3	5	8	11.67	11.65	1	9	8	1.28*	0.42	4	-5	9	3.16	2.93	-6	0	9	11.84	11.35	3	3	9	2.60	2.53
4	5	8	6.84	7.16	2	9	8	1.58*	1.21	-6	-4	9	5.14	5.24	-5	0	9	3.81	2.13	4	3	9	1.17*	0.46
5	5	8	12.21	12.35	3	9	8	6.62	6.41	-5	-4	9	0.79*	0.09	-4	0	9	4.45	2.45	5	3	9	17.73	19.19
6	5	8	4.87	5.45	4	9	8	6.38	6.63	-4	-4	9	6.57	5.16	-3	0	9	0.74*	1.10	6	3	9	7.66	7.94
7	5	8	8.54	8.23	5	9	8	2.49*	2.67	-3	-4	9	0.77*	0.66	-2	0	9	4.97	4.20	7	3	9	2.20*	2.19
8	5	8	7.50	7.48	6	9	8	2.75	1.91	-2	-4	9	0.77*	0.90	-1	0	9	0.72*	0.09	8	3	9	3.76	3.40
9	5	8	1.31*	2.19	7	9	8	5.11	4.93	-1	-4	9	3.22	3.06	0	0	9	4.78	3.93	9	3	9	1.46*	1.33
-6	6	8	1.77*	1.38	8	9	8	6.55	6.60	0	-4	9	12.28	12.22	1	0	9	22.58	23.11	-6	4	9	2.94	2.36
-5	6	8	2.11*	2.09	-3	10	8	4.57	4.11	1	-4	9	8.55	9.32	2	0	9	7.11	7.04	-5	4	9	0.78*	0.64
-4	6	8	1.46*	1.93	-2	10	8	5.87	5.36	2	-4	9	4.38	3.87	3	0	9	7.79	8.09	-4	4	9	0.78*	0.67
-3	6	8	11.01	10.35	-1	10	8	7.53	7.81	3	-4	9	10.15	10.22	4	0	9	3.75	3.89	-3	4	9	7.74	7.64
-2	6	8	1.09*	2.87	0	10	8	5.45	5.09	4	-4	9	2.16*	0.52	5	0	9	1.58*	0.45	-2	4	9	6.75	6.96
-1	6	8	43.82	44.74	1	10	8	1.47*	1.13	5	-4	9	19.72	19.48	6	0	9	6.15	5.46	-1	4	9	14.98	15.41
0	6	8	28.57	28.15	2	10	8	6.50	6.65	-7	-3	9	6.73	5.49	7	0	9	2.21*	0.82	0	4	9	5.68	5.90
1	6	8	7.02	7.22	3	10	8	9.31	8.97	-6	-3	9	4.43	6.42	8	0	9	5.45	4.55	1	4	9	12.71	12.66
2	6	8	6.29	7.34	4	10	8	4.16	4.12	-5	-3	9	3.01	0.99	-7	1	9	0.83*	1.93	2	4	9	10.36	11.18
3	6	8	14.23	14.97	5	10	8	5.79	5.68	-4	-3	9	1.65*	1.18	-6	1	9	4.62	4.00	3	4	9	13.79	14.08
4	6	8	24.57	25.31	6	10	8	3.07	2.89	-3	-3	9	5.29	4.31	-5	1	9	0.78*	0.40	4	4	9	7.81	8.06
5	6	8	17.88	18.19	7	10	8	3.11	3.22	-2	-3	9	6.05	6.64	-4	1	9	6.09	7.01	5	4	9	17.39	17.07
6	6	8	7.13	6.09	8	10	8	8.99	8.32	-1	-3	9	8.74	9.22	-3	1	9	5.13	5.89	6	4	9	2.74	2.08
7	6	8	2.30*	1.77	-1	11	8	0.82*	0.33	0	-3	9	5.80	5.52	-2	1	9	0.74*	0.20	7	4	9	3.41	2.55
8	6	8	1.48*	1.50	0	11	8	1.58*	2.48	1	-3	9	0.74*	0.37	-1	1	9	3.51	4.75	8	4	9	0.79*	0.01
9	6	8	1.85*	0.53	1	11	8	1.19*	0.59	2	-3	9	9.87	9.25	0	1	9	18.86	18.80	9	4	9	0.82*	0.27
-5	7	8	8.50	8.48	2	11	8	2.20*	1.95	3	-3	9	2.41*	4.21	1	1	9	3.33	5.03	-6	5	9	10.11	9.88
-4	7	8	2.52*	2.97	3	11	8	4.50	4.74	4	-3	9	2.62	2.07	2	1	9	19.00	19.77	-5	5	9	6.73	6.01
-3	7	8	0.77*	0.44	4	11	8	3.01	3.20	5	-3	9	12.21	12.38	3	1	9	17.83	17.34	-4	5	9	6.74	6.72
-2	7	8	0.75*	0.72	5	11	8	7.27	7.04	6	-3	9	2.57*	1.29	4	1	9	1.85*	1.99	-3	5	9	6.05	5.68
-1	7	8	0.77*	1.72	6	11	8	2.88	3.66	-7	-2	9	8.12	6.78	5	1	9	3.24	2.20	-2	5	9	3.81	3.94
0	7	8	4.38	4.05	7	11	8	3.01	3.20	-6	-2	9	4.99	4.25	6	1	9	10.34	9.70	-1	5	9	1.60*	2.19
1	7	8	37.73	39.27	1	12	8	0.82*	0.76	-5	-2	9	9.58	10.44	7	1	9	3.33	3.34	0	5	9	5.56	5.52
2	7	8	22.94	22.51	2	12	8	4.90	5.28	-4	-2	9	5.67	4.99	8	1	9	2.15*	3.12	1	5	9	7.86	6.98
3	7	8	16.88	16.46	3	12	8	1.47*	1.63	-3	-2	9	7.08	6.84	-7	2	9	4.62	4.24	2	5	9	2.58	2.92
4	7	8	2.46	2.03	4	12	8	0.82*	1.30	-2	-2	9	1.89*	1.76	-6	2	9	9.77	9.61	3	5	9	1.07*	1.01
5	7	8	2.13*	2.25	5	12	8	0.84*	1.72	-1	-2	9	28.61	28.18	-5	2	9	2.21*	2.60	4	5	9	1.71*	1.59
6	7	8	5.08	5.52	-3	-7	9	9.77	9.28	0	-2	9	15.22	15.67	-4	2	9	16.72	16.78	5	5	9	1.51*	1.53
7	7	8	3.43	2.85	-2	-7	9	5.06	5.63	1	-2	9	10.92	11.15	-3	2	9	3.01	4.12	6	5	9	9.51	9.16
8	7	8	3.13	3.44	-1	-7	9	1.85*	1.03	2	-2	9	9.13	8.29	-2	2	9	9.45	7.96	7	5	9	13.66	14.32
9	7	8	2.00*	0.23	0	-7	9	4.52	5.02	3	-2	9	2.06*	1.02	-1	2	9	5.75	4.13	8	5	9	8.04	7.63
-5	8	8	1.84*	1.65	1	-7	9	0.82*	0.13	4	-2	9	5.06	6.16	0	2	9	9.73	8.09	9	5	9	5.16	5.05
-4	8	8	4.44	5.46	-5	-6	9	3.76	2.20	5	-2	9	14.42	13.96	1	2	9	2.31	0.76	-5	6	9	7.62	7.82
-3	8	8	1.79*	2.49	-4	-6	9	6.36	5.73	6	-2	9	8.35	8.21	2	2	9	1.50*	0.24	-4	6	9	7.43	7.62
-2	8	8	2.62	2.43	-3	-6	9	0.80*	2.63	7	-2	9	7.22	7.68	3	2	9	8.45	9.58	-3	6	9	6.35	7.05
-1	8	8	5.29	5.97	-2	-6	9	8.07	7.86	-7	-1	9	6.93	7.31	4	2	9	1.12*	0.51	-2	6	9	5.36	5.31
0	8	8	0.75*	0.47	-1	-6	9	10.74	9.80	-6	-1	9	7.51	7.66	5	2	9	12.69	12.43	-1	6	9	0.75*	1.08
1	8	8	15.06	14.91	0	-6	9	3.12	3.18	-5	-1	9	10.52	9.82	6	2	9	6.83	6.51	0	6	9	2.35*	2.25
2	8	8	1.40*	0.12	1	-6	9	4.38	3.55	-4	-1	9	1.67*	2.87	7	2	9	1.65*	0.45	1	6	9	11.12	11.01
3	8	8	11.61	12.60	2	-6	9	6.89	6.88	-3	-1	9	2.82	1.10	8	2	9	11.70	11.93	2	6	9	9.01	9.06
4	8	8	12.60	12.28	3	-6	9	2.79	3.66	-2	-1	9	2.30*	0.21	9	2	9	3.95	3.83	3	6	9	3.42	2.94
5	8	8	15.95	16.21	-6	-5	9	5.95	5.20	-1	-1	9	19.53	18.23	-7	3	9	2.31*	2.60	4	6	9	2.69	2.18
6	8	8	4.96	4.48	-5	-5	9	1.53*	2.65	0	-1	9	18.33	18.74	-6	3	9	1.53*	1.99	5	6	9	0.74*	0.30
7	8	8	3.92	3.35	-4	-5	9	5.73	5.10	1	-1	9	18.33	18.10	-5	3	9	3.37	2.78	6	6	9	0.77*	0.52

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	6	9	13.47	14.15	6	11	9	6.51	6.78	5	-1	10	4.87	5.24	6	3	10	4.43	4.42	-2	8	10	3.08	3.11
8	6	9	2.02*	1.81	-2	-6	10	3.71	4.02	6	-1	10	7.42	6.65	7	3	10	0.79*	0.83	-1	8	10	5.43	5.16
9	6	9	7.27	7.28	-1	-6	10	3.19	2.83	7	-1	10	8.21	8.63	8	3	10	4.78	4.29	0	8	10	3.57	3.88
-5	7	9	0.83*	0.55	0	-6	10	6.30	5.98	-6	0	10	6.60	7.30	-5	4	10	0.80*	0.99	1	8	10	3.46	2.52
-4	7	9	7.57	7.44	1	-6	10	3.52	3.59	-5	0	10	7.60	6.18	-4	4	10	1.36*	0.05	2	8	10	3.06	3.55
-3	7	9	20.25	19.65	-4	-5	10	2.57*	1.93	-4	0	10	4.70	2.78	-3	4	10	2.13*	2.52	3	8	10	15.00	15.89
-2	7	9	8.13	8.22	-3	-5	10	6.04	5.32	-3	0	10	5.97	4.86	-2	4	10	4.77	4.89	4	8	10	13.40	13.48
-1	7	9	6.77	7.26	-2	-5	10	7.80	8.62	-2	0	10	7.11	7.62	-1	4	10	12.94	13.11	5	8	10	6.26	5.57
0	7	9	4.46	4.65	-1	-5	10	7.06	6.59	-1	0	10	6.59	6.57	0	4	10	8.34	9.52	6	8	10	0.82*	0.56
1	7	9	19.73	18.71	0	-5	10	5.94	6.44	0	0	10	1.82*	0.24	1	4	10	3.50	2.22	7	8	10	6.82	6.84
2	7	9	3.72	3.63	1	-5	10	7.04	7.06	1	0	10	24.33	23.96	2	4	10	9.72	8.82	-2	9	10	1.52*	2.18
3	7	9	11.79	11.10	2	-5	10	2.10*	0.87	2	0	10	28.39	27.53	3	4	10	6.77	6.54	-1	9	10	2.92	2.54
4	7	9	1.99*	1.73	3	-5	10	0.82*	0.01	3	0	10	21.60	21.00	4	4	10	8.04	8.00	0	9	10	2.33*	2.11
5	7	9	1.76*	1.74	-5	-4	10	0.80*	0.12	4	0	10	14.97	14.86	5	4	10	0.78*	1.84	1	9	10	2.64	2.43
6	7	9	3.43	3.17	-4	-4	10	0.79*	0.70	5	0	10	3.92	3.51	6	4	10	4.72	4.93	2	9	10	0.78*	0.14
7	7	9	5.56	5.56	-3	-4	10	12.33	10.75	6	0	10	1.55*	1.22	7	4	10	0.78*	0.45	3	9	10	14.63	14.18
8	7	9	3.82	3.43	-2	-4	10	8.14	8.83	7	0	10	1.41*	0.44	8	4	10	0.80*	0.11	4	9	10	4.90	5.06
-4	8	9	7.32	6.86	-1	-4	10	2.45*	1.41	-6	1	10	1.87*	0.09	-5	5	10	1.53*	0.81	5	9	10	12.68	12.89
-3	8	9	4.24	4.32	0	-4	10	4.40	4.14	-5	1	10	3.12	2.04	-4	5	10	0.78*	0.04	6	9	10	16.61	16.12
-2	8	9	2.26*	2.85	1	-4	10	4.59	3.54	-4	1	10	7.76	8.45	-3	5	10	2.88	3.26	7	9	10	3.38	3.44
-1	8	9	10.25	10.67	2	-4	10	5.86	4.94	-3	1	10	4.98	4.14	-2	5	10	0.75*	0.33	0	10	10	4.36	4.87
0	8	9	7.62	7.22	3	-4	10	14.79	14.56	-2	1	10	0.74*	1.46	-1	5	10	1.53*	0.35	1	10	10	4.16	4.30
1	8	9	11.22	11.47	4	-4	10	2.83	2.87	-1	1	10	3.81	3.56	0	5	10	6.72	5.97	2	10	10	4.30	3.97
2	8	9	8.10	7.34	-5	-3	10	2.94	1.89	0	1	10	9.55	9.74	1	5	10	10.05	9.70	3	10	10	6.51	6.58
3	8	9	21.96	21.45	-4	-3	10	4.60	2.89	1	1	10	14.81	14.15	2	5	10	7.82	8.76	4	10	10	3.12	3.57
4	8	9	7.87	7.61	-3	-3	10	4.78	3.70	2	1	10	4.64	4.96	3	5	10	0.74*	0.47	5	10	10	6.24	6.68
5	8	9	2.48*	2.99	-2	-3	10	8.77	8.62	3	1	10	9.22	8.91	4	5	10	12.69	13.37	6	10	10	1.58*	2.43
6	8	9	7.94	8.46	-1	-3	10	13.17	12.91	4	1	10	12.26	11.18	5	5	10	17.74	16.90	2	11	10	5.63	5.72
7	8	9	0.79*	1.50	0	-3	10	14.45	13.99	5	1	10	5.28	5.24	6	5	10	5.37	5.53	3	11	10	6.51	6.02
8	8	9	3.92	3.60	1	-3	10	9.99	9.99	6	1	10	10.23	9.78	7	5	10	8.06	7.72	-3	-4	11	5.19	3.20
-3	9	9	2.92	3.11	2	-3	10	3.63	3.63	7	1	10	4.05	4.18	8	5	10	0.82*	1.36	-2	-4	11	2.82	2.54
-2	9	9	2.44*	1.15	3	-3	10	4.54	3.99	-6	2	10	7.63	7.75	-4	6	10	5.43	4.77	-1	-4	11	2.67	3.23
-1	9	9	2.18*	2.02	4	-3	10	3.32	2.96	-5	2	10	7.57	7.02	-3	6	10	2.29*	2.20	0	-4	11	8.73	8.40
0	9	9	0.77*	0.05	5	-3	10	1.47*	0.23	-4	2	10	5.14	6.78	-2	6	10	0.78*	0.96	1	-4	11	3.75	4.42
1	9	9	4.49	5.16	-6	-2	10	0.82*	1.93	-3	2	10	0.77*	2.49	-1	6	10	0.77*	0.57	2	-4	11	0.80*	1.25
2	9	9	2.00*	1.12	-5	-2	10	4.05	3.70	-2	2	10	14.14	14.28	0	6	10	5.56	5.77	-4	-3	11	5.70	6.74
3	9	9	11.71	12.11	-4	-2	10	1.91*	2.66	-1	2	10	9.66	11.18	1	6	10	5.50	5.24	-3	-3	11	8.24	7.66
4	9	9	12.45	12.08	-3	-2	10	8.26	8.32	0	2	10	4.69	4.06	2	6	10	16.43	16.55	-2	-3	11	3.57	3.42
5	9	9	12.38	11.89	-2	-2	10	0.77*	0.00	1	2	10	2.26*	0.17	3	6	10	1.81*	1.53	-1	-3	11	6.05	6.31
6	9	9	8.98	8.24	-1	-2	10	0.77*	1.82	2	2	10	3.95	4.56	4	6	10	2.02*	1.45	0	-3	11	8.87	8.76
7	9	9	2.63	2.57	0	-2	10	12.69	12.13	3	2	10	10.01	9.02	5	6	10	1.86*	1.54	1	-3	11	2.63	2.83
8	9	9	4.20	4.92	1	-2	10	0.77*	1.48	4	2	10	2.11*	1.92	6	6	10	2.55	2.01	2	-3	11	0.80*	2.10
-2	10	9	6.10	5.79	2	-2	10	7.06	6.85	5	2	10	6.80	6.47	7	6	10	3.99	3.98	3	-3	11	1.19*	0.03
-1	10	9	7.76	7.61	3	-2	10	5.04	5.20	6	2	10	7.87	7.13	8	6	10	8.59	8.27	4	-3	11	2.58*	2.50
0	10	9	4.69	4.70	4	-2	10	4.31	4.68	7	2	10	8.77	7.80	-4	7	10	0.83*	0.28	-4	-2	11	5.52	4.35
1	10	9	6.68	6.55	5	-2	10	4.41	4.57	8	2	10	6.49	6.88	-3	7	10	0.82*	1.73	-3	-2	11	0.80*	0.41
2	10	9	3.90	4.25	6	-2	10	4.14	4.15	-6	3	10	4.85	4.41	-2	7	10	3.71	2.99	-2	-2	11	4.54	5.56
3	10	9	3.60	4.04	-6	-1	10	2.15*	1.44	-5	3	10	0.79*	0.99	-1	7	10	2.02*	0.35	-1	-2	11	7.86	6.95
4	10	9	3.92	3.29	-5	-1	10	0.80*	1.27	-4	3	10	10.57	10.00	0	7	10	8.30	8.16	0	-2	11	4.94	6.90
5	10	9	4.89	5.16	-4	-1	10	6.73	4.92	-3	3	10	7.11	7.85	1	7	10	8.57	8.94	1	-2	11	5.77	5.59
6	10	9	2.18*	0.63	-3	-1	10	8.58	6.67	-2	3	10	13.46	14.82	2	7	10	10.79	10.69	2	-2	11	12.45	12.58
7	10	9	0.83*	1.72	-2	-1	10	8.46	6.89	-1	3	10	3.51	3.73	3	7	10	1.19*	0.86	3	-2	11	6.69	6.99
0	11	9	3.33	3.36	-1	-1	10	3.21	4.43	0	3	10	1.89*	0.25	4	7	10	0.77*	1.71	4	-2	11	0.82*	0.51
1	11	9	3.02	2.61	0	-1	10	10.28	9.79	1	3	10	8.51	8.11	5	7	10	9.08	7.96	5	-2	11	0.83*	0.75
2	11	9	4.72	4.51	1	-1	10	20.80	20.78	2	3	10	0.74*	0.67	6	7	10	4.68	4.23	-5	-1	11	2.39*	1.03
3	11	9	0.80*	1.18	2	-1	10	19.30	19.46	3	3	10	6.94	7.44	7	7	10	6.26	6.36	-4	-1	11	1.70*	1.89
4	11	9	3.97	3.31	3	-1	10	1.60*	1.45	4	3	10	0.74*	0.29	8	7	10	3.09	3.38	-3	-1	11	3.75	1.50
5	11	9	10.92	10.46	4	-1	10	1.55*	2.11	5	3	10	4.85	4.75	-3	8	10	2.97	3.32	-2	-1	11	3.84	2.51

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-1	-1	11	5.06	5.91	-3	4	11	5.33	5.32	4	9	11	0.80*	0.10	-1	4	12	3.66	3.91	-1	4	13	7.72	7.45
0	-1	11	6.50	6.45	-2	4	11	1.72*	0.78	5	9	11	12.06	12.00	0	4	12	12.88	12.91	0	4	13	4.48	5.02
1	-1	11	3.92	4.63	-1	4	11	7.08	7.00	2	10	11	0.82*	1.05	1	4	12	5.48	6.21	1	4	13	0.83*	0.97
2	-1	11	8.77	9.00	0	4	11	7.19	7.96	3	10	11	3.43	3.05	2	4	12	4.45	3.24	2	4	13	2.57*	2.92
3	-1	11	0.78*	1.06	1	4	11	5.65	4.86	0	-3	12	0.83*	1.21	3	4	12	5.06	4.40	3	4	13	4.79	5.35
4	-1	11	0.79*	0.08	2	4	11	8.14	7.99	-2	-2	12	7.31	6.52	4	4	12	7.67	7.79	4	4	13	0.80*	0.23
5	-1	11	8.90	8.13	3	4	11	4.48	4.66	-1	-2	12	8.41	8.27	5	4	12	1.71*	0.75	0	5	13	8.90	7.88
-5	0	11	5.23	5.88	4	4	11	6.24	6.23	0	-2	12	11.75	10.87	6	4	12	3.82	3.83	1	5	13	9.62	9.76
-4	0	11	9.86	8.32	5	4	11	2.40*	2.36	1	-2	12	8.31	8.15	-3	5	12	0.80*	0.78	2	5	13	5.87	5.75
-3	0	11	1.32*	0.61	6	4	11	3.51	3.20	2	-2	12	6.38	5.80	-2	5	12	1.42*	0.43	3	5	13	1.76*	1.24
-2	0	11	2.64	2.44	7	4	11	2.82	2.49	3	-2	12	2.92	3.50	-1	5	12	7.72	7.08	4	5	13	2.08*	2.80
-1	0	11	3.60	2.95	-4	5	11	0.80*	0.01	-3	-1	12	2.41*	3.08	0	5	12	2.58	3.00	1	6	13	2.70	1.84
0	0	11	7.70	7.74	-3	5	11	3.22	3.64	-2	-1	12	2.89	3.23	1	5	12	5.40	5.16	2	6	13	8.02	7.10
1	0	11	5.68	5.44	-2	5	11	3.13	2.64	-1	-1	12	1.81*	1.99	2	5	12	7.35	7.87	3	6	13	7.41	7.05
2	0	11	7.99	7.84	-1	5	11	6.54	6.78	0	-1	12	6.62	6.81	3	5	12	5.68	5.63					
3	0	11	8.63	9.53	0	5	11	6.97	5.90	1	-1	12	2.35*	2.06	4	5	12	0.80*	0.35	4016	REFLECTIONS			
4	0	11	14.42	14.57	1	5	11	3.02	4.64	2	-1	12	3.33	3.18	5	5	12	1.27*	0.82					
5	0	11	5.76	5.64	2	5	11	11.17	10.86	3	-1	12	4.18	3.96	6	5	12	0.83*	0.80					
6	0	11	0.83*	1.74	3	5	11	6.21	6.24	4	-1	12	8.13	7.83	-2	6	12	3.53	2.61					
-5	1	11	0.82*	0.95	4	5	11	5.02	4.68	-3	0	12	0.82*	0.73	-1	6	12	3.68	2.33					
-4	1	11	3.55	3.21	5	5	11	7.13	7.58	-2	0	12	1.89*	1.57	0	6	12	0.82*	1.21					
-3	1	11	0.78*	2.19	6	5	11	3.50	2.58	-1	0	12	0.79*	1.27	1	6	12	4.62	4.31					
-2	1	11	7.85	6.64	7	5	11	5.67	6.15	0	0	12	4.46	4.50	2	6	12	0.79*	0.95					
-1	1	11	4.07	4.00	-3	6	11	3.13	3.54	1	0	12	1.58*	0.36	3	6	12	4.83	4.66					
0	1	11	5.65	4.20	-2	6	11	6.59	6.72	2	0	12	3.80	3.28	4	6	12	7.45	7.38					
1	1	11	1.40*	2.63	-1	6	11	1.16*	2.12	3	0	12	11.89	11.12	5	6	12	10.43	9.42					
2	1	11	8.75	8.26	0	6	11	0.79*	0.08	4	0	12	6.59	6.66	6	6	12	6.38	5.71					
3	1	11	12.67	12.89	1	6	11	4.05	3.74	-4	1	12	0.82*	1.91	-1	7	12	6.34	5.64					
4	1	11	7.14	7.90	2	6	11	2.40*	1.63	-3	1	12	5.37	4.39	0	7	12	5.12	5.54					
5	1	11	5.42	5.67	3	6	11	2.41*	2.35	-2	1	12	7.76	8.60	1	7	12	5.80	5.57					
6	1	11	6.25	6.92	4	6	11	5.40	5.40	-1	1	12	12.13	11.43	2	7	12	3.66	3.57					
-5	2	11	2.30*	2.93	5	6	11	5.07	4.89	0	1	12	2.70	2.12	3	7	12	1.51*	1.05					
-4	2	11	0.79*	0.27	6	6	11	9.35	9.44	1	1	12	4.04	3.74	4	7	12	2.30*	1.00					
-3	2	11	8.48	7.50	7	6	11	6.33	6.11	2	1	12	8.45	8.26	5	7	12	3.77	3.34					
-2	2	11	5.80	7.28	-3	7	11	5.92	5.40	3	1	12	8.35	8.20	0	8	12	1.50*	2.70					
-1	2	11	9.63	8.50	-2	7	11	6.12	5.56	4	1	12	3.95	3.56	1	8	12	2.89	3.56					
0	2	11	5.09	4.97	-1	7	11	8.16	7.77	5	1	12	13.64	13.51	2	8	12	6.70	6.07					
1	2	11	6.40	7.23	0	7	11	12.09	11.97	-3	2	12	2.99	2.28	3	8	12	2.65	2.23					
2	2	11	3.42	2.88	1	7	11	2.58	2.57	-2	2	12	1.47*	0.77	4	8	12	3.53	2.73					
3	2	11	3.12	2.72	2	7	11	9.07	8.91	-1	2	12	3.02	2.78	0	0	13	6.24	5.87					
4	2	11	4.28	4.44	3	7	11	1.28*	1.63	0	2	12	9.47	7.93	1	0	13	4.06	3.89					
5	2	11	16.48	15.85	4	7	11	2.91	3.14	1	2	12	5.60	6.74	2	0	13	7.71	6.94					
6	2	11	10.88	11.08	5	7	11	1.30*	2.90	2	2	12	4.19	4.26	-1	1	13	1.77*	1.91					
7	2	11	1.82*	1.84	6	7	11	0.82*	1.03	3	2	12	3.70	3.96	0	1	13	6.06	5.53					
-5	3	11	3.06	2.83	7	7	11	0.83*	0.54	4	2	12	7.81	8.18	1	1	13	5.17	4.34					
-4	3	11	0.79*	1.88	-2	8	11	3.09	2.43	5	2	12	13.54	13.32	2	1	13	0.82*	0.54					
-3	3	11	3.82	3.17	-1	8	11	3.45	3.82	-3	3	12	1.16*	1.48	3	1	13	0.83*	0.79					
-2	3	11	8.87	8.92	0	8	11	2.41*	1.98	-2	3	12	5.28	5.15	-1	2	13	7.18	6.40					
-1	3	11	1.86*	3.61	1	8	11	7.86	8.23	-1	3	12	0.80*	0.57	0	2	13	8.83	9.13					
0	3	11	8.97	9.66	2	8	11	2.19*	3.32	0	3	12	3.24	3.58	1	2	13	11.77	11.40					
1	3	11	6.78	6.85	3	8	11	3.70	3.92	1	3	12	2.25*	2.12	2	2	13	7.32	6.36					
2	3	11	12.26	12.68	4	8	11	2.84	2.30	2	3	12	0.79*	1.52	3	2	13	4.35	3.28					
3	3	11	0.77*	0.78	5	8	11	0.82*	0.50	3	3	12	0.79*	0.91	-1	3	13	3.66	3.24					
4	3	11	2.24*	3.11	6	8	11	3.68	3.09	4	3	12	6.51	6.79	0	3	13	2.79	2.78					
5	3	11	7.66	7.84	0	9	11	2.87	2.30	5	3	12	3.48	3.89	1	3	13	1.43*	2.42					
6	3	11	4.60	3.88	1	9	11	0.80*	0.58	6	3	12	7.38	7.32	2	3	13	3.19	3.65					
7	3	11	7.56	7.90	2	9	11	0.80*	1.04	-3	4	12	1.72*	0.58	3	3	13	2.04*	2.92					
-4	4	11	6.39	5.73	3	9	11	3.03	2.75	-2	4	12	2.34*	2.45	4	3	13	4.63	4.19					

Appendix B

STRUCTURE FACTORS FOR 1,2,4-TRIAZOLE

* denotes weak reflection.

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	0	0	3.49	3.03	5	3	1	10.89	10.33	1	2	2	15.00	15.57	4	9	2	6.37	6.25	1	8	3	0.78*	1.59
6	0	0	11.83	11.65	6	3	1	12.56	12.69	2	2	2	8.25	8.04	0	10	2	5.78	6.01	2	8	3	0.88*	1.05
8	0	0	1.53*	1.58	7	3	1	1.50*	1.22	3	2	2	5.57	5.70	1	10	2	1.52*	2.08	3	8	3	1.40*	1.40
0	2	0	19.06	20.36	8	3	1	1.35*	0.98	4	2	2	18.29	17.86	2	10	2	1.77	2.15	4	8	3	4.20	3.82
3	2	0	3.30	3.09	1	4	1	6.52	6.04	5	2	2	6.67	6.39	3	10	2	1.75	1.89	5	8	3	3.41	3.24
4	2	0	38.30	38.30	2	4	1	1.50	0.88	6	2	2	3.66	3.48	2	0	3	8.09	7.93	1	9	3	2.64	2.81
5	2	0	1.12*	0.27	3	4	1	10.65	10.45	7	2	2	3.81	3.91	4	0	3	19.42	19.18	2	9	3	0.47*	0.07
6	2	0	3.90	3.98	4	4	1	5.50	5.62	8	2	2	0.50*	0.06	6	0	3	7.64	7.77	3	9	3	2.36	2.46
7	2	0	2.29	1.99	5	4	1	13.57	13.86	0	3	2	8.91	8.98	8	0	3	0.91*	1.38	4	9	3	2.14	1.90
8	2	0	1.22*	1.74	6	4	1	2.47	1.94	1	3	2	9.02	8.56	1	1	3	0.34*	0.44	1	10	3	1.80	2.11
0	4	0	13.61	11.85	7	4	1	1.56	1.09	2	3	2	11.82	11.38	2	1	3	3.86	3.75	2	10	3	2.12	1.80
1	4	0	25.85	24.81	1	5	1	16.61	16.18	3	3	2	30.59	29.72	3	1	3	4.02	3.82	3	10	3	2.95	2.74
2	4	0	4.88	4.08	2	5	1	6.18	6.07	4	3	2	7.76	7.40	4	1	3	5.90	5.57	0	0	4	36.95	36.69
3	4	0	48.75	49.33	3	5	1	1.97	2.65	5	3	2	6.88	6.85	5	1	3	5.42	5.28	2	0	4	13.05	11.90
4	4	0	0.70*	0.95	4	5	1	6.05	5.53	6	3	2	3.80	3.64	6	1	3	1.10*	0.80	4	0	4	7.67	7.69
5	4	0	3.91	3.92	5	5	1	17.85	18.35	7	3	2	0.74*	0.48	7	1	3	3.62	3.51	6	0	4	8.57	8.40
6	4	0	8.00	8.28	6	5	1	1.64	1.92	8	3	2	0.78*	1.04	8	1	3	0.50*	1.04	8	0	4	3.80	3.94
7	4	0	9.38	9.74	7	5	1	3.37	3.56	0	4	2	4.40	4.15	1	2	3	0.34*	0.83	0	1	4	15.93	14.86
0	6	0	13.50	13.12	1	6	1	10.29	9.70	1	4	2	6.15	5.74	2	2	3	24.12	22.86	1	1	4	12.23	12.93
1	6	0	24.01	23.75	2	6	1	3.76	4.08	2	4	2	1.37	1.62	3	2	3	11.09	10.96	2	1	4	4.29	4.39
2	6	0	14.95	13.98	3	6	1	5.04	5.03	3	4	2	15.60	15.12	4	2	3	5.81	5.80	3	1	4	1.43	1.39
3	6	0	11.29	11.51	4	6	1	8.98	9.08	4	4	2	6.21	6.05	5	2	3	9.11	8.93	4	1	4	2.19	1.30
4	6	0	2.47	2.06	5	6	1	4.20	4.12	5	4	2	9.09	9.14	6	2	3	0.46*	0.07	5	1	4	5.47	5.43
5	6	0	1.18*	0.56	6	6	1	2.50	3.05	6	4	2	0.47*	0.50	7	2	3	0.79*	0.91	6	1	4	1.56	0.74
6	6	0	9.03	9.33	7	6	1	0.50*	0.47	7	4	2	0.48*	1.08	8	2	3	1.36*	1.29	7	1	4	3.81	4.05
7	6	0	6.40	6.63	1	7	1	12.29	12.68	0	5	2	7.92	7.77	1	3	3	0.83*	0.77	0	2	4	7.40	7.84
0	8	0	17.16	16.73	2	7	1	4.43	3.71	1	5	2	20.83	19.71	2	3	3	3.76	3.85	1	2	4	36.26	35.85
1	8	0	12.21	12.36	3	7	1	9.98	10.06	2	5	2	7.52	6.44	3	3	3	3.82	4.27	2	2	4	1.47	1.38
2	8	0	1.67	2.04	4	7	1	7.29	7.50	3	5	2	3.84	3.42	4	3	3	2.75	2.42	3	2	4	11.13	10.32
3	8	0	3.40	3.57	5	7	1	1.26*	0.93	4	5	2	3.16	2.71	5	3	3	1.29*	1.78	4	2	4	3.21	3.03
4	8	0	9.54	9.76	6	7	1	4.54	4.80	5	5	2	6.66	6.93	6	3	3	6.46	6.52	5	2	4	3.24	2.98
5	8	0	3.91	3.75	1	8	1	3.92	4.10	6	5	2	0.48*	0.01	7	3	3	1.57	1.45	6	2	4	5.88	5.71
0	10	0	14.80	15.26	2	8	1	9.07	9.17	7	5	2	7.64	7.67	1	4	3	16.48	15.46	7	2	4	2.71	2.98
1	10	0	3.83	3.74	3	8	1	4.69	4.95	0	6	2	0.41*	0.54	2	4	3	8.86	8.80	0	3	4	24.19	23.63
2	10	0	3.54	3.72	4	8	1	1.01*	0.70	1	6	2	3.78	3.52	3	4	3	13.63	13.15	1	3	4	6.65	5.98
3	10	0	0.49*	0.63	5	8	1	0.98*	0.93	2	6	2	3.30	2.65	4	4	3	3.15	2.59	2	3	4	13.43	12.62
4	0	1	5.75	5.17	1	9	1	2.26	2.35	3	6	2	5.50	5.56	5	4	3	0.47*	1.88	3	3	4	3.48	2.73
6	0	1	1.05*	0.30	2	9	1	10.81	10.95	4	6	2	4.11	3.64	6	4	3	0.47*	0.48	4	3	4	3.53	3.08
8	0	1	2.00	2.01	3	9	1	1.96	1.97	5	6	2	0.47*	0.08	7	4	3	1.46*	1.34	5	3	4	4.39	4.29
1	1	1	26.85	27.46	4	9	1	1.64	1.79	6	6	2	2.71	2.74	1	5	3	0.40*	0.16	6	3	4	3.92	3.96
3	1	1	23.09	22.61	1	10	1	2.81	2.86	7	6	2	2.85	3.05	2	5	3	1.19*	1.22	7	3	4	1.98	2.38
4	1	1	1.08*	0.67	2	10	1	3.60	3.62	0	7	2	12.37	11.65	3	5	3	0.67*	0.59	0	4	4	24.86	23.96
5	1	1	6.39	6.22	3	10	1	2.88	3.34	1	7	2	1.14*	0.67	4	5	3	1.53	1.30	1	4	4	18.09	17.34
6	1	1	2.69	2.96	1	11	1	2.32	2.14	2	7	2	2.63	2.01	5	5	3	3.62	3.76	2	4	4	22.77	22.10
7	1	1	5.19	5.12	0	0	2	35.14	37.76	3	7	2	11.05	11.25	6	5	3	0.48*	0.47	3	4	4	8.43	8.83
8	1	1	5.41	5.46	2	0	2	19.69	20.27	4	7	2	0.47*	0.20	7	5	3	4.49	4.66	4	4	4	10.90	11.21
1	2	1	31.53	31.68	4	0	2	4.67	4.36	5	7	2	5.50	5.44	1	6	3	5.61	5.10	5	4	4	0.46*	0.11
2	2	1	10.23	10.24	6	0	2	9.23	9.53	6	7	2	4.71	4.44	2	6	3	8.37	7.71	6	4	4	2.66	3.12
3	2	1	23.34	23.26	8	0	2	3.58	3.64	0	8	2	0.45*	0.68	3	6	3	1.37*	0.15	7	4	4	4.14	4.37
4	2	1	15.28	15.12	0	1	2	49.34	53.45	1	8	2	4.91	5.05	4	6	3	5.29	5.69	0	5	4	3.73	3.37
5	2	1	0.44*	1.15	2	1	2	8.03	8.12	2	8	2	2.12	2.08	5	6	3	4.40	4.23	1	5	4	15.49	14.72
6	2	1	4.60	4.40	3	1	2	11.34	10.91	3	8	2	0.98*	0.97	6	6	3	2.29	2.21	2	5	4	3.48	4.15
7	2	1	1.54	1.47	4	1	2	14.09	13.28	4	8	2	1.25*	0.40	1	7	3	1.16*	1.69	3	5	4	6.66	6.85
8	2	1	2.74	2.83	5	1	2	5.85	5.42	5	8	2	1.08*	0.70	2	7	3	3.52	3.43	4	5	4	0.47*	1.02
1	3	1	30.84	30.71	6	1	2	5.54	5.51	0	9	2	3.53	3.62	3	7	3	1.74	1.85	5	5	4	0.47*	0.26
2	3	1	3.81	3.38	7	1	2	4.20	3.93	1	9	2	3.89	4.25	4	7	3	1.02*	0.93	6	5	4	2.79	3.36
3	3	1	10.47	10.64	8	1	2	1.39*	0.88	2	9	2	5.02	4.61	5	7	3	1.26*	0.74	7	5	4	0.51*	0.70
4	3	1	22.03	21.99	0	2	2	10.59	8.78	3	9	2	2.47	2.63	6	7	3	2.12	1.69	0	6	4	27.29	27.05

H	K	L	FO	FC
1	6	4	2.16	1.73
2	6	4	18.78	19.08
3	6	4	5.22	5.55
4	6	4	8.43	8.40
5	6	4	3.91	4.31
6	6	4	1.57*	1.72
0	7	4	2.16	1.25
1	7	4	8.00	8.17
2	7	4	4.06	4.03
3	7	4	5.78	5.71
4	7	4	2.77	3.04
5	7	4	0.84*	0.91
0	8	4	10.36	10.78
1	8	4	13.40	14.09
2	8	4	8.21	8.25
3	8	4	6.36	6.40
4	8	4	3.26	2.91
5	8	4	1.85	1.56
0	9	4	6.99	6.93
1	9	4	4.43	4.64
2	9	4	4.03	3.73
3	9	4	0.49*	0.39
4	9	4	0.50*	0.58
0	10	4	0.90*	1.56
1	10	4	7.60	7.49
2	10	4	0.50*	0.26
2	0	5	7.23	7.31
4	0	5	6.22	6.08
6	0	5	1.02*	0.75
1	1	5	19.30	18.47
2	1	5	26.77	26.59
3	1	5	24.92	24.60
4	1	5	5.97	5.74
5	1	5	11.04	11.12
6	1	5	0.47*	0.85
7	1	5	4.61	4.80
1	2	5	0.81*	0.54
2	2	5	0.40*	0.98
3	2	5	4.71	4.62
4	2	5	0.71*	0.88
5	2	5	2.59	2.46
6	2	5	1.32*	1.31
7	2	5	1.43*	1.32
1	3	5	9.19	9.46
2	3	5	10.91	10.45
3	3	5	3.43	3.16
4	3	5	19.14	18.76
5	3	5	5.74	5.96
6	3	5	9.70	10.29
7	3	5	0.50*	0.10
1	4	5	3.25	3.58
2	4	5	1.93	1.89
3	4	5	1.91	2.08
4	4	5	1.60	1.46
5	4	5	0.47*	0.49
6	4	5	0.72*	1.14
7	4	5	0.99*	1.13
1	5	5	1.38	1.71
2	5	5	5.12	5.75
3	5	5	8.45	8.05
4	5	5	6.72	7.53
5	5	5	12.77	12.91
6	5	5	3.98	3.63
1	6	5	1.03*	0.84
2	6	5	5.21	5.55
3	6	5	2.05	2.29
4	6	5	0.47*	0.66
5	6	5	0.48*	0.39
6	6	5	0.50*	0.14
1	7	5	7.59	7.76
2	7	5	1.48	1.51
3	7	5	9.80	10.25
4	7	5	4.88	5.02
5	7	5	3.53	3.47
1	8	5	2.43	2.10
2	8	5	0.47*	0.19
3	8	5	1.84	2.02
4	8	5	2.18	2.53
1	9	5	0.87*	0.36
2	9	5	7.82	8.13
3	9	5	0.50*	0.16
0	0	6	24.65	23.96
2	0	6	3.09	2.24
4	0	6	9.80	9.47
6	0	6	3.64	3.59
0	1	6	20.24	19.14
1	1	6	2.40	2.51
2	1	6	1.48	1.23
3	1	6	7.92	7.71
4	1	6	6.91	7.12
5	1	6	8.82	8.62
6	1	6	0.97*	1.09
7	1	6	4.55	4.43
0	2	6	19.41	18.73
1	2	6	18.05	16.88
2	2	6	0.42*	0.29
3	2	6	2.79	2.66
4	2	6	4.49	5.09
5	2	6	1.26*	1.75
6	2	6	5.21	5.17
7	2	6	2.44	2.44
0	3	6	4.08	3.99
1	3	6	12.63	11.54
2	3	6	6.43	6.15
3	3	6	2.61	2.20
4	3	6	0.76*	0.15
5	3	6	2.88	3.10
6	3	6	4.83	4.99
0	4	6	11.04	10.49
1	4	6	3.81	3.95
2	4	6	10.96	10.52
3	4	6	13.59	13.81
4	4	6	7.30	7.62
5	4	6	1.82	1.77
6	4	6	2.56	2.20
0	5	6	5.26	5.49
1	5	6	7.73	7.28
2	5	6	0.94*	0.64
3	5	6	9.64	9.74
4	5	6	3.44	3.40
5	5	6	2.54	2.87
6	5	6	2.67	3.04
0	6	6	4.69	4.67
1	6	6	1.47	1.55
2	6	6	10.78	10.88
3	6	6	8.75	8.97
4	6	6	8.90	8.78
5	6	6	1.53*	1.53
0	7	6	2.53	2.50
1	7	6	10.92	11.42
2	7	6	3.03	3.15
3	7	6	1.76	1.66
4	7	6	2.23	2.71
0	8	6	10.23	10.23
1	8	6	7.31	7.58
2	8	6	1.98	1.53
3	8	6	3.08	2.92
4	8	6	0.99*	0.89
0	9	6	7.26	7.56
1	9	6	2.29	2.66
2	9	6	3.09	3.76
2	0	7	15.46	14.87
4	0	7	6.05	6.38
6	0	7	5.19	5.51
1	1	7	1.80	0.81
2	1	7	7.12	7.17
3	1	7	1.49	1.76
4	1	7	3.51	3.38
5	1	7	0.47*	0.60
6	1	7	0.49*	0.59
1	2	7	7.24	6.91
2	2	7	11.59	12.16
3	2	7	1.32*	0.87
4	2	7	3.67	3.17
5	2	7	5.91	6.07
6	2	7	3.26	3.39
1	3	7	7.56	7.52
2	3	7	6.33	6.72
3	3	7	3.28	3.13
4	3	7	0.71*	0.78
5	3	7	3.69	3.27
6	3	7	3.71	3.41
1	4	7	10.92	10.96
2	4	7	4.05	4.31
3	4	7	5.29	5.41
4	4	7	0.82*	0.43
5	4	7	5.43	5.26
6	4	7	1.28*	0.56
1	5	7	6.64	6.71
2	5	7	3.91	3.72
3	5	7	2.18	2.45
4	5	7	0.48*	0.89
5	5	7	4.81	4.61
1	6	7	6.56	7.10
2	6	7	4.00	3.72
3	6	7	2.98	3.38
4	6	7	0.49*	0.30
5	6	7	4.22	4.10
1	7	7	1.35*	1.38
2	7	7	2.95	2.81
3	7	7	0.94*	1.09
4	7	7	2.87	2.83
1	8	7	2.21	2.10
2	8	7	4.34	4.35
0	0	8	15.57	16.37
2	0	8	13.50	13.77
4	0	8	7.83	8.33
6	0	8	2.74	2.83
0	1	8	8.27	7.74
1	1	8	15.15	15.74
2	1	8	7.66	8.00
3	1	8	12.36	12.50
4	1	8	8.43	8.56
5	1	8	0.49*	1.32
6	1	8	5.53	5.27
0	2	8	10.14	10.05
1	2	8	8.67	8.78
2	2	8	7.96	8.49
3	2	8	5.86	6.19
4	2	8	5.05	5.11
5	2	8	2.42	2.50
6	2	8	2.58	2.70
0	3	8	20.61	21.80
1	3	8	13.78	13.62
2	3	8	6.76	7.34
3	3	8	3.15	3.38
4	3	8	3.36	3.70
5	3	8	2.83	2.47
0	4	8	1.05*	0.43
1	4	8	6.78	7.34
2	4	8	0.47*	0.05
3	4	8	5.12	5.21
4	4	8	0.49*	1.19
5	4	8	2.48	2.61
0	5	8	7.93	7.95
1	5	8	8.55	8.62
2	5	8	4.60	4.70
3	5	8	9.52	9.39
4	5	8	1.30*	1.33
0	6	8	2.29	2.54
1	6	8	0.48*	0.90
2	6	8	1.40*	1.86
3	6	8	0.94*	1.08
4	6	8	0.87*	0.51
0	7	8	4.85	4.68
1	7	8	1.12*	1.43
2	7	8	1.95	1.91
3	7	8	3.37	3.52
0	8	8	0.85*	0.57
2	0	9	4.08	3.92
4	0	9	5.79	5.95
1	1	9	3.35	3.55
2	1	9	0.88*	0.49
3	1	9	9.23	9.45
4	1	9	7.70	7.46
5	1	9	7.54	7.90
1	2	9	1.71	1.73
2	2	9	7.15	7.34
3	2	9	2.36	2.05
4	2	9	1.10*	0.64
5	2	9	4.14	4.21
1	3	9	3.04	3.47
2	3	9	11.25	11.23
3	3	9	0.48*	0.91
4	3	9	8.24	8.32
1	4	9	6.37	6.22
2	4	9	3.59	3.85
3	4	9	4.39	4.39
4	4	9	1.22*	0.88
1	5	9	6.36	6.32
2	5	9	3.38	3.80
3	5	9	7.43	7.35
1	6	9	3.82	3.91
2	6	9	3.05	2.73
0	0	10	15.03	14.13
2	0	10	15.85	15.66
4	0	10	8.13	8.39
0	1	10	4.28	4.05
1	1	10	6.36	6.19
2	1	10	1.59	0.92
3	1	10	2.15	2.23
4	1	10	1.36*	1.48
0	2	10	14.76	14.89
1	2	10	9.35	9.07
2	2	10	7.98	7.97
3	2	10	7.04	7.06
4	2	10	2.64	2.93
0	3	10	2.44	2.60
1	3	10	2.20	2.40
2	3	10	2.43	2.68
3	3	10	2.12	2.36
0	4	10	2.21	1.96
1	4	10	10.50	10.90
2	4	10	0.49*	0.84
3	4	10	2.52	2.61
0	5	10	3.78	4.48
1	5	10	1.08*	0.91
2	5	10	1.48*	1.74
2	0	11	2.43	2.17
1	1	11	0.47*	0.35
2	1	11	0.88*	0.52
1	2	11	1.05*	0.70
2	2	11	0.49*	1.05
1	3	11	0.49*	0.52

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