*Acta Cryst.* (1964). **17**, 1033

# The Crystal and Molecular Structure of Hexacrylonitrile*

By Marvin J. Kornblau† and R. E. Hughes

*Department of Chemistry and Laboratory for Research on the Structure of Matter,*
*University of Pennsylvania, Philadelphia 4, Pennsylvania, U.S.A.*

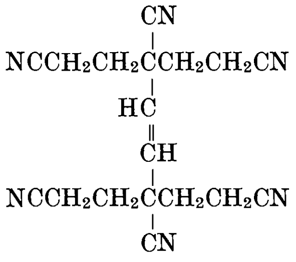
(*Received* 6 *May* 1963)

The crystal structure of a hexamer of acrylonitrile has been determined by two-dimensional Fourier and three-dimensional Patterson analyses. The crystals are monoclinic, in space group $P2_1/a$, and $a=15{\cdot}56\pm0{\cdot}02$, $b=6{\cdot}42\pm0{\cdot}02$, $c=9{\cdot}24\pm0{\cdot}02$ Å; $\beta=108{\cdot}3°\pm0{\cdot}1°$; $Z=2$. The structure was refined by a full-matrix three-dimensional least-squares analysis of 1445 reflections, 1123 of which were observed. The reliability index ($R$) for the full data is 0·131; for the observed data only it is 0·110.

All of the atoms in the molecule lie in three planes. Two of the nitrile groups lie in the plane of the *trans* carbon double bond. All other carbon atoms lie in planar arrays of *trans*, staggered, single bonds.

## Introduction

In a study of the stereospecific polymerization of acrylonitrile, Takashina & Price (1962) utilized a triphenylphosphine initiator and isolated a crystalline hexamer which melted sharply at 240 °C without decompositon. Physical and chemical evidence indicated that the compound has a somewhat unusual structure (I) which can be formally described by the appellation 1,1,4,4-tetra-(2-cyanoethyl)-1,4-dicyano-*trans*-2-butene, but will hereinafter be simply called hexacrylonitrile. The compound is thermally and chemically stable and the double bond appears to be particularly inaccessible to attack, even to bromine and permanganate. This structure investigation was undertaken to corroborate and extend the results of the chemical study.



$$\begin{array}{c} \mathrm{CN} \\ | \\ \mathrm{NCCH_2CH_2CCH_2CH_2CN} \\ | \\ \mathrm{HC} \\ \| \\ \mathrm{CH} \\ | \\ \mathrm{NCCH_2CH_2CCH_2CH_2CN} \\ | \\ \mathrm{CN} \end{array}$$

(I)

## Experimental

Although hexacrylonitrile is insoluble in most common solvents, it was possible to recrystallize it from acetonitrile and from *N*,*N*-dimethylformamide to yield crystals approximately 0·8 × 0·4 × 0·1 mm with the crystallographic $b$ axis along the long axis. The lattice constants $a$, $c$ and $\beta$ of the monoclinic cell were determined from calibrated Weissenberg photographs about [010] with the use of Cr $K\alpha$ radiation and combined film shrinkage and radius corrections. The $b$ dimension was obtained from an average of measurements on precession photographs about [100] and [001] and oscillation photographs about [010]. The values thus obtained are:

$$a=15{\cdot}56\pm0{\cdot}02,\ \ b=6{\cdot}42\pm0{\cdot}02,\ \ c=9{\cdot}24\pm0{\cdot}02\ \text{Å};$$
$$\beta=108{\cdot}3°\pm0{\cdot}1°$$

The density calculated for $Z=2$ is 1·20 g.cm$^{-3}$ which corresponds to the value determined by a flotation method.

The observed systematic extinctions of $h0l$ reflections with $h$ odd and of $0k0$ with $k$ odd uniquely correspond to the space group $P2_1/a$.

The intensity data were recorded with a few exceptions, on multiple equi-inclination Weissenberg photographs about $b(k=0,\cdots,4)$ utilizing Ni filtered Cu $K\alpha$ radiation. Eight low angle reflections were measured on precession photographs which were cross correlated with the other data. Intensities were measured by visual comparison with a series of 30 carefully timed exposures of a typical reflection of the crystal. Lorentz and polarization factors were applied and, on the upper level data, spot extension corrections (Phillips, 1954) were made. Scale factors between layers were derived from photographs about the $c$ axis. Of the 1445 reflections investigated in this way, 1123 were measurable and 322 were carried through the analysis as unobserved data.

## Determination of the structure

Initially, attempts were made to solve the structure by trial and error methods. Half of one molecule represents

---

* Supported in part by the Advanced Research Projects Agency, Contract SD-69.

† Present address: Aerojet General Corp., Sacramento, California, U.S.A.

the asymmetric unit with the center of the double bond located at the center of symmetry. It was assumed that the five contiguous carbon atoms were in a planar zigzag array coplanar with the two pendant nitrile groups and that the double bond was in its usual planar configuration. The intense 10, 0, 3 reflection has a very high unitary structure factor, and it appeared that this fact, along with a few other strong reflections and some simple packing arguments, would serve to determine the orientation of the molecule. Despite the fact that all of the assumptions were later shown to have been essentially correct, it was not possible to achieve a satisfactory model in this way.

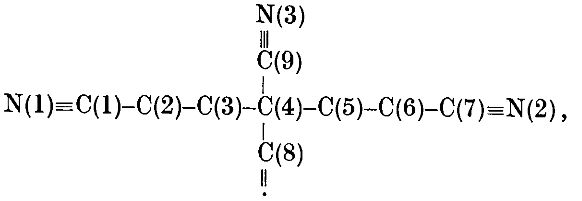
All of the data were utilized to calculate a three-dimensional sharpened Patterson synthesis at intervals of 0·01 along *a*, 0·03 along *b* and 0·02 along *c*. The sections were computed to the limits $a=\frac{1}{2}$, $b=\frac{1}{2}$ and $c=1$ on an IBM 1620 computer with the program of van der Helm & Patterson (1961). The synthesis required about 20 hours of machine time to sum the 1123 data at 42,500 points. The function was sharpened by dividing the $F^2$ by the squared average of the form factors for carbon and nitrogen (Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal, 1955).

The zero sections ($b=0$) of the Patterson synthesis showed a well defined linear array of peaks extending from the origin which could be identified as being produced by a C–C≡N group perpendicular to the *b* axis. Preserving the assumption of the planar zigzag conformation for the carbon backbone, it was possible to interpret another linear array of peaks extending upwards from the origin into the cell. These two constraints led to a model which was in reasonable accord with a rather complex and ambiguous Harker section at $b=\frac{1}{2}$ and, using it, it was possible to analyze satisfactory the principal features of the Patterson synthesis.

An electron density projection on (010) reproduced the essential features of the model. Several Fourier refinements, neglecting hydrogen and utilizing a single isotropic temperature factor, reduced $R$ to 0·21 for the projection. Substantial coordinate shifts were involved in this initial refinement.

## Three-dimensional refinement

At this point it was decided to continue the refinement by three-dimensional least-squares analysis. For the asymmetric half of the molecule,



$$\begin{array}{c} \mathrm{N(3)} \\ ||| \\ \mathrm{N(1)}\equiv\mathrm{C(1)}-\mathrm{C(2)}-\mathrm{C(3)}-\overset{\overset{\mathrm{C(9)}}{|}}{\underset{\underset{\underset{\|}{\mathrm{C(8)}}}{|}}{\mathrm{C(4)}}}-\mathrm{C(5)}-\mathrm{C(6)}-\mathrm{C(7)}\equiv\mathrm{N(2)}, \\ \cdot \end{array}$$

the *x* and *z* coordinates of atoms C(9) and N(5) were the least reliable because of severe overlap in the projection. Nevertheless, all coordinates were known with sufficient accuracy to make it possible to compute relative *y* coordinates by using conventionally accepted values of bond lengths and angles. The molecule was then placed in the cell by setting $y=0·0$ for C(8) since the projected length of the double bond was 1·3 Å, close to the expected value.

The full-matrix least-squares program used for the refinement was written by Gantzel, Sparks & Trueblood at the University of California and modified by Y. Okaya (1962) at the IBM Laboratories. Each iteration using the full set of data (1445) and 120 parameters required 14 minutes on an IBM 7090 computer. The unobserved data were introduced in each case as 0·28 times the minimum observable $F(hkl)$ and the appropriate correction factors were then applied. The weighting system used in all of the refinements,

$$\begin{aligned} F_o &\le 10·0\,, & \sqrt{w} &= 0·00895F_o\,; \\ 50·0 > F_o &> 10·0\,, & \sqrt{w} &= 0·0283\sqrt{F_o}\,; \\ F_o &\ge 50·0\,, & \sqrt{w} &= 10·0F_o{}^{-1}\,, \end{aligned}$$

involved a reasonably continuous function of $F_o$.

A series of preliminary least-squares analyses with selected groups of data led to better values for the *y* parameters and, in general, an improved coordinate set. Hydrogen atom positions were then estimated and included in the final complete refinement. Atomic form factors were those of Berghuis *et.al.* (1955) for carbon and nitrogen and McWeeny (1951) for hydrogen. Since the program could treat a maximum of 128 parameters, only atoms N(1), C(1), N(3), C(9), N(2), C(7) and C(8) were given full anisotropic temperature factors. The hydrogen atoms were arbitrarily assigned fixed isotropic temperature factors of $B=4·0$ and all other atoms were refined with a simple isotropic factor.

The refinement proceeded smoothly through five iterations and a final value of $R=0·131$ was obtained for all data including the unobserved. A value of $R=0·110$ was calculated utilizing only the observed data. A detailed comparison of $F_{\text{obs}}$ and $F_{\text{calc}}$ is presented in Table 1 for all of the data.

## Discusions of the structure

### *Bond lengths, bond angles and thermal parameters*

The final positional parameters are recorded in Table 2 along with the estimated standard deviations calculated from the least-squares analysis. In Table 3, a listing of all bond lengths in the molecule, the hydrogen atoms are numbered to correspond to the carbon to which they are bound. If two hydrogen atoms are on a carbon atom, one is designated by a primed number. Atom C(8′) is centrosymmetrically related to atom C(8). The least-squares analysis yielded an estimated standard deviation for bond C(8)–C(8′) of 0·016 Å; for all C–H bonds it is 0·07 Å and for all other bonds not involving hydrogen it is

0·008 Å. All bond angles and their estimated standard deviations are given in Table 4.

The average of the three C–N bond lengths, 1·123 Å is slightly shorter than the usually accepted value of about 1·14 Å (*Tables of Interatomic Distances*, 1958). Low values could be expected for two reasons. First, since there is a concentration of electron density in the triple bond, the use of spherically symmetric atomic

Table 1. *Observed and calculated structure factors*

| h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 1 | 29.8 | 27.0 | 12 | 0 | -2 | 6.6 | 6.5 | 4 | 1 | -2 | 37.6 | 38.9 | 16 | 1 | -5 | 6.5 | 4.9 | 2 | 1 | -10 | 2.5 | -3.0 | 5 | 2 | 3 | 20.6 | 21.5 | 16 | 2 | -6 | 3.4 | 0.9 |
| 0 | 0 | 2 | 57.4 | -58.6 | 12 | 0 | -3 | 3.0 | 3.2 | 5 | 1 | -2 | 40.6 | 42.0 | 18 | 1 | -5 | 4.7 | -2.8 | 3 | 1 | -10 | 2.9 | 2.9 | 4 | 2 | 3 | 20.3 | -20.7 | 18 | 2 | -6 | 3.8 | -3.0 |
| 0 | 0 | 3 | 28.5 | -27.8 | 12 | 0 | -4 | 6.2 | 5.4 | 6 | 1 | -2 | 11.0 | 11.2 | 12 | 1 | 6 | 6.8 | 6.9 | 4 | 1 | -10 | 2.5 | -1.2 | 3 | 2 | 3 | 13.0 | -12.2 | 10 | 2 | 7 | 2.5 | -1.2 |
| 0 | 0 | 4 | 6.4 | 6.8 | 12 | 0 | -5 | 19.5 | 21.6 | 7 | 1 | -2 | 5.6 | 5.7 | 11 | 1 | 6 | 6.8 | -5.6 | 5 | 1 | -10 | 6.2 | -4.6 | 2 | 2 | 3 | 5.5 | 5.3 | 7 | 2 | 7 | 3.6 | 2.3 |
| 0 | 0 | 5 | 21.4 | -21.1 | 12 | 0 | -7 | 12.2 | -11.6 | 8 | 1 | -2 | 5.3 | -3.6 | 10 | 1 | 6 | 4.7 | -5.0 | 6 | 1 | -10 | 6.2 | 6.2 | 1 | 2 | 3 | 10.1 | -9.6 | 6 | 2 | 7 | 3.8 | 3.3 |
| 0 | 0 | 6 | 11.8 | -13.6 | 12 | 0 | -8 | 3.8 | 2.2 | 9 | 1 | -2 | 3.1 | 2.0 | 9 | 1 | 6 | 4.1 | 4.4 | 7 | 1 | -10 | 3.6 | -2.6 | 0 | 2 | 3 | 6.8 | 5.5 | 5 | 2 | 7 | 5.0 | -6.3 |
| 0 | 0 | 7 | 5.3 | -4.8 | 12 | 0 | -9 | 8.0 | -7.3 | 10 | 1 | -2 | 3.4 | -3.4 | 8 | 1 | 6 | 2.8 | 1.6 | 8 | 1 | -10 | 2.9 | -2.5 | 1 | 2 | -3 | 23.0 | 22.7 | 4 | 2 | 7 | 3.1 | 2.8 |
| 0 | 0 | 9 | 6.2 | -5.9 | 14 | 0 | 0 | 5.1 | -4.5 | 12 | 1 | -2 | 3.5 | -2.9 | 7 | 1 | 6 | 4.8 | -4.2 | 10 | 1 | -10 | 2.7 | 1.3 | 2 | 2 | -3 | 19.1 | -16.2 | 3 | 2 | 7 | 3.1 | -1.7 |
| 2 | 0 | 0 | 35.8 | 36.9 | 14 | 0 | 1 | 6.7 | -5.5 | 13 | 1 | -2 | 5.2 | 5.0 | 6 | 1 | 6 | 6.3 | 6.1 | 13 | 1 | -10 | 9.6 | -9.2 | 3 | 2 | -3 | 13.2 | -12.7 | 2 | 2 | 7 | 8.7 | -8.7 |
| 2 | 0 | 1 | 45.5 | -45.8 | 14 | 0 | 2 | 8.7 | -7.4 | 14 | 1 | -2 | 8.7 | 8.3 | 5 | 1 | 6 | 8.2 | -7.9 | 15 | 1 | -10 | 1.9 | -2.2 | 4 | 2 | -3 | 7.5 | 5.9 | 1 | 2 | 7 | 10.1 | 9.2 |
| 2 | 0 | 2 | 34.4 | -33.3 | 14 | 0 | 4 | 3.0 | 3.3 | 15 | 1 | -2 | 12.2 | 13.4 | 4 | 1 | 6 | 8.8 | 10.2 | 0 | 1 | -11 | 2.5 | -2.7 | 5 | 2 | -3 | 2.8 | 0.5 | 0 | 2 | 7 | 8.4 | -7.5 |
| 2 | 0 | 3 | 4.8 | -4.4 | 14 | 0 | 5 | 3.9 | 4.3 | 16 | 1 | -2 | 4.1 | -3.5 | 3 | 1 | 6 | 7.2 | -7.3 | 2 | 1 | -11 | 3.5 | -2.8 | 6 | 2 | -3 | 2.8 | 0.6 | 1 | 2 | -7 | 19.7 | -20.6 |
| 2 | 0 | 4 | 24.8 | -23.2 | 14 | 0 | -1 | 8.6 | 8.2 | 17 | 1 | -2 | 2.9 | -1.5 | 2 | 1 | 6 | 2.7 | -1.2 | 5 | 1 | -11 | 4.0 | -4.6 | 8 | 2 | -3 | 4.5 | 4.3 | 2 | 2 | -7 | 20.3 | -21.7 |
| 2 | 0 | 6 | 2.9 | 2.7 | 14 | 0 | -2 | 10.3 | 13.1 | 19 | 1 | -2 | 5.0 | 1.0 | 1 | 1 | 6 | 3.0 | 4.1 | 7 | 1 | -11 | 5.3 | -5.3 | 9 | 2 | -3 | 20.0 | 20.1 | 4 | 2 | -7 | 3.4 | 3.9 |
| 2 | 0 | 7 | 9.3 | -8.7 | 14 | 0 | -3 | 4.3 | -2.2 | 15 | 1 | 3 | 5.2 | -4.3 | 0 | 1 | 6 | 9.2 | -8.5 | 8 | 1 | -11 | 8.5 | -6.8 | 10 | 2 | -3 | 19.8 | 18.8 | 5 | 2 | -7 | 3.4 | 2.7 |
| 2 | 0 | 8 | 3.7 | -3.0 | 14 | 0 | -4 | 15.9 | -16.4 | 14 | 1 | 3 | 2.5 | 1.7 | 3 | 1 | -6 | 12.5 | 10.6 | 9 | 1 | -11 | 3.8 | -3.8 | 11 | 2 | -3 | 5.3 | 3.9 | 6 | 2 | -7 | 6.0 | -4.9 |
| 2 | 0 | -1 | 9.5 | 7.5 | 14 | 0 | -5 | 15.6 | 18.3 | 13 | 1 | 3 | 4.9 | -4.8 | 4 | 1 | -6 | 17.5 | 16.3 | 10 | 1 | -11 | 4.7 | -6.0 | 12 | 2 | -3 | 7.2 | -6.3 | 7 | 2 | -7 | 15.2 | 15.6 |
| 2 | 0 | -2 | 74.8 | 74.6 | 14 | 0 | -6 | 4.3 | 3.3 | 12 | 1 | 3 | 6.2 | -7.4 | 5 | 1 | -6 | 8.4 | -8.5 | 11 | 1 | -11 | 6.2 | 5.3 | 13 | 2 | -3 | 10.3 | -9.5 | 8 | 2 | -7 | 20.2 | -20.9 |
| 2 | 0 | -3 | 60.1 | 60.5 | 14 | 0 | -8 | 5.3 | -7.0 | 10 | 1 | 3 | 6.6 | 5.4 | 6 | 1 | -6 | 24.6 | 23.8 | 12 | 1 | -11 | 5.5 | -7.0 | 16 | 2 | -3 | 10.4 | 9.3 | 9 | 2 | -7 | 13.7 | 13.2 |
| 2 | 0 | -4 | 18.1 | 18.1 | 14 | 0 | -10 | 3.3 | -2.8 | 9 | 1 | 3 | 10.0 | -10.9 | 7 | 1 | -6 | 15.5 | -14.8 | 2 | 2 | 0 | 13.7 | -13.8 | 17 | 2 | -3 | 3.4 | -2.3 | 10 | 2 | -7 | 5.1 | 3.5 |
| 2 | 0 | -5 | 30.4 | -28.8 | 16 | 0 | 0 | 5.4 | -5.3 | 8 | 1 | 3 | 5.8 | 5.3 | 8 | 1 | -6 | 8.9 | 7.6 | 3 | 2 | 0 | 47.8 | 51.8 | 18 | 2 | -3 | 5.8 | 5.5 | 12 | 2 | -7 | 5.5 | 4.3 |
| 2 | 0 | -6 | 10.2 | -9.6 | 16 | 0 | 1 | 8.6 | 6.5 | 7 | 1 | 3 | 5.4 | 6.0 | 9 | 1 | -6 | 3.1 | -1.9 | 4 | 2 | 0 | 16.7 | 14.8 | 19 | 2 | -3 | 8.0 | 1.6 | 13 | 2 | -7 | 5.9 | -5.3 |
| 2 | 0 | -8 | 11.1 | -11.9 | 16 | 0 | -1 | 14.0 | -12.5 | 5 | 1 | 3 | 14.7 | -14.3 | 10 | 1 | -6 | 2.8 | -1.8 | 5 | 2 | 0 | 21.1 | 18.8 | 14 | 2 | 4 | 5.8 | -5.3 | 14 | 2 | -7 | 4.7 | 4.2 |
| 2 | 0 | -9 | 6.1 | -5.1 | 16 | 0 | -2 | 8.5 | 7.7 | 4 | 1 | 3 | 24.7 | -24.5 | 11 | 1 | -6 | 10.6 | -10.3 | 6 | 2 | 0 | 18.9 | 16.1 | 12 | 2 | 4 | 2.7 | 1.8 | 16 | 2 | -7 | 3.1 | 1.0 |
| 2 | 0 | -10 | 7.0 | 5.6 | 16 | 0 | -3 | 12.5 | 10.5 | 3 | 1 | 3 | 9.7 | 9.2 | 12 | 1 | -6 | 11.9 | -11.6 | 8 | 2 | 0 | 9.6 | 7.4 | 10 | 2 | 4 | 3.9 | -3.6 | 17 | 2 | -7 | 9.8 | 9.1 |
| 4 | 0 | 0 | 36.5 | -36.3 | 16 | 0 | -5 | 5.3 | 5.9 | 2 | 1 | 3 | 22.7 | -21.6 | 13 | 1 | -6 | 4.8 | 5.8 | 9 | 2 | 0 | 5.3 | -4.4 | 9 | 2 | 4 | 3.1 | 1.7 | 9 | 2 | 8 | 3.1 | 4.5 |
| 4 | 0 | 1 | 5.5 | 3.8 | 16 | 0 | -7 | 3.5 | 4.9 | 1 | 1 | 3 | 23.3 | 20.9 | 14 | 1 | -6 | 9.6 | -9.5 | 11 | 2 | 0 | 10.4 | -9.6 | 8 | 2 | 4 | 13.8 | -15.1 | 8 | 2 | 8 | 6.4 | -7.3 |
| 4 | 0 | 2 | 25.7 | -25.1 | 16 | 0 | -8 | 4.8 | -5.4 | 0 | 1 | 3 | 31.6 | 30.6 | 15 | 1 | -6 | 9.6 | 7.8 | 12 | 2 | 0 | 10.2 | 10.6 | 7 | 2 | 4 | 13.7 | -14.5 | 7 | 2 | 8 | 5.3 | 7.0 |
| 4 | 0 | 3 | 23.8 | 22.0 | 18 | 0 | 1 | 3.6 | -2.8 | 1 | 1 | -3 | 1.9 | -1.4 | 17 | 1 | -6 | 4.3 | 3.9 | 15 | 2 | 0 | 2.9 | 1.6 | 6 | 2 | 4 | 3.8 | 2.9 | 5 | 2 | 8 | 4.4 | -5.4 |
| 4 | 0 | 4 | 6.9 | -6.1 | 18 | 0 | -1 | 2.9 | 2.2 | 2 | 1 | -3 | 18.4 | 16.2 | 18 | 1 | -6 | 2.0 | 2.3 | 16 | 2 | 1 | 4.8 | -4.9 | 5 | 2 | 4 | 3.5 | -2.3 | 3 | 2 | 8 | 2.9 | -3.1 |
| 4 | 0 | 5 | 9.3 | 10.6 | 18 | 0 | -2 | 8.3 | 7.7 | 3 | 1 | -3 | 10.6 | -8.5 | 19 | 1 | -6 | 2.9 | -1.4 | 15 | 2 | 1 | 3.3 | 2.1 | 4 | 2 | 4 | 13.8 | -12.6 | 2 | 2 | 8 | 7.2 | -6.9 |
| 4 | 0 | 6 | 5.9 | -6.9 | 18 | 0 | -3 | 4.1 | -2.8 | 4 | 1 | -3 | 46.3 | 45.4 | 11 | 1 | 7 | 3.6 | -3.5 | 10 | 2 | 1 | 4.2 | -4.5 | 3 | 2 | 4 | 14.5 | 13.9 | 1 | 2 | 8 | 7.3 | -7.2 |
| 4 | 0 | 7 | 10.7 | -9.3 | 18 | 0 | -6 | 5.9 | 5.9 | 5 | 1 | -3 | 23.3 | 21.4 | 10 | 1 | 7 | 2.0 | -2.1 | 9 | 2 | 1 | 6.8 | -7.7 | 1 | 2 | 4 | 8.5 | 9.3 | 0 | 2 | 8 | 5.6 | -7.3 |
| 4 | 0 | 8 | 7.7 | 8.2 | 18 | 0 | -7 | 3.8 | 3.4 | 6 | 1 | -3 | 3.5 | 3.3 | 7 | 1 | 7 | 3.1 | 3.8 | 8 | 2 | 1 | 2.6 | 0.8 | 0 | 2 | 4 | 7.8 | -7.0 | 1 | 2 | -8 | 5.9 | 4.9 |
| 4 | 0 | 9 | 7.7 | 5.5 | 18 | 0 | -8 | 5.2 | 6.1 | 7 | 1 | -3 | 14.0 | 14.1 | 6 | 1 | 7 | 7.7 | -8.3 | 7 | 2 | 1 | 10.3 | -9.4 | 1 | 2 | -4 | 26.6 | 24.7 | 2 | 2 | -8 | 8.6 | -9.9 |
| 4 | 0 | 10 | 6.0 | -7.3 | 20 | 0 | -4 | 6.7 | 7.2 | 8 | 1 | -3 | 2.2 | -0.1 | 5 | 1 | 7 | 3.6 | -0.2 | 6 | 2 | 1 | 21.3 | -20.0 | 2 | 2 | -4 | 5.4 | 5.2 | 4 | 2 | -8 | 7.9 | 9.2 |
| 4 | 0 | -1 | 21.2 | 21.2 | 2 | 1 | 0 | 24.8 | 26.9 | 9 | 1 | -3 | 2.3 | 3.1 | 3 | 1 | 7 | 16.5 | -18.3 | 5 | 2 | 1 | 14.7 | -12.6 | 3 | 2 | -4 | 2.2 | 2.2 | 5 | 2 | -8 | 4.1 | -3.6 |
| 4 | 0 | -2 | 10.1 | 12.8 | 3 | 1 | 0 | 2.8 | 4.2 | 12 | 1 | -3 | 7.2 | -7.1 | 1 | 1 | 7 | 6.2 | -6.1 | 4 | 2 | 1 | 16.7 | 15.8 | 4 | 2 | -4 | 8.6 | -6.4 | 6 | 2 | -8 | 9.5 | 9.9 |
| 4 | 0 | -3 | 18.7 | 18.6 | 4 | 1 | 0 | 19.6 | -20.9 | 13 | 1 | -3 | 11.2 | -10.6 | 0 | 1 | 7 | 2.8 | 0.8 | 3 | 2 | 1 | 7.5 | -7.1 | 5 | 2 | -4 | 14.0 | -12.5 | 7 | 2 | -8 | 9.9 | -8.2 |
| 4 | 0 | -4 | 19.8 | -17.2 | 5 | 1 | 0 | 42.8 | 43.6 | 14 | 1 | -3 | 7.2 | -7.8 | 1 | 1 | -7 | 2.8 | 0.2 | 2 | 2 | 1 | 21.6 | -20.2 | 6 | 2 | -4 | 11.3 | -12.7 | 8 | 2 | -8 | 6.7 | -8.2 |
| 4 | 0 | -5 | 6.3 | -4.6 | 6 | 1 | 0 | 19.3 | -18.0 | 15 | 1 | -3 | 9.4 | 10.5 | 2 | 1 | -7 | 2.7 | -1.2 | 1 | 2 | 1 | 49.2 | -49.5 | 7 | 2 | -4 | 7.3 | -6.3 | 10 | 2 | -8 | 8.3 | -9.3 |
| 4 | 0 | -6 | 17.7 | 19.1 | 7 | 1 | 0 | 7.9 | -6.4 | 16 | 1 | -3 | 10.3 | -11.5 | 3 | 1 | -7 | 10.3 | -9.1 | 0 | 2 | 1 | 34.5 | 34.9 | 8 | 2 | -4 | 8.8 | 7.3 | 12 | 2 | -8 | 3.6 | -3.1 |
| 4 | 0 | -7 | 19.0 | 20.3 | 8 | 1 | 0 | 3.3 | -3.3 | 17 | 1 | -3 | 6.2 | 6.5 | 4 | 1 | -7 | 6.5 | 5.9 | 1 | 2 | -1 | 19.1 | -21.4 | 9 | 2 | -4 | 16.3 | 15.6 | 13 | 2 | -8 | 2.7 | 2.3 |
| 4 | 0 | -8 | 22.3 | -27.2 | 9 | 1 | 0 | 9.7 | -7.6 | 19 | 1 | -3 | 5.3 | 5.2 | 6 | 1 | -7 | 21.1 | -20.8 | 2 | 2 | -1 | 48.8 | 54.8 | 10 | 2 | -4 | 16.5 | 15.9 | 14 | 2 | -8 | 4.1 | 4.3 |
| 4 | 0 | -9 | 10.7 | -8.5 | 10 | 1 | 0 | 3.5 | 1.5 | 15 | 1 | 4 | 2.4 | 2.9 | 7 | 1 | -7 | 9.4 | -8.6 | 3 | 2 | -1 | 46.7 | -50.3 | 11 | 2 | -4 | 19.7 | 20.5 | 16 | 2 | -8 | 3.4 | -2.2 |
| 4 | 0 | -10 | 4.1 | 2.1 | 11 | 1 | 0 | 3.4 | 3.1 | 13 | 1 | 4 | 3.1 | -2.7 | 8 | 1 | -7 | 4.3 | -3.8 | 4 | 2 | -1 | 14.0 | -13.7 | 12 | 2 | -4 | 18.1 | 18.6 | 17 | 2 | -8 | 3.6 | 3.3 |
| 6 | 0 | 0 | 12.0 | -10.0 | 13 | 1 | 0 | 8.1 | 8.7 | 12 | 1 | 4 | 13.3 | -16.1 | 9 | 1 | -7 | 5.7 | 5.7 | 5 | 2 | -1 | 3.7 | 3.1 | 15 | 2 | -4 | 4.2 | 1.8 | 6 | 2 | 9 | 3.0 | -3.8 |
| 6 | 0 | 1 | 18.0 | 17.5 | 14 | 1 | 0 | 8.5 | -8.7 | 11 | 1 | 4 | 2.8 | 3.3 | 10 | 1 | -7 | 4.6 | 6.0 | 6 | 2 | -1 | 18.5 | 18.0 | 16 | 2 | -4 | 3.9 | 3.9 | 5 | 2 | 9 | 3.1 | 2.8 |
| 6 | 0 | 3 | 22.9 | 22.5 | 15 | 1 | 0 | 6.0 | -6.1 | 10 | 1 | 4 | 7.6 | -8.3 | 11 | 1 | -7 | 2.9 | -2.3 | 7 | 2 | -1 | 27.3 | 27.5 | 17 | 2 | -4 | 12.8 | -11.2 | 4 | 2 | 9 | 3.5 | 3.5 |
| 6 | 0 | 4 | 11.1 | 11.1 | 18 | 1 | 0 | 4.5 | -4.2 | 9 | 1 | 4 | 13.0 | -13.5 | 12 | 1 | -7 | 5.5 | 6.8 | 8 | 2 | -1 | 13.7 | 13.9 | 18 | 2 | -4 | 9.1 | 8.9 | 2 | 2 | 9 | 5.8 | 7.1 |
| 6 | 0 | 5 | 7.5 | -5.2 | 15 | 1 | 1 | 5.9 | -4.4 | 8 | 1 | 4 | 5.6 | -5.6 | 13 | 1 | -7 | 4.3 | -4.0 | 9 | 2 | -1 | 3.9 | 2.5 | 19 | 2 | -4 | 5.1 | -4.2 | 1 | 2 | 9 | 4.7 | -4.9 |
| 6 | 0 | 6 | 11.6 | -11.5 | 14 | 1 | 1 | 7.4 | -8.3 | 7 | 1 | 4 | 10.2 | -8.7 | 14 | 1 | -7 | 2.7 | 0.8 | 11 | 2 | -1 | 14.6 | -14.9 | 13 | 2 | 5 | 3.0 | 4.4 | 0 | 2 | 9 | 3.7 | -4.4 |
| 6 | 0 | 7 | 7.0 | -6.5 | 12 | 1 | 1 | 6.2 | 6.0 | 6 | 1 | 4 | 11.1 | 10.3 | 16 | 1 | -7 | 4.8 | -4.4 | 12 | 2 | -1 | 3.0 | 3.2 | 12 | 2 | 5 | 5.1 | -6.6 | 1 | 2 | -9 | 3.8 | 4.0 |
| 6 | 0 | 9 | 3.6 | -4.9 | 11 | 1 | 1 | 7.6 | 5.8 | 5 | 1 | 4 | 13.4 | -12.1 | 17 | 1 | -7 | 3.4 | 2.5 | 13 | 2 | -1 | 4.3 | 4.6 | 10 | 2 | 5 | 4.7 | -4.8 | 3 | 2 | -9 | 7.7 | -8.5 |
| 6 | 0 | -1 | 17.3 | 15.3 | 10 | 1 | 1 | 4.0 | -3.8 | 3 | 1 | 4 | 12.6 | -10.0 | 19 | 1 | -7 | 1.9 | -1.7 | 14 | 2 | -1 | 5.3 | 5.8 | 8 | 2 | 5 | 4.4 | -4.6 | 4 | 2 | -9 | 5.4 | -5.6 |
| 6 | 0 | -2 | 41.3 | -42.0 | 9 | 1 | 1 | 15.4 | 15.5 | 2 | 1 | 4 | 12.6 | -12.9 | 9 | 1 | 8 | 1.6 | -1.5 | 16 | 2 | -1 | 4.2 | 3.9 | 7 | 2 | 5 | 11.2 | -11.6 | 8 | 2 | -9 | 3.7 | 3.4 |
| 6 | 0 | -3 | 27.6 | 25.5 | 8 | 1 | 1 | 15.9 | -16.4 | 1 | 1 | 4 | 15.1 | 14.9 | 7 | 1 | 8 | 2.2 | 2.2 | 17 | 2 | -1 | 3.7 | 3.3 | 6 | 2 | 5 | 3.8 | -4.0 | 9 | 2 | -9 | 8.3 | 7.6 |
| 6 | 0 | -4 | 38.4 | 37.3 | 7 | 1 | 1 | 23.3 | -24.4 | 0 | 1 | 4 | 7.2 | 6.3 | 6 | 1 | 8 | 4.9 | -5.1 | 17 | 2 | 2 | 3.9 | -3.9 | 4 | 2 | 5 | 3.8 | -3.9 | 10 | 2 | -9 | 8.9 | -8.2 |
| 6 | 0 | -5 | 22.1 | -20.1 | 6 | 1 | 1 | 42.2 | -43.9 | 1 | 1 | -4 | 13.3 | -11.0 | 5 | 1 | 8 | 5.2 | 6.0 | 16 | 2 | 2 | 4.2 | -4.0 | 3 | 2 | 5 | 6.3 | 6.3 | 12 | 2 | -9 | 6.2 | -5.5 |
| 6 | 0 | -6 | 29.2 | -30.1 | 5 | 1 | 1 | 21.7 | -21.2 | 2 | 1 | -4 | 4.3 | -3.0 | 3 | 1 | 8 | 5.6 | -5.9 | 13 | 2 | 2 | 5.7 | 4.3 | 2 | 2 | 5 | 11.2 | -10.6 | 13 | 2 | -9 | 3.7 | -3.3 |
| 6 | 0 | -7 | 9.2 | 9.4 | 4 | 1 | 1 | 14.2 | 13.5 | 3 | 1 | -4 | 32.3 | -30.9 | 1 | 1 | 8 | 10.9 | -11.3 | 12 | 2 | 2 | 8.5 | -8.9 | 1 | 2 | 5 | 11.4 | -11.0 | 15 | 2 | -9 | 6.5 | -5.4 |
| 6 | 0 | -9 | 5.1 | 4.7 | 3 | 1 | 1 | 21.2 | 18.9 | 4 | 1 | -4 | 39.9 | -38.0 | 0 | 1 | 8 | 3.3 | 2.6 | 11 | 2 | 2 | 10.6 | 12.2 | 0 | 2 | 5 | 8.6 | -9.1 | 16 | 2 | -9 | 6.5 | -5.4 |
| 6 | 0 | -10 | 7.4 | -8.3 | 2 | 1 | 1 | 92.1 | 104.2 | 5 | 1 | -4 | 2.0 | 3.2 | 1 | 1 | -8 | 3.3 | -1.0 | 10 | 2 | 2 | 8.4 | -8.7 | 1 | 2 | -5 | 20.2 | 20.9 | 3 | 2 | 10 | 4.6 | 3.9 |
| 8 | 0 | 0 | 3.5 | 5.3 | 1 | 1 | 1 | 19.2 | -16.8 | 7 | 1 | -4 | 37.3 | 36.7 | 2 | 1 | -8 | 8.4 | -5.6 | 9 | 2 | 2 | 16.0 | -16.0 | 2 | 2 | -5 | 30.1 | 30.5 | 2 | 2 | 10 | 6.8 | 9.1 |
| 8 | 0 | 1 | 32.5 | 31.3 | 0 | 1 | 1 | 26.6 | 25.7 | 8 | 1 | -4 | 5.0 | 4.5 | 3 | 1 | -8 | 14.4 | -13.5 | 8 | 2 | 2 | 5.0 | 4.7 | 3 | 2 | -5 | 7.8 | 6.9 | 1 | 2 | 10 | 6.9 | 5.9 |
| 8 | 0 | 2 | 34.0 | 32.0 | 1 | 1 | -1 | 49.5 | 53.5 | 9 | 1 | -4 | 4.8 | -3.5 | 4 | 1 | -8 | 9.2 | -7.4 | 7 | 2 | 2 | 12.3 | -11.4 | 5 | 2 | -5 | 5.0 | -3.4 | 0 | 2 | 10 | 3.8 | -2.9 |
| 8 | 0 | 3 | 17.5 | -18.5 | 2 | 1 | -1 | 25.9 | -25.4 | 10 | 1 | -4 | 2.9 | -2.3 | 5 | 1 | -8 | 3.8 | 3.1 | 6 | 2 | 2 | 2.8 | -2.5 | 6 | 2 | -5 | 9.6 | -8.7 | 2 | 2 | -10 | 5.8 | -5.5 |
| 8 | 0 | 4 | 13.5 | -14.9 | 3 | 1 | -1 | 21.5 | 21.1 | 11 | 1 | -4 | 9.6 | 9.3 | 6 | 1 | -8 | 10.2 | -9.1 | 5 | 2 | 2 | 13.2 | -11.1 | 7 | 2 | -5 | 4.8 | 3.2 | 4 | 2 | -10 | 9.0 | -8.4 |
| 8 | 0 | 5 | 15.7 | -16.9 | 4 | 1 | -1 | 19.9 | 22.8 | 13 | 1 | -4 | 7.2 | 6.4 | 7 | 1 | -8 | 2.9 | 1.7 | 4 | 2 | 2 | 16.2 | 16.4 | 8 | 2 | -5 | 16.3 | 15.1 | 6 | 2 | -10 | 3.4 | 0.5 |
| 8 | 0 | 6 | 9.2 | -8.9 | 5 | 1 | -1 | 42.1 | 43.6 | 14 | 1 | -4 | 3.5 | 3.9 | 8 | 1 | -8 | 8.7 | 8.4 | 3 | 2 | 2 | 12.2 | -10.9 | 9 | 2 | -5 | 17.8 | -16.2 | 7 | 2 | -10 | 7.8 | -7.8 |
| 8 | 0 | 8 | 6.4 | 7.4 | 6 | 1 | -1 | 12.9 | 10.8 | 16 | 1 | -4 | 13.2 | 10.6 | 9 | 1 | -8 | 4.8 | -5.3 | 2 | 2 | 2 | 11.3 | 10.7 | 11 | 2 | -5 | 9.7 | -7.7 | 10 | 2 | -10 | 7.7 | -7.5 |
| 8 | 0 | -1 | 9.0 | 7.4 | 7 | 1 | -1 | 9.6 | 7.9 | 17 | 1 | -4 | 2.5 | 3.0 | 11 | 1 | -8 | 7.6 | -8.4 | 1 | 2 | 2 | 11.4 | -10.1 | 12 | 2 | -5 | 8.7 | 9.3 | 11 | 2 | -10 | 4.7 | 3.6 |
| 8 | 0 | -2 | 8.6 | 8.1 | 8 | 1 | -1 | 11.1 | -10.9 | 19 | 1 | -4 | 5.3 | 1.5 | 15 | 1 | -8 | 2.7 | 1.9 | 0 | 2 | 2 | 24.0 | 22.9 | 14 | 2 | -5 | 8.7 | -8.3 | 12 | 2 | -10 | 7.1 | -8.2 |
| 8 | 0 | -4 | 6.9 | 6.7 | 9 | 1 | -1 | 3.1 | -2.6 | 13 | 1 | 5 | 2.8 | -6.2 | 17 | 1 | -8 | 3.3 | 3.2 | 1 | 2 | -2 | 7.2 | 4.8 | 15 | 2 | -5 | 10.0 | 8.7 | 13 | 2 | -10 | 6.4 | 6.5 |
| 8 | 0 | -5 | 14.1 | -14.7 | 10 | 1 | -1 | 2.4 | 0.5 | 12 | 1 | 5 | 7.8 | 4.5 | 18 | 1 | -8 | 5.1 | 6.0 | 2 | 2 | -2 | 19.4 | 18.5 | 16 | 2 | -5 | 6.0 | -4.6 | 14 | 2 | -10 | 2.3 | -3.0 |
| 8 | 0 | -6 | 6.8 | 7.4 | 11 | 1 | -1 | 7.6 | 6.7 | 11 | 1 | 5 | 4.3 | -0.4 | 7 | 1 | 9 | 1.7 | -1.5 | 3 | 2 | -2 | 19.9 | -19.1 | 17 | 2 | -5 | 3.8 | 2.3 | 4 | 2 | -11 | 2.8 | -5.0 |
| 8 | 0 | -8 | 6.6 | -5.9 | 12 | 1 | -1 | 5.5 | 6.2 | 9 | 1 | 5 | 6.9 | 7.0 | 6 | 1 | 9 | 6.0 | 5.9 | 4 | 2 | -2 | 2.3 | 1.3 | 18 | 2 | -5 | 5.5 | 5.1 | 5 | 2 | -11 | 2.3 | -2.0 |
| 8 | 0 | -9 | 10.3 | -9.9 | 13 | 1 | -1 | 15.0 | 14.4 | 7 | 1 | 5 | 8.6 | -7.3 | 4 | 1 | 9 | 4.7 | 4.1 | 5 | 2 | -2 | 10.5 | 10.4 | 19 | 2 | -5 | 4.5 | 0.9 | 7 | 2 | -11 | 3.1 | -3.3 |
| 8 | 0 | -10 | 4.0 | -5.8 | 14 | 1 | -1 | 8.3 | 9.0 | 6 | 1 | 5 | 5.1 | 4.9 | 3 | 1 | 9 | 9.4 | 8.0 | 6 | 2 | -2 | 15.8 | 16.5 | 12 | 2 | 6 | 3.2 | -3.2 | 8 | 2 | -11 | 4.2 | -2.3 |
| 10 | 0 | 0 | 10.2 | 9.4 | 17 | 1 | -1 | 4.5 | -3.7 | 5 | 1 | 5 | 11.1 | -12.2 | 2 | 1 | 9 | 7.5 | 6.9 | 7 | 2 | -2 | 5.1 | -3.9 | 11 | 2 | 6 | 2.9 | 2.7 | 9 | 2 | -11 | 2.5 | -1.2 |
| 10 | 0 | 1 | 8.6 | 9.6 | 17 | 1 | 2 | 3.1 | -2.1 | 4 | 1 | 5 | 3.9 | 4.2 | 1 | 1 | 9 | 2.6 | -2.5 | 8 | 2 | -2 | 10.5 | 12.3 | 9 | 2 | 6 | 3.6 | 3.7 | 10 | 3 | -3 | 20.9 | 23.2 |
| 10 | 0 | 2 | 3.8 | -4.1 | 16 | 1 | 2 | 3.9 | -3.5 | 3 | 1 | 5 | 9.9 | -8.9 | 0 | 1 | 9 | 2.7 | -2.0 | 9 | 2 | -2 | 5.9 | -4.7 | 8 | 2 | 6 | 3.7 | 4.5 | 6 | 3 | -4 | 5.6 | 5.5 |
| 10 | 0 | 3 | 40.9 | -43.5 | 15 | 1 | 2 | 6.0 | -5.7 | 2 | 1 | 5 | 2.1 | 1.3 | 1 | 1 | -9 | 3.8 | 3.4 | 10 | 2 | -2 | 7.2 | 7.5 | 6 | 2 | 6 | 4.4 | -3.3 | 9 | 3 | -8 | 3.0 | 0.4 |
| 10 | 0 | 4 | 5.3 | -4.0 | 13 | 1 | 2 | 6.2 | -6.8 | 1 | 1 | 5 | 10.0 | 9.6 | 2 | 1 | -9 | 9.7 | 9.8 | 11 | 2 | -2 | 10.7 | -10.9 | 3 | 2 | 6 | 3.6 | 3.0 | 2 | 3 | 0 | 2.7 | 2.1 |
| 10 | 0 | 5 | 14.8 | 13.1 | 12 | 1 | 2 | 3.6 | 3.9 | 0 | 1 | 5 | 14.4 | -11.9 | 3 | 1 | -9 | 3.8 | -3.7 | 12 | 2 | -2 | 15.1 | -15.4 | 2 | 2 | 6 | 9.5 | -8.1 | 3 | 3 | 0 | 6.2 | 5.9 |
| 10 | 0 | 7 | 4.2 | -2.4 | 11 | 1 | 2 | 5.2 | -5.0 | 1 | 1 | -5 | 4.2 | -2.2 | 4 | 1 | -9 | 6.2 | 5.9 | 13 | 2 | -2 | 3.1 | -2.4 | 1 | 2 | 6 | 10.1 | 9.5 | 4 | 3 | 0 | 22.2 | 21.8 |
| 10 | 0 | -1 | 6.1 | 5.3 | 10 | 1 | 2 | 7.2 | 9.6 | 2 | 1 | -5 | 4.0 | 1.8 | 5 | 1 | -9 | 10.7 | -11.1 | 14 | 2 | -2 | 4.9 | 3.8 | 0 | 2 | 6 | 8.8 | -8.1 | 5 | 3 | 0 | 6.7 | 7.6 |
| 10 | 0 | -2 | 27.1 | 25.5 | 9 | 1 | 2 | 5.7 | 4.7 | 3 | 1 | -5 | 9.7 | -8.7 | 6 | 1 | -9 | 5.6 | 4.6 | 15 | 2 | -2 | 6.8 | -7.4 | 1 | 2 | -6 | 6.4 | -6.7 | 6 | 3 | 0 | 9.7 | -10.5 |
| 10 | 0 | -3 | 12.2 | 12.1 | 8 | 1 | 2 | 24.6 | 24.7 | 4 | 1 | -5 | 25.2 | -23.6 | 7 | 1 | -9 | 3.6 | -4.4 | 16 | 2 | -2 | 3.7 | 3.1 | 2 | 2 | -6 | 5.5 | 5.2 | 7 | 3 | 0 | 9.0 | -6.2 |
| 10 | 0 | -4 | 4.5 | 3.5 | 7 | 1 | 2 | 3.0 | 2.9 | 5 | 1 | -5 | 29.6 | -27.4 | 8 | 1 | -9 | 3.5 | -5.4 | 17 | 2 | -2 | 3.3 | 4.3 | 3 | 2 | -6 | 20.4 | 20.4 | 8 | 3 | 0 | 9.2 | 9.3 |
| 10 | 0 | -5 | 7.1 | -7.1 | 6 | 1 | 2 | 7.7 | 7.2 | 6 | 1 | -5 | 10.2 | 8.7 | 10 | 1 | -9 | 4.4 | -4.3 | 18 | 2 | -2 | 3.9 | -3.5 | 4 | 2 | -6 | 6.9 | 7.4 | 9 | 3 | 0 | 8.1 | 7.2 |
| 10 | 0 | -6 | 9.6 | 10.1 | 5 | 1 | 2 | 6.8 | 4.8 | 7 | 1 | -5 | 15.3 | 13.6 | 11 | 1 | -9 | 3.7 | -2.8 | 19 | 2 | -2 | 7.1 | 7.0 | 5 | 2 | -6 | 3.2 | 3.2 | 10 | 3 | 0 | 6.5 | -7.2 |
| 10 | 0 | -7 | 11.8 | -14.1 | 4 | 1 | 2 | 26.4 | -25.1 | 8 | 1 | -5 | 8.1 | -6.1 | 12 | 1 | -9 | 8.8 | 9.0 | 16 | 2 | 3 | 2.5 | -1.5 | 6 | 2 | -6 | 11.5 | -12.0 | 11 | 3 | 0 | 12.6 | 13.4 |
| 10 | 0 | -9 | 6.1 | -5.1 | 3 | 1 | 2 | 67.9 | 64.3 | 9 | 1 | -5 | 9.0 | 8.7 | 13 | 1 | -9 | 6.4 | -6.0 | 15 | 2 | 3 | 4.4 | -4.1 | 8 | 2 | -6 | 14.0 | -14.6 | 12 | 3 | 0 | 4.7 | -3.7 |
| 10 | 0 | -10 | 10.4 | 9.7 | 2 | 1 | 2 | 42.0 | -42.3 | 10 | 1 | -5 | 3.7 | 4.8 | 14 | 1 | -9 | 4.1 | 5.3 | 14 | 2 | 3 | 5.3 | -4.9 | 9 | 2 | -6 | 12.0 | -10.3 | 13 | 3 | 0 | 4.7 | -4.3 |
| 10 | 0 | -11 | 4.6 | -6.3 | 1 | 1 | 2 | 29.0 | -28.2 | 11 | 1 | -5 | 6.9 | 6.3 | 15 | 1 | -9 | 4.4 | -4.4 | 13 | 2 | 3 | 8.1 | -7.9 | 10 | 2 | -6 | 4.2 | -3.8 | 15 | 3 | 0 | 5.9 | -4.4 |
| 12 | 0 | 0 | 6.8 | -6.4 | 0 | 1 | 2 | 26.5 | -24.2 | 12 | 1 | -5 | 12.1 | 11.0 | 16 | 1 | -9 | 4.1 | -3.5 | 10 | 2 | 3 | 3.1 | 3.2 | 11 | 2 | -6 | 3.1 | 3.7 | 16 | 3 | 0 | 2.8 | 2.4 |
| 12 | 0 | 1 | 8.5 | -6.1 | 1 | 1 | -2 | 35.5 | -35.0 | 13 | 1 | -5 | 11.4 | 11.0 | 4 | 1 | 10 | 3.7 | -4.7 | 8 | 2 | 3 | 3.4 | 3.5 | 12 | 2 | -6 | 4.1 | 5.1 | 16 | 3 | 1 | 3.2 | 2.7 |
| 12 | 0 | 3 | 7.1 | -6.0 | 2 | 1 | -2 | 36.5 | -35.7 | 14 | 1 | -5 | 4.0 | 3.1 | 3 | 1 | 10 | 3.7 | 3.5 | 7 | 2 | 3 | 18.2 | 18.3 | 13 | 2 | -6 | 6.1 | 6.7 | 15 | 3 | 1 | 3.0 | -2.0 |
| 12 | 0 | 6 | 4.0 | -2.3 | 3 | 1 | -2 | 18.8 | 17.7 | 15 | 1 | -5 | 4.7 | -4.6 | 1 | 1 | -10 | 3.0 | -2.8 | 6 | 2 | 3 | 7.5 | 8.0 | 14 | 2 | -6 | 3.9 | 4.5 | 14 | 3 | 1 | 2.7 | 2.3 |

Table 1. (*cont.*)

| h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal | h | k | ℓ | kFob | Fcal |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 3 | 1 | 6.2 | -7.2 | 9 | 3 | 5 | 6.3 | -6.1 | 11 | 3 | -10 | 2.2 | 3.2 | 5 | 4 | -4 | 3.4 | -0.4 | 0 | 0 | 10 | 0.5 | 1.7 | 17 | 2 | 0 | 1.0 | -0.7 | 16 | 3 | -5 | 1.1 | -1.5 |
| 11 | 3 | 1 | 3.1 | -2.5 | 7 | 3 | 5 | 12.1 | -12.1 | 6 | 3 | -11 | 5.6 | -1.0 | 6 | 4 | -4 | 6.9 | 5.3 | 0 | 0 | 11 | 0.3 | -1.0 | 18 | 2 | 0 | 0.7 | 1.2 | 10 | 3 | 6 | 1.0 | -0.2 |
| 9 | 3 | 1 | 5.3 | -3.9 | 6 | 3 | 5 | 9.9 | -9.7 | 7 | 3 | -11 | 1.7 | -2.1 | 7 | 4 | -4 | 4.1 | 5.8 | 2 | 0 | 5 | 0.5 | 4.5 | 18 | 2 | 1 | 0.5 | -3.2 | 9 | 3 | 6 | 1.1 | 0.4 |
| 8 | 3 | 1 | 2.8 | -1.9 | 4 | 3 | 5 | 3.8 | 2.4 | 8 | 3 | -11 | 1.5 | -2.5 | 8 | 4 | -4 | 17.4 | -16.3 | 2 | 0 | 9 | 0.6 | -0.2 | 17 | 2 | 1 | 0.8 | -0.9 | 8 | 3 | 6 | 1.2 | 0.1 |
| 7 | 3 | 1 | 9.5 | 8.0 | 3 | 3 | 5 | 2.9 | -0.1 | 2 | 4 | 0 | 3.0 | -2.3 | 9 | 4 | -4 | 8.1 | -4.7 | 9 | 0 | 10 | 0.5 | 2.7 | 14 | 2 | 1 | 1.2 | -0.2 | 7 | 3 | 6 | 1.3 | 0.4 |
| 6 | 3 | 1 | 19.8 | -19.1 | 2 | 3 | 5 | 5.7 | -6.6 | 3 | 4 | 0 | 12.7 | -12.1 | 10 | 4 | -4 | 3.8 | -3.8 | 2 | 0 | -7 | 0.6 | -1.8 | 13 | 2 | 1 | 1.3 | -0.1 | 6 | 3 | 6 | 1.4 | -1.8 |
| 5 | 3 | 1 | 34.1 | 38.6 | 1 | 3 | 5 | 6.4 | -6.5 | 4 | 4 | 0 | 9.2 | 8.4 | 11 | 4 | -4 | 4.3 | -1.5 | 2 | 0 | -11 | 0.4 | -1.2 | 12 | 2 | 1 | 1.3 | -3.1 | 4 | 3 | 6 | 1.4 | 0.4 |
| 4 | 3 | 1 | 4.9 | -8.0 | 0 | 3 | 5 | 3.8 | 5.9 | 5 | 4 | 0 | 3.7 | -5.9 | 12 | 4 | -4 | 4.9 | 4.1 | 4 | 0 | -11 | 0.4 | 2.6 | 11 | 2 | 1 | 1.3 | 1.9 | 1 | 3 | 6 | 1.7 | -0.7 |
| 3 | 3 | 1 | 20.2 | 21.0 | 1 | 3 | -5 | 2.7 | 0.3 | 6 | 4 | 0 | 13.2 | 16.5 | 13 | 4 | -4 | 4.7 | -4.2 | 6 | 0 | 2 | 0.5 | 0.3 | 10 | 2 | -1 | 1.2 | 1.1 | 2 | 3 | -6 | 1.3 | 0.6 |
| 2 | 3 | 1 | 6.5 | 4.8 | 2 | 3 | -5 | 13.5 | 13.1 | 7 | 4 | 0 | 8.0 | -9.9 | 14 | 4 | -4 | 7.0 | 6.9 | 6 | 0 | 8 | 0.6 | 1.2 | 15 | 2 | -1 | 1.3 | 0.2 | 11 | 3 | -6 | 1.4 | -1.5 |
| 1 | 3 | 1 | 12.3 | -11.9 | 3 | 3 | -5 | 2.7 | -2.7 | 8 | 4 | 0 | 3.5 | 2.7 | 15 | 4 | -4 | 7.8 | 6.9 | 6 | 0 | -8 | 0.6 | -1.2 | 18 | 2 | -1 | 0.9 | 0.2 | 13 | 3 | -6 | 1.3 | -2.2 |
| 0 | 3 | 1 | 2.9 | -2.1 | 4 | 3 | -5 | 15.1 | 15.8 | 9 | 4 | 0 | 12.7 | -14.7 | 16 | 4 | -4 | 8.5 | 7.3 | 6 | 0 | -11 | 0.5 | -0.1 | 19 | 2 | -1 | 0.5 | -4.1 | 15 | 3 | -6 | 1.7 | 2.9 |
| 1 | 3 | -1 | 2.0 | -0.9 | 6 | 3 | -5 | 2.8 | 4.4 | 10 | 4 | 0 | 4.7 | 6.2 | 17 | 4 | -4 | 4.5 | 3.3 | 8 | 0 | 7 | 0.6 | -0.7 | 15 | 2 | 2 | 1.1 | -1.0 | 18 | 3 | -6 | 0.6 | 1.3 |
| 2 | 3 | -1 | 6.2 | 7.7 | 7 | 3 | -5 | 6.2 | 7.2 | 12 | 4 | 0 | 4.2 | -3.8 | 12 | 4 | 5 | 2.5 | -2.4 | 8 | 0 | -3 | 0.5 | 1.3 | 14 | 2 | 2 | 1.2 | 0.4 | 9 | 3 | 7 | 0.8 | -1.3 |
| 3 | 3 | -1 | 1.7 | 2.0 | 8 | 3 | -5 | 16.1 | -16.9 | 13 | 4 | 0 | 4.0 | 4.0 | 11 | 4 | 5 | 2.8 | -3.8 | 8 | 0 | -7 | 0.6 | -1.1 | 12 | 2 | 3 | 1.3 | 3.3 | 7 | 3 | 7 | 1.1 | -0.4 |
| 4 | 3 | -1 | 11.9 | 12.5 | 9 | 3 | -5 | 7.4 | -7.1 | 14 | 4 | 0 | 4.4 | -5.2 | 8 | 4 | 5 | 4.3 | -3.8 | 8 | 0 | -11 | 0.4 | -2.9 | 11 | 2 | 3 | 1.3 | -2.3 | 3 | 3 | 7 | 1.4 | 0.1 |
| 5 | 3 | -1 | 8.1 | -7.7 | 10 | 3 | -5 | 11.4 | -10.8 | 16 | 4 | 0 | 3.4 | 2.7 | 5 | 4 | 5 | 3.8 | 4.3 | 10 | 0 | 6 | 0.6 | 1.7 | 9 | 2 | 3 | 1.3 | -1.4 | 5 | 3 | -7 | 1.4 | -1.3 |
| 6 | 3 | -1 | 10.1 | -10.0 | 11 | 3 | -5 | 13.1 | -13.6 | 16 | 4 | 1 | 2.0 | 2.9 | 4 | 4 | 5 | 3.8 | 2.4 | 10 | 0 | 8 | 0.2 | 0.3 | 7 | 2 | -3 | 1.0 | 0.8 | 14 | 3 | -7 | 1.2 | 2.1 |
| 7 | 3 | -1 | 2.4 | 1.4 | 12 | 3 | -5 | 9.0 | 9.8 | 15 | 4 | 1 | 3.4 | -4.1 | 3 | 4 | 5 | 5.7 | 5.1 | 10 | 0 | -8 | 0.6 | 1.1 | 14 | 2 | -3 | 1.3 | 1.2 | 4 | 3 | -8 | 1.4 | -2.7 |
| 8 | 3 | -1 | 3.0 | 4.5 | 13 | 3 | -5 | 3.8 | 4.5 | 14 | 4 | 1 | 4.7 | -2.8 | 2 | 4 | 5 | 10.2 | -11.1 | 12 | 0 | 2 | 0.6 | -1.1 | 15 | 2 | -3 | 1.3 | -2.3 | 14 | 3 | -8 | 1.5 | -1.1 |
| 9 | 3 | -1 | 5.5 | 4.2 | 14 | 3 | -5 | 6.5 | 6.1 | 12 | 4 | 1 | 4.1 | -4.1 | 1 | 4 | 5 | 5.1 | 4.8 | 12 | 0 | 4 | 0.6 | 0.2 | 15 | 2 | 4 | 0.6 | 2.6 | 16 | 3 | -8 | 0.7 | 2.0 |
| 10 | 3 | -1 | 10.2 | -10.5 | 15 | 3 | -5 | 13.7 | 12.1 | 10 | 4 | 1 | 3.8 | 4.2 | 0 | 4 | 5 | 3.6 | -4.8 | 12 | 0 | 5 | 0.5 | 1.7 | 13 | 2 | 4 | 1.1 | -0.2 | 5 | 3 | 9 | 0.7 | -0.3 |
| 11 | 3 | -1 | 3.0 | -2.2 | 17 | 3 | -5 | 3.6 | 3.7 | 9 | 4 | 1 | 6.8 | -7.3 | 1 | 4 | -5 | 10.2 | 9.9 | 12 | 0 | -1 | 0.6 | 1.9 | 11 | 2 | 4 | 1.3 | -1.2 | 3 | 3 | -9 | 1.2 | 0.6 |
| 13 | 3 | -1 | 3.9 | 3.2 | 18 | 3 | -5 | 2.0 | -2.7 | 8 | 4 | 1 | 3.6 | -4.4 | 5 | 4 | -5 | 4.2 | -5.3 | 12 | 0 | -6 | 0.6 | -0.2 | 2 | 2 | 4 | 1.0 | -1.7 | 8 | 3 | -9 | 1.2 | 1.2 |
| 14 | 3 | -1 | 5.9 | -7.5 | 11 | 3 | 6 | 3.0 | -1.6 | 6 | 4 | 1 | 8.7 | 10.7 | 6 | 4 | -5 | 5.0 | 4.1 | 12 | 0 | -10 | 0.5 | 1.8 | 13 | 2 | -4 | 1.3 | 2.6 | 9 | 3 | -9 | 1.2 | 0.1 |
| 18 | 3 | -1 | 5.0 | 3.7 | 5 | 3 | 6 | 10.5 | -9.9 | 5 | 4 | 1 | 10.2 | -12.4 | 7 | 4 | -5 | 11.1 | 11.9 | 14 | 0 | 3 | 0.6 | 0.0 | 14 | 2 | -4 | 1.3 | -0.6 | 15 | 3 | -9 | 0.6 | -1.3 |
| 15 | 3 | 2 | 2.7 | 2.4 | 3 | 3 | 6 | 7.7 | -7.5 | 4 | 4 | 1 | 5.3 | 6.1 | 8 | 4 | -5 | 3.7 | 1.9 | 14 | 0 | -7 | 0.6 | 0.5 | 14 | 2 | 5 | 0.6 | -1.5 | 2 | 3 | 10 | 0.6 | 4.9 |
| 14 | 3 | 2 | 3.2 | -4.5 | 2 | 3 | 6 | 5.1 | -6.2 | 3 | 4 | 1 | 15.7 | 16.3 | 9 | 4 | -5 | 7.5 | 9.0 | 14 | 0 | -9 | 0.5 | -2.3 | 11 | 2 | 5 | 1.2 | -0.8 | 0 | 3 | 10 | 0.8 | -0.4 |
| 13 | 3 | 2 | 2.8 | 3.4 | 0 | 3 | 6 | 16.9 | 17.0 | 2 | 4 | 1 | 9.7 | 9.2 | 11 | 4 | -5 | 16.9 | 16.6 | 16 | 0 | 2 | 0.5 | 0.9 | 9 | 2 | 5 | 1.3 | 2.4 | 1 | 3 | -10 | 0.9 | 1.7 |
| 11 | 3 | 2 | 3.9 | -4.4 | 1 | 3 | -6 | 15.9 | -15.9 | 1 | 4 | 1 | 10.0 | 8.4 | 12 | 4 | -5 | 6.0 | -6.8 | 16 | 0 | 3 | 0.4 | 0.9 | 5 | 2 | 5 | 1.3 | 0.1 | 2 | 3 | -10 | 1.0 | 2.7 |
| 8 | 3 | 2 | 5.8 | -6.8 | 3 | 3 | -6 | 16.1 | -16.1 | 0 | 4 | 1 | 13.6 | 15.2 | 13 | 4 | -5 | 3.5 | -2.4 | 16 | 0 | 4 | 0.2 | -1.1 | 4 | 2 | -5 | 1.1 | 0.7 | 8 | 3 | -10 | 1.0 | 1.3 |
| 7 | 3 | 2 | 2.2 | -0.9 | 4 | 3 | -6 | 4.0 | 4.1 | 1 | 4 | -1 | 5.3 | -4.8 | 14 | 4 | -5 | 4.9 | 4.8 | 16 | 0 | -4 | 0.6 | 0.9 | 10 | 2 | -5 | 1.3 | 2.5 | 9 | 3 | -10 | 1.0 | -1.4 |
| 5 | 3 | 2 | 28.4 | -30.3 | 5 | 3 | -6 | 7.0 | -6.0 | 2 | 4 | -1 | 8.4 | 9.0 | 10 | 4 | 6 | 2.6 | -4.1 | 16 | 0 | -6 | 0.6 | 0.4 | 13 | 2 | -5 | 1.3 | -0.1 | 12 | 3 | -10 | 0.7 | -0.7 |
| 4 | 3 | 2 | 30.2 | -32.6 | 6 | 3 | -6 | 8.9 | 9.6 | 3 | 4 | -1 | 8.4 | 8.1 | 8 | 4 | 6 | 2.9 | -3.3 | 18 | 0 | 0 | 0.4 | -0.9 | 10 | 2 | 6 | 1.1 | -0.9 | 13 | 3 | -10 | 0.5 | 0.4 |
| 3 | 3 | 2 | 14.7 | -13.1 | 7 | 3 | -6 | 13.7 | 14.0 | 4 | 4 | -1 | 10.5 | -11.6 | 7 | 4 | 6 | 3.2 | -3.3 | 18 | 0 | -4 | 0.5 | -0.3 | 7 | 2 | 6 | 1.3 | -3.1 | 4 | 3 | -11 | 0.5 | -1.0 |
| 2 | 3 | 2 | 3.3 | 4.6 | 8 | 3 | -6 | 5.8 | 4.3 | 5 | 4 | -1 | 17.9 | 21.6 | 6 | 4 | 6 | 3.4 | -3.0 | 18 | 0 | -5 | 0.5 | 0.6 | 5 | 2 | 6 | 1.3 | -2.1 | 5 | 3 | -11 | 0.6 | 7.2 |
| 1 | 3 | 2 | 12.6 | 10.6 | 9 | 3 | -6 | 20.2 | 21.5 | 6 | 4 | -1 | 12.2 | -12.3 | 5 | 4 | 6 | 4.5 | -3.3 | 20 | 0 | -2 | 0.2 | 0.3 | 4 | 2 | 6 | 1.3 | 0.1 | 9 | 3 | -11 | 0.4 | -4.8 |
| 0 | 3 | 2 | 2.7 | 2.3 | 10 | 3 | -6 | 12.6 | -13.5 | 7 | 4 | -1 | 6.9 | -7.1 | 4 | 4 | 6 | 4.2 | -3.9 | 20 | 0 | -3 | 0.3 | 1.8 | 7 | 2 | -6 | 1.3 | 1.9 | 5 | 4 | -10 | 1.0 | 3.3 |
| 1 | 3 | -2 | 22.8 | 21.6 | 12 | 3 | -6 | 7.2 | 7.5 | 8 | 4 | -1 | 11.5 | 11.8 | 3 | 4 | 6 | 6.2 | 6.9 | 20 | 0 | -5 | 0.3 | 2.0 | 15 | 2 | -6 | 1.2 | 0.4 | 11 | 4 | 0 | 1.7 | 0.9 |
| 2 | 3 | -2 | 4.3 | -2.8 | 14 | 3 | -6 | 3.9 | 3.5 | 9 | 4 | -1 | 11.4 | -11.8 | 0 | 4 | 6 | 13.6 | -13.5 | 12 | 1 | 0 | 1.3 | -0.6 | 17 | 2 | -6 | 1.0 | -0.3 | 15 | 4 | 0 | 1.3 | -2.2 |
| 3 | 3 | -2 | 22.4 | 22.8 | 16 | 3 | -6 | 6.1 | 6.3 | 10 | 4 | -1 | 3.7 | 1.2 | 1 | 4 | -6 | 8.9 | 10.5 | 16 | 1 | 0 | 1.2 | 0.7 | 9 | 2 | 7 | 1.0 | 1.2 | 13 | 4 | 1 | 1.5 | 1.3 |
| 4 | 3 | -2 | 11.1 | -10.4 | 17 | 3 | -6 | 3.0 | -0.8 | 11 | 4 | -1 | 4.8 | -4.4 | 2 | 4 | -6 | 11.3 | -12.2 | 17 | 1 | 0 | 1.0 | -0.9 | 8 | 2 | 7 | 1.1 | -1.5 | 11 | 4 | 1 | 1.7 | -0.2 |
| 6 | 3 | -2 | 2.3 | -4.2 | 8 | 3 | 7 | 3.1 | 3.0 | 15 | 4 | 2 | 4.2 | -4.6 | 3 | 4 | -6 | 8.2 | 8.9 | 19 | 1 | 0 | 0.5 | -2.0 | 3 | 2 | -7 | 1.3 | 0.5 | 7 | 4 | 1 | 1.6 | 0.1 |
| 7 | 3 | -2 | 6.8 | 6.1 | 6 | 3 | 7 | 3.8 | 3.2 | 14 | 4 | 2 | 4.8 | 5.1 | 4 | 4 | -6 | 3.7 | 0.3 | 18 | 1 | 1 | 0.7 | 0.4 | 11 | 2 | -7 | 1.3 | -1.1 | 12 | 4 | -1 | 1.7 | -0.4 |
| 8 | 3 | -2 | 3.3 | 1.7 | 5 | 3 | 7 | 5.7 | -6.5 | 13 | 4 | 2 | 5.1 | -6.0 | 5 | 4 | -6 | 5.0 | -6.8 | 17 | 1 | 1 | 0.9 | -1.0 | 15 | 2 | -7 | 1.1 | 0.4 | 13 | 4 | -1 | 1.7 | 1.2 |
| 9 | 3 | -2 | 7.7 | 8.5 | 4 | 3 | 7 | 3.0 | -2.2 | 10 | 4 | 2 | 8.1 | -7.8 | 6 | 4 | -6 | 5.7 | 4.8 | 16 | 1 | 1 | 1.1 | -1.9 | 6 | 2 | 8 | 1.1 | -1.3 | 14 | 4 | -1 | 1.5 | -0.6 |
| 10 | 3 | -2 | 2.9 | 1.2 | 2 | 3 | 7 | 3.1 | -3.8 | 9 | 4 | 2 | 4.4 | 3.1 | 7 | 4 | -6 | 10.8 | 9.9 | 13 | 1 | 1 | 1.3 | -1.5 | 4 | 2 | 8 | 1.2 | 2.0 | 15 | 4 | -1 | 1.4 | -2.9 |
| 11 | 3 | -2 | 3.8 | -1.6 | 1 | 3 | 7 | 7.7 | 10.0 | 8 | 4 | 2 | 4.3 | -3.1 | 8 | 4 | -6 | 7.9 | 8.3 | 15 | 1 | -1 | 1.3 | -1.1 | 3 | 2 | -8 | 1.3 | -0.6 | 16 | 4 | -1 | 1.1 | -0.3 |
| 12 | 3 | -2 | 5.6 | -6.0 | 0 | 3 | 7 | 9.3 | 8.2 | 7 | 4 | 2 | 9.6 | 9.3 | 9 | 4 | -6 | 8.9 | 8.7 | 16 | 1 | -1 | 1.2 | 3.3 | 9 | 2 | -8 | 1.3 | 1.5 | 17 | 4 | -1 | 0.8 | 1.9 |
| 13 | 3 | -2 | 7.4 | 6.7 | 1 | 3 | -7 | 6.1 | -4.1 | 5 | 4 | 2 | 7.3 | -7.3 | 12 | 4 | -6 | 3.5 | -3.0 | 18 | 1 | -1 | 0.9 | -1.1 | 11 | 2 | -8 | 1.3 | 0.6 | 12 | 4 | 2 | 1.6 | -0.3 |
| 14 | 3 | -2 | 7.9 | -9.0 | 2 | 3 | -7 | 10.2 | -11.2 | 4 | 4 | 2 | 4.2 | -5.7 | 13 | 4 | -6 | 8.8 | -6.9 | 19 | 1 | -1 | 0.7 | -0.3 | 15 | 2 | -8 | 1.0 | 0.9 | 11 | 4 | 2 | 1.7 | 1.4 |
| 15 | 3 | -2 | 2.8 | 1.7 | 3 | 3 | -7 | 5.9 | -6.3 | 3 | 4 | 2 | 3.4 | -2.5 | 14 | 4 | -6 | 8.0 | 5.4 | 14 | 1 | 2 | 1.2 | -1.7 | 3 | 2 | 9 | 1.1 | 0.9 | 6 | 4 | 2 | 1.6 | -2.5 |
| 17 | 3 | -2 | 3.1 | -3.1 | 4 | 3 | -7 | 4.3 | 3.5 | 2 | 4 | 2 | 8.4 | 7.0 | 15 | 4 | -6 | 3.7 | 2.9 | 11 | 1 | -2 | 1.2 | 0.6 | 2 | 2 | -9 | 1.3 | -1.7 | 10 | 4 | -2 | 1.7 | 2.5 |
| 18 | 3 | -2 | 8.6 | 8.3 | 6 | 3 | -7 | 11.2 | 12.9 | 1 | 4 | 2 | 8.2 | -5.9 | 6 | 4 | 7 | 2.8 | -1.5 | 18 | 1 | -2 | 1.0 | 1.2 | 5 | 2 | -9 | 1.3 | -0.2 | 15 | 4 | -2 | 1.4 | 0.4 |
| 15 | 3 | 3 | 2.1 | -1.5 | 7 | 3 | -7 | 5.6 | -5.5 | 0 | 4 | 2 | 3.5 | -3.4 | 5 | 4 | 7 | 3.1 | -2.8 | 16 | 1 | 3 | 0.8 | 0.6 | 6 | 2 | -9 | 1.3 | 0.3 | 16 | 4 | -2 | 1.2 | -4.3 |
| 14 | 3 | 3 | 4.8 | -4.9 | 8 | 3 | -7 | 11.7 | 13.1 | 1 | 4 | -2 | 6.2 | 5.0 | 4 | 4 | 7 | 3.8 | -4.1 | 11 | 1 | 3 | 1.3 | -0.6 | 7 | 2 | -9 | 1.3 | 0.8 | 14 | 4 | 3 | 0.9 | 0.2 |
| 11 | 3 | 3 | 5.7 | -5.5 | 9 | 3 | -7 | 7.4 | -5.2 | 2 | 4 | -2 | 8.7 | 6.3 | 3 | 4 | 7 | 3.7 | 4.2 | 6 | 1 | 3 | 1.0 | -1.1 | 11 | 2 | -9 | 1.2 | -0.5 | 12 | 4 | 3 | 1.4 | 0.7 |
| 9 | 3 | 3 | 6.7 | -5.6 | 10 | 3 | -7 | 3.9 | -4.1 | 3 | 4 | -2 | 9.9 | -8.9 | 2 | 4 | 7 | 8.2 | 9.3 | 10 | 1 | -3 | 1.1 | 1.5 | 14 | 2 | -9 | 0.9 | 1.1 | 10 | 4 | 3 | 1.7 | -2.0 |
| 8 | 3 | 3 | 3.8 | -2.7 | 11 | 3 | -7 | 4.0 | -5.1 | 4 | 4 | -2 | 10.2 | 8.4 | 1 | 4 | 7 | 7.3 | -6.9 | 11 | 1 | -3 | 1.2 | 1.6 | 4 | 2 | 10 | 0.5 | 0.8 | 1 | 4 | -3 | 1.3 | 3.0 |
| 7 | 3 | 3 | 2.9 | -0.4 | 12 | 3 | -7 | 2.9 | 2.0 | 5 | 4 | -2 | 8.9 | 10.3 | 1 | 4 | -7 | 3.7 | 4.5 | 18 | 1 | -3 | 1.0 | -0.5 | 1 | 2 | -10 | 1.0 | 0.5 | 6 | 4 | -3 | 1.5 | -0.5 |
| 6 | 3 | 3 | 13.8 | 14.3 | 13 | 3 | -7 | 2.7 | -3.4 | 6 | 4 | -2 | 3.1 | -3.6 | 2 | 4 | -7 | 5.7 | -4.9 | 14 | 1 | 4 | 1.0 | -0.3 | 3 | 2 | -10 | 1.1 | 1.9 | 8 | 4 | -3 | 1.6 | -0.7 |
| 5 | 3 | 3 | 8.0 | -8.1 | 15 | 3 | -7 | 3.6 | 3.0 | 7 | 4 | -2 | 10.9 | 9.9 | 3 | 4 | -7 | 9.9 | 10.9 | 4 | 1 | 4 | 1.0 | -0.9 | 5 | 2 | -10 | 1.1 | 1.4 | 13 | 4 | -3 | 1.7 | -1.4 |
| 4 | 3 | 3 | 12.1 | -11.1 | 16 | 3 | -7 | 7.1 | 7.8 | 8 | 4 | -2 | 13.8 | 13.3 | 4 | 4 | -7 | 10.3 | -9.5 | 6 | 1 | -4 | 0.9 | -0.5 | 8 | 2 | -10 | 1.1 | 0.2 | 14 | 4 | -3 | 1.6 | -0.6 |
| 3 | 3 | 3 | 12.7 | 9.1 | 17 | 3 | -7 | 7.0 | 6.7 | 9 | 4 | -2 | 10.4 | 10.0 | 5 | 4 | -7 | 7.8 | -8.4 | 12 | 1 | -4 | 1.2 | -1.1 | 9 | 2 | -10 | 1.1 | -1.8 | 15 | 4 | -3 | 1.4 | 2.3 |
| 2 | 3 | 3 | 6.8 | 7.2 | 8 | 3 | 8 | 4.2 | 5.0 | 11 | 4 | -2 | 9.4 | -9.5 | 6 | 4 | -7 | 7.8 | -6.3 | 15 | 1 | -4 | 1.3 | 1.2 | 0 | 2 | 11 | 0.5 | 5.4 | 16 | 4 | -3 | 1.2 | -0.1 |
| 1 | 3 | 3 | 3.0 | 2.7 | 7 | 3 | 8 | 3.0 | -2.5 | 12 | 4 | -2 | 5.4 | 7.3 | 7 | 4 | -7 | 10.2 | -9.6 | 18 | 1 | -4 | 1.0 | 1.3 | 1 | 2 | -11 | 0.6 | 0.1 | 0 | 4 | 4 | 1.5 | 0.6 |
| 0 | 3 | 3 | 5.1 | -3.2 | 6 | 3 | 8 | 5.4 | 5.0 | 13 | 4 | -2 | 4.2 | 3.6 | 9 | 4 | -7 | 3.6 | 5.5 | 10 | 1 | 5 | 1.2 | 0.4 | 2 | 2 | -11 | 0.7 | -1.3 | 2 | 4 | -4 | 1.5 | -0.8 |
| 1 | 3 | -3 | 23.1 | -23.0 | 5 | 3 | 8 | 2.9 | -2.1 | 14 | 4 | -2 | 3.4 | 2.5 | 10 | 4 | -7 | 3.5 | 4.0 | 8 | 1 | 5 | 1.3 | -1.6 | 3 | 2 | -11 | 0.8 | 0.8 | 10 | 4 | 5 | 1.3 | -0.3 |
| 2 | 3 | -3 | 10.2 | 9.4 | 4 | 3 | 8 | 3.1 | -1.4 | 17 | 4 | -2 | 4.4 | -4.9 | 14 | 4 | -7 | 6.7 | -7.0 | 17 | 1 | -5 | 1.1 | 1.6 | 6 | 2 | -11 | 0.8 | 1.0 | 9 | 4 | 5 | 1.8 | 0.7 |
| 3 | 3 | -3 | 4.4 | 3.4 | 3 | 3 | 8 | 3.3 | -2.2 | 13 | 4 | 3 | 3.2 | -2.6 | 6 | 4 | 8 | 2.5 | -3.3 | 19 | 1 | -5 | 0.8 | 3.8 | 10 | 2 | -11 | 0.7 | -0.2 | 7 | 4 | 5 | 1.7 | 0.3 |
| 4 | 3 | -3 | 2.2 | -0.1 | 2 | 3 | 8 | 6.3 | -5.2 | 11 | 4 | 3 | 4.9 | 5.5 | 5 | 4 | 8 | 2.8 | -1.7 | 1 | 1 | -6 | 1.1 | -0.3 | 11 | 2 | -11 | 0.6 | 1.4 | 6 | 4 | 5 | 1.7 | -2.3 |
| 5 | 3 | -3 | 26.7 | 27.5 | 1 | 3 | 8 | 3.6 | 2.5 | 9 | 4 | 3 | 3.7 | -1.9 | 3 | 4 | 8 | 5.6 | 5.9 | 2 | 1 | -6 | 1.1 | -0.5 | 12 | 2 | -11 | 0.3 | -1.7 | 2 | 4 | -5 | 1.6 | -0.8 |
| 7 | 3 | -3 | 8.7 | 7.2 | 0 | 3 | 8 | 13.8 | -13.0 | 8 | 4 | 3 | 5.2 | 5.2 | 1 | 4 | 8 | 3.7 | 4.7 | 16 | 1 | -6 | 1.1 | 0.7 | 14 | 3 | 0 | 1.3 | 1.0 | 3 | 4 | -5 | 1.6 | 0.1 |
| 8 | 3 | -3 | 7.0 | -6.5 | 1 | 3 | -8 | 13.3 | 10.9 | 7 | 4 | 3 | 11.0 | -12.2 | 1 | 4 | -8 | 9.0 | -8.7 | 9 | 1 | 7 | 1.0 | 0.3 | 17 | 3 | 0 | 0.8 | 1.4 | 4 | 4 | -5 | 1.6 | -0.3 |
| 9 | 3 | -3 | 2.8 | 0.9 | 2 | 3 | -8 | 14.0 | -12.2 | 6 | 4 | 3 | 7.3 | -6.7 | 2 | 4 | -8 | 3.5 | 4.5 | 8 | 1 | 7 | 1.1 | -1.4 | 18 | 3 | 0 | 0.3 | -3.0 | 10 | 4 | -5 | 1.7 | -2.4 |
| 11 | 3 | -3 | 16.3 | 18.0 | 3 | 3 | -8 | 5.5 | -4.5 | 5 | 4 | 3 | 4.5 | -4.9 | 4 | 4 | -8 | 4.1 | -5.4 | 4 | 1 | 7 | 1.3 | 0.5 | 17 | 3 | 1 | 0.6 | -0.7 | 15 | 4 | -5 | 1.3 | 0.5 |
| 13 | 3 | -3 | 12.6 | 14.1 | 5 | 3 | -8 | 14.5 | -16.0 | 4 | 4 | 3 | 13.6 | -13.8 | 5 | 4 | -8 | 3.5 | 1.7 | 2 | 1 | 7 | 1.3 | -1.6 | 12 | 3 | 1 | 1.4 | -0.4 | 16 | 4 | -5 | 1.1 | 1.1 |
| 15 | 3 | -3 | 3.6 | 3.0 | 6 | 3 | -8 | 3.8 | 4.4 | 3 | 4 | 3 | 14.8 | -16.7 | 6 | 4 | -8 | 3.5 | -2.0 | 5 | 1 | -7 | 1.2 | -1.1 | 10 | 3 | 1 | 1.4 | 0.1 | 17 | 4 | -5 | 0.8 | 2.2 |
| 16 | 3 | -3 | 7.1 | -5.9 | 7 | 3 | -8 | 8.0 | -7.4 | 2 | 4 | 3 | 4.4 | -4.6 | 7 | 4 | -8 | 3.5 | -3.5 | 15 | 1 | -7 | 1.2 | 0.8 | 12 | 3 | -1 | 1.4 | -1.4 | 9 | 4 | 6 | 1.2 | -1.3 |
| 17 | 3 | -3 | 5.8 | -4.7 | 8 | 3 | -8 | 5.5 | 7.6 | 1 | 4 | 3 | 9.6 | -10.5 | 8 | 4 | -8 | 8.3 | -6.7 | 18 | 1 | -7 | 0.8 | 0.7 | 15 | 3 | -1 | 1.2 | -0.2 | 2 | 4 | 6 | 1.7 | 2.8 |
| 18 | 3 | -3 | 2.9 | -1.6 | 10 | 3 | -8 | 3.5 | 2.3 | 0 | 4 | 3 | 6.4 | 4.9 | 9 | 4 | -8 | 11.1 | 8.6 | 8 | 1 | 8 | 0.9 | -0.9 | 16 | 3 | -1 | 1.1 | -1.8 | 1 | 4 | 6 | 1.7 | 0.9 |
| 14 | 3 | 4 | 2.7 | 3.9 | 11 | 3 | -8 | 4.1 | 4.2 | 2 | 4 | -3 | 10.0 | 8.5 | 10 | 4 | -8 | 11.1 | -7.1 | 4 | 1 | 8 | 1.2 | -0.6 | 17 | 3 | -1 | 0.9 | 0.9 | 10 | 4 | -6 | 1.7 | 0.5 |
| 13 | 3 | 4 | 8.7 | -7.7 | 12 | 3 | -8 | 5.4 | -4.6 | 3 | 4 | -3 | 13.3 | -12.5 | 11 | 4 | -8 | 8.0 | 7.1 | 2 | 1 | 8 | 1.3 | 0.2 | 16 | 3 | 2 | 0.7 | -0.0 | 11 | 4 | -6 | 1.7 | 0.8 |
| 12 | 3 | 4 | 4.1 | -3.7 | 13 | 3 | -8 | 7.8 | -7.5 | 4 | 4 | -3 | 13.6 | 10.9 | 13 | 4 | -8 | 3.0 | 3.4 | 10 | 1 | -8 | 1.3 | 0.3 | 12 | 3 | 2 | 1.4 | 0.5 | 16 | 4 | -6 | 1.0 | 1.3 |
| 8 | 3 | 4 | 3.6 | 3.4 | 15 | 3 | -8 | 10.9 | -11.2 | 5 | 4 | -3 | 4.3 | -0.5 | 14 | 4 | -8 | 5.6 | -5.1 | 12 | 1 | -8 | 1.2 | 1.1 | 10 | 3 | 2 | 1.4 | 0.8 | 9 | 4 | 7 | 0.3 | 2.4 |
| 5 | 3 | 4 | 8.8 | 8.4 | 4 | 3 | 9 | 2.7 | 2.7 | 7 | 4 | -3 | 8.9 | 8.3 | 3 | 4 | 9 | 2.6 | 1.7 | 13 | 1 | -8 | 1.2 | -2.1 | 9 | 3 | 2 | 1.4 | 1.2 | 8 | 4 | 7 | 0.9 | -1.0 |
| 3 | 3 | 4 | 2.7 | 2.2 | 3 | 3 | 9 | 7.5 | -7.1 | 9 | 4 | -3 | 8.8 | 7.4 | 2 | 4 | 9 | 6.5 | -7.5 | 14 | 1 | -8 | 1.1 | -1.1 | 6 | 3 | 2 | 1.5 | -0.1 | 7 | 4 | 7 | 1.2 | -1.7 |
| 2 | 3 | 4 | 8.2 | -7.2 | 2 | 3 | 9 | 2.8 | 0.8 | 10 | 4 | -3 | 13.4 | 13.2 | 1 | 4 | 9 | 7.6 | 8.1 | 16 | 1 | -8 | 0.9 | -0.6 | 5 | 3 | -2 | 1.0 | -0.5 | 0 | 4 | 7 | 1.7 | 1.3 |
| 1 | 3 | 4 | 3.5 | -3.0 | 1 | 3 | 9 | 14.3 | -12.3 | 11 | 4 | -3 | 11.4 | -12.9 | 1 | 4 | -9 | 3.4 | 1.1 | 5 | 1 | 9 | 0.9 | 0.1 | 16 | 3 | -2 | 1.2 | -1.8 | 8 | 4 | -7 | 1.7 | -1.0 |
| 0 | 3 | 4 | 7.1 | -5.4 | 0 | 3 | 9 | 12.3 | -11.2 | 12 | 4 | -3 | 11.2 | 13.3 | 3 | 4 | -9 | 3.6 | 5.1 | 9 | 1 | -9 | 1.2 | 0.4 | 13 | 3 | 3 | 1.1 | 1.0 | 11 | 4 | -7 | 1.6 | 2.1 |
| 1 | 3 | -4 | 4.8 | 3.5 | 1 | 3 | -9 | 3.3 | 0.5 | 17 | 4 | -3 | 5.0 | -5.5 | 4 | 4 | -9 | 5.1 | -3.0 | 17 | 1 | -9 | 0.5 | -4.1 | 12 | 3 | 3 | 1.3 | -2.5 | 12 | 4 | -7 | 2.1 | 3.0 |
| 2 | 3 | -4 | 5.9 | 7.5 | 2 | 3 | -9 | 5.3 | -5.0 | 13 | 4 | 4 | 3.1 | -3.8 | 6 | 4 | -9 | 6.7 | -5.6 | 2 | 1 | 10 | 0.9 | 0.6 | 10 | 3 | 3 | 1.4 | -0.2 | 13 | 4 | -7 | 1.4 | 0.7 |
| 3 | 3 | -4 | 3.3 | -1.3 | 4 | 3 | -9 | 6.8 | -6.1 | 12 | 4 | 4 | 4.7 | -4.7 | 7 | 4 | -9 | 7.9 | -9.0 | 1 | 1 | 10 | 1.0 | -1.0 | 6 | 3 | -3 | 1.1 | -1.6 | 15 | 4 | -7 | 1.0 | -1.6 |
| 4 | 3 | -4 | 13.0 | 12.6 | 5 | 3 | -9 | 4.6 | -5.4 | 11 | 4 | 4 | 4.8 | -4.9 | 9 | 4 | -9 | 3.9 | -4.2 | 0 | 1 | 10 | 1.0 | 0.9 | 12 | 3 | -3 | 1.4 | 0.1 | 16 | 4 | -7 | 0.7 | -0.9 |
| 5 | 3 | -4 | 8.8 | 7.3 | 6 | 3 | -9 | 6.2 | -5.2 | 10 | 4 | 4 | 3.3 | -1.7 | 11 | 4 | -9 | 7.8 | 7.1 | 9 | 1 | -10 | 1.1 | 0.3 | 14 | 3 | -3 | 1.4 | -0.2 | 4 | 4 | 8 | 1.2 | -2.3 |
| 7 | 3 | -4 | 2.7 | -1.7 | 7 | 3 | -9 | 3.4 | -0.2 | 9 | 4 | 4 | 3.5 | -1.6 | 13 | 4 | -9 | 7.7 | 10.7 | 11 | 1 | -10 | 1.0 | -1.2 | 11 | 3 | 4 | 1.2 | 0.0 | 2 | 4 | 8 | 1.4 | -1.5 |
| 8 | 3 | -4 | 12.2 | -10.6 | 10 | 3 | -9 | 3.1 | 2.8 | 8 | 4 | 4 | 3.7 | -2.4 | 1 | 4 | -10 | 2.5 | 0.9 | 12 | 1 | -10 | 0.9 | 0.7 | 10 | 3 | 4 | 1.3 | 0.4 | 0 | 4 | 8 | 1.5 | 3.4 |
| 9 | 3 | -4 | 8.7 | -9.9 | 11 | 3 | -9 | 3.7 | -2.2 | 7 | 4 | 4 | 3.8 | -1.3 | 2 | 4 | -10 | 3.8 | -3.6 | 14 | 1 | -10 | 0.8 | 2.7 | 9 | 3 | 4 | 1.4 | 0.6 | 3 | 4 | -8 | 1.6 | 1.5 |
| 10 | 3 | -4 | 14.7 | 16.5 | 12 | 3 | -9 | 2.7 | -2.2 | 6 | 4 | 4 | 3.8 | 2.9 | 4 | 4 | -10 | 3.9 | 5.5 | 1 | 1 | -11 | 0.7 | 1.5 | 7 | 3 | 4 | 1.4 | -1.2 | 12 | 4 | -8 | 1.3 | 0.5 |
| 11 | 3 | -4 | 5.8 | 3.8 | 13 | 3 | -9 | 2.5 | -2.3 | 5 | 4 | 4 | 14.1 | 14.8 | 7 | 4 | -10 | 2.9 | -2.6 | 3 | 1 | -11 | 0.8 | 1.8 | 6 | 3 | 4 | 1.4 | 1.6 | 0 | 4 | 9 | 1.2 | -1.7 |
| 12 | 3 | -4 | 3.9 | 4.3 | 14 | 3 | -9 | 3.4 | 2.3 | 4 | 4 | 4 | 10.8 | 12.3 | 8 | 4 | -10 | 2.4 | -2.1 | 4 | 1 | -11 | 0.9 | 2.4 | 4 | 3 | 4 | 1.3 | -0.1 | 2 | 4 | -9 | 1.3 | 1.1 |
| 13 | 3 | -4 | 3.1 | 0.0 | 3 | 3 | -10 | 2.7 | 2.9 | 3 | 4 | 4 | 7.5 | -8.5 | 9 | 4 | -10 | 4.0 | -5.1 | 6 | 1 | -11 | 0.9 | 1.5 | 12 | 3 | 5 | 0.9 | -1.2 | 5 | 4 | -9 | 2.1 | 2.6 |
| 14 | 3 | -4 | 3.0 | 3.1 | 4 | 3 | -10 | 5.5 | -5.0 | 2 | 4 | 4 | 8.7 | -9.3 |  |  |  |  |  | 7 | 2 | 0 | 0.9 | 0.1 | 11 | 3 | 5 | 1.1 | -0.4 | 8 | 4 | -9 | 1.3 | -1.9 |
| 15 | 3 | -4 | 3.4 | 3.1 | 5 | 3 | -10 | 5.6 | -4.4 | 1 | 4 | 4 | 13.4 | -14.4 | Unobserved Data |  |  |  |  | 10 | 2 | 0 | 1.2 | -1.0 | 10 | 3 | 5 | 1.2 | -1.1 | 10 | 4 | -9 | 1.2 | -0.8 |
| 16 | 3 | -4 | 7.5 | -7.2 | 6 | 3 | -10 | 5.1 | -5.8 | 1 | 4 | -4 | 10.7 | 10.9 |  |  |  |  |  | 13 | 2 | 0 | 1.3 | 0.2 | 8 | 3 | 5 | 1.4 | -0.8 | 12 | 4 | -9 | 1.0 | 1.8 |
| 17 | 3 | -4 | 8.5 | 8.4 | 7 | 3 | -10 | 11.3 | -11.4 | 3 | 4 | -4 | 4.3 | -5.6 |  |  |  |  |  | 14 | 2 | 0 | 1.3 | 1.1 | 5 | 3 | 5 | 1.4 | 1.4 | 3 | 4 | -10 | 0.9 | 0.5 |
| 18 | 3 | -4 | 6.2 | -6.5 | 10 | 3 | -10 | 2.4 | 2.7 | 4 | 4 | -4 | 7.2 | 6.2 | 0 | 0 | 8 | 0.6 | 2.9 | 16 | 2 | 0 | 1.1 | -0.2 | 5 | 3 | -5 | 1.2 | 1.1 | 6 | 4 | -10 | 1.0 | -0.7 |

Table 2. *Final position parameters and their estimated standard deviations**

| | $x$ | $y$ | $z$ | $\sigma(x)$ | $\sigma(y)$ | $\sigma(z)$ |
|---|---|---|---|---|---|---|
| C(1) | 9264 | 6766 | 4011 | 0004 | 0012 | 0007 |
| C(2) | 9661 | 7112 | 2742 | 0004 | 0012 | 0007 |
| C(3) | 0494 | 8451 | 3276 | 0004 | 0012 | 0006 |
| C(4) | 0880 | 8970 | 1938 | 0003 | 0010 | 0006 |
| C(5) | 1758 | 0256 | 2634 | 0004 | 0012 | 0007 |
| C(6) | 2243 | 0797 | 1457 | 0004 | 0011 | 0006 |
| C(7) | 2995 | 2258 | 2095 | 0004 | 0013 | 0007 |
| C(8) | 0183 | 0293 | 0725 | 0003 | 0010 | 0005 |
| C(9) | 1095 | 7043 | 1290 | 0003 | 0010 | 0005 |
| N(1) | 8944 | 6500 | 4914 | 0004 | 0011 | 0006 |
| N(2) | 3573 | 3337 | 2561 | 0004 | 0012 | 0006 |
| N(3) | 1278 | 5526 | 0802 | 0004 | 0009 | 0005 |
| H(2) | 911 | 808 | 196 | 004 | 012 | 007 |
| H(2′) | 982 | 591 | 240 | 004 | 012 | 007 |
| H(3) | 024 | 006 | 363 | 004 | 012 | 007 |
| H(3′) | 109 | 755 | 405 | 004 | 012 | 007 |
| H(5) | 152 | 169 | 281 | 004 | 013 | 007 |
| H(5′) | 220 | 902 | 353 | 004 | 011 | 007 |
| H(6) | 176 | 191 | 047 | 004 | 012 | 007 |
| H(6′) | 253 | 939 | 095 | 004 | 011 | 007 |
| H(8) | 999 | 194 | 117 | 004 | 012 | 007 |

* Decimal point on left omitted.

form factors results in an apparent shortening of the bond. Further, any libration of the C–C–N group generates mean positions which correspond to a bond length significantly shorter than the actual one. Calculations of this effect have not been made in the present case, but Bekoe & Trueblood (1959) obtained corrections of 0·02 Å in this way for the case of tetracyanoethylene.

Table 3. *Bond lengths and their estimated standard deviations*

| Bond | Length (Å) | σ (Å) | Bond | Length (Å) | σ σ |
|---|---|---|---|---|---|
| N(1)–C(1) | 1·112 | 0·008 | C(8)–C(8′) | 1·335 | 0·016 |
| N(2)–C(7) | 1·110 | 0·008 | | | |
| N(3)–C(9) | 1·146 | 0·008 | H(2)–C(2) | 1·12 | 0·07 |
| C(1)–C(2) | 1·503 | 0·008 | H(2′)–C(2) | 0·89 | 0·07 |
| C(6)–C(7) | 1·471 | 0·008 | H(3)–C(3) | 1·19 | 0·07 |
| C(4)–C(9) | 1·458 | 0·008 | H(3′)–C(3) | 1·13 | 0·07 |
| C(2)–C(3) | 1·503 | 0·008 | H(5)–C(5) | 1·03 | 0·07 |
| C(3)–C(4) | 1·571 | 0·008 | H(5′)–C(5) | 1·19 | 0·07 |
| C(4)–C(5) | 1·553 | 0·008 | H(6)–C(6) | 1·21 | 0·07 |
| C(5)–C(6) | 1·546 | | H(6′)–C(6) | 1·17 | 0·07 |
| C(4)–C(8) | 1·547 | 0·008 | H(8)–C(8) | 1·21 | 0·07 |

Table 4. *Bond angles and their estimated standard deviations*

| | Angle | e.s.d. |
|---|---|---|
| N(1)–C(1)–C(2) | 177·7° | 0·7° |
| N(2)–C(7)–C(6) | 178·5 | 0·7 |
| N(3)–C(9)–C(4) | 178·8 | 0·7 |
| C(1)–C(2)–C(3) | 110·6 | 0·5 |
| C(2)–C(3)–C(4) | 111·5 | 0·5 |
| C(8)–C(4)–C(3) | 109·4 | 0·5 |
| C(8)–C(4)–C(5) | 109·5 | 0·5 |
| C(9)–C(4)–C(3) | 109·7 | 0·5 |
| C(9)–C(4)–C(5) | 109·6 | 0·5 |
| C(3)–C(4)–C(5) | 106·9 | 0·5 |
| C(9)–C(4)–C(8) | 111·5 | 0·5 |
| C(4)–C(5)–C(6) | 112·8 | 0·5 |
| C(5)–C(6)–C(7) | 111·3 | 0·5 |
| C(4)–C(8)–C(8′) | 123·7 | 0·6 |
| H(8)–C(8)–C(8′) | 121·0 | 3·4 |
| H(8)–C(8)–C(4) | 115·3 | 3·4 |
| H(3)–C(3)–C(2) | 105·2 | 3·4 |
| H(3)–C(3)–C(4) | 105·8 | 3·4 |
| H(3′)–C(3)–C(2) | 111·2 | 3·6 |
| H(3′)–C(3)–C(4) | 99·6 | 3·6 |
| H(3′)–C(3)–H(3) | 123·2 | 4·9 |
| H(2)–C(2)–C(1) | 99·7 | 4·0 |
| H(2)–C(2)–C(3) | 107·3 | 3·6 |
| H(2′)–C(2)–C(1) | 111·6 | 3·5 |
| H(2′)–C(2)–C(3) | 108·0 | 4·5 |
| H(2′)–C(2)–H(2) | 119·4 | 5·8 |
| H(5)–C(5)–C(4) | 103·1 | 3·9 |
| H(5)–C(5)–C(6) | 101·3 | 3·9 |
| H(5′)–C(5)–C(4) | 100·2 | 3·4 |
| H(5′)–C(5)–H(5) | 130·0 | 5·2 |
| H(5′)–C(5)–C(6) | 109·3 | 3·4 |
| H(6)–C(6)–C(7) | 98·7 | 3·3 |
| H(6)–C(6)–C(5) | 109·9 | 3·3 |
| H(6′)–C(6)–C(5) | 116·2 | 3·5 |
| H(6′)–C(6)–C(7) | 107·2 | 3·5 |
| H(6′)–C(6)–H(6) | 112·0 | 4·8 |

The C–C bond length in the C–C–N groups is reported to be 1·45–1·46 Å (*Tables of Interatomic Distances*, 1958). Bonds C(6)–C(7) and C(4)–C(9) are substantially in agreement with these values, but bond C(1)–C(2) is longer. This difference is probably not meaningful. It should be noted for example, that the bond adjacent to this one, C(2)–C(3), is shorter than the generally accepted value of 1·54 Å for a normal carbon–carbon bond. The average found for all the normal C–C bonds is 1·544 Å, in excellent agreement with the expected value. The length of the double bond C(8)–C(8′) agrees well with the value 1·33 Å, usually reported for this type of bond.

As would be expected, considerable variation appeared in the carbon–hydrogen bond lengths, and the estimated standard deviations were large; nevertheless, the average value, 1·13 Å, is in excellent accord with the usual value, 1·09 Å.

Turning to a consideration of the bond angles, we note that Parkes & Hughes (1963) reported a linear C–C≡N group in cyanogen; Hannan & Collin (1953) assumed it in the structure of dicyanoacetylene and Luxmoore & Truter (1962) found a value of 178° for the sequence in tetracarbonyl (acrylonitrile) iron. As can be seen from the results listed in Table 4, the slight deviations from linearity for the three groups in the present structure appear to be of doubtful significance.

The values found for the normal C–C–C bond angles average 110·3° corresponding, as would be expected, rather closely to the tetrahedral angle. At the double bond, the angle C(4)–C(8)–C(8′) is nearly identical with the values reported for tetramethylethylene and isobutene (Pauling, 1960). The deviations of the angles involving hydrogen atoms are consistent with the difficulties associated with the precise location of such light atoms.

The variations found in the structure for a few of the bond lengths and bond angles from the generally accepted values suggest the possibility of some small but systematic errors in the data. The principal source of such errors appears to be the lack of data beyond the fourth layer about the $b$ axis. Some evidence for this was observed in the analysis of the Patterson synthesis. For example, a peak observed on the $b$ axis 1·7 Å from the origin was shifted to a more reasonable distance of 1·5 Å by assuming normal fall-off for the data and including estimated values for the missing fifth and sixth levels. The effects would, of course, be strongest along $b$ but they were noted elsewhere as well. Although a detailed analysis of the effects of such omissions is not possible, it is not unreasonable to assume that some coordinates and, more certainly, some temperature factors could be affected.

The final thermal parameters and their estimated standard deviations are listed in Table 5. A complete analysis of these parameters was undertaken to calculate the mean-square displacements of the atoms in different directions in the structure. The results of these calculations are not presented here because, of the seven atoms treated anisotropically, two, C(8) and C(9), were characterized by imaginary solutions for the atomic vibration ellipsoids. Therefore, although the calculated displacements for the other atoms were, in fact, not unreasonable, they are of doubtful significance.

Table 5. *Final thermal parameters and their estimated standard deviations**

| | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|
| C(1) | 0044 | 0233 | 0113 | −0044 | 0075 | −0068 |
| | 3 | 28 | 9 | 16 | 10 | 26 |
| C(7) | 0038 | 0241 | 0108 | −0035 | 0041 | 0081 |
| | 3 | 31 | 9 | 16 | 9 | 25 |
| C(8) | 0026 | 0106 | 0093 | 0004 | 0058 | 0017 |
| | 3 | 24 | 8 | 12 | 8 | 22 |
| C(9) | 0033 | 0063 | 0055 | −0000 | 0044 | 0060 |
| | 3 | 25 | 7 | 12 | 7 | 19 |
| N(1) | 0064 | 0329 | 0159 | −0033 | 0134 | 0005 |
| | 4 | 28 | 10 | 15 | 10 | 25 |
| N(2) | 0055 | 0382 | 0166 | −0130 | 0055 | −0009 |
| | 4 | 30 | 17 | 17 | 10 | 28 |
| N(3) | 0068 | 0128 | 0106 | 0069 | 0064 | −0044 |
| | 4 | 25 | 8 | 14 | 9 | 21 |

| | $B$ | $\sigma$ | | $B$ | $\sigma$ |
|---|---|---|---|---|---|
| C(2) | 3·133 | 0·135 | C(5) | 2·813 | 0·123 |
| C(3) | 2·776 | 0·122 | C(6) | 2·833 | 0·121 |
| C(4) | 2·009 | 0·107 | | | |

* In the case of the anisotropic parameters, the decimal point on the left is omitted and the estimated standard deviations are recorded directly below the appropriate values in the correct decimal position. A value of $B=4{\cdot}0$ was used for all hydrogen atoms.

*The molecular structure*

The molecule consists of two centrosymmetric halves with a double bond connecting two carbon atoms at the center. The sequence of atoms,

$$\mathrm{N(3)\equiv C(9)\text{–}C(4)\text{–}C(8)=C(8')\text{–}C(4')\text{–}C(9')\equiv N(3)'}\ ,$$

which crosses the molecule through its center is almost exactly planar within experimental error. The orientation is such that the plane is essentially parallel to the crystallographic $(34\bar{3})$ plane. The planar *trans* configuration about the double bond is, of course, not unexpected, but there appears to be no obvious requirement that the nitrile groups should lie in this plane.

The principal sequence in the molecule,

$$\mathrm{N(1)\equiv C(1)\text{–}C(2)\text{–}C(3)\text{–}C(4)\text{–}C(5)\text{–}C(6)\text{–}C(7)\equiv N(2)}\ ,$$

as well as its centrosymmetric mate, is also very close to planar. This corresponds to *trans* staggered configurations about each of the carbon–carbon bonds in the array. Deviations from the plane range from 0·002 to 0·072 Å and the average deviation is 0·034 Å. A least-squares analysis yielded an equation for the plane,

$$-0{\cdot}521x+0{\cdot}794y-0{\cdot}134z = -1{\cdot}550\ ,$$

where $x$, $y$, and $z$ are in Å and are measured along the crystallographic axes. The distance from the plane to the origin is 1·550 Å; hence, the perpendicular distance

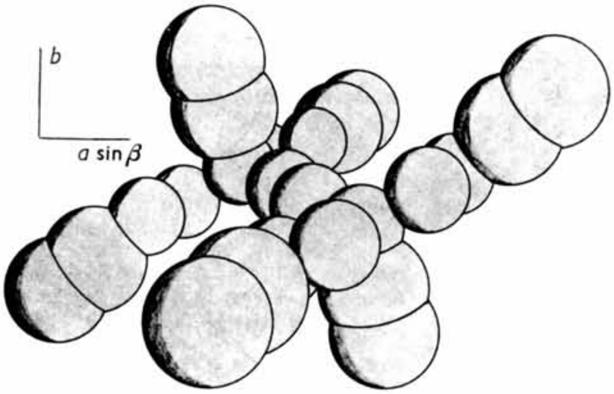


Fig. 1. A view of the molecule projected down the $c$ axis. (Hydrogen atoms omitted for clarity).

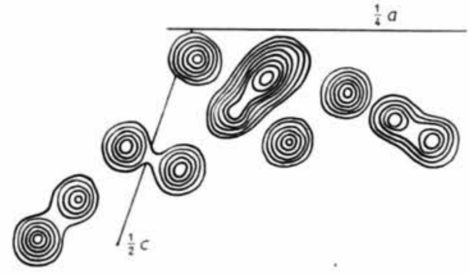


Fig. 2. Final electron density projection down the $b$ axis, with contours drawn at arbitrary intervals.

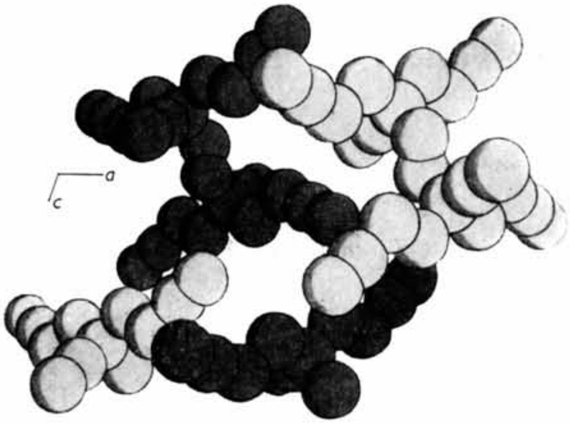


Fig. 3. A view of the structure projected along the screw axis.

between the two centrosymmetrically related planes of atoms in the molecule is 3·10 Å.

Fig. 1 shows a view of the molecule without hydrogen atoms as seen down the *c* axis. The three major planes of atoms in the molecule are clearly visible. The final electron density projection of the asymmetric half of the molecule down the *b* axis is shown in Fig. 2. A perspective view of the molecule down the same axis can be seen in Fig. 3.

### *The crystal structure*

The molecular packing can be seen in Fig. 3 where the structure is viewed in projection down the screw axis. An interesting feature of the packing is the antiparallel array of nitrile groups which is almost parallel to (10, 0, 3). The antiparallel configuration suggests dipole–dipole interactions among these highly polar groups.

Table 6. *Intermolecular distances*

| Contact | Distances (Å) | | | | | |
|---|---|---|---|---|---|---|
| $N \cdots N$ | 3·84 | 3·77 | 3·73 | 3·71 | 3·66 | |
| $N \cdots C$ | 3·84 | 3·58 | 3·52 | 3·45 | 3·40 | 3·38 |
| | 3·31 | | | | | |
| $C \cdots C$ | 3·39 | | | | | |
| $N \cdots CH$ | 3·55 | | | | | |
| $N \cdots CH_2$ | 3·87 | 3·75 | 3·66 | 3·63 | 3·57 | 3·56 |
| | 3·52 | 3·50 | 3·44 | 3·36 | 3·36 | |

In Table 6 is a listing of all significant intermolecular distances which are less than 3·9 Å. The average of the $N \cdots N$ contact distance is 3·74 Å, for $N \cdots C$ it is 3·50 Å, and for $N \cdots CH_2$ it is 3·56 Å.

Pauling (1960) gives a value of 1·5 ± 0·2 Å for the van der Waals radius of nitrogen. The $N \cdots N$ contacts listed in Table 6 are significantly longer than would be predicted from this figure. Nevertheless they are more nearly in accord with results reported in other structures. The range of value observed can be seen in that Bekoe & Trueblood (1958) reported an $N \cdots N$ distance of 3·41 Å in tetracyanoethylene, Parkes & Hughes (1963) found a value of 3·54 Å in cyanogen, Hannan & Collin (1953) reported 3·60 Å in dicyanoacetylene and Shallcross & Carpenter (1958) obtained 3·7 Å in cyanoacetylene.

Closest contact distances for $N \cdots C$ of 3·12 Å in tetracyanoethylene, 3·25 Å in cyanogen and 3·30 Å in dicyanoacetylene have been reported. Although most of the values given in Table 6 are larger, the closest contact, 3·31 Å, is in agreement with that found in tetracyanoethylene.

The higher values of the $N \cdots CH_2$ and $N \cdots CH$ distances are reasonable in terms of the van der Waals radius of 2·0 ± 0·1 Å given to both the methyl and methylene groups by Pauling (1960). The shorter values listed are of interest. Shallcross & Carpenter reported a value of 3·27 Å for a $N \cdots CH$ contact in cyanoacetylene and suggested that this distance involved hydrogen bonding even though it is a little longer than the 3·18 Å reported for the hydrogen bonding HCN by Dulmage & Lipscomb (1951). Considering the high melting point of hexacrylonitrile, it is possible that the short van der Waals distances are due to this effect.

## References

Bekoe, D. A. & Trueblood, K. N. (1959). *Z. Kristallogr.* **113**, 1.

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Dulmage, W. J. & Lipscomb, W. N. (1951). *Acta Cryst.* **4**, 330.

Hannan, R. B. & Collin, R. L. (1953). *Acta Cryst.* **6**, 350.

Luxmoore, A. R. & Truter, M. R. (1962). *Acta Cryst.* **15**, 1117.

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

Okaya, Y. (1962). Private communication.

Parkes, A. S. & Hughes, R. E. (1963). *Acta Cryst.* **16**, 734.

Pauling, L. (1960). *The Nature of the Chemical Bond*: Ithaca: Cornell Univ. Press.

Philips, D. C. (1954). *Acta Cryst.* **7**, 746.

Shallcross, F. V. & Carpenter, G. B. (1958). *Acta Cryst.* **11**, 490.

*Tables of Interatomic Distances* (1958). London: The Chemical Society.

Takashina, N. & Price, C. C. (1962). *J. Amer. Chem. Soc.* **84**, 489.

Van der Helm, D. & Patterson, A. L. (1961). *Amer. Cryst. Assoc. Computer Program Listing*, 2nd Ed., No. 354.