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The Crystal Structure of Myo-Inositol

By I. N. Rabinowitz* and J. Kraut†

Department of Biochemistry, University of Washington, Seattle 5, Washington, U.S.A.

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The crystal structure of myo-inositol has been determined by three-dimensional Patterson superposition methods, and refined by full-matrix and block-diagonal least-squares computations. The final R index is 5·5% for 2968 reflections with measurable intensities. The space group is $P2_1/c$, with unit cell dimensions $a = 6{\cdot}640$, $b = 12{\cdot}084$, $c = 19{\cdot}681$ Å and $\beta = 105^\circ\ 50'$. There are two molecules per asymmetric unit. All twenty-four hydrogen atoms have been located and their parameters refined.

Both molecules are found in the expected chair form with one hydroxyl group axial, but small measurable distortions from the perfect chair conformation are observed. The two molecules of the asymmetric unit are almost identical, to the extent that these small distortions appear to occur in the same way in both. No unusual bond lengths or angles are present.

Introduction

Among biologically important compounds, myo-inositol has been known for a relatively long time, having been first isolated from meat extracts by Scherer as early as 1850 (Bartow & Walker, 1938). Since it is without optical activity, Scherer originally named the compound *meso*-inositol. However six other inositols are also in the *meso* form, and this particular member of the family is now more commonly known as myo-inositol, following the suggestion by Fletcher, Anderson & Lardy (1951).

The inositols are hexahydroxycyclohexanes, of which there are eight possible *cis-trans* isomers. Seven are *meso* forms, and one is a DL pair, giving a total of nine stereoisomers (Eliel, 1962, p. 183). Four of these, scyllo-, myo-, D- and L-inositol are found to occur naturally; the others have been synthesized in the laboratory. Myo-inositol is the isomer with a single axial hydroxyl group. It is therefore somewhat higher in energy than scyllo-inositol in which all the hydroxyl groups are equatorial. Nevertheless, of the three naturally occurring *cis-trans* isomers, myo-inositol is by far the most abundant, having been found in all plant or animal tissues which have been assayed for its presence (Angyal & Anderson, 1959).

The chemical structure of myo-inositol has been known since 1887, and excellent reviews of the chemistry of the inositols can be found in articles by Lohmar (1957) and by Angyal & Anderson (1959). The conformation, on the other hand, has presented a somewhat more difficult problem. Various lines of evidence have pointed to a chair conformation with a single axial hydroxyl group, in full accord with the X-ray diffraction results presented here. It is interesting that Magasanick (1956) was able to arrive at the correct conformation through enzyme specificity studies. The stereochemistry of six-membered rings in general has been reviewed by Orloff (1954), and quite recently by Eliel (1962). A discussion of some aspects of the biological role of myo-inositol can be found in the review by Angyal & Anderson (1959).

During the final stages of this work we learned that the crystal structure of myo-inositol hydrate had recently been solved by Beevers (1962) and coworkers. At the time this manuscript was being prepared the details of the hydrate structure were not yet available to us for comparison.

Experimental

The myo-inositol sample used in this study was obtained from the California Corporation for Biochemical Research, who prepared the material according to the method of Bartow & Walker (1938). The commercial product was recrystallized from water–ethanol solutions. Large well formed flattened monoclinic prisms were readily obtained. They were elongated in the a direction and displayed prominent ((010)) faces. Unit-cell parameters, as measured with a G.E. XRD 5 single-crystal diffractometer, were

$$a = 6{\cdot}640 \pm 0{\cdot}005,\ b = 12{\cdot}084 \pm 0{\cdot}005,$$
$$c = 19{\cdot}681 \pm 0{\cdot}005\ \text{Å};\ \beta = 105^\circ\ 50' \pm 2'\ .$$

The indicated uncertainties are estimated standard deviations. A weighted mean wavelength for Cu $K\alpha_1$ and Cu $K\alpha_2$ was taken to be $\lambda = 1{\cdot}5418$ Å. These parameters are in good agreement with those reported by White (1931).

The crystal density, determined by the method of free flotation with a mixture of carbon tetrachloride and xylene, was 1·57 g.cm^{-3}, with an estimated standard deviation of 0·01 g.cm^{-3}. The calculated density

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* Present address: Department of Agricultural Biochemistry, Rutgers University, New Brunswick, New Jersey, U.S.A.

† Present address: Department of Chemistry, University of California at San Diego, California, U.S.A.

for eight molecules of myo-inositol per unit cell is 1·575 g.cm^{-3}.

Reflections observed to be systematically absent were $h0l$ with l odd and $0k0$ with k odd, confirming the space group $P2_1/c$ reported by White (1931). The density indicates that there are two molecules of myo-inositol per asymmetric unit, with no water of crystallization.

Copper $K\alpha$ intensity data were collected on the diffractometer by a 2θ-scanning technique in which the background correction was made by consideration of the mean background on either side of the peak. Goniostat settings were calculated using U.W. program 0014. A total of 3344 intensities were measured, accounting for all reflections within the range of the instrument ($2\theta \leq 161°$). No absorption corrections were applied, but a small crystal fragment of approximate dimensions 0·10 by 0·07 by 0·08 mm was used to minimize the resultant errors. The number of reflections which proved too weak to measure was 1376 or 41% of the total. This large proportion of unobserved reflections was due to the small size of the crystal and to the application of a rather conservative criterion for the acceptance of a reflection intensity as significantly different from background.

During data reduction with U.W. program 0029 the customary Lorenz and polarization corrections were made, and an estimate of the standard deviation for each reflection intensity was arrived at on the basis of counting statistics. The criterion that I/σ should be greater than 2 was used to decide whether or not an intensity was significantly different from background. The quantity I is understood to be the net relative intensity above background, and σ is its estimated standard deviation. The relative average standard deviation of the reflection amplitudes for the reflections satisfying this criterion, as calculated by the formula $R_p = \Sigma\sigma(F)/\Sigma F$, was 4·7%. This figure may, for the want of an established expression, be referred to as the 'Poisson R'; it represents something in the nature of a minimum meaningful R index for the data in hand. When reflection amplitudes were not significantly above background, the estimated *minimum observable* amplitude was stored by the data reduction program in the location reserved for the observed amplitude, and the reflection suitably flagged. At data-reduction time the atomic scattering factors were also interpolated from tables given by Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for carbon and oxygen, and McWeeny (1951) for hydrogen.

Determination of the structure

The structure was solved by machine vector-coincidence methods applied to a sharpened, origin-removed Patterson function, with the use of a generalization of the scheme applied to the solution of the structures of 2-aminoethanol phosphate (Kraut, 1961), thiamine hydrochloride (Kraut & Reed, 1962) and adenosine-5′-phosphate (Kraut & Jensen, 1963). In this case, however, we were dealing with a 24-light-atom structure consisting of a pair of molecules in unknown relative orientations. It was thus felt that myo-inositol presented a fairly stringent challenge to the method.

As before, the first step was the attempt to identify some Patterson peak as arising from the interaction of a pair of atoms. In a centrosymmetric structure containing heavy atoms the natural procedure is to look for a heavy-atom to heavy-atom interaction across a center of symmetry. It is well known that correct identification of such an interaction and use of the corresponding vector as the basis of a superposition function may well provided the solution of a structure almost at once in favorable cases. Where no heavy atoms are present however, it is obviously necessary to settle for a piecemeal approach to the problem. In the first place, even if a vector between a pair of centrosymmetrically related atoms could be found, the resulting superposition map would certainly not be expected to contain the entire structure since there is now no dominant set of heavy-atom to light-atom Patterson peaks to image the structure. Secondly, it is unlikely in the general case that such vectors would be represented by readily identifiable peaks in the Patterson map since they are of half-weight compared with the other types of vectors and greatly outnumbered by them. In fact, the invisibility of these 'centric vectors' leads to an ambiguity in the interpretation of sets of Patterson peaks which initially caused us to make a disappointing and protracted false start, as will be described below.

In view of these considerations the procedure followed was this. Reasoning that any prominent Patterson peak was likely to be the locus of at least one vector between a pair of atoms, we selected such peaks essentially at random and then inspected the Patterson map for additional peaks associated with vectors between atoms related by symmetry to the original pair. When such a self-consistent set of vectors was found, the locations of the corresponding *possible* pair of atoms were used to calculate a multiple superposition function in the usual way. The qualifier 'possible' is used here advisedly. It is very easy, owing to the invisibility of the centric vectors belonging to the given set (alluded to above) mistakenly to identify a peak as belonging to the set which in actuality is related to the correct peak by the mirror plane of the Patterson space group $P2/m$. This error leads to an exchange of the y coordinates of the corresponding atom pair and, in our case, to a superposition map based on these false coordinates which contained convincing images of inositol rings, but which ultimately could not be interpreted as a stereochemically satisfying overall structure.

When finally a correct pair of atom coordinates, derived from a different set of Patterson peaks, were used in an eightfold minimum-function superposi-

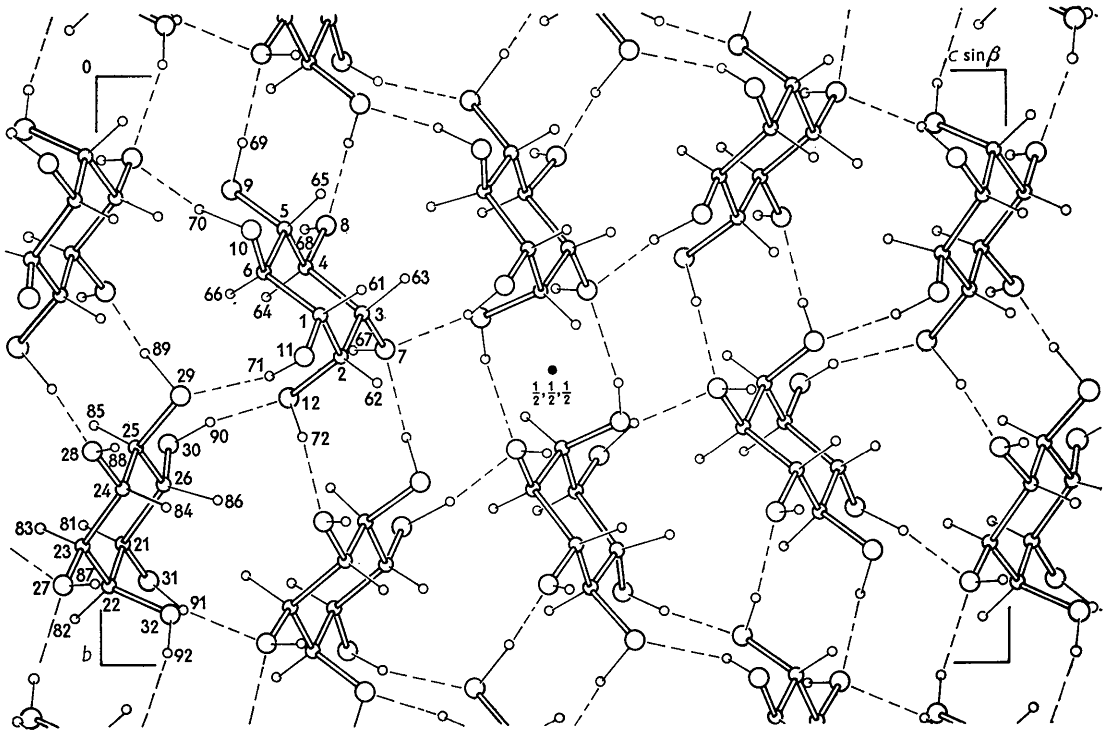

Fig. 1. Orthographic projection along the *a* axis of the unit cell of myo-inositol.

tion, eighteen of the twenty-four atoms of the asymmetric unit could be picked out without great difficulty. The coordinates of these eighteen atoms were then used to calculate a 72-fold minimum-(9)-function which yielded all twenty-four atoms of the asymmetric unit and incidentally revealed our original mistake in interchanging the *y* coordinates of the first pair of atoms. The minimum-(9)-function refers to the fact that the smallest 9 out of the 72 Patterson points contributing to each point of the superposition function were added to obtain the value of the superposition function at that point. The correctly identified pair of atoms used in the successful eightfold minimum function turned out to be those labeled 23 and 25 in Fig. 1.

A preliminary round of structure factor calculations for the inner half of the data ($\sin\theta/\lambda \le 0{\cdot}51$) based on atom coordinates from the final superposition map gave an *R* index of 0·35.

Refinement

Refinement was carried out entirely by the method of least-squares and proceeded in a fairly routine manner. A weighting scheme similar to Hughes's (1941) was applied, with the weight assigned to a particular reflection taken as the smaller of the two quantities $[\sigma(F)]^{-2}$ or $(0{\cdot}05F)^{-2}$, where $\sigma(F)$ was estimated from counting statistics. Reflections flagged during data reduction as not having intensities significantly above the background level were given zero weight whenever the calculated amplitude dropped below the inserted minimum observable value. A single overall scale factor was carried through all refinement computations as an adjustable parameter.

The first stages of the calculations were made with the Busing & Levy (1959) program ORXLS adapted for the IBM 709. Two cycles of refinement on atomic positional parameters and the overall isotropic temperature factor brought the *R* index down to 0·21. This was followed by three more cycles in which refinement of both positional parameters and individual anisotropic temperature factors for the twelve oxygen atoms was alternated with the same calculations for the twelve carbon atoms. *R* was now 0·11 for the observed reflections.

A difference-Fourier synthesis calculated at this point revealed all twenty-four hydrogen atoms with peak heights ranging from 0·3 e.Å^{-3} to 0·8 e.Å^{-3}.

Refinement was continued after introduction of the hydrogen atom positions. A modified version of the UCLA block-diagonal least-squares program (Gantzel, Sparks & Trueblood, 1961) was used henceforth, with the important convenience that all parameters could be refined simultaneously. In the final cycles of calculations all parameters, including coordinates and isotropic temperature factors for hydrogen atoms, were simultaneously adjusted until the last shift in any parameter was less than or comparable to its estimated standard deviation.

The mean last shift in non-hydrogen atom coordinates, in terms of their standard deviations, was $0{\cdot}2\sigma$, with the maximum shift equal to $0{\cdot}8\sigma$. For hydrogen atom coordinates, the corresponding mean and maximum were $0{\cdot}4\sigma$ and $1{\cdot}6\sigma$. For thermal parameters the mean and maximum last changes were $0{\cdot}4\sigma$, $1{\cdot}4\sigma$ for the non-hydrogen atom β_{ij}'s, and $0{\cdot}2\sigma$, $0{\cdot}5\sigma$ for the hydrogen atom B's. The final R index for 2968 reflections with amplitudes significantly above background was 0·055, if contributing reflections are considered to have equal weight.

A final difference-Fourier synthesis calculated from structure factors for non-hydrogen atoms only showed

Table 1. *Positional parameters of non-hydrogen atoms, in fractional coordinates* × 10⁴, *and their estimated standard deviations*

Atom	x/a	y/b	z/c
C(1)	3948 ± 4	4077 ± 3	2435 ± 2
C(2)	2320 ± 4	4768 ± 2	2663 ± 1
C(3)	796 ± 4	4009 ± 2	2902 ± 1
C(4)	−316 ± 4	3251 ± 2	2297 ± 1
C(5)	1297 ± 5	2569 ± 2	2059 ± 1
C(6)	2879 ± 4	3301 ± 2	1844 ± 1
O(7)	−656 ± 3	4653 ± 2	3159 ± 1
O(8)	−1713 ± 3	2552 ± 2	2529 ± 1
O(9)	272 ± 3	1895 ± 2	1470 ± 1
O(10)	4444 ± 3	2631 ± 2	1673 ± 1
O(11)	5479 ± 3	4762 ± 2	2267 ± 1
O(12)	1204 ± 3	5451 ± 2	2093 ± 1
C(21)	1226 ± 4	7934 ± 2	251 ± 1
C(22)	2935 ± 4	8664 ± 2	113 ± 1
C(23)	4352 ± 4	7968 ± 2	−217 ± 1
C(24)	5335 ± 4	7012 ± 2	262 ± 1
C(25)	3621 ± 4	6304 ± 2	410 ± 1
C(26)	2126 ± 4	6946 ± 3	716 ± 1
O(27)	5909 ± 3	8635 ± 2	−404 ± 1
O(28)	6574 ± 3	6375 ± 2	−79 ± 1
O(29)	4527 ± 4	5424 ± 2	887 ± 1
O(30)	424 ± 3	6253 ± 2	764 ± 1
O(31)	−183 ± 3	8567 ± 2	528 ± 1
O(32)	4128 ± 3	9127 ± 2	772 ± 1

Table 3. *Positional parameters of hydrogen atoms, in fractional coordinates* × 10³, *and their estimated standard deviations; isotropic temperature factors for these atoms and their estimated standard deviations*

Atom	x/a	y/b	z/c	Isotropic temperature factor (Å²)
H(61)	473 ± 6	360 ± 3	289 ± 2	2·7 ± 0·8
H(62)	305 ± 5	522 ± 3	307 ± 2	1·5 ± 0·7
H(63)	168 ± 6	346 ± 3	338 ± 2	3·5 ± 0·9
H(64)	−115 ± 5	374 ± 3	187 ± 2	1·8 ± 0·7
H(65)	214 ± 5	199 ± 3	246 ± 2	2·9 ± 0·8
H(66)	215 ± 6	370 ± 3	145 ± 2	2·5 ± 0·8
H(67)	−189 ± 6	465 ± 3	279 ± 2	4·4 ± 1·0
H(68)	−310 ± 6	258 ± 3	228 ± 2	3·3 ± 0·9
H(69)	350 ± 7	114 ± 4	161 ± 2	5·2 ± 1·1
H(70)	370 ± 7	223 ± 4	113 ± 3	6·4 ± 1·3
H(71)	508 ± 6	508 ± 3	189 ± 2	3·9 ± 1·0
H(72)	138 ± 7	613 ± 4	223 ± 2	6·1 ± 1·3
H(81)	34 ± 6	760 ± 3	−19 ± 2	2·7 ± 0·8
H(82)	221 ± 6	924 ± 3	−29 ± 2	3·8 ± 1·0
H(83)	348 ± 5	765 ± 3	−66 ± 2	1·6 ± 0·7
H(84)	633 ± 4	733 ± 2	75 ± 1	0·7 ± 0·6
H(85)	269 ± 5	591 ± 3	−5 ± 2	2·2 ± 0·8
H(86)	295 ± 5	720 ± 2	130 ± 2	1·6 ± 0·7
H(87)	703 ± 6	861 ± 3	−6 ± 2	3·7 ± 1·0
H(88)	799 ± 5	629 ± 3	17 ± 2	2·0 ± 0·7
H(89)	416 ± 8	470 ± 4	51 ± 3	8·3 ± 1·6
H(90)	71 ± 8	589 ± 4	122 ± 3	7·2 ± 1·4
H(91)	51 ± 8	908 ± 4	91 ± 2	6·7 ± 1·3
H(92)	440 ± 6	981 ± 3	73 ± 2	3·4 ± 0·9

Table 2. *Thermal parameters of non-hydrogen atoms and their estimated standard deviations*

β as given here is defined by:

$$T=\exp\{10^{-5}(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\}$$

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	1621 ± 68	583 ± 22	233 ± 8	−70 ± 32	184 ± 20	42 ± 11
C(2)	1786 ± 67	546 ± 21	189 ± 8	2 ± 32	184 ± 18	33 ± 10
C(3)	1543 ± 63	490 ± 20	222 ± 8	−31 ± 29	276 ± 18	20 ± 10
C(4)	1541 ± 64	457 ± 19	231 ± 8	−45 ± 29	225 ± 19	30 ± 10
C(5)	1998 ± 72	536 ± 20	191 ± 8	113 ± 33	195 ± 19	−1 ± 11
C(6)	1784 ± 70	595 ± 22	221 ± 8	118 ± 33	286 ± 20	7 ± 11
O(7)	1891 ± 51	486 ± 14	254 ± 6	110 ± 23	306 ± 15	−29 ± 8
O(8)	1726 ± 51	504 ± 15	301 ± 7	−109 ± 23	291 ± 15	30 ± 8
O(9)	2533 ± 60	519 ± 15	222 ± 6	−60 ± 27	156 ± 16	−42 ± 8
O(10)	1760 ± 52	846 ± 20	286 ± 7	200 ± 27	285 ± 16	−148 ± 10
O(11)	1686 ± 51	712 ± 18	261 ± 7	−214 ± 25	285 ± 15	32 ± 9
O(12)	2290 ± 56	451 ± 14	223 ± 6	14 ± 24	159 ± 15	81 ± 8
C(21)	1648 ± 65	530 ± 21	214 ± 8	20 ± 31	214 ± 19	−33 ± 10
C(22)	1841 ± 71	501 ± 20	208 ± 8	70 ± 31	143 ± 19	−8 ± 11
C(23)	1734 ± 65	490 ± 20	192 ± 8	−71 ± 30	216 ± 18	29 ± 10
C(24)	1599 ± 65	456 ± 19	222 ± 8	24 ± 30	210 ± 19	−16 ± 10
C(25)	1852 ± 69	446 ± 19	222 ± 8	−28 ± 30	235 ± 19	9 ± 10
C(26)	1740 ± 67	587 ± 21	197 ± 8	−72 ± 33	209 ± 19	34 ± 11
O(27)	1825 ± 52	528 ± 15	252 ± 6	−91 ± 23	285 ± 15	31 ± 8
O(28)	1759 ± 50	549 ± 15	275 ± 7	116 ± 24	277 ± 15	−53 ± 9
O(29)	2715 ± 63	442 ± 14	247 ± 7	−14 ± 26	211 ± 16	62 ± 8
O(30)	1671 ± 53	781 ± 19	289 ± 7	−327 ± 26	216 ± 16	100 ± 10
O(31)	1716 ± 50	726 ± 17	250 ± 6	155 ± 25	286 ± 15	−41 ± 9
O(32)	2208 ± 57	503 ± 15	223 ± 6	−67 ± 24	145 ± 15	−3 ± 8

Table 4. *Observed reflection amplitudes and calculated structure factors*

Within each group of constant h and k, the columns contain, from left to right: l, $10F_o$ and $10F_c$. An asterisk indicates the estimated minimum observable $10F_o$ for reflections which were too weak to be measured.

0,0,L		
2	37*	-14
4	1703	1895
6	268	-274
8	340	-349
10	88	-88
12	260	245
14	110	111
16	72	-90
18	148	-153
20	88	-81
22	47*	-20
24	29*	8
0,1,L		
1	30	24
2	38	39
3	85	79
4	1282	1383
5	65	80
6	285	292
7	283	281
8	370	-380
9	444	-446
10	169	-176
11	50	-44
12	36*	-23
13	200	-187
14	85	-66
15	47	32
16	111	122
17	44*	36
18	44*	48
19	41*	-13
20	42*	15
21	33*	14
22	80	-66
23	41*	-35
24	30*	-25
0,2,L		
0	566	-610
1	534	572
2	651	-700
3	924	-1005
4	168	-164
5	91	95
6	613	-650
7	80	-92
8	268	-261
9	87	-90
10	441	436
11	37*	-23
12	68	-53
13	109	112
14	122	114
15	92	-83
16	46*	-0
17	98	108
18	73	73
19	148	148
20	36*	5
21	58	64
22	125	128
23	85	92
24	26*	24
0,3,L		
1	215	-218
2	1088	1144
3	207	-231
4	287	-293
5	119	110
6	378	380
7	95	-90
8	380	-381
9	50	-56
10	366	-356
11	347	341
12	40*	-22
13	32	42
14	43*	-4
15	42*	14
16	156	164
17	199	203
18	93	-87
19	160	-157
20	58	62
21	44*	16
22	68	-52
23	33*	-17
0,4,L		
0	149	-156
1	226	225
2	1332	-1400
3	191	204
4	112	-107
5	139	137
6	72	-70
7	32*	9
8	119	123
9	218	212
10	59	60
11	210	-195
12	66	68
13	40*	-0
14	111	-115
15	44*	41
16	85	-80
17	100	112
18	42*	-52
19	40*	-9
20	63	-69
21	44*	-19
22	52	-61
23	46	-36
0,5,L		
1	67	-67
2	193	201
3	113	116
4	218	-230
5	35*	24
6	35*	27
7	519	497
8	191	-186
9	35	-9
10	42	32
11	44	-35
12	137	133
13	43*	-28
14	80	75
15	40*	-49
16	41*	31
17	39*	14
18	53*	28
19	44	-41
20	127	-119
21	88	80
22	33*	18
0,6,L		
0	97	109
1	33*	34
2	301	306
3	296	-283
4	76	77
5	61	59
6	285	277
7	76	72
8	38*	-6
9	37	38
10	63	-58
11	143	-133
12	122	-113
13	42*	37
14	42*	-2
15	242	-235
16	42*	-13
17	113	-118
18	60	62
19	36*	-14
20	46*	-39
21	143	-131
22	120	117
0,7,L		
1	63	-55
2	78	85
3	43	-45
4	106	-105
5	37*	1
6	109	107
7	102	-97
8	39*	-26
9	106	-104
10	106	-111
11	109	-111
12	189	184
13	42*	-80
14	43*	-33
15	47	-34
16	37*	-13
17	45	49
18	47*	-21
19	95	84
20	40*	5
21	30*	17
0,8,L		
0	241	230
1	40*	-9
2	81	82
3	113	-120
4	302	301
5	40*	-35
6	42*	-29
7	131	130
8	42*	11
9	144	142
10	68	-64
11	41*	29
12	40*	4
13	55	41
14	54	-59
15	84	-79
16	86	84
17	46	45
18	93	80
19	116	122
20	76	78
0,9,L		
1	42*	40
2	75	79
3	41*	-10
4	83	-80
5	87	93
6	75	-68
7	125	-132
8	44*	2
9	193	180
10	41*	-13
11	44*	9
12	42*	-43
13	52*	-13
14	50*	10
15	47*	-19
16	54	-54
17	44*	-46
18	41*	15
19	40*	-22
0,10,L		
0	142	-146
1	59	57
2	113	102
3	170	-193
4	54	-57
5	140	-136
6	44*	1
7	44*	13
8	85	91
9	112	112
10	64	-78
11	53*	6
12	54*	5
13	52*	17
14	47*	58
15	36*	25
16	53	-48
17	39*	-9
18	73	-74
0,11,L		
1	88	95
2	120	119
3	85	-103
4	32	-30
5	69	-70
6	160	164
7	44*	-40
8	50*	-11
9	63	65
10	42*	-34
11	66	67
12	76	80
13	88	91
14	44*	0
15	66	67
16	34*	22
17	139	-141
0,12,L		
0	192	-197
1	76	75
2	273	-289
3	131	-138
4	49*	-52
5	86	94
6	114	-118
7	82	-82
8	47*	22
9	47	-49
10	61	-63
11	40*	38
12	46	57
13	40*	-19
14	37*	-2
15	37	-37
0,13,L		
1	57	65
2	59	-66
3	80	85
4	42*	26
5	88	-102
6	60	-69
7	149	-158
8	39*	6
9	38*	4
10	42*	-35
11	40*	-12
12	35*	-4
13	30*	26
0,14,L		
0	91	-89
1	200	225
2	278	275
3	39*	9
4	38*	26
5	122	134
6	70	76
7	42*	4
8	42*	43
9	35*	-1
10	33	-38
0,15,L		
1	37*	21
2	38*	12
3	33*	-12
4	35*	-26
5	37*	28
1,0,L		
-24	37	-37
-22	76	-68
-20	126	121
-18	49	50
-16	315	319
-14	240	259
-12	112	-104
-10	214	-234
-8	156	-148
-6	457	512
-4	30*	-38
-2	53	-57
0	65	-64
2	1894	-2083
4	449	-485
6	463	-489
8	388	-386
10	137	129
12	409	-412
14	224	220
16	49	-50
18	44*	-3
20	70	78
22	41*	-14
1,1,L		
-24	36*	-36
-23	44*	29
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1	42*	-5
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3	93	99
4	48	46
5	73	-82
6	43*	9
7	65	-67
8	44*	-37
9	41*	-16
10	86	-87
11	40	-38
12	36*	16
13	35*	-1
14	40*	-24
15	30*	1
16	72	83
17	28*	-19
2,10,L		
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-18	38*	-12
-17	36*	27
-16	52	-42
-15	48*	7
-14	121	106
-13	61*	-34
-12	87	80
-11	101	-106
-10	44*	24
-9	46*	-36
-8	433	435
-7	279	-258
-6	92	83
-5	233	220
-4	369	365
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1	81	84
2	47*	-42
3	74	-86
4	85	-100
5	156	-169
6	91	115
7	41*	4
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9	52	-62
10	39*	-34
11	47	-55
12	86	-81
13	51*	-63
14	43	-52
15	100	-101
2,11,L		
-17	73	-81
-16	33*	-0
-15	42*	33
-14	63	50
-13	49*	44
-12	92	-96
-11	151	146
-10	109	112
-9	53	58
-8	111	-105
-7	40*	-19
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-5	54	-62
-4	60	-54
-3	192	-191
-2	106	107
-1	94	95
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1	42	47
2	46*	60
3	44*	39
4	53	-56
5	82	-85
6	48*	18
7	52*	16
8	72	-64
9	59	-54
10	37*	11
11	52	53
12	50	26
13	100	111
14	30*	7
2,12,L		
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-14	40*	27
-13	41*	21
-12	44*	-6
-11	49*	30
-10	36*	15
-9	81	82
-8	81	82
-7	127	119
-6	68	-76
-5	44*	-53
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-3	54	59
-2	101	-96
-1	93	-54
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1	44*	-15
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3	41*	-35
4	42*	-37
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6	51*	48
7	48*	18
8	48*	11
9	47*	-40
10	41*	-24
11	74	82
12	31*	19
2,13,L		
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-12	35*	-23
-11	38*	-7
-10	44	-31
-9	48*	55
-8	36*	-11
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-1	46*	32
0	46	-54
1	40*	12
2	47*	-50
3	122	129
4	44*	-11
5	38	-34
6	44*	-22
7	43*	-27
8	80	85
9	34*	22
10	81	-98
2,14,L		
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-9	33*	27
-8	35*	-27
-7	39*	-3
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-5	37*	30
-4	42*	30
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-1	68	-62
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2	50	62
3	36*	45
4	39*	-4
5	46	49
6	32*	24
2,15,L		
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-1	29*	8
3,0,L		
-24	85	-86
-22	102	106
-20	58*	-43
-18	44*	17
-16	166	167
-14	158	159
-12	41*	29
-10	447	-448
-8	68	-73
-6	437	443
-4	45	-44
-2	1230	1269
0	113	120
2	31*	-36
4	209	-215
6	136	141
8	53	-34
10	117	112
12	45*	48
14	39*	17
16	119	113
18	130	109
20	148	127
3,1,L		
-25	145	-163
-24	115	-123
-23	89	91
-22	93	91
-21	150	-160
-20	182	-187
-19	108	118
-18	48*	4
-17	69	-60
-16	54	69
-15	97	-105
-14	177	171
-13	43*	36
-12	80	80
-11	169	-182
-10	440	437
-9	33*	21
-8	33*	25
-7	33*	-41
-6	215	-247
-5	36*	-2
-4	126	-133
-3	323	-319
-2	109	112
-1	275	278
0	150	-149
1	44	-34
2	35	28
3	145	-148
4	111	110
5	40*	42
6	111	-104
7	210	-209
8	49	-40
9	44*	-42
10	43*	-12
11	76	65
12	42	40
13	43*	-33
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15	77	83
16	38*	-35
17	38*	-45
18	82	-86
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20	29*	-28
3,2,L		
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-23	169	-177
-22	99	-106
-21	130	-123
-20	132	-112
-19	220	-239
-18	42	45
-17	47*	-16
-16	163	162
-15	42*	25
-14	195	-192
-13	44*	32
-12	235	223
-11	95	88
-10	227	-219
-9	34*	20
-8	196	-198
-7	126	129
-6	321	315
-5	465	-463
-4	450	428
-3	195	188
-2	253	251
-1	339	-325
0	30*	-20
1	119	-121
2	172	-154
3	36*	26
4	52	-48
5	88	77
6	77	-75
7	163	179
8	151	143
9	41*	-26
10	41	26
11	191	191
12	43*	-7
13	127	115
14	134	-139
15	39*	-5
16	37*	10
17	78	81
18	147	-137
19	37*	-18
20	29*	31
3,3,L		
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-23	100	100
-22	49	14
-21	50*	38
-20	47*	-29
-19	52*	13
-18	64	-72
-17	55	47
-16	47*	14
-15	80	-85
-14	137	137
-13	97	88
-12	293	307
-11	150	141
-10	54	64
-9	334	327
-8	575	-538
-7	290	-284
-6	294	-281
-5	357	343
-4	744	-709
-3	355	-333
-2	267	-260
-1	151	142
0	451	451
1	35*	-16
2	109	-103
3	176	168
4	48	-60
5	126	124
6	92	-94
7	110	-102
8	131	-131
9	142	151
10	88	76
11	98	104
12	64	60
13	42*	-33
14	89	92
15	42*	-24
16	36*	-26
17	39*	2

Table 4 (*cont.*)

3,3,L		
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-20	54	42
-19	55	64
-18	54*	-13
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-16	42*	-14
-15	49	-58
-14	47	-51
-13	41*	16
-12	40	16
-11	58	59
-10	37*	-6
-9	190	-175
-8	151	-125
-7	83	84
-6	164	162
-5	176	173
-4	1158	-1127
-3	237	-231
-2	36*	-34
-1	211	-204
0	951	-950
1	33*	8
2	175	-169
3	111	-105
4	41*	30
5	259	-250
6	79	72
7	39*	-7
8	37*	5
9	162	-149
10	75	61
11	45*	-5
12	130	-127
13	44*	3
14	41*	13
15	40*	33
16	35*	-18
17	94	85
18	37*	6
19	104	-103
3,5,L		
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-22	55	49
-21	46*	-21
-20	50*	-21
-19	44	44
-18	53*	-71
-17	45*	-18
-16	40	-51
-15	49	54
-14	46*	-18
-13	68	64
-12	148	-143
-11	38*	13
-10	38*	31
-9	40*	-9
-8	112	-110
-7	35	-37
-6	41	-35
-5	137	127
-4	559	539
-3	329	-336
-2	188	182
-1	538	519
0	321	328
1	155	-154
2	64	68
3	130	128
4	177	-176
5	157	-153
6	125	-124
7	42*	16
8	44*	34
9	131	-120
10	43*	44
11	41*	-12
12	42*	-0
13	63	56
14	45	47
15	40*	33
16	38*	-25
17	51	-51
18	34*	24
3,6,L		
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-22	37*	33
-21	42*	31
-20	44	55
-19	48	-42
-18	101	-104
-17	53*	-4
-16	48	50
-15	49*	-61
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-13	142	-142
-12	72	68
-11	41	-40
-10	61	61
-9	43*	24
-8	80	90
-7	41*	43
-6	37	-22
-5	126	117
-4	103	91
-3	118	107
-2	279	-276
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0	339	330
1	371	353
2	61	62
3	308	309
4	96	95
5	230	228
6	145	141
7	43*	38
8	49	-61
9	300	-288
10	98	-101
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12	43*	-3
13	64	-73
14	48	38
15	37	-35
16	41*	22
17	34*	-4
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3,7,L		
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-21	37*	17
-20	44*	-7
-19	47*	-34
-18	52*	-14
-17	64	-46
-16	47	51
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1	232	-226
2	591	-614
3	298	287
4	247	244
5	44*	6
6	48	-43
7	42*	19
8	41*	23
9	60	-56
10	110	110
11	68	-73
12	41*	-10
13	51	-40
14	77	-74
15	43*	27
16	68	-72
17	91	89
3,8,L		
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-20	63	-59
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-18	40*	47
-17	52*	41
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-15	80	80
-14	48	42
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-12	47*	-18
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-10	95	95
-9	65	63
-8	42*	-2
-7	41*	-10
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-5	41*	30
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1	154	-160
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3	76	-71
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5	44*	-17
6	81	-84
7	125	130
8	106	-113
9	55	-47
10	85	79
11	46*	-29
12	38*	-25
13	37*	-40
14	38*	19
15	40*	35
16	30*	25
3,9,L		
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-19	44	-38
-18	41*	-19
-17	47*	21
-16	37*	24
-15	44*	19
-14	43*	46
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-10	43*	-5
-9	44*	10
-8	77	-83
-7	44*	-33
-6	243	-245
-5	98	105
-4	43*	-51
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1	45*	30
2	77	-77
3	117	-115
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5	45*	29
6	41*	-3
7	71	71
8	81	76
9	50*	16
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14	36*	-13
15	27*	-30
3,10,L		
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-16	47	-42
-15	66	-67
-14	46	39
-13	41*	-35
-12	67	-68
-11	41*	-23
-10	42*	-32
-9	44*	6
-8	68	67
-7	47	51
-6	258	-243
-5	215	227
-4	40*	-14
-3	214	-212
-2	388	-368
-1	42	31
0	43*	-28
1	174	-190
2	161	-160
3	59	-63
4	124	-122
5	42*	-2
6	45*	40
7	90	101
8	48*	0
9	44*	5
10	39*	15
11	46*	38
12	68	65
13	33*	-9
3,11,L		
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-15	132	123
-14	53	-48
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-12	38*	11
-11	59	-51
-10	38*	-9
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-8	43*	21
-7	69	70
-6	50*	3
-5	43	-29
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-3	177	177
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-1	88	76
0	102	110
1	60	-45
2	57	-46
3	43*	-37
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5	46	-54
6	39*	5
7	88	81
8	49*	-32
9	44*	32
10	38*	-3
11	36*	18
12	28*	-4
3,12,L		
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-12	37	-40
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-10	40	45
-9	37*	18
-8	37*	-0
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1	77	80
2	40*	35
3	68	75
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6	36*	26
7	36*	-12
8	38*	-24
9	46	-40
10	29*	18
3,13,L		
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-10	47	-42
-9	77	-68
-8	34*	14
-7	41	-43
-6	41*	-7
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-4	41	37
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-2	47*	42
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1	34*	-1
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6	36*	-16
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3,14,L		
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1	36*	9
2	35*	49
3	33*	-6
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-22	229	204
-20	105	-112
-18	252	275
-16	139	151
-14	155	148
-12	452	446
-10	65	61
-8	179	192
-6	34*	-8
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-2	39	-43
0	54	-52
2	44	50
4	66	-69
6	86	-80
8	149	-153
10	203	-236
12	47*	-30
14	49*	-10
16	44*	-32
18	29*	-26
4,1,L		
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-22	42*	15
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-19	71	67
-18	54	61
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-14	42*	-27
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-11	181	-176
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-9	85	92
-8	62	-56
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-6	36*	18
-5	78	-71
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-1	35*	-37
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2	39*	16
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5	330	329
6	173	178
7	78	-74
8	80	-71
9	40	-31
10	55	-38
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12	42*	-14
13	105	-97
14	89	-88
15	37*	26
16	42	-22
17	37*	1
18	43	46
4,2,L		
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-20	39*	-1
-19	41*	25
-18	89	84
-17	301	312
-16	228	-256
-15	166	188
-14	97	-83
-13	53	42
-12	167	-175
-11	90	95
-10	49	-41
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-8	38*	32
-7	38*	-11
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-5	54	47
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-2	49	50
-1	37*	-36
0	46	-37
1	37*	-32
2	60	-48
3	42*	26
4	368	356
5	212	204
6	132	-154
7	238	244
8	128	134
9	74	68
10	60	50
11	143	156
12	88	92
13	117	-118
14	44*	-30
15	78	-78
16	86	86
17	43	-34
4,3,L		
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-23	39*	-42
-22	89	-100
-21	149	-144
-20	91	101
-19	232	-240
-18	203	-216
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-15	266	-266
-14	256	-262
-13	48	58
-12	45*	42
-11	42*	40
-10	176	-185
-9	122	-124
-8	81	-72
-7	38*	12
-6	41*	30
-5	189	177
-4	37*	11
-3	153	150
-2	38*	7
-1	37*	7
0	37*	10
1	43	-36
2	41*	-25
3	222	-222
4	217	215
5	41*	-5
6	98	-108
7	227	-242
8	176	187
9	137	149
10	77	-75
11	54*	-29
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13	54	-44
14	46*	9
15	49	4
16	37*	8
17	32*	-16
4,4,L		
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-22	68	68
-21	43*	7
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-18	47*	-45
-17	45*	-47
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-14	183	-179
-13	59	63
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-10	165	150
-9	70	-52
-8	59	57
-7	38*	26
-6	205	208
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-4	41*	19
-3	80	-81
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-1	65	61
0	149	48
1	104	102
2	93	80
3	94	-93
4	124	109
5	43*	36
6	118	-118
7	120	119
8	125	126
9	95	-103
10	155	-167
11	52*	22
12	78	-77
13	49*	-19
14	45*	-11
15	43*	-13
16	37*	-21
17	26*	-14
4,5,L		
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-21	42*	5
-20	81	81
-19	85	79
-18	77	92
-17	43*	-23
-16	154	171
-15	230	235
-14	76	-67
-13	41*	-12
-12	41*	-3
-11	80	-69
-10	78	71
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2	335	-337
3	227	-221
4	159	-147
5	186	-182
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7	125	-129
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11	45	-48
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13	68	66
14	43*	-8
15	41*	-18
16	32*	16
4,6,L		
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-20	43*	-6
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-17	42*	29
-16	57	61
-15	38*	-9
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-12	81	99
-11	106	106
-10	91	-78
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-8	44*	-38
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-6	117	-111
-5	93	-93
-4	57	-69
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-2	68	-53
-1	99	-88
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1	43*	30
2	375	-354
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5	194	-201
6	198	-199
7	397	-416
8	42*	-8
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4	248	259
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8	42*	6
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0	45*	19
1	38*	-2
2	182	-183
3	276	300
4	108	103
5	69	-61
6	155	-164
7	72	84
7,2,L		
-19	26*	27
-18	35*	28
-17	47	-57
-16	44*	9
-15	37	43
-14	88	101
-13	102	-111
-12	85	83
-11	120	118
-10	43	51
-9	44	52
-8	50	44
-7	83	85
-6	67	-69
-5	55	51
-4	44	-32
-3	43*	-34
-2	58	58
-1	41*	-22
0	99	-106
1	43*	-2
2	63	58
3	96	104
4	96	-91
5	113	118
6	105	-111
7	64	73
7,3,L		
-18	46	-42
-17	38*	-18
-16	118	-122
-15	40*	-4
-14	75	-78
-13	63	-57
-12	39*	18

Table 4 (*cont.*)

7,3,L		
-11	41	44
-10	36*	32
-9	38*	-33
-8	35*	-21
-7	71	73
-6	53	49
-5	51*	10
-4	52	-40
-3	94	-93
-2	49*	-11
-1	133	-135
0	50	55
1	204	-191
2	50	50
3	105	-109
4	40*	14
5	91	-91
6	31*	1
7	26*	-24
7,4,L		
-17	35*	22
-16	204	-205
-15	43*	-12
-14	34*	25
-13	35*	-5
-12	81	-65
-11	60	-50
-10	32*	5
-9	88	-76
-8	78	88
-7	40*	37
-6	43*	15
-5	49*	35
-4	54	51
-3	90	-87
-2	44*	-24
-1	64	59
0	42	43
1	87	-97
2	48	-38
3	45	-26
4	36*	8
5	35*	16
6	30*	26
7,5,L		
-16	60	60
-15	62	58
-14	35*	14
-13	46	-44
-12	40	39
-11	42	-39
-10	32*	-18
-9	33*	21
-8	56	71
-7	37*	11
-6	37*	-14
-5	37	31
-4	45*	-18
-3	40*	-30
-2	46*	-24
-1	44*	31
0	45*	39
1	56	-68
2	50	-38
3	35*	7
4	70	79
5	30*	-29
7,6,L		
-15	31*	-35
-14	35*	-5
-13	39*	33
-12	31*	-26
-11	43	16
-10	30*	-22
-9	40	-43
-8	38*	-22
-7	45*	-14
-6	35*	-27
-5	43*	-7
-4	43*	6
-3	41*	-2
-2	42*	6
-1	40*	11
0	38*	-14
1	37*	-27
2	33*	8
3	33*	-31
4	26*	5
7,7,L		
-13	30*	-4
-12	33*	27
-11	36*	-22
-10	35*	2
-9	40*	-21
-8	33*	-5
-7	33*	-6
-6	38*	-8
-5	41*	1
-4	40	-36
-3	38*	6
-2	36*	4
-1	37*	24
0	43	-36
1	36*	45
2	29*	-13
7,8,L		
-11	26*	-20
-10	27*	-23
-9	33*	-32
-8	54	-53
-7	32*	11
-6	34*	20
-5	35*	15
-4	33*	-11
-3	51	43
-2	30*	-3
-1	29*	20
8,0,L		
-14	33	40
-12	111	-114
-10	36*	4
-8	32*	-4
-6	32*	24
-4	38*	-13
-2	68	63
0	64	-65
8,1,L		
-14	30*	4
-13	53	59
-12	38	37
-11	33*	-2
-10	39*	33
-9	33*	15
-8	40*	-7
-7	36*	-2
-6	32*	-34
-5	33*	-41
-4	48	48
-3	31*	42
-2	35*	-22
-1	34*	9
0	30*	26
1	28*	-20
8,2,L		
-14	26*	9
-13	28*	-32
-12	42	-27
-11	83	83
-10	36*	-41
-9	31*	-4
-8	38*	-11
-7	39*	-27
-6	41*	33
-5	46	-42
-4	36*	16
-3	72	-104
-2	32*	-10
-1	33*	-19
0	29*	2
1	31*	-55
8,3,L		
-13	55	66
-12	72	80
-11	56	-55
-10	42	-44
-9	33*	12
-8	33*	7
-7	34*	6
-6	36*	8
-5	36*	-13
-4	36	-37
-3	46	49
-2	66	66
-1	31*	-28
0	26*	-8
8,4,L		
-11	26*	2
-10	155	160
-9	35	44
-8	34*	7
-7	49	43
-6	33*	5
-5	68	60
-4	32*	-15
-3	30*	3
-2	27*	-18
8,5,L		
-8	57	-51
-7	91	-91
-6	28*	8
-5	27*	18

no positive regions other than hydrogen peaks exceeding 0·3 e.Å^{-3}. Hydrogen atom peak heights ranged from 0·3 e.Å^{-3} to 0·7 e.Å^{-3}. A final difference-Fourier synthesis based on structure factors for *all* atoms showed no positive or negative regions with absolute electron density exceeding 0·3 e.Å^{-3}.

Atomic parameters resulting from the last round of block-diagonal least-squares refinement are given in Tables 1, 2 and 3. The estimated standard deviations are those calculated from the diagonal elements of the inverse block-diagonal matrix. Observed reflection amplitudes versus structure factors calculated from these parameters are listed in Table 4.

Results and discussion

The crystal structure of myo-inositol as viewed in orthographic projection along the *a* axis is illustrated in Fig. 1. The numbering of atoms is arbitrary and is simply a carryover from the system used for atom identification during the computations. Note that atoms in molecule 2 have identification numbers which are obtained by adding 20 to the identification numbers of corresponding atoms in molecule 1, and that hydrogen atom identification numbers are obtained by adding 60 to the identification numbers of the atoms to which they are covalently bonded. The labeling does, however, provide for the carbon atom carrying an axial hydroxyl group to be numbered 2 (or 22) in deference to the two most commonly used myo-inositol ring numbering systems.

In Fig. 2 a single asymmetric unit is shown in

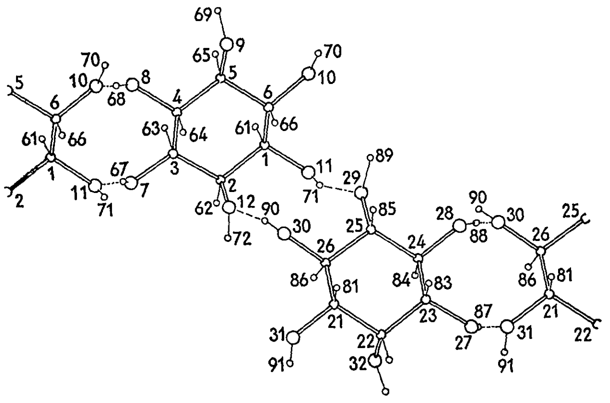

Fig. 2. Orthographic projection of the asymmetric unit of myo-inositol. The projection direction is parallel to the vector [0·550, −0·024, 0·226].

Table 5. *Bond lengths of covalent bonds and their estimated standard deviations*

Bond	Length (Å)	Bond	Length (Å)
C(1)–C(2)	1·527 ± 0·005	C(21)–C(22)	1·519 ± 0·004
C(2)–C(3)	1·532 ± 0·004	C(22)–C(23)	1·533 ± 0·004
C(3)–C(4)	1·524 ± 0·004	C(23)–C(24)	1·521 ± 0·004
C(4)–C(5)	1·523 ± 0·005	C(24)–C(25)	1·514 ± 0·004
C(5)–C(6)	1·518 ± 0·005	C(25)–C(26)	1·508 ± 0·005
C(6)–C(1)	1·512 ± 0·004	C(26)–C(21)	1·523 ± 0·004
C(1)–O(11)	1·419 ± 0·004	C(21)–O(31)	1·427 ± 0·004
C(2)–O(12)	1·426 ± 0·003	C(22)–O(32)	1·436 ± 0·003
C(3)–O(7)	1·435 ± 0·004	C(23)–O(27)	1·436 ± 0·004
C(4)–O(8)	1·421 ± 0·004	C(24)–O(28)	1·421 ± 0·004
C(5)–O(9)	1·428 ± 0·003	C(25)–O(29)	1·438 ± 0·003
C(6)–O(10)	1·428 ± 0·004	C(26)–O(30)	1·430 ± 0·004
C(1)–H(61)	1·06 ± 0·03	C(21)–H(81)	0·98 ± 0·03
C(2)–H(62)	0·99 ± 0·03	C(22)–H(82)	1·07 ± 0·04
C(3)–H(63)	1·17 ± 0·03	C(23)–H(83)	0·98 ± 0·03
C(4)–H(64)	1·05 ± 0·03	C(24)–H(84)	1·08 ± 0·02
C(5)–H(65)	1·09 ± 0·03	C(25)–H(85)	1·06 ± 0·03
C(6)–H(66)	0·93 ± 0·03	C(26)–H(86)	1·17 ± 0·03
O(7)–H(67)	0·93 ± 0·03	O(27)–H(87)	0·85 ± 0·03
O(8)–H(68)	0·92 ± 0·03	O(28)–H(88)	0·94 ± 0·03
O(9)–H(69)	0·95 ± 0·04	O(29)–H(89)	1·14 ± 0·05
O(10)–H(70)	1·15 ± 0·05	O(30)–H(90)	0·97 ± 0·05
O(11)–H(71)	0·81 ± 0·04	O(31)–H(91)	0·98 ± 0·05
O(12)–H(72)	0·86 ± 0·05	O(32)–H(92)	0·85 ± 0·04

Table 6. *Bond angles for covalent bonds not including hydrogen atoms*

The estimated standard deviation is 0·3° for all angles in the table

Angle		Angle	
C(6)–C(1)–C(2)	110·1°	C(26)–C(21)–C(22)	111·9°
C(1)–C(2)–C(3)	110·0	C(21)–C(22)–C(23)	109·4
C(2)–C(3)–C(4)	109·8	C(22)–C(23)–C(24)	111·3
C(3)–C(4)–C(5)	109·5	C(23)–C(24)–C(25)	109·3
C(4)–C(5)–C(6)	111·6	C(24)–C(25)–C(26)	113·4
C(5)–C(6)–C(1)	111·2	C(25)–C(26)–C(21)	110·9
C(6)–C(1)–O(11)	113·4	C(26)–C(21)–O(31)	112·4
C(1)–C(2)–O(12)	110·1	C(21)–C(22)–O(32)	108·6
C(2)–C(3)–O(7)	110·3	C(22)–C(23)–O(27)	111·6
C(3)–C(4)–O(8)	109·0	C(23)–C(24)–O(28)	108·9
C(4)–C(5)–O(9)	109·8	C(24)–C(25)–O(29)	109·9
C(5)–C(6)–O(10)	109·8	C(25)–C(26)–O(30)	110·1
C(2)–C(1)–O(11)	111·0	C(22)–C(21)–O(31)	110·9
C(1)–C(6)–O(10)	108·3	C(21)–C(26)–O(30)	108·1
C(6)–C(5)–O(9)	108·6	C(26)–C(25)–O(29)	108·8
C(5)–C(4)–O(8)	110·7	C(25)–C(24)–O(28)	110·3
C(4)–C(3)–O(7)	111·9	C(24)–C(23)–O(27)	111·6
C(3)–C(2)–O(12)	110·1	C(23)–C(22)–O(32)	110·2

orthographic projection parallel the vector direction [0·550, −0·024, 0·226]. Portions of both molecules of the asymmetric unit translated along the *a* axis are also shown, allowing the hydrogen bonds between O(8)–O(10), O(7)–O(11), O(28)–O(30) and O(27)–O(31) to be displayed. These hydrogen bonds cannot be seen in Fig. 1.

Bond lengths and angles for covalent bonds are given in Tables 5 and 6. Hydrogen bond lengths are given in Table 7. The estimated standard deviations are calculated from the standard deviations in positional parameters listed in Tables 1 and 3, with due allowance for error in the unit-cell parameters. Corrections have not been made in bond lengths to allow for the effects of rotational oscillations of the molecules (Cruickshank 1956, 1961); these would probably result in increases of a few thousandths of an Ångström unit at most.

Table 7. *Hydrogen bond lengths*

The estimated standard deviation is 0·003 Å for all bond lengths in the table

Bond	Length
O(7)–O(11)	2·688
O(8)–O(10)	2·648
O(9)–O(7)	2·800
O(10)–O(27)	2·884
O(11)–O(29)	2·734
O(12)–O(8)	2·641
O(27)–O(31)	2·739
O(28)–O(30)	2·645
O(29)–O(28)	2·675
O(30)–O(12)	2·704
O(31)–O(7)	2·814
O(32)–O(27)	2·799

Qualitatively it is apparent that these results completely corroborate the conclusion, drawn from more indirect evidence, that myo-inositol exists in the chair form with a single axial hydroxyl group. Bond lengths are almost normal, although perhaps the C–C bonds are slightly short; the mean C–C bond length is 1·521 ± 0·007 Å, and the mean C–O bond length is 1·429 ± 0·006 Å. The uncertainties here are r.m.s. deviations from the mean among the 12 bonds of each type. It is noteworthy that they are only about 1½ times the rather surprisingly small individual bond-length standard deviations calculated from the least-squares result, lending a degree of credibility to the latter. The mean of twelve C–C–C bond-angles within the rings is 110·7 ± 1·2°, and the mean of twenty-four C–C–O bond angles is 110·2 ± 1·3°. As might be expected, the r.m.s. deviations from the mean among the observed bond angles is about four times as large as their individual estimated standard deviations, indicating small but real distortions from the perfect chair conformation. Such distortions of the bond angles as observed here, giving rise to deviations from the expected 109·47° of not more than 3·9° (at C atoms 24, 25, 26), could easily result from the forces involved in hydrogen-bonding and molecular packing if we accept $17{\cdot}5\theta^2$ cal.mole^{-1} as the energy of bending (Westheimer, 1956, p. 533). It is interesting, however, that the smallest and largest angles of both kinds, rings and external, occur at the same places in both molecules of the asymmetric unit, suggesting the possibility that we are really observing small conformational perturbations characteristic of the myo-inositol molecule. Obviously such questions can only be settled by examining the molecular parameters in a variety of different crystal structures.

Looking at the myo-inositol molecule in another way, if it were to have a perfect chair conformation the plane formed by C atoms 1, 3, and 5 would be exactly parallel to the plane of atoms 2, 4 and 6. In fact it is observed that the dihedral angle between these planes is 1° 27′ in the first molecule and 1° 14′ in the second. The estimated standard deviation of these angles is only about 0° 10′. Again, the distortion is small but measurable.

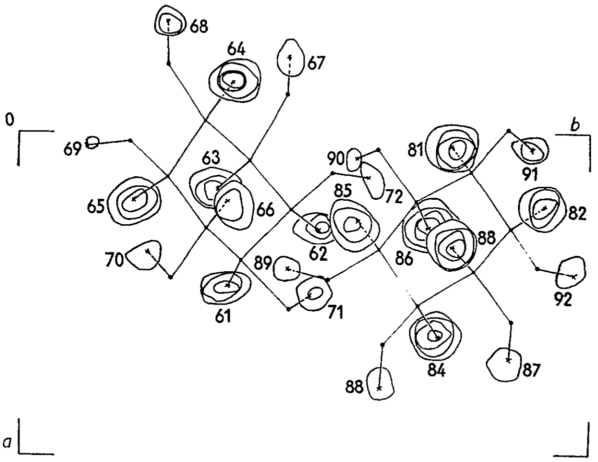

Fig. 3. Composite of difference-Fourier synthesis showing electron density peaks corresponding to hydrogen atoms in one asymmetric unit. View is along the *c* axis. Crosses represent positions of hydrogen atoms calculated by least squares.

Fig. 3 is a composite projection of levels of constant *Z* from the final difference-Fourier synthesis and shows electron density peaks corresponding to hydrogen atoms in one asymmetric unit. Contours are drawn at intervals of 0·1 e.Å^{-3} between 0·27 and 0·67 e.Å^{-3}. Least-squares positions for the hydrogen atoms are indicated by crosses. It is evident that these positions do not always coincide with the maxima of the associated difference-Fourier peaks. The average of the twelve C–H distances is 1·05 ± 0·08 Å, and the average of the twelve O–H distances is 0·95 ± 0·11 Å. The observed r.m.s. deviations from the mean accompanying these averages are about three times as large as the individual estimated standard deviations derived from the least-squares results, suggesting that block-diagonal treatment of hydrogen atom parame-

Table 8. *Magnitudes and direction cosines of the principal axes of thermal vibration ellipsoids*

	Axis *i*	B_i	C_{ia}	C_{ib}	C_{ic}		Axis *i*	B_i	C_{ia}	C_{ib}	C_{ic}
C(1)	1	3·82	−0·2188	0·7543	0·6552	C(21)	1	3·39	0·0456	−0·7088	0·6648
	2	3·07	−0·3465	0·5330	−0·6480		2	2·94	−0·5338	−0·6129	−0·4148
	3	2·47	−0·9122	−0·3834	0·3883		3	2·38	−0·8444	0·3492	0·6213
C(2)	1	3·34	−0·0074	0·9011	0·4191	C(22)	1	3·32	−0·7464	−0·5357	0·5836
	2	2·93	−0·9006	0·1824	−0·1336		2	2·92	−0·2668	−0·3027	−0·8074
	3	2·48	−0·4346	−0·3934	0·8980		3	2·74	−0·6098	0·7881	0·0859
C(3)	1	3·41	−0·3387	0·2143	0·7889	C(23)	1	3·10	−0·3596	0·8649	0·4349
	2	2·89	−0·2877	0·9507	−0·0330		2	3·02	−0·6657	0·0250	−0·5358
	3	1·94	−0·8958	−0·2243	0·6136		3	2·17	−0·6539	−0·5012	0·7237
C(4)	1	3·42	0·1029	0·3130	0·8802	C(24)	1	3·24	0·1601	−0·2116	0·8838
	2	2·75	−0·5447	0·8119	−0·0532		2	2·71	0·4981	0·8606	−0·0343
	3	2·15	−0·8323	−0·4927	0·4716		3	2·37	−0·8520	0·4637	0·4665
C(5)	1	3·55	−0·7450	−0·6425	0·0310	C(25)	1	3·34	0·4901	0·0221	0·7046
	2	2·90	−0·4402	0·6755	−0·4489		2	2·80	0·7102	−0·5898	−0·5637
	3	2·60	−0·5012	0·3618	0·8930		3	2·50	−0·5055	−0·8072	0·4311
C(6)	1	3·75	0·4610	0·7269	0·3638	C(26)	1	3·61	−0·2454	0·9254	0·3447
	2	3·28	−0·2254	0·6506	−0·6361		2	3·02	−0·6549	0·0612	−0·5459
	3	2·20	−0·8583	0·2196	0·6804		3	2·33	−0·7148	−0·3739	0·7637
O(7)	1	3·88	0·3855	−0·0761	0·7794	O(27)	1	3·80	0·2675	0·2313	0·8268
	2	3·20	0·5721	0·8016	−0·3231		2	3·31	0·5439	−0·8376	−0·0989
	3	2·16	−0·7239	0·5930	0·5368		3	2·28	−0·7953	−0·4950	0·5537
O(8)	1	4·38	0·0911	0·1604	0·9206	O(28)	1	4·18	0·0148	−0·4382	0·8606
	2	3·21	0·5674	−0·8194	−0·0769		2	3·40	−0·6000	−0·7229	−0·1658
	3	2·23	−0·8184	−0·5503	0·3828		3	2·19	−0·7998	0·5342	0·4815
O(9)	1	4·29	−0·9949	0·0374	0·3615	O(29)	1	4·49	−0·9940	0·1089	0·2774
	2	3·50	−0·0479	0·6408	−0·7241		2	3·80	−0·0511	−0·4136	−0·8605
	3	2·70	0·0886	0·7668	0·5874		3	2·30	−0·0964	−0·9039	0·4272
O(10)	1	6·08	−0·2019	−0·8205	0·5697	O(30)	1	5·71	−0·3572	0·7970	0·5660
	2	3·66	−0·5499	−0·3570	−0·5763		2	3·72	−0·3700	0·3580	−0·7237
	3	1·93	−0·8105	0·4466	0·5859		3	1·94	−0·8576	−0·4864	0·3948
O(11)	1	4·49	−0·3141	0·9263	0·2859	O(31)	1	4·50	−0·2229	−0·9335	0·3311
	2	3·83	−0·3144	0·1053	−0·8218		2	3·70	−0·4025	−0·1743	−0·7547
	3	2·04	−0·8958	−0·3618	0·4928		3	2·13	−0·8879	0·3133	0·5664
O(12)	1	3·97	−0·8211	0·3510	0·6572	O(32)	1	3·83	−0·9435	0·2108	0·5035
	2	3·58	−0·5691	−0·4425	−0·5114		2	3·17	−0·1915	0·2827	−0·8519
	3	2·12	−0·0440	−0·8252	0·5537		3	2·87	0·2704	0·9358	0·1437

ters may underestimate the associated errors. In the interest of saving space, covalent bond angles involving hydrogen atoms are not listed in the tables. There are no significant variations from normal tetrahedral angles, if due allowance is made for the rather large errors involved.

Hydrogen bonds are shown as dashed lines in Figs. 1 and 2. There is no evidence of a systematic difference between hydrogen bonding of the axial as distinguished from the equatorial hydroxyl groups. Nor does there seem to be any particular preference for hydrogen bonding between molecules related by symmetry on the one hand or between those not so related, on the other. All hydroxyl groups in the structure contribute their hydrogen atoms to hydrogen bonds. Two oxygen atoms, 7 and 27, accept two hydrogen bonds each, and in compensation oxygen atoms 9 and 32 accept no hydrogen bonds. All other oxygen atoms accept one hydrogen bond. Hydrogen bond distances and angles are unexceptional.

Hydrogen bond angles of the type C(2)–O(12)–O(30) tend to be roughly tetrahedral, as would be expected, but very large variations are found. For example, in the particular case cited, the angle is 152·8 ± 0·5°. As usual, the hydrogen atoms are found to be somewhat off of the internuclear O · · · O axis, the most extreme cases being hydrogen atoms 70 and 91, which form H–O · · · O angles of 20° and 22°.

The magnitudes and direction cosines of the principal axes of the ellipsoids of thermal vibration are given in Table 8. The quantities C_{ia}, C_{ib} and C_{ic} are cosines of the angles between the *i*th principal axis and the *a*, *b* and *c* axes of the unit cell. The B_i are given in Å^2. All atoms were found to be vibrating with *significant* anisotropy in the sense that at least one of the β_{ij} for every atom differs by more than 2σ (see Table 2) from the value it would have if the atom were actually vibrating isotropically with B equal to the mean principal axis B_i. As would be expected, the hydroxyl groups have a greater tendency than the ring atoms to be vibrating anisotropically. There are, however, no atoms in the structure with exceptionally large anisotropies. No effort has been made to analyse the thermal parameters in terms of oscillations or rotations of whole molecules.

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Molecular Complexes Exhibiting Polarization Bonding. IV. The Crystal Structure of the Anthracene-s-trinitrobenzene Complex

BY D. S. BROWN, S. C. WALLWORK AND (IN PART) A. WILSON

Department of Chemistry, University of Nottingham, England

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The crystal structure of the 1:1 complex formed between anthracene and *s*-trinitrobenzene has been determined at room temperature and at low temperature (*ca.* −100 °C). The structure is basically the same at the two temperatures though there are small differences in atomic positions. The crystals are monoclinic with four molecules of complex in a cell of dimensions $a = 11{\cdot}70$, $b = 16{\cdot}20$, $c = 13{\cdot}22$, all $\pm 0{\cdot}02$ Å, $\beta = 132{\cdot}8^\circ \pm 0{\cdot}5^\circ$ at room temperature, and $a = 11{\cdot}35$, $b = 16{\cdot}27$, $c = 13{\cdot}02$, all $\pm 0{\cdot}02$ Å, $\beta = 133{\cdot}2^\circ \pm 0{\cdot}5^\circ$ at low temperature, giving the maximum contraction approximately along the $[10\bar{3}]$ crystal direction. The space group is $C2/c$. The structure has been determined at each temperature by three-dimensional Fourier and least-squares methods. The component molecules are stacked alternately, each in two different orientations, in infinite columns along the c axis and the most important intermolecular contacts are approximately along this direction.

Introduction

The complex between anthracene, $C_{14}H_{10}$, and *s*-trinitrobenzene, $C_6H_3(NO_2)_3$, is one of the series of trinitrobenzene complexes discussed briefly in part III (Wallwork, 1961). The conclusion drawn for the series as a whole was that if there are charge transfer forces operating in the crystal lattices, they must be weak. On the other hand the orange colour of the crystals of the anthracene complex and the evidence from spectroscopic studies of the complex in solution (Briegleb & Czekalla, 1955; McGlynn & Boggus, 1958) suggest that there is a certain amount of charge transfer. Since this complex is one of the more highly coloured and one of the more stable of the aromatic hydrocarbon–trinitrobenzene series, it was felt that a detailed crystallographic examination would be of interest.

Experimental

Crystals were deposited slowly as orange needles after warm solutions of the components in ethanol had been mixed and allowed to cool. In polarized light at room temperature, the crystals exhibited pleochroism (with colours ranging from orange to yellow) with the maximum absorption of light when the electric vector was parallel to the needle axis. At the low temperature (*ca.* −100 °C) attained by blowing the vapour from boiling liquid nitrogen over the crystal, its general