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The Crystal Structure of Protopine, $C_{20}H_{19}O_5N$

BY S. R. HALL* AND F. R. AHMED

Pure Physics Division, National Research Council of Canada, Ottawa 7, Canada

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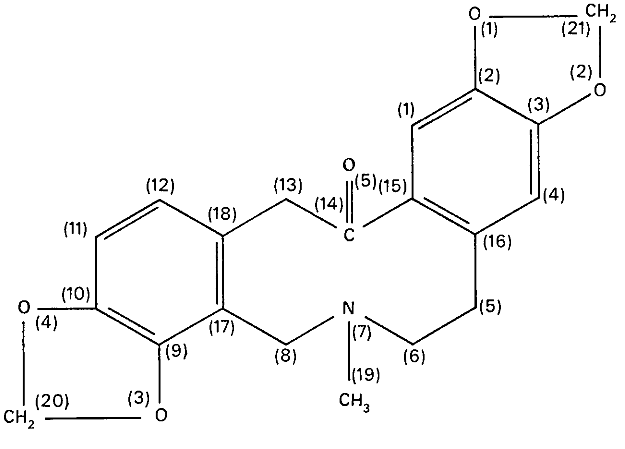
The crystal structure of protopine, $C_{20}H_{19}O_5N$, has been determined by the symbolic addition procedure, and has been refined by least squares to an R index of 0·043, with use of counter data for 2904 observed reflexions. The space group is $P2_1/n$ and the cell constants are $a=13{\cdot}610$, $b=17{\cdot}445$, $c=7{\cdot}102$ Å, $\beta=96{\cdot}75°$. The ten-membered ring in the molecule is severely buckled and contains a short distance across the ring of only 2·555 Å between the C atom of the carbonyl group and the tertiary nitrogen atom. Each of the two benzene rings has a very slight boat form, and the normals to their mean planes are at an angle of 27·8° from each other. The carbonyl group is about 37·4° out of the mean plane of its nearest benzene ring. The carbonyl oxygen atom and the methyl group are on the same side of the ten-membered ring.

Introduction

A natural group of alkaloids in opium is presented by the two members: protopine, $C_{20}H_{19}O_5N$, and cryptopine, $C_{21}H_{23}O_5N$. Protopine is almost the typical alkaloid of the poppy order (Papavaraceae) since it has been found in most species of this order. Molecules in this group are characterized by the presence of a ten-membered *N*-hetero-ring containing one carbonyl group (Manske & Holmes, 1954). The carbonyl group and the tertiary amino function are held very closely together across this medium-sized ring, and it is of interest to define the degree of interaction between them. The two functional groups have been found to interact when a proton is added to the carbonyl oxygen, as for example in protopine hydriodide, with the net result of transforming the ten-membered ring into two six-membered rings. This interaction was studied by Mottus, Schwarz & Marion (1953), and by Anet & Marion (1954) from the ultraviolet and infrared spectra. The molecular structure for the protopine base is shown in (I); the numbering of the atoms is based on that given by Henry (1949), p. 300.



(I) Protopine

X-ray analysis of protopine and cryptopine has been undertaken in order to determine their structures and

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* National Research Council Postdoctorate Fellow. Present address: Department of Physics, The University of Western Australia, Nedlands, Western Australia.

in particular the shape and dimensions of the central ten-membered ring, and the orientation of the carbonyl group relative to the rings. In each case, the analysis has been carried out on the base, since the heavy atom derivatives have been expected to involve steric change or complete closure of the ten-membered ring. In addition to the chemical interest in the two structures, they have been considered by the authors to be very suitable for trying out a self-consistent set of crystallographic programs developed by Ahmed, Hall, Pippy & Huber (1966) in FORTRAN IV for use on the IBM 360 system, and in particular a program for the direct method of phase determination by the symbolic addition procedure for centrosymmetric crystals. The structure of protopine is reported in this paper and that of cryptopine will be described in a separate communication.

Crystal data

Space group and unit-cell data for protopine, based on precession photographs, have been reported by Barnes & Forsyth (1954) as follows: space group $P2_1/c$; $a=7{\cdot}10_9$, $b=17{\cdot}44$, $c=16{\cdot}08$ Å, $\beta=122°45'$, $Z=4$; $D_c=1{\cdot}399$ g.cm^{-3}, $D_o=1{\cdot}393$ g.cm^{-3}.

For the present X-ray analysis the space group has been changed to $P2_1/n$, and the cell constants as remeasured on the General Electric XRD 5 diffractometer using a 1° take-off angle, 0·02° and 0·05° slits and Cu radiation (λ, $K\alpha_1=1{\cdot}54050$ Å, $K\alpha_2=1{\cdot}54434$ Å) are $a=13{\cdot}610$ ($\sigma=0{\cdot}003$), $b=17{\cdot}445$ ($\sigma=0{\cdot}004$), $c=7{\cdot}102$ Å ($\sigma=0{\cdot}003$), $\beta=96°45'$ ($\sigma=3'$); $U=1674{\cdot}5$ Å^3, mol. wt. $=353{\cdot}36$, $D_c=1{\cdot}401$ g.cm^{-3}; μ(Cu) $=8{\cdot}48$ cm^{-1}, $F(000)=744$. For this space group, the systematic absences are the $h0l$ with $h+l=2n+1$, and the $0k0$ when k is odd.

Intensity data

Cu radiation, Ni filters, and a prismatic crystal of dimensions between 0·2 and 0·3 mm were employed for the intensity data collection by the moving-crystal moving-counter method (Furnas, 1957). The crystal was mounted with the b axis along the direction of the fibre, the take-off angle was set at 2°, and the integrated intensity was measured at each lattice site within the range of the instrument. The 2θ scan was varied between 2° for the low-angle reflexions and 4° for the high-angle reflexions, and the background was measured at the beginning and at the end of each scan on the Laue streak through the reflexion. The mA setting was reduced for the strong reflexions instead of using attenuators, and when the peak height exceeded 20000 counts per second the intensity was corrected for nonlinearity of the counter by an empirically evaluated function. The intensity of the 400 reflexion was measured at short intervals of time during the data collection and employed for scaling of the intensities. Many of the weak reflexions were remeasured prior to the final stages of refinement in order to improve their counting statistics. The 1/Lp corrections were applied to the net counts (total – background), and the absorption corrections were ignored since $(\mu t)_{\text{av}}=0{\cdot}21$ (Jeffrey & Rose, 1964).

In the reciprocal space corresponding to $2\theta_{\max}$ of about 161° ($\sin\theta/\lambda=0{\cdot}64$), there are 3705 non-equivalent lattice sites excluding those prohibited by the space group, and of these, 2904 reflexions (78·4%) were observed above threshold.

Structure determination by symbolic addition

The structure was determined by the symbolic addition procedure for centrosymmetric crystals (Hauptman & Karle, 1953), using a program written by S.R.H. for the IBM 360 system in FORTRAN IV, which performs all the necessary operations automatically. The program starts with the $|F_o|$ data on some arbitrary scale and the $f(hkl)$ values at zero temperature, as output from the data reduction program, and concludes by supplying the signed $E(hkl)$ data in the appropriate order on magnetic tape which can be used directly as input to the Fourier program for calculation of the E map. However, human intervention is made possible at various stages in the program if need be.

The scale of the $|F_o|$ data, K', and the overall temperature factor, B, were estimated from the Wilson plot. In this calculation all the non-equivalent observed and accidentally unobserved reflexions were included, and appropriate allowances were made for the equivalent reflexions and for the systematic absences. The scattering factor curves employed in this and all other calculations were those derived by Hanson, Herman, Lea & Skillman (1964), except that the hydrogen curve was modified by a temperature factor of $-2{\cdot}5$ Å^2 as suggested by Jensen (1965). The normalized structure factor amplitudes $|E_{\mathbf{h}}|$ were calculated from the expression

$$|E_{\mathbf{h}}|^2=K(s)|F_{\mathbf{h}}|^2/\varepsilon \sum_j f_j^2(s)$$

where $|F_{\mathbf{h}}|$ are on the assumed original scale, $s=\sin\theta/\lambda$, $K(s)=K'^2 . \exp(2Bs^2)$, and ε for space group $P2_1/n$ was taken as 2 for the $h0l$ and $0k0$ reflexions and as 1 for all the others. The computed values for the distribution and statistics of $|E|$ for this structure, and the corresponding theoretical values which were calculated by Karle, Hauptman, Karle & Wing (1958), given in parentheses, were as follows: $\langle|E|\rangle=0{\cdot}803$ (0·798), $\langle|E|^2\rangle=0{\cdot}989$ (1·000), $\langle|E^2-1|\rangle=0{\cdot}954$ (0·968); reflexions with $|E|>3$ were 0·30% (0·3%), reflexions with $|E|>2$ were 4·67% (5·0%), and reflexions with $|E|>1$ were 30·4% (32·0%).

The 478 reflexions with $|E|>1{\cdot}50$ were then separated from the rest of the data, sorted in descending order of $|E|$, and each of them was assigned one of the eight parities in order to simplify the search operation. The search for sets of reflexions which satisfy the Σ_2 relationship

$$sE_{\mathbf{h}} \sim s \sum_{\mathbf{h}} E_{\mathbf{h}'} \cdot E_{\mathbf{h}-\mathbf{h}'}$$

was performed for all values of $|E_{\mathbf{h}}| > 1{\cdot}50$ but limiting $|E_{\mathbf{h}'}|$ and $|E_{\mathbf{h}-\mathbf{h}'}|$ to values more than 2·0 each. The three origin-defining reflexions $\bar{8}74$, 735, and 12,6,1 were selected by the program from the first ten reflexions with the largest $|E|$'s, and it was found necessary to select the 1,14,4 reflexion to define a symbol A. The first stage of sign determination was limited to the 178 reflexions with $|E| > 2{\cdot}0$, but it was possible to fix the signs of only 164 of these reflexions, and it was found later that 14 of them were wrongly signed. The sign determination was then extended to include the remainder of the 478 reflexions with $|E| > 1{\cdot}50$. Altogether, the signs were deduced for a total of 453 reflexions, of which 47 signs were later found to be wrong. However, the E map which was evaluated with these 453 reflexions gave the structure (excluding the hydrogen atoms) without any ambiguity as shown in Fig. 1, and there were no spurious peaks in the map as high as those selected for the molecule. The relatively high percentage of incorrect signs can be attributed to the unsuitability of the scheme adopted in the program for acceptance or rejection of the signs, and steps are now being taken to modify this part of the program.

The structure factors calculated for the trial model, assuming isotropic temperature factors, gave an R index of 0·27.

Refinement

The structure was refined by successive cycles of block-diagonal least squares, employing only the observed reflexions and evaluating matrices of sizes 4×4, 9×9, or (3×3 and 6×6) per atom. After two cycles of isotropic refinement, the R index was reduced to 0·14, and after three more cycles of anisotropic refinement, it was reduced further to 0·09. A difference map was computed and positions of all the hydrogen atoms were derived from it. In cycles six to nine, the C, N, and O atoms were refined anisotropically and the H atoms isotropically, and the R index was brought to 0·05. It was obvious at this stage that the structure amplitudes for some of the weak reflexions were not as accurate as the rest of the data, and the very strong reflexions were affected by extinction. The intensities of most of the weak reflexions were remeasured and their structure amplitudes were modified accordingly. The structure factors were recalculated without the contributions of the H atoms giving an R index of 0·074, a second difference map was evaluated omitting the 101, $\bar{2}21$, 310, 320, and $\bar{3}21$ reflexions which had appreciable extinction errors, and new positions for the hydrogen atoms were derived from it. A composite drawing of this difference map is presented in Fig. 2. The peak heights for the hydrogen atoms were between 0·4 and 0·7 e.Å^{-3}, the residual electron densities on some of the bonds were as high as 0·2 or 0·25 e.Å^{-3}, and the background elsewhere was quite flat and within ±0·15 e.Å^{-3}.

The final three cycles of refinement were carried out on all atoms, with the revised data but excluding the five strong reflexions with appreciable extinction errors. The final shifts in the parameters were much smaller than their e.s.d.'s, the final R index for all the observed

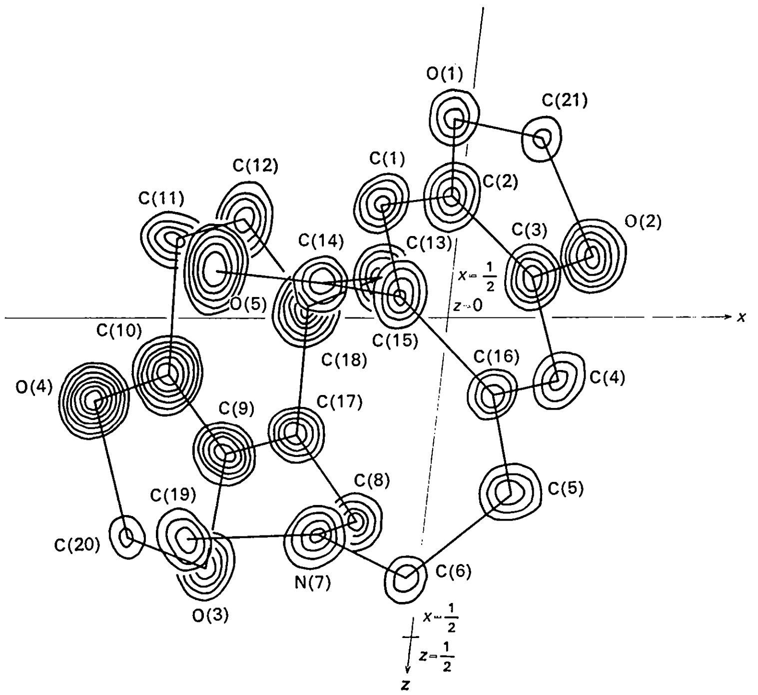

Fig. 1. Composite drawing of the E map as evaluated with 453 reflexions, of which 47 had wrong signs.

data was 0·043, and it was only 0·041 without the five aforementioned reflexions. The $|F_c|$ values for the large majority of the unobserved reflexions were below the threshold amplitudes, and the rest were only very slightly above them. The weights employed in the refinement were calculated by the expression

$$w = 1/\{1+[(|F_o|-60)/40]^2\}\,.$$

Results

The refined parameters of the C, N, and O atoms are listed in Table 1, and those of the H atoms are given in Table 2. The e.s.d.'s in Tables 1 and 2 were calculated with expression 6.4.3(6) of *International Tables for X-ray Crystallography* (1959, p.330), and increased by 30% in order to allow for omission of the unobserved reflexions and of the interaction between the atoms. The molecule in perspective as viewed from two directions at right angles to each other is shown in Fig. 3.

The observed structure amplitudes, and the calculated structure factors based on the parameters in Tables 1 and 2, are listed in Table 3. A summary of the agreement between $|F_o|$ and $|F_c|$ (Ahmed & Barnes, 1963) is presented in Table 4. Of the 3705 reflexions, only two observed reflexions show high discrepancy; both of these are very strong and are obviously affected by extinction.

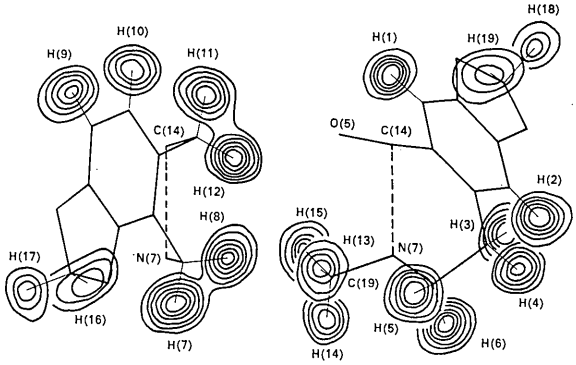

Fig. 2. The second difference map, showing the hydrogen atoms, with the contour lines at intervals of 0·1 e.Å^{-3}, starting at 0·2 e.Å^{-3}. For clarity, the molecule has been divided at the dotted line.

Table 1. *Fractional coordinates, vibration tensor components* (Å^2) *for the expression* $T=\exp[-2\pi^2(U_{11}a^{*2}h^2+\ldots+2U_{23}b^*c^*kl+\ldots)]$, *and their e.s.d.'s* (*all quantities* × 10^4)

	x	y	z	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{13}$	$2U_{12}$
C(1)	4352 (2)	3173 (1)	−1807 (3)	335 (12)	361 (14)	357 (13)	87 (20)	67 (20)	88 (20)
C(2)	4930 (2)	3808 (1)	−1872 (4)	402 (14)	412 (14)	425 (14)	283 (23)	163 (23)	63 (23)
C(3)	5712 (2)	3951 (1)	−508 (4)	367 (13)	398 (14)	546 (16)	241 (24)	150 (24)	−152 (23)
C(4)	5964 (2)	3462 (1)	974 (4)	339 (13)	427 (14)	443 (14)	166 (23)	−7 (22)	−152 (22)
C(5)	5709 (2)	2263 (1)	2749 (3)	334 (12)	399 (14)	384 (13)	189 (22)	−114 (21)	−118 (22)
C(6)	4882 (2)	2108 (1)	3971 (3)	483 (14)	330 (12)	298 (12)	−4 (20)	3 (21)	−208 (23)
N(7)	4137 (1)	1587 (1)	3037 (2)	316 (10)	259 (10)	303 (9)	−3 (15)	68 (15)	−6 (16)
C(8)	4441 (2)	781 (1)	3222 (3)	357 (12)	276 (12)	294 (11)	34 (19)	−6 (19)	6 (19)
C(9)	3313 (2)	−326 (1)	2099 (3)	338 (12)	274 (12)	376 (13)	42 (19)	88 (20)	64 (19)
C(10)	2738 (2)	−731 (1)	699 (4)	341 (12)	267 (12)	490 (14)	−11 (21)	117 (21)	−51 (20)
C(11)	2682 (2)	−535 (1)	−1168 (4)	432 (14)	373 (14)	429 (14)	−186 (23)	20 (23)	−122 (23)
C(12)	3248 (2)	94 (1)	−1611 (3)	423 (13)	381 (14)	322 (12)	−99 (21)	75 (21)	−38 (22)
C(13)	4433 (2)	1178 (1)	−738 (3)	341 (12)	313 (12)	295 (11)	−6 (19)	137 (19)	6 (20)
C(14)	3945 (2)	1948 (1)	−473 (3)	304 (11)	333 (12)	275 (11)	44 (19)	7 (18)	7 (19)
C(15)	4603 (2)	2644 (1)	−313 (3)	297 (11)	278 (12)	329 (12)	39 (19)	90 (19)	51 (19)
C(16)	5406 (2)	2782 (1)	1062 (3)	280 (11)	331 (12)	354 (12)	85 (19)	69 (19)	−21 (19)
C(17)	3858 (2)	303 (1)	1711 (3)	308 (11)	234 (10)	317 (11)	−39 (18)	59 (18)	53 (19)
C(18)	3830 (2)	505 (1)	−216 (3)	317 (12)	267 (10)	340 (12)	−52 (19)	142 (19)	54 (19)
C(19)	3158 (2)	1697 (1)	3636 (4)	413 (14)	365 (14)	474 (15)	−6 (23)	259 (23)	75 (23)
C(20)	2574 (2)	−1283 (2)	3487 (4)	754 (22)	566 (18)	642 (20)	498 (32)	−336 (34)	−621 (34)
C(21)	5682 (3)	4875 (2)	−2694 (5)	692 (22)	646 (22)	840 (24)	693 (38)	15 (37)	−364 (36)
O(1)	4843 (1)	4391 (1)	−3201 (3)	584 (12)	593 (12)	659 (13)	707 (23)	−45 (21)	−220 (20)
O(2)	6151 (2)	4635 (1)	−886 (3)	614 (13)	555 (12)	802 (15)	641 (23)	−119 (23)	−460 (22)
O(3)	3227 (1)	−651 (1)	3848 (2)	587 (12)	387 (10)	421 (10)	173 (16)	57 (17)	−284 (19)
O(4)	2246 (1)	−1316 (1)	1517 (3)	609 (12)	409 (10)	566 (12)	88 (18)	27 (19)	−418 (19)
O(5)	3052 (1)	2023 (1)	−805 (2)	296 (8)	413 (10)	535 (10)	80 (17)	−121 (15)	25 (16)

The bond lengths and their e.s.d.'s as calculated by the expression of Ahmed & Cruickshank (1953) are shown in Fig.4(*a*). The bond angles and their e.s.d.'s (*International Tables for X-ray Crystallography*, 1959, p.331) are given in Fig.4(*b*). These results are based on the refined coordinates and do not include the corrections for thermal vibration. The angles which have been omitted from Fig.4(*b*) for simplicity, and their e.s.d.'s, are: C(16)–C(5)–H(4), 106·9° (1·4); C(6)–C(5)–H(3), 110·5° (1·4); N(7)–C(6)–H(5), 105·9° (1·4); C(5)–C(6)–H(6), 108·6° (1·3); N(7)–C(8)–H(8), 110·0° (1·3); C(17)–C(8)–H(7), 109·6° (1·3); C(18)–C(13)–H(12), 111·5° (1·3); C(14)–C(13)–H(11), 102·1° (1·5); N(7)–C(19)–H(14), 111·8° (1·6); H(13)–C(19)–H(15), 105·3° (2·1); O(3)–C(20)–H(17), 115·5° (2·0); O(4)–C(20)–H(16), 106·7° (1·8); O(1)–C(21)–H(19), 112·4° (2·1); O(2)–C(21)–H(18), 103·9° (1·8).

Table 2. *Fractional coordinates* $(\times 10^3)$ *and isotropic temperature factors* (Å^2) *of the hydrogen atoms, and their e.s.d.'s*

	x	*y*	*z*	*B*
H(1)	375 (2)	304 (1)	−276 (3)	3·4 (0·5)
H(2)	655 (2)	359 (1)	194 (3)	3·1 (0·5)
H(3)	600 (2)	175 (1)	231 (3)	3·6 (0·6)
H(4)	629 (2)	252 (1)	353 (3)	3·6 (0·5)
H(5)	451 (2)	260 (1)	425 (3)	3·6 (0·6)
H(6)	519 (2)	187 (1)	527 (3)	3·4 (0·5)
H(7)	436 (2)	56 (1)	450 (3)	3·1 (0·5)
H(8)	520 (2)	73 (1)	308 (3)	3·0 (0·5)
H(9)	224 (2)	−82 (1)	−218 (4)	4·4 (0·6)
H(10)	320 (2)	26 (1)	−297 (4)	3·9 (0·6)
H(11)	448 (2)	117 (1)	−213 (4)	3·9 (0·6)
H(12)	511 (2)	117 (1)	−4 (3)	2·6 (0·5)
H(13)	293 (2)	227 (2)	343 (4)	4·9 (0·7)
H(14)	314 (2)	155 (2)	506 (4)	6·0 (0·7)
H(15)	264 (2)	138 (2)	285 (4)	4·8 (0·6)
H(16)	292 (2)	−180 (2)	384 (4)	7·0 (0·9)
H(17)	196 (3)	−127 (2)	417 (5)	8·6 (1·0)
H(18)	619 (2)	471 (2)	−365 (5)	7·0 (0·9)
H(19)	549 (3)	543 (2)	−259 (5)	9·3 (1·0)

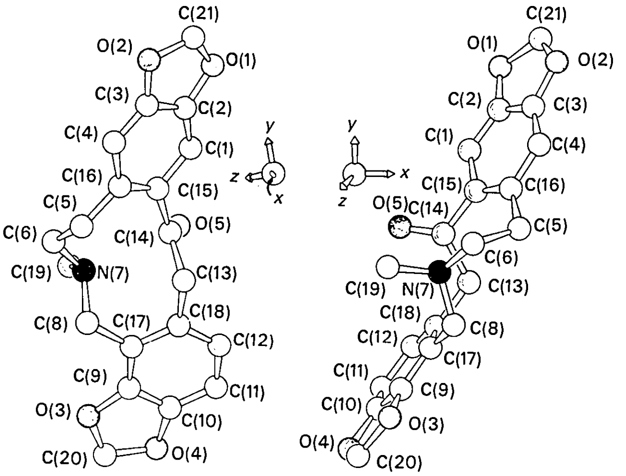

Fig.3. Two perspective views of the molecule at 90° from each other.

The distance N(7)$\cdots$C(14) across the ten-membered ring is only 2·555 Å, and it makes angles of 106·0°, 108·6°, and 105·1° with the three bonds N(7)–C(6), N(7)–C(8), and N(7)–C(19), respectively. It also makes angles of 84·7, 97·7, and 101·6° with the three bonds C(14)–C(13), C(14)–C(15), and C(14)–O(5), respectively.

Discussion

Bond lengths and angles

The various types of bond in this structure have mean values which are about the same as the corresponding average values given by Sutton (1965), which are quoted here in parentheses. The aromatic C–C bonds in the two benzene rings vary in length from 1·363 to 1·418 Å; the mean is 1·388 Å (1·394 ± 0·005 Å). The C–C single bonds in the ten-membered ring are in the range 1·504 to 1·525 Å, mean is 1·512 Å (1·506 ± 0·005 Å for a C–C single bond shortened in the presence of a carbon–oxygen double bond, and 1·53 ± 0·01 Å in the presence of an aromatic bond). The three C–N bonds are between 1·458 and 1·466 Å; the mean is 1·462 Å (1·472 ± 0·005 Å for a trivalent nitrogen atom). The carbon–oxygen double bond is 1·218 Å, which indicates clearly that it has ketonic character for which the average distance is 1·215 ± 0·005 Å, as compared with the average distance of 1·145 ± 0·01 Å for a carbonyl group (Sutton, 1965). The C–O single bonds are of two types; the first type involves the C-atom of an aromatic ring and varies in length between 1·375 and 1·385 Å, mean is 1·381 Å (1·371 ± 0·016 Å in conjugated heterocyclic compounds), and the second type involves the C-atom of a CH_2 group and ranges from 1·419 to 1·431 Å, mean is 1·425 Å (1·426 ± 0·005 Å in saturated heterocyclic compounds). Finally, the C–H bonds are between 1·00 and 1·06 Å, mean is 1·02 Å (1·06 to 1·09 Å).

The mean angle at each of the twelve carbon atoms in the benzene rings is between 119·98 and 120·00°, thus showing that the three bonds at each of these atoms are nearly planar. At C(14), the mean angle is only 119·3°, and that atom is about 0·11 Å away from the plane through atoms C(13), C(15), and O(5). The four bonds at each of the other carbon atoms are very nearly tetrahedrally arranged; mean angle at each atom is between 109·3 and 109·4°. The three bonds at N(7) and the short distance N(7)$\cdots$C(14) across the ten-membered ring are arranged nearly tetrahedrally around the nitrogen atom; these angles range from 105·1 to 113·2° and their mean is 109·4°. Therefore, it seems that in derivatives of protopine in which the nitrogen atom is tetravalent, the direction of the fourth bond for least steric change would be across the ring in the direction of N(7)$\cdots$C(14), thus transforming it into two six-membered rings. The other alternative, in which a fourth atom other than C(14) is attached to N(7), would certainly require a conformational change in the ten-membered ring and a considerable increase in the N(7)$\cdots$C(14) distance. It is of interest to men-

Table 3. *Observed structure amplitudes and calculated structure factors* (× 10)

(* indicates unobserved reflexion and $|F_{th}|$ in place of $|F_o|$).

K	FO	FC
H=	0, L=	0
2	441	451
4	46	37
6	19*	0
8	371	-359
10	262	-254
12	347	-352
14	82	93
16	65	67
18	83	76
20	96	-100
22	73	-73
H=	0, L=	1
1	97	91
2	384	-382
3	593	608
4	70	-72
5	23	-14
6	513	-515
7	53	-59
8	89	-87
9	49	-47
10	241	234
11	50	44
12	30*	-14
13	253	-257
14	158	-163
15	282	283
16	168	173
17	34*	-25
18	32*	21
19	30*	-8
20	37	-27
21	39	32
22	25	22
H=	0, L=	2
0	308	-306
1	885	900
2	424	-425
3	177	-173
4	21	13
5	360	-352
6	417	-398
7	49	-35
8	181	-180
9	83	-88
10	120	118
11	327	310
12	103	-109
13	139	133
14	34*	-32
15	42	-42
16	48	54
17	45	49
18	31*	31
19	29*	-12
20	113	112
21	20*	-19
H=	0, L=	3
1	21*	9
2	629	627
3	769	-756
4	321	-317
5	65	-51
6	25*	18
7	209	-205
8	188	-185
9	184	-180
10	96	-86
11	97	100
12	157	-158
13	68	67
14	78	-81
15	67	65
16	115	115
17	63	55
18	103	103
19	51	57
20	73	71
21	47	-47
H=	0, L=	4
0	546	-541
1	48	41
2	68	-51
3	64	52
4	193	193
5	377	372
6	29*	12
7	35	37
8	125	134
9	83	-82
10	42	47
11	207	216
12	68	63
13	90	-91
14	124	-125
15	83	-76
16	57	-46
17	46	35
18	38	-27
19	74	-67
20	49	46
H=	0, L=	5
1	162	162
2	143	141
3	309	315
4	25	25
5	134	139
6	210	219
7	46	-46
8	45	40
9	78	-82
10	227	-235
11	146	-147
12	64	64
13	76	-81
14	98	-97
15	51	-49
16	26*	-17
17	73	-68
18	43	-41
H=	0, L=	6
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1	278	286
2	138	149
3	118	114
4	74	-77
5	119	128
6	56	57
7	38	-27
8	40	37
9	34*	-11
10	85	-80
11	40	-37
12	79	85
13	35	-36
14	66	-51
15	30	-28
16	48	44
H=	0, L=	7
1	34*	3
2	127	-124
3	33*	29
4	33*	-34
5	33*	14
6	54	42
7	70	75
8	30	30
9	29*	4
10	53	48
11	54	-56
12	37	37
13	60	57
14	89	-92
H=	0, L=	8
0	121	-126
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2	28*	-20
3	27*	11
4	64	64
5	26*	8
6	30	-28
7	23*	-2
8	21*	-4
9	19*	-16
10	44	-39
H=	0, L=	9
1	34	-37
2	36	36
H=	1, L=	0
1	170	-175
2	38	38
3	178	186
4	687	709
5	204	-213
6	363	-370
7	252	253
8	207	-208
9	165	158
10	79	-68
11	70	-74
12	338	-345
13	32*	-1
14	176	-182
15	99	-95
16	34*	10
17	126	131
18	179	177
19	37	-32
20	77	-68
21	85	88
22	38	-31
H=	1, L=	1
0	1438	-1662
1	142	149
2	429	-434
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6	102	-100
7	153	-153
8	341	-335
9	195	192
10	196	199
11	413	-423
12	243	238
13	59	61
14	238	239
15	318	334
16	69	60
17	190	-201
18	69	53
19	30*	2
20	78	84
21	97	-94
22	22	17
H=	-1, L=	1
0	366	-366
1	238	239
2	553	558
3	984	-1030
4	488	-486
5	44	-47
6	20*	20
7	99	-95
8	181	-163
9	168	-170
10	353	-346
11	29*	-7
12	165	169
13	75	-71
14	182	180
15	189	189
16	34*	-39
17	51	-56
18	101	-102
19	46	-39
20	139	-139
21	22*	9
22	63	-67
H=	1, L=	2
1	414	406
2	683	-692
3	50	-49
4	479	489
5	174	179
6	370	-370
7	245	-239
8	213	199
9	44	-53
10	90	-94
11	30*	1
12	115	109
13	199	201
14	89	81
15	176	-181
16	70	-74
17	33*	11
18	113	111
19	72	71
20	47	-50
21	20*	-10
H=	-1, L=	2
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2	133	-134
3	34	41
4	167	162
5	145	-155
6	59	-56
7	326	324
8	145	139
9	253	244
10	245	230
11	144	-149
12	279	269
13	299	311
14	228	-229
15	345	-358
16	157	-160
17	197	-196
18	31*	-22
19	190	-190
20	160	-154
21	24	-31
H=	1, L=	3
0	470	-469
1	378	-376
2	184	-175
3	246	-239
4	206	201
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6	561	550
7	27*	-20
8	196	192
9	30*	2
10	205	207
11	88	93
12	211	-207
13	55	54
14	132	-136
15	144	149
16	40	-51
17	73	68
18	53	-53
19	56	53
20	80	60
H=	-1, L=	3
0	504	-506
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2	248	240
3	182	-180
4	157	-138
5	223	-217
6	112	104
7	197	186
8	177	174
9	110	103
10	54	52
11	95	-92
12	39	-33
13	141	-141
14	111	-110
15	40	34
16	33*	27
17	108	-107
18	29*	-20
19	48	-43
20	122	-120
21	17	-23
H=	1, L=	4
1	186	175
2	192	-176
3	123	110
4	55	66
5	174	165
6	202	200
7	61	-73
8	73	72
9	144	146
10	31	-26
11	34*	2
12	34*	-23
13	252	-264
14	347	353
15	32*	26
16	31*	-26
17	33	-30
18	44	-39
19	43	-35
H=	-1, L=	4
1	182	-161
2	144	143
3	96	90
4	590	583
5	152	-139
6	36	-39
7	114	112
8	57	61
9	32	25
10	136	-138
11	213	216
12	246	-258
13	288	298
14	40	38
15	72	70
16	31*	9
17	51	50
18	49	52
19	21*	0
20	16	16
H=	1, L=	5
0	330	326
1	159	-150
2	179	-189
3	33	-33
4	205	-205
5	103	-103
6	33*	4
7	50	-46
8	36	-33
9	117	-122
10	113	-130
11	75	-73
12	50	-37
13	53	-44
14	76	77
15	29*	24
16	32	-40
17	19	22
18	18	17
H=	-1, L=	5
0	119	-116
1	173	-167
2	193	193
3	51	-53
4	96	87
5	34	29
6	33*	-24
7	44	44
8	34*	19
9	34*	23
10	49	-47
11	119	-129
12	169	167
13	33	-28
14	78	73
15	29*	8
16	91	-81
17	25	-21
18	69	62
H=	1, L=	6
1	156	-156
2	34*	-8
3	254	-265
4	278	-286
5	44	-42
6	164	-175
7	38	-34
8	138	-139
9	119	126
10	147	147
11	31*	20
12	62	59
13	75	-75
14	28	-23
15	85	84
16	18*	-4
H=	-1, L=	6
1	45	40
2	89	-92
3	34*	-29
4	34*	34
5	34*	-25
6	34*	23
7	168	-172
8	70	-72
9	34*	16
10	33*	-9
11	36	-26
12	30*	4
13	73	-63
14	113	118
15	42	46
16	19*	-10
H=	1, L=	7
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1	146	-141
2	33*	21
3	33*	18
4	55	-46
5	101	-96
6	32*	-5
7	31*	-8
8	30*	-24
9	28*	-15
10	90	82
11	26	-34
12	22*	-9
13	18	20
H=	-1, L=	7
0	55	47
1	218	-214
2	34*	-17
3	202	208
4	158	-156
5	57	56
6	32*	-5
7	42	47
8	46	48
9	66	67
10	37	26
11	80	-90
12	47	-48
13	82	77
14	26	-22
H=	1, L=	8
1	63	47
2	95	104
3	25	22
4	61	66
5	35	39
6	40	42
7	32	35
8	46	-39
9	27	22
10	119	123
H=	-1, L=	8
1	28*	-15
2	28*	5
3	34	-26
4	110	-105
5	26	-23
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7	24*	7
8	32	-28
9	20*	-4
10	76	80
H=	-1, L=	9
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1	50	-55
2	75	-73
3	38	44
H=	2, L=	0
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1	552	572
2	567	-582
3	229	-233
4	289	297
5	448	-471
6	350	-346
7	232	224
8	142	128
9	214	-217
10	161	162
11	80	78
12	59	58
13	36	30
14	97	-90
15	108	-110
16	122	-119
17	84	85
18	107	115
19	30*	-14
20	27*	-26
21	27	27
22	17*	-11
H=	2, L=	1
1	148	-151
2	372	-376
3	119	-121
4	19	-18
5	408	-417
6	200	195
7	283	276
8	49	42
9	688	-694
10	109	90
11	92	92
12	121	120
13	32*	11
14	111	-114
15	114	-108
16	110	-116
17	34*	-24
18	172	-174
19	60	-48
20	26*	20
21	87	-87
22	76	77
H=	-2, L=	1
1	612	-618
2	1435	-1745
3	642	638
4	483	-475
5	268	-257
6	504	-497
7	410	394
8	50	-26
9	271	255
10	334	-328
11	84	73
12	31*	-14
13	206	-211
14	242	245
15	105	106
16	140	-137
17	137	140
18	41	-37
19	61	57
20	35	-25
21	57	57
22	15*	-14
H=	2, L=	2
0	1018	-1031
1	222	226
2	295	286
3	111	-108
4	307	295
5	307	301
6	205	-194
7	217	-210
8	468	468
9	39	-39
10	40	-47
11	148	144
12	218	-218
13	127	-136
14	286	-298
15	214	-219
16	166	-168
17	37	-34
18	105	-102
19	28*	-9
20	24*	-2
21	28	24
H=	-2, L=	2
0	782	785
1	48	53
2	687	-689
3	591	594
4	324	-313
5	220	-220
6	253	250
7	159	-157
8	167	156
9	37	-41
10	74	63
11	83	-77
12	75	68
13	125	123
14	96	95
15	73	-71
16	65	73
17	47	-48
18	60	60
19	52	42
20	45	37
21	37	35
H=	2, L=	3
1	98	-92
2	177	177
3	184	-170
4	184	-181
5	25*	17
6	26*	8
7	128	120
8	285	283
9	125	121
10	102	-109
11	33*	-10
12	94	96
13	250	253
14	34*	23
15	38	38
16	176	-177
17	31*	34
18	56	-52
19	25*	-2
20	20*	10
H=	-2, L=	3
1	412	395
2	234	-232
3	196	-188
4	133	142
5	107	94
6	75	-81
7	202	192
8	154	153
9	130	131
10	285	281
11	32*	-6
12	116	-117
13	373	-382
14	68	66
15	34*	21
16	71	-70
17	103	-101
18	76	64
19	26*	14
20	21*	-9
21	14*	16
H=	2, L=	4
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1	35	-35
2	235	227
3	205	204
4	267	-259
5	297	294
6	119	131
7	81	71
8	109	111
9	151	160
10	73	-71
11	92	-82
12	198	195
13	124	-132
14	33*	19
15	140	-132
16	113	116
17	68	-64
18	47	47
19	30	-31
H=	-2, L=	4
0	478	464
1	120	-118
2	32	-25
3	42	-37
4	172	169
5	28*	19
6	80	-78
7	52	-47
8	37	-37
9	185	180
10	135	-136
11	247	249
12	192	-191
13	141	138
14	34*	-28
15	33*	-17
16	131	129
17	28*	1
18	25*	16
19	47	39
20	40	38
H=	2, L=	5
1	211	-223
2	73	-72
3	167	158
4	113	120
5	70	62
6	201	-202
7	38*	-20
8	34	-27
9	34*	9
10	40	31
11	105	-103
12	33	34
13	72	74
14	124	-124
15	86	85
16	43	47
17	50	-49
18	84	64
H=	-2, L=	5
1	196	194
2	377	385
3	87	-82
4	32*	3
5	207	208
6	153	-153
7	252	-255
8	110	110
9	47	-40
10	34*	-17
11	48	-55
12	34*	8
13	78	-80
14	58	-58
15	56	53
16	76	77
17	91	-87
18	47	47
H=	2, L=	6
0	40	37
1	245	253
2	136	144
3	32	30
4	34*	16
5	36	-28
6	148	-156
7	34*	22
8	153	-156
9	112	115
10	48	-33
11	59	-59
12	79	75
13	105	106
14	24*	8
15	60	60
16	16*	-6
H=	-2, L=	6
0	34*	-14
1	34*	19
2	34*	-10
3	212	-224
4	44	-40
5	245	-252
6	77	-72
7	260	-269
8	249	-255
9	64	-60
10	44	-33
11	42	37
12	79	75
13	28*	20
14	33	-28
15	26	-24
16	78	84
H=	2, L=	7
1	44	40
2	141	-144
3	51	-43
4	43	43
5	32	27
6	41	42
7	46	-54
8	62	60
9	32	-45
10	26*	-17
11	24*	4
12	28	23
13	36	38
H=	-2, L=	7
1	32	29
2	112	-119
3	72	-65
4	148	-157
5	33*	4
6	32*	-2
7	94	-88
8	107	-105
9	29*	-16
10	28*	3
11	26*	20
12	53	60
13	33	38
14	52	-52
H=	2, L=	8
0	143	-142
1	83	-82
2	69	-61
3	31	-33
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5	33	22
6	23	19
7	48	-42
8	28	30
9	26	29
H=	-2, L=	8
0	57	-60
1	96	98
2	28*	-23
3	28*	-11
4	158	160
5	33	29
6	25*	3
7	25	24
8	22*	1
9	29	-31
10	32	37
H=	-2, L=	9
1	75	73
2	40	40
3	29	25
H=	3, L=	0
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2	1342	-1528
3	240	251
4	824	-862
5	469	472
6	145	139
7	359	-357
8	432	-421
9	219	-220
10	183	-187
11	29*	-11
12	80	75
13	44	35
14	76	76
15	34*	16
16	76	-75
17	112	117
18	70	71
19	29*	-9
20	61	-61
21	21*	1
22	54	43
H=	3, L=	1
0	520	524
1	68	-72
2	478	-489
3	237	-230
4	19*	-2
5	340	342
6	29	35
7	153	141
8	200	-197
9	137	-144
10	87	81
11	113	129
12	256	-257
13	33*	8
14	119	122
15	332	337
16	99	101
17	89	-89
18	69	-55
19	71	-65
20	23	20
21	32	33
H=	-3, L=	1
0	15*	-7
1	50	49
2	1058	1166
3	169	-164
4	822	846
5	705	718
6	257	258
7	246	235
8	508	-495
9	156	-145
10	101	116
11	40	35
12	31*	-14
13	111	-100
14	34*	12
15	34*	14
16	198	-198
17	128	128
18	124	-115
19	36	-30
20	155	150
21	42	-32
H=	3, L=	2
1	187	-173
2	397	-389
3	218	-216
4	600	-604
5	477	-460
6	416	-406
7	273	-263
8	242	247
9	28*	26
10	30*	5
11	72	70
12	204	210
13	107	106
14	214	222
15	120	116
16	61	60
17	32*	-9
18	30*	-5
19	27*	-3
20	39	-40
21	27	26
H=	-3, L=	2
1	431	-436
2	97	103
3	317	-324
4	493	-487
5	408	411
6	42	29
7	349	-345
8	43	-42
9	37	32
10	57	-56
11	60	-58
12	298	310
13	143	143
14	42	-46
15	30	-27
16	132	-132
17	55	47
18	31*	-4
19	28*	7
20	24*	-6
21	93	94
H=	3, L=	3
0	160	150
1	146	151
2	311	-308
3	61	-64
4	551	-548
5	188	189
6	172	170
7	170	169
8	55	61
9	82	-80
10	39	-35
11	255	258
12	93	95
13	99	-99
14	66	67
15	34*	-15
16	118	111
17	30*	31
18	42	38
19	24*	-3
20	38	-42
H=	-3, L=	3
0	328	-320
1	363	365
2	289	-289
3	22*	-13
4	122	-117
5	304	295
6	35	-25
7	156	151
8	117	-120
9	290	-295
10	67	73
11	146	-138
12	192	-190
13	303	-310
14	129	-135
15	82	78
16	33*	22
17	31*	13
18	52	46
19	25*	6
20	20*	20
H=	3, L=	4
1	123	117
2	276	272
3	147	144
4	67	65
5	40	40
6	123	118
7	50	52
8	122	-115
9	160	162
10	40	49
11	65	-72
12	247	-259
13	307	-310
14	33*	-27
15	61	-61
16	29*	21
17	26*	-29
18	23*	24
19	71	-68
H=	-3, L=	4
1	307	-297
2	197	-199
3	115	-107
4	28*	10
5	53	-43
6	100	98
7	136	132
8	96	-88
9	49	-41
10	322	-324
11	160	-165
12	60	63
13	132	130
14	34*	0
15	28	-28
16	87	78
17	81	-82
18	22	-18
19	71	67
H=	3, L=	5
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1	47	-38
2	231	242
3	196	193
4	196	201
5	131	-126
6	150	-155
7	53	52
8	183	-186
9	84	-95
10	153	-157
11	95	-105
12	48	39
13	31*	-20
14	29*	-11
15	34	-31
16	24	-26
17	20*	15
H=	-3, L=	5
0	31*	25
1	244	247
2	252	244
3	125	-125
4	70	-69
5	99	109
6	61	61
7	212	204
8	66	61
9	57	59
10	61	-65
11	156	161
12	34*	37
13	33*	-22
14	31*	-8
15	63	-59
16	26*	13
17	54	-48
18	35	26
H=	3, L=	6
1	241	252
2	134	135
3	34*	-12
4	34*	13
5	34*	-6
6	108	112
7	45	43
8	83	-79
9	87	-84
10	27	26
11	30*	2
12	28*	-14
13	42	-50
14	47	-48
15	21	-15
H=	-3, L=	6
1	59	-58
2	97	99
3	104	105
4	75	59
5	99	95
6	113	113
7	100	97
8	43	-41
9	112	115
10	100	96
11	47	-43
12	77	-79
13	28*	-9
14	56	-49
15	65	-68
16	58	54
H=	3, L=	7
0	76	-78
1	117	-121
2	32*	23
3	32*	23
4	33	24
5	38	-35
6	30*	-1
7	51	-53
8	28*	12
9	41	-41
10	24*	19
11	22*	8
12	44	-40
13	43	42
H=	-3, L=	7
0	82	-90
1	110	-107
2	73	72
3	37	32
4	81	-78
5	97	-92
6	32*	-13
7	122	123
8	122	124
9	60	63
10	27*	22
11	64	-64
12	63	67
13	66	67
14	43	40
H=	3, L=	8
1	25*	8
2	67	73
3	24*	-15
4	27	-26
5	28	-31
6	23	22
7	70	-69
8	42	-45
H=	-3, L=	8
1	36	-32
2	42	-37
3	32	34
4	39	-39
5	45	-39
6	99	97
7	44	46
8	35	-37
9	27	-31
10	38	35
H=	-3, L=	9
0	63	-69
1	59	-67
2	22	-17
3	65	70
H=	4, L=	0
0	242	238
1	17*	5
2	373	-366
3	668	678
4	505	-515
5	407	410
6	591	-605
7	150	139
8	189	184
9	122	-121
10	104	98
11	379	-381
12	101	-96
13	87	-82
14	250	261
15	158	-164
16	203	208
17	77	87
18	71	69
19	28*	-17
20	86	-82
21	31	-30
H=	4, L=	1
1	239	236
2	176	178
3	205	-200
4	96	-93
5	253	-249
6	326	-324
7	131	128
8	234	229
9	319	-318
10	222	220
11	62	59
12	137	136
13	150	148
14	106	107
15	124	113
16	98	-96
17	38	-40
18	51	-54
19	28*	19
20	25	-26
21	17	-14
H=	-4, L=	1
1	206	208
2	172	-170
3	441	449
4	379	-366
5	449	-449
6	69	64
7	103	92
8	124	109
9	218	-210
10	100	102
11	34	-38
12	32*	-23
13	65	56
14	42	49
15	61	-58
16	129	134
17	33*	28
18	58	49
19	28*	-25
20	85	-84
21	61	-57
H=	4, L=	2
0	22*	-4
1	22*	22
2	41	48
3	297	-297
4	293	290
5	57	-60
6	81	72
7	418	-411
8	28*	-10
9	82	85
10	64	67
11	53	51
12	73	67
13	40	-39
14	44	46
15	96	97
16	33*	-5
17	122	122
18	29*	12
19	87	89
20	21*	-6
21	15	-16
H=	-4, L=	2
0	243	-252
1	155	144
2	500	-494
3	177	173
4	153	149
5	501	-492
6	24*	-4
7	26*	-4
8	147	149
9	103	-95
10	45	43
11	76	64
12	203	196
13	49	52
14	34*	-16
15	127	143
16	208	-211
17	32*	12
18	60	-58
19	93	-87
20	115	-114
21	22	-23
H=	4, L=	3
1	156	-162
2	342	328
3	72	70
4	281	281
5	425	423
6	238	-240
7	86	80
8	36	41
9	476	481
10	45	-30
11	62	-66
12	136	137
13	34*	0
14	47	-48
15	78	-80
16	110	116
17	147	-144
18	102	102
19	60	-58
20	16*	3
H=	-4, L=	3
1	40	37
2	319	-315
3	105	-92
4	226	227
5	435	-429
6	99	88
7	229	227
8	37	29
9	70	66
10	260	256
11	228	235
12	40	-31
13	164	-166
14	34*	20
15	41	-45
16	149	-146
17	30*	2
18	28*	-9
19	68	-70
20	77	-77
H=	4, L=	4
0	193	-199
1	125	131
2	125	116
3	209	-214
4	36	-20
5	137	-144
6	143	136
7	36	42
8	141	-145
9	40	40
10	34*	26
11	138	-135
12	150	145
13	33*	16
14	122	-123
15	75	82
16	92	-91
17	38	-40
18	96	-88
19	14*	1
H=	-4, L=	4
0	262	-262
1	95	-94
2	28*	-5
3	109	110
4	122	122
5	173	167
6	37	-41
7	103	-103
8	254	267
9	194	-202
10	106	-105
11	258	-264
12	104	97
13	68	-72
14	33*	-2
15	77	75
16	30	37
17	27	29
18	24	23
19	82	73
H=	4, L=	5
1	410	-425
2	180	-177
3	153	-160
4	188	199
5	79	82
6	147	151
7	71	-69
8	129	-127
9	34*	-22
10	51	-54
11	33*	16
12	32*	-4
13	87	92
14	49	-48
15	25*	-13
16	33	27
17	18	-18
H=	-4, L=	5
1	43	38
2	119	107
3	90	-76
4	32*	-1
5	33*	16
6	144	-149
7	34*	20
8	47	-44
9	222	225
10	125	-127
11	111	105
12	33*	-7
13	44	35
14	148	148
15	54	57
16	25*	3
17	22*	9
18	68	72
H=	4, L=	6
0	194	-194
1	75	74
2	96	-91
3	62	-61
4	97	-93
5	49	58
6	54	-55
7	51	-51
8	138	147
9	31*	-29
10	41	43
11	38	-36
12	42	-41
13	24*	15
14	36	24
15	21	22
H=	-4, L=	6
0	252	257
1	172	-167
2	69	61
3	95	97
4	153	-159
5	34*	5
6	58	65
7	158	-164
8	34*	-30
9	81	79
10	100	-98
11	31*	23
12	56	54
13	27*	8
14	46	-34
15	86	-74
16	103	105
H=	4, L=	7
1	57	50
2	49	-49
3	31*	5
4	102	-100
5	30*	-2
6	29*	-3
7	28*	2
8	96	95
9	25*	-22
10	72	-78
11	48	-48
12	16*	0
H=	-4, L=	7
1	143	-149
2	42	47
3	52	-59
4	69	66
5	32*	-9
6	62	-63
7	31*	-4
8	30*	15
9	64	69
10	92	91
11	33	-26
12	22*	5
13	79	-76
H=	4, L=	8
0	68	63
1	110	-111
2	35	34
3	22*	-12
4	21*	4
5	79	76
6	123	123
7	36	-35
H=	-4, L=	8
0	28*	-25
1	67	71
2	87	-95
3	27*	10
4	73	79
5	35	-23
6	24*	-15
7	23*	11
8	66	-68
9	59	59
10	15*	4
H=	-4, L=	9
1	40	44
2	14*	-11
H=	5, L=	0
1	302	-298
2	214	219
3	136	-123
4	103	-98
5	414	-412
6	244	239
7	101	106
8	239	235
9	70	74
10	47	42
11	180	-186
12	102	-107
13	34*	-25
14	117	-121
15	54	-43
16	78	-76
17	102	89
18	103	94
19	50	-49
20	98	-98
21	32	24
H=	5, L=	1
0	674	669
1	90	-82
2	106	102
3	65	53
4	118	122
5	133	126
6	38	-38
7	28	-16
8	405	-407
9	245	-245
10	269	-274
11	36	24
12	225	-232
13	129	-131
14	239	-249
15	34*	19
16	59	-45
17	32*	7
18	65	67
19	26*	-9
20	22*	-16
21	16*	14
H=	-5, L=	1
0	400	413
1	352	-359
2	275	265
3	585	-590
4	403	-404
5	476	-467
6	307	290
7	163	-160
8	116	105
9	111	116
10	30*	-15
11	240	240
12	33*	31
13	162	160
14	87	90
15	195	-211
16	45	40
17	32*	4
18	72	-62
19	27*	-20
20	69	70
21	78	-73
H=	5, L=	2
1	190	-190
2	24*	-8
3	317	313
4	116	122
5	164	-157
6	288	-293
7	96	94
8	185	176
9	31*	-8
10	127	-122
11	59	57
12	215	-222
13	178	-182
14	34*	14
15	34*	-7
16	32*	-5
17	30*	-15
18	32	28
19	24*	13
20	34	-28
H=	-5, L=	2
1	259	-254
2	149	164
3	155	155
4	115	-126
5	476	474
6	697	-687
7	68	-64
8	28*	0
9	30*	-15
10	42	38
11	82	80
12	141	-141
13	82	81
14	134	-136
15	47	54
16	86	-75
17	69	80
18	55	52
19	79	-71
20	34	40
21	123	122
H=	5, L=	3
0	46	37
1	61	60
2	59	67
3	28*	-2
4	82	77
5	92	-97
6	88	82
7	131	128
8	111	112
9	104	108
10	34*	9
11	231	241
12	34	40
13	61	56
14	34*	-19
15	171	-168
16	30*	3
17	135	-138
18	107	103
19	26	-20
H=	-5, L=	3
0	158	-168
1	255	239
2	48	-45
3	112	113
4	29	26
5	221	223
6	81	66
7	29*	-14
8	82	78
9	180	184
10	177	179
11	31	27
12	34*	-28
13	57	-60
14	69	-67
15	56	46
16	70	-57
17	65	-69
18	26*	-11
19	28	22
20	74	77
H=	5, L=	4
1	88	76
2	143	-149
3	207	-217
4	56	52
5	168	169
6	248	251
7	33*	1
8	71	-72
9	34*	14
10	85	-75
11	30	33
12	97	-97
13	67	-63
14	31	23
15	38	45
16	62	-62
17	104	107
18	35	33
H=	-5, L=	4
1	337	329
2	30	-29
3	59	38
4	193	188
5	208	207
6	91	80
7	338	-337
8	360	368
9	330	-337
10	121	-124
11	178	-180
12	145	137
13	147	145
14	72	-76
15	31*	9
16	29*	-15
17	40	-46
18	24	14
19	39	35
H=	5, L=	5
0	100	-99
1	159	-165
2	34	-28
3	251	259
4	53	57
5	34	-33
6	92	-88
7	34*	25
8	83	88
9	34*	12
10	39	38
11	38	44
12	69	-61
13	79	72
14	26*	19
15	35	-31
16	78	70
H=	-5, L=	5
0	164	-172
1	112	106
2	126	127
3	32*	-1
4	109	105
5	212	215
6	79	-78
7	43	45

Table 3 (*cont.*)

K	FO	FC
H= -5, L= 5		
8	336	-337
9	34*	11
10	76	70
11	79	84
12	33*	2
13	31*	-4
14	42	-35
15	29	25
16	77	73
17	43	44
18	14*	1
H= 5, L= 6		
1	231	236
2	127	128
3	34*	-14
4	209	-211
5	61	-61
6	33*	7
7	32*	-18
8	31*	9
9	81	-81
10	132	128
11	45	-52
12	41	39
13	27	-24
14	22	-18
H= -5, L= 6		
1	108	113
2	66	-71
3	34*	2
4	125	-129
5	34	34
6	55	62
7	115	-117
8	68	-66
9	35	-29
10	113	-116
11	111	-113
12	38	-33
13	41	-36
14	62	61
15	25	21
16	22	23
H= 5, L= 7		
0	30*	2
1	30*	11
2	75	-77
3	29*	10
4	29*	17
5	28*	1
6	43	39
7	26*	15
8	24*	6
9	22*	-6
10	29	-26
11	36	36
H= -5, L= 7		
0	199	207
1	33	-34
2	49	50
3	62	-66
4	88	-78
5	88	-92
6	61	-56
7	30*	-7
8	77	-78
9	140	-142
10	80	-77
11	89	-90
12	21*	-2
13	17*	-13
H= 5, L= 8		
1	66	-69
2	38	37
3	23	28
4	20	15
5	23	-20
6	14*	6
H= -5, L= 8		
1	37	-32
2	36	-35
3	41	44
4	48	-50
5	36	29
6	105	107
7	35	32
8	64	-67
9	35	34
H= 6, L= 0		
0	391	-389
1	395	397
2	145	140
3	23*	-6
4	351	348
5	268	-267
6	160	-143
7	107	-104
8	170	-162
9	73	77
10	119	117
11	57	53
12	39	-41
13	34*	42
14	42	44
15	45	-43
16	47	49
17	67	62
18	39	28
19	27	17
20	21*	-12
21	13*	-20
H= 6, L= 1		
1	23*	8
2	59	-62
3	28*	-22
4	124	-120
5	26*	0
6	117	115
7	88	-92
8	64	-69
9	123	-115
10	111	115
11	104	101
12	126	126
13	95	105
14	117	115
15	84	-92
16	51	54
17	30*	-20
18	28*	-19
19	24*	-3
20	59	50
H= -6, L= 1		
1	85	-77
2	113	103
3	42	49
4	323	334
5	61	68
6	756	755
7	522	518
8	379	375
9	308	312
10	108	-104
11	47	47
12	33	38
13	53	-46
14	238	250
15	96	-99
16	47	-59
17	79	-87
18	25	-21
19	32	28
20	80	-77
H= 6, L= 2		
0	751	-745
1	26*	-19
2	236	-235
3	515	-499
4	74	-74
5	77	-75
6	84	86
7	28	25
8	31*	-22
9	324	317
10	33*	-8
11	287	293
12	245	255
13	96	91
14	105	105
15	88	82
16	41	-45
17	105	-99
18	26*	1
19	23	-29
20	59	52
H= -6, L= 2		
0	735	742
1	58	-40
2	444	-439
3	76	67
4	185	186
5	96	-97
6	153	160
7	158	161
8	64	54
9	33	-31
10	32*	-15
11	124	121
12	106	-102
13	47	-38
14	75	73
15	52	-46
16	55	-56
17	43	-38
18	27*	9
19	27	-19
20	99	-92
H= 6, L= 3		
1	29*	-18
2	191	-183
3	145	156
4	262	256
5	31*	10
6	31*	-5
7	130	-135
8	33*	-1
9	61	61
10	129	-136
11	112	-113
12	157	161
13	34*	21
14	54	-48
15	74	-70
16	29*	-18
17	26*	10
18	35	-28
19	21	-21
H= -6, L= 3		
1	211	-207
2	136	-127
3	176	-172
4	296	286
5	364	-370
6	29*	7
7	170	175
8	128	-126
9	114	117
10	99	52
11	42	38
12	159	-156
13	195	-193
14	180	-182
15	33	35
16	55	-54
17	28*	-16
18	48	44
19	50	47
H= 6, L= 4		
0	58	-70
1	32*	-10
2	205	200
3	225	-235
4	270	-276
5	33*	4
6	113	110
7	34*	-12
8	45	40
9	75	-72
10	91	-100
11	241	-239
12	33*	-6
13	60	-60
14	88	-80
15	84	86
16	24*	16
17	48	-46
18	127	-131
H= -6, L= 4		
0	209	-210
1	186	193
2	85	-79
3	128	-124
4	31*	21
5	224	-220
6	53	-52
7	146	139
8	176	173
9	118	-122
10	169	-166
11	183	-181
12	185	-184
13	66	-73
14	82	-81
15	44	45
16	38	-36
17	44	-45
18	20*	9
H= 6, L= 5		
1	173	180
2	34*	-18
3	88	90
4	34*	-6
5	82	85
6	136	-148
7	99	-101
8	48	46
9	109	-116
10	41	33
11	91	-88
12	45	-47
13	36	29
14	27	27
15	21*	-10
16	26	-24
H= -6, L= 5		
1	136	132
2	122	127
3	112	-117
4	94	-99
5	34*	3
6	50	-41
7	153	-156
8	110	-108
9	80	-83
10	164	161
11	86	78
12	41	32
13	112	106
14	28*	0
15	26*	17
16	37	-32
17	51	46
H= 6, L= 6		
0	143	145
1	114	-117
2	87	86
3	40	34
4	33*	20
5	70	66
6	32	-27
7	102	-101
8	31	-23
9	28*	-22
10	27*	-8
11	55	-66
12	21	-18
13	20	13
H= -6, L= 6		
0	84	-83
1	198	-202
2	53	56
3	42	50
4	34*	-11
5	55	60
6	34*	-1
7	44	38
8	199	195
9	147	141
10	69	64
11	137	134
12	108	104
13	25*	-3
14	26	-25
15	19	-11
H= 6, L= 7		
1	28*	5
2	28*	-4
3	27*	-18
4	55	-53
5	62	-58
6	43	-40
7	28	-32
8	54	55
9	19*	16
10	37	-33
H= -6, L= 7		
1	66	-72
2	47	42
3	78	79
4	100	-94
5	51	-40
6	30*	-5
7	56	59
8	33	33
9	127	129
10	25*	25
11	22*	20
12	50	53
13	22	-21
H= 6, L= 8		
0	61	57
1	54	-54
2	35	-39
3	31	-28
H= -6, L= 8		
0	71	74
1	26*	8
2	44	-44
3	25*	24
4	45	-44
5	34	29
6	40	34
7	39	-45
8	18*	0
9	21	27
H= 7, L= 0		
1	163	153
2	86	85
3	117	-108
4	375	365
5	170	-158
6	321	318
7	256	-263
8	363	370
9	176	-177
10	32*	-21
11	91	-90
12	27*	-19
13	116	108
14	34*	12
15	47	61
16	128	-124
17	54	57
18	66	-56
19	27	24
20	99	-86
H= 7, L= 1		
0	492	479
1	284	-277
2	105	-122
3	327	-325
4	27*	12
5	63	-67
6	39	-36
7	90	87
8	93	83
9	214	-217
10	179	185
11	218	227
12	98	-99
13	101	88
14	42	43
15	33	-32
16	37	25
17	29*	12
18	26*	10
19	66	-57
20	16*	-4
H= -7, L= 1		
0	24*	0
1	112	-96
2	170	-158
3	113	-111
4	39	-38
5	31	-32
6	236	-238
7	29*	15
8	349	-349
9	56	-51
10	153	163
11	75	80
12	112	110
13	88	99
14	45	33
15	33*	3
16	28	27
17	108	113
18	28	24
19	23*	-17
20	36	36
H= 7, L= 2		
1	169	174
2	51	47
3	133	119
4	52	-48
5	77	79
6	31*	8
7	54	49
8	70	-64
9	77	-82
10	38	-37
11	217	215
12	36	-33
13	43	26
14	93	95
15	173	173
16	30*	13
17	54	-51
18	40	40
19	59	-53
H= -7, L= 2		
1	257	-256
2	70	59
3	212	215
4	32	33
5	175	173
6	35	-39
7	69	69
8	31*	7
9	78	79
10	33*	-7
11	36	-35
12	34*	31
13	196	-209
14	109	115
15	37	-42
16	31*	26
17	29*	-2
18	48	-45
19	76	-73
20	53	56
H= 7, L= 3		
0	258	253
1	198	190
2	31*	-3
3	31*	8
4	32*	-10
5	112	-110
6	57	-58
7	33*	-24
8	344	351
9	134	-134
10	115	109
11	56	52
12	84	-76
13	100	-96
14	31*	-14
15	29*	-16
16	84	-85
17	23*	-2
18	62	-68
H= -7, L= 3		
0	235	229
1	279	282
2	28*	13
3	114	-109
4	341	-342
5	148	143
6	90	100
7	185	-184
8	65	63
9	41	-40
10	113	-113
11	147	154
12	88	88
13	43	38
14	42	33
15	50	52
16	29*	-12
17	43	-33
18	25	19
19	57	49
H= 7, L= 4		
1	139	-145
2	148	146
3	322	-319
4	139	-142
5	34*	-22
6	136	140
7	100	103
8	34*	-14
9	71	63
10	66	67
11	49	-40
12	31*	1
13	28	28
14	113	-117
15	25*	13
16	21*	1
17	40	-42
H= -7, L= 4		
1	29	-31
2	95	-94
3	51	46
4	130	134
5	161	159
6	39	-32
7	43	-40
8	81	79
9	82	99
10	162	-174
11	80	-76
12	34*	8
13	51	45
14	107	-110
15	29*	-19
16	93	88
17	26	-20
18	28	31
H= 7, L= 5		
0	325	-329
1	75	84
2	49	-41
3	381	388
4	34*	14
5	131	129
6	93	-88
7	51	55
8	58	-53
9	30	-22
10	30	-29
11	29*	-3
12	113	103
13	65	-70
14	62	-61
15	51	-50
H= -7, L= 5		
0	249	-255
1	110	103
2	104	97
3	107	-101
4	91	86
5	196	-199
6	140	149
7	274	-279
8	34*	-38
9	76	-72
10	49	37
11	32*	21
12	31*	-22
13	62	60
14	59	-58
15	66	55
16	58	60
17	27	21
H= 7, L= 6		
1	89	-92
2	80	78
3	72	74
4	38	-36
5	124	-120
6	84	81
7	29*	5
8	81	-85
9	40	39
10	75	66
11	22*	9
12	56	-57
H= -7, L= 6		
1	85	86
2	34	28
3	58	-66
4	34*	-24
5	63	58
6	102	-98
7	46	38
8	57	64
9	63	-64
10	30*	-8
11	41	31
12	38	-32
13	96	96
14	45	39
15	15*	-17
H= 7, L= 7		
0	46	42
1	41	40
2	25	27
3	25*	-8
4	57	59
5	43	-47
6	49	44
7	20*	10
8	53	48
9	17	10
H= -7, L= 7		
0	150	-149
1	77	-69
2	53	-48
3	77	-74
4	58	61
5	71	64
6	25	-21
7	28*	16
8	53	-49
9	25*	10
10	24	25
11	20*	15
12	16*	-12
H= -7, L= 8		
1	75	-82
2	34	-35
3	40	-39
4	62	-61
5	21*	26
6	67	70
7	55	-51
8	43	45
H= 8, L= 0		
0	301	-296
1	27*	-18
2	279	265
3	109	114
4	68	-71
5	186	185
6	46	-47
7	109	-113
8	50	-49
9	33*	26
10	214	-221
11	108	-108
12	239	-242
13	32	27
14	34*	-21
15	32*	11
16	30*	11
17	28*	9
18	59	-64
19	72	69
H= 8, L= 1		
1	327	323
2	146	-139
3	79	80
4	80	-77
5	93	-93
6	191	-188
7	375	-379
8	87	-90
9	149	-149
10	305	-319
11	113	-129
12	120	-120
13	34*	20
14	133	138
15	32*	-13
16	29*	3
17	102	100
18	98	93
19	63	-54
H= -8, L= 1		
1	27*	8
2	76	72
3	28*	-18
4	509	-518
5	117	-113
6	194	-194
7	57	57
8	32*	20
9	315	-328
10	33*	-6
11	140	139
12	34	44
13	202	214
14	117	117
15	83	-76
16	30*	-21
17	35	32
18	24*	12
19	26	24
H= 8, L= 2		
0	137	145
1	127	-131
2	34	33
3	30*	11
4	31*	-14
5	58	50
6	288	293
7	87	-82
8	170	-172
9	139	150
10	164	-164
11	92	-93
12	34*	26
13	44	-43
14	32*	15
15	66	66
16	27*	11
17	45	-42
18	34	-28
H= -8, L= 2		
0	88	95
1	296	-286
2	129	139
3	116	-123
4	435	429
5	151	148
6	79	-82
7	32*	-11
8	89	-85
9	111	-112
10	99	115
11	32	26
12	120	122
13	215	-225
14	35	34
15	32*	-13
16	56	-60
17	27*	16
18	30	25
19	39	-30
H= 8, L= 3		
1	32*	1
2	108	-106
3	33*	-22
4	76	76
5	72	66
6	319	-324
7	34*	-21
8	128	130
9	215	221
10	34*	6
11	83	-70
12	97	94
13	115	-118
14	29*	1
15	36	33
16	24*	14
17	46	37
H= -8, L= 3		
1	88	-85
2	50	-51
3	191	191
4	31*	29
5	186	-181
6	38	-43
7	226	232
8	50	51
9	146	138
10	169	-176
11	34*	-21
12	34*	-9
13	92	-81
14	65	61
15	30*	21
16	95	-92
17	24*	4
18	20*	8
H= 8, L= 4		
0	150	-157
1	88	91
2	38	-32
3	38	-34
4	23*	-15
5	173	184
6	88	91
7	95	99
8	137	-132
9	33*	-1
10	108	112
11	57	-52
12	43	38
13	27*	15
14	25*	3
15	55	56
16	86	82
H= -8, L= 4		
0	181	187
1	52	49
2	32*	4
3	161	156
4	84	-88
5	165	158
6	41	-38
7	397	409
8	74	-75
9	34*	-25
10	101	-93
11	126	-127
12	50	50
13	31*	17
14	29*	9
15	37	38
16	40	36
17	20*	6
H= 8, L= 5		
1	61	64
2	34*	-7
3	81	-79
4	33*	-20
5	223	229
6	45	38
7	79	-78
8	55	61
9	57	58
10	28*	-18
11	26*	1
12	24*	4
13	53	-55
14	37	32
H= -8, L= 5		
1	63	63
2	34*	-4
3	102	-102
4	281	291
5	85	-85
6	195	193
7	100	-108
8	142	-151
9	71	-67
10	98	99
11	31*	-9
12	49	-43
13	27*	5
14	25*	-8
15	44	40
16	30	-34
H= 8, L= 6		
0	97	98
1	103	-101
2	30*	-3
3	33	-28
4	29*	17
5	28*	-27
6	32	25
7	26*	4
8	25*	-11
9	27	-33
10	21*	15
11	17*	17
H= -8, L= 6		
0	34*	23
1	32	-35
2	36	26
3	83	85
4	73	-76
5	119	-116
6	138	-135
7	77	79
8	177	174
9	58	60
10	34	-31
11	26*	1
12	98	-105
13	21*	4
14	17*	-16
H= 8, L= 7		
1	34	36
2	68	65
3	21*	-25
4	29	-30
5	44	-39
6	119	120
7	14*	7
H= -8, L= 7		
1	80	83
2	119	126
3	29*	13
4	29*	-10
5	64	48
6	32	30
7	26*	0
8	47	-46
9	37	-33
10	87	-86
11	40	-42
H= -8, L= 8		
0	42	47
1	30	-25
2	28	31
3	30	33
4	20*	-6
5	19*	15
6	23	25
7	61	-68
H= 9, L= 0		
1	185	190
2	354	350
3	63	63
4	106	-109
5	251	-261
6	102	-98
7	205	210
8	120	124
9	34*	30
10	50	-40
11	53	-46
12	34*	32
13	34*	24
14	32*	31
15	30*	6
16	40	32
17	23	23
18	21*	3
19	38	-40
H= 9, L= 1		
0	49	-59
1	75	73
2	111	-108
3	31*	-16
4	106	-111
5	121	117
6	32*	-10
7	251	255
8	239	240
9	34*	0
10	34*	11
11	179	187
12	46	48
13	79	-77
14	37	-36
15	30*	8
16	27	-20
17	48	44
18	109	99
H= -9, L= 1		
0	232	-235
1	29*	-22
2	388	-382
3	132	133
4	30*	12
5	227	-223
6	42	44
7	30	28
8	345	356
9	301	306
10	258	262
11	49	44
12	91	-88
13	191	204
14	44	39
15	44	-41
16	28*	0
17	34	-31
18	36	-43
19	15*	-13
H= 9, L= 2		
1	205	-197
2	93	88
3	132	129
4	33*	5
5	70	-71
6	34*	-6
7	224	225
8	36	-29
9	89	-81
10	292	300
11	34*	4
12	89	85
13	66	-64
14	30*	14
15	27*	-13
16	45	-45
17	21*	-19
18	45	37
H= -9, L= 2		
1	122	-119
2	86	92
3	122	-115
4	239	231
5	164	161
6	109	-108
7	203	210
8	312	326
9	34*	16
10	244	251
11	129	129
12	36	29
13	45	30
14	32*	3
15	47	-45
16	38	-25
17	29	-29
18	19*	-4
H= 9, L= 3		
0	146	-136
1	41	37
2	57	53
3	38	48
4	40	31
5	267	-275
6	259	-277
7	168	-170
8	76	72
9	46	36
10	47	-52
11	32	-31
12	92	90
13	34	-28
14	82	-83
15	24*	-7
16	43	-47
17	30	-28
H= -9, L= 3		
0	32*	-21
1	90	90
2	32*	10
3	35	37
4	75	-77
5	140	144
6	33*	-6
7	204	-212
8	34*	-8
9	34*	-22
10	34*	20
11	34*	-23
12	39	32
13	118	-118
14	30*	-8
15	49	-47
16	77	-68
17	20	-15
18	47	-52
H= 9, L= 4		
1	135	-137
2	187	-192
3	34*	26
4	40	-43
5	36	27
6	34*	-25
7	107	98
8	43	-45
9	46	-45
10	34	-29
11	45	-37
12	27*	-3
13	38	32
14	21*	-13
15	66	-66
H= -9, L= 4		
1	108	-110
2	133	-135
3	34*	8
4	123	-118
5	86	101
6	126	-125
7	237	-241
8	75	78
9	142	146
10	90	-93
11	69	-66
12	31*	9
13	94	-92
14	60	-55
15	24*	-11
16	68	-59
17	14	-16
H= 9, L= 5		
0	33*	2
1	129	-128
2	120	118
3	32*	23
4	32*	-5
5	91	-98
6	63	62
7	133	-139
8	29*	17
9	27*	12
10	84	-86
11	41	-34
12	80	70
13	89	84
H= -9, L= 5		
0	61	57
1	77	77
2	34*	10
3	34*	-19
4	34*	5
5	34*	-16
6	68	61
7	135	-135
8	221	-217
9	32*	-71
10	108	-103
11	31	-21
12	78	79
13	25*	-13
14	22*	11
15	18*	11
H= 9, L= 6		
1	28*	-8
2	27*	-12
3	52	55
4	50	52
5	25*	-5
6	41	-39
7	76	-76
8	21*	-7
9	34	31
10	77	76
H= -9, L= 6		
1	33*	22
2	53	-54
3	58	-58
4	52	52
5	75	-80
6	62	-57
7	30*	-14
8	29*	25
9	90	88
10	27	26
11	72	70
12	79	82
13	94	96
H= 9, L= 7		
0	46	44
1	52	-61
2	73	-70
3	39	-27
4	14*	-5
H= -9, L= 7		
0	59	-64
1	28*	18
2	28*	-4
3	126	-132
4	50	55
5	26*	29
6	28	34
7	24*	11
8	22*	-3
9	58	59
10	49	50
H= -9, L= 8		
1	19*	-10
2	38	33
3	27	-29
4	16*	-2
5	68	66
H= 10, L= 0		
0	174	168
1	35	45
2	32	-34
3	73	76
4	32*	-25
5	172	179
6	226	234
7	113	-115
8	186	-188
9	131	132
10	34*	2
11	120	117
12	88	-90
13	64	-73
14	30*	-7
15	31	-24
16	55	-43
17	34	-26
18	29	-16
H= 10, L= 1		
1	32*	-15
2	88	-86
3	62	62
4	100	-95
5	180	177
6	103	110
7	254	-267
8	112	123
9	314	317
10	124	-117
11	34*	4
12	33*	28
13	53	41
14	29	-31
15	48	51
16	24*	7
17	20*	11
H= -10, L= 1		
1	31*	18
2	82	-87
3	149	-148
4	40	29
5	37	31
6	33*	-6
7	173	-175
8	281	-294
9	185	-188
10	138	-139
11	32	31
12	42	-34
13	56	-53
14	30*	15
15	28*	20
16	69	56
17	22*	0
18	60	59
H= 10, L= 2		
0	215	207
1	115	112
2	145	155
3	174	-173
4	87	82
5	125	-127
6	142	138
7	34*	28
8	274	-276
9	116	-114
10	63	55
11	70	63
12	123	117
13	43	-36
14	37	35
15	42	-37
16	37	34
17	41	-49
H= -10, L= 2		
0	109	-111
1	103	98
2	166	-173
3	95	-95
4	46	44
5	85	86
6	34*	8
7	56	57
8	63	52
9	34*	19
10	108	95
11	207	215
12	174	-180
13	98	-105
14	43	40
15	35	34
16	24*	-13
17	20*	0
18	39	-40
H= 10, L= 3		
1	57	-54
2	88	-86
3	143	-155
4	34*	-28
5	34*	41
6	76	76
7	34*	23
8	33*	-6
9	83	82
10	68	-60
11	30*	21
12	28*	-24
13	26*	3
14	84	-81
15	53	-45
H= -10, L= 3		
1	61	60
2	245	244
3	26	22
4	109	-111
5	83	87
6	34*	27
7	61	59
8	133	144
9	134	-134
10	70	-69
11	96	-106
12	32*	15
13	30*	-23
14	28*	28
15	25*	-6
16	22*	3
17	51	51
H= 10, L= 4		
0	127	-131
1	130	123
2	34*	28
3	68	-72
4	95	-85
5	280	248
6	88	-82
7	204	196
8	46	49
9	103	-94
10	29	-23
11	73	72
12	86	-84
13	20*	-7
14	38	32
H= -10, L= 4		
0	57	68
1	66	-68
2	34*	4
3	32	-27
4	34*	14
5	57	59
6	30	23
7	97	92
8	70	-65
9	161	-164
10	38	34
11	34	31
12	29	38
13	62	-56
14	31	-20
15	74	73
16	17	18
H= 10, L= 5		
1	99	94
2	176	178
3	88	-84
4	30*	7
5	77	-72
6	147	145
7	78	-73
8	50	52
9	43	-39
10	36	-33
11	18*	-16
12	13*	-12
H= -10, L= 5		
1	40	41
2	99	-98
3	166	164
4	178	-184
5	62	54
6	42	-32
7	32*	14
8	108	-108
9	81	-81
10	77	79
11	34	-32
12	25*	3
13	49	-44
14	60	52
H= 10, L= 6		
0	57	-54
1	47	-37
2	53	52
3	80	69
4	37	-37
5	22*	-16
6	20*	5
7	38	31
8	40	41
H= -10, L= 6		
0	60	59
1	30	-29
2	91	78
3	58	-53
4	31*	7
5	149	-156
6	56	-66
7	61	57
8	74	78
9	38	-36
10	29	-20
11	21*	-13
12	28	-29
H= -10, L= 7		
1	26*	10
2	42	-40
3	76	-69
4	27	-22
5	23*	2
6	108	114
7	29	27
8	41	-40
9	28	23
H= -10, L= 8		
0	17	-12
1	36	-40
H= 11, L= 0		
1	31	-26
2	71	-65
3	145	145
4	141	150
5	343	-352
6	363	-368
7	34	36
8	88	-90
9	50	-56
10	59	-74
11	33*	23
12	31*	-16
13	35	-32
14	57	42
15	46	52
16	21*	-3
17	16*	7
H= 11, L= 1		
0	172	170
1	53	-49
2	78	78
3	101	-98
4	34*	-18
5	232	-233
6	186	-189
7	34*	-15
8	121	-125
9	53	45
10	105	-101
11	124	-118
12	64	60
13	71	62
14	63	59
15	54	47
16	30	30
H= -11, L= 1		
0	65	59
1	33	47
2	63	-62
3	120	-122
4	154	147
5	123	-134
6	117	-120
7	80	85
8	73	-67
9	59	-66
10	93	-91
11	69	-81
12	32*	4
13	53	57
14	46	-53
15	25*	-16
16	21*	-17
17	77	-76
H= 11, L= 2		
1	34*	24
2	133	-133
3	34*	-6
4	147	153
5	170	172
6	107	-109
7	34*	-3
8	199	-201
9	141	-141
10	67	65
11	30*	18
12	28	32
13	31	-25
14	72	69
15	20*	-1
16	63	-65
H= -11, L= 2		
1	123	127
2	70	-67
3	56	53
4	211	224
5	212	-215
6	33	28
7	232	230
8	133	-137
9	34*	7
10	77	-75
11	32*	26
12	36	-37
13	47	51
14	83	-84
15	37	-47
16	51	47
17	27	20
H= 11, L= 3		
0	67	77
1	129	-138
2	108	-108
3	100	109
4	34*	-7
5	49	-49
6	74	-80
7	32*	-33
8	99	95
9	129	119
10	74	65
11	27*	-19
12	25*	-4
13	89	85
14	39	37
H= -11, L= 3		
0	34*	-4
1	120	116
2	241	240
3	40	39
4	34*	6
5	34*	-3
6	34*	-2
7	30	-28
8	229	227
9	33*	-23
10	45	-40
11	31*	-33
12	59	-51
13	27*	-3
14	25*	-14
15	80	-75
16	25	23
H= 11, L= 4		
1	44	38
2	81	80
3	32*	0
4	31	22
5	103	99
6	30*	-18
7	32	-29
8	94	96
9	28	24
10	26	18
11	22*	14
12	19*	-8
H= -11, L= 4		
1	34*	-5
2	34*	25
3	55	-57
4	99	100
5	34*	-11
6	36	-31
7	33*	-15
8	93	89
9	31*	30
10	30*	-10
11	28*	16
12	34	-26
13	28	18
14	21*	2
15	24	-21
H= 11, L= 5		
0	28*	9
1	26*	9
2	67	-64
3	27*	-10
4	44	42
5	45	38
6	149	153
7	69	-70
8	21*	-17
9	30	-28
10	15*	-6
H= -11, L= 5		
0	213	-212
1	84	86
2	107	-99
3	180	183
4	81	-76
5	143	139
6	31	31
7	76	-73
8	64	64
9	82	83
10	73	-70
11	24*	-15
12	83	84
13	45	-40
H= 11, L= 6		
1	20	16
2	40	35
3	18*	11
4	17*	9
5	76	79
H= -11, L= 6		
1	79	-77
2	39	30
3	29*	-12
4	67	64
5	62	-67
6	109	-106
7	67	-64
8	80	81
9	57	60
10	19*	-6
11	15*	6
H= -11, L= 7		
0	60	-62
1	23*	9
2	22*	-16
3	44	-44
4	49	48
5	84	87
6	82	85
7	16*	1
H= 12, L= 0		
0	68	55
1	138	142
2	67	67
3	50	-51
4	134	-141
5	168	156
6	137	136
7	88	84
8	34	37
9	67	-59
10	32*	12
11	56	52
12	57	54
13	35	-40
14	22	23
15	20*	19
16	15*	-12
H= 12, L= 1		
1	34*	9
2	34*	9
3	98	94
4	214	218
5	42	36
6	281	284
7	34*	20
8	139	136
9	41	43
10	111	-107
11	161	-158
12	27*	16
13	91	79
14	32	-25
15	112	-106
H= -12, L= 1		
1	190	-199
2	150	-153
3	110	110
4	72	79
5	98	98
6	204	-211
7	76	-74
8	43	45
9	33	29
10	102	112
11	97	105
12	53	56
13	81	78
14	63	66
15	21*	-3
16	27	-26

Table 3 (*cont.*)

K	FO	FC
H= 12, L= 2		
0	237	-243
1	48	53
2	163	172
3	77	-84
4	108	-110
5	33*	-23
6	37	-37
7	50	55
8	40	33
9	121	-116
10	29*	-14
11	57	58
12	25*	-16
13	35	26
14	35	-41
H= -12, L= 2		
0	184	-182
1	50	-46
2	127	-123
3	96	-95
4	57	-52
5	54	-50
6	34*	18
7	34*	22
8	73	-65
9	189	193
10	135	146
11	75	91
12	94	92
13	89	82
14	68	66
15	74	72
H= 12, L= 3		
1	33*	-8
2	33*	-21
3	163	-164
4	105	-106
5	117	-116
6	119	-116
7	116	109
8	58	56
9	27*	2
10	25*	15
11	47	-38
12	89	-86
13	20	17
H= -12, L= 3		
1	34*	-29
2	34*	-9
3	61	-69
4	139	142
5	96	96
6	34*	15
7	33*	3
8	78	63
9	59	49
10	79	-75
11	28*	-10
12	32	-25
13	24*	5
14	78	75
15	16*	9
H= 12, L= 4		
0	188	-183
1	58	-62
2	29*	-7
3	29*	4
4	26	27
5	29	-27
6	26*	11
7	102	-107
8	153	151
9	64	-50
10	19*	-3
11	26	-24
H= -12, L= 4		
0	195	191
1	123	-126
2	33*	-25
3	60	-52
4	33*	18
5	32*	-21
6	32*	-13
7	56	-54
8	145	-139
9	130	-127
10	37	40
11	25*	-2
12	47	-47
13	19*	-10
14	19	17
H= 12, L= 5		
1	27	-26
2	39	-47
3	30	28
4	22*	-18
5	32	-38
6	19*	-10
7	20	24
H= -12, L= 5		
1	43	44
2	38	-33
3	31*	17
4	53	-53
5	31	27
6	29*	-23
7	70	-70
8	26*	-3
9	78	-85
10	22*	-3
11	20*	10
12	77	-76
H= -12, L= 6		
0	27	27
1	33	22
2	35	-32
3	32	29
4	25*	-27
5	45	-47
6	23*	-18
7	22*	1
8	29	28
9	67	-72
H= -12, L= 7		
1	46	45
2	25	-28
3	83	-93
4	72	-73
H= 13, L= 0		
1	85	85
2	34*	27
3	40	-44
4	261	260
5	33*	-19
6	33*	-21
7	85	76
8	75	-69
9	30*	-13
10	31	34
11	106	100
12	25*	-8
13	167	-165
14	83	-78
H= 13, L= 1		
0	127	129
1	76	74
2	34*	-11
3	108	-102
4	125	125
5	62	-66
6	32*	-6
7	47	47
8	30*	22
9	64	62
10	27*	19
11	36	-34
12	58	-54
13	70	-59
14	75	79
H= -13, L= 1		
0	177	182
1	34*	-11
2	204	-216
3	34*	-18
4	168	162
5	67	62
6	76	74
7	41	-35
8	35	-32
9	66	-67
10	48	-45
11	40	-35
12	137	-129
13	86	-90
14	55	-49
H= 13, L= 2		
1	36	30
2	75	77
3	72	-66
4	169	-167
5	114	116
6	73	-68
7	65	-59
8	69	-66
9	27*	-22
10	25*	13
11	23*	19
12	29	18
13	16*	-9
H= -13, L= 2		
1	47	-54
2	88	85
3	38	-44
4	71	-66
5	79	-82
6	33*	15
7	32*	15
8	58	-56
9	30*	-9
10	28*	-3
11	34	-31
12	24*	4
13	59	-64
14	71	-78
H= 13, L= 3		
0	30*	8
1	30*	-21
2	32	-35
3	77	71
4	29*	20
5	75	71
6	25	19
7	26*	-2
8	79	-72
9	23*	15
10	42	-38
11	89	84
H= -13, L= 3		
0	33*	15
1	65	75
2	33*	-7
3	60	-53
4	33*	27
5	33	25
6	77	-71
7	211	213
8	36	-35
9	28*	9
10	40	26
11	39	36
12	29	-35
13	19*	-5
H= 13, L= 4		
1	25*	-6
2	38	30
3	99	98
4	57	-59
5	27	-22
6	73	72
7	114	-109
8	63	57
9	17	-22
H= -13, L= 4		
1	59	58
2	32*	17
3	31*	-12
4	31*	16
5	30*	-11
6	67	69
7	49	36
8	48	-45
9	25*	-21
10	23*	5
11	21*	-10
12	17*	-2
H= 13, L= 5		
0	17*	6
1	73	68
2	17*	11
3	74	-66
4	14*	-11
H= -13, L= 5		
0	44	46
1	96	90
2	119	119
3	69	-74
4	27*	17
5	26*	-18
6	45	-44
7	24*	-10
8	44	48
9	20*	-8
10	100	-99
H= -13, L= 6		
1	122	130
2	22*	-5
3	65	65
4	21*	4
5	38	-33
6	45	-45
7	44	-48
H= 14, L= 0		
0	104	-102
1	84	-86
2	36	-31
3	93	-88
4	162	-155
5	69	-68
6	68	-68
7	56	-56
8	58	50
9	40	35
10	83	83
11	22*	-8
12	25	21
13	15*	-11
H= 14, L= 1		
1	35	34
2	149	-148
3	62	-55
4	31*	-4
5	32	-27
6	161	-157
7	28*	21
8	86	83
9	25*	-4
10	72	-74
11	95	-92
12	17*	2
H= -14, L= 1		
1	65	-67
2	33*	-24
3	32*	29
4	83	81
5	33	-22
6	44	43
7	28	-27
8	25	21
9	27*	-3
10	25	23
11	23*	-17
12	21	22
13	105	98
H= 14, L= 2		
0	96	-86
1	30*	18
2	88	89
3	31	27
4	30	-28
5	28*	15
6	63	-61
7	39	-38
8	42	-44
9	23	-19
10	92	87
11	46	50
H= -14, L= 2		
0	132	-128
1	159	157
2	126	129
3	98	88
4	62	-71
5	38	-30
6	81	85
7	91	-91
8	72	77
9	26*	7
10	49	-49
11	22	-23
12	21	-18
13	91	-93
H= 14, L= 3		
1	55	49
2	51	-58
3	25*	-19
4	24*	-5
5	55	54
6	22*	14
7	31	-28
8	60	55
9	50	53
H= -14, L= 3		
1	31*	-15
2	31*	23
3	92	91
4	55	63
5	75	78
6	28*	-24
7	89	91
8	26*	19
9	24*	20
10	31	-37
11	31	-26
12	23	-27
H= 14, L= 4		
0	108	107
1	51	-45
2	39	-33
3	69	65
4	18*	-4
5	48	-44
H= -14, L= 4		
0	29*	-9
1	68	-65
2	39	37
3	28*	25
4	53	47
5	56	50
6	25*	19
7	32	-37
8	60	-58
9	20*	5
10	18*	9
H= -14, L= 5		
1	196	-199
2	41	-42
3	24*	12
4	23*	8
5	27	-29
6	76	-74
7	28	24
8	74	78
H= -14, L= 6		
0	78	-78
1	41	-40
2	86	-97
3	16*	4
4	66	-67
H= 15, L= 0		
1	97	99
2	105	109
3	98	94
4	80	87
5	42	-42
6	90	95
7	43	31
8	23*	-10
9	82	-81
10	24	25
11	82	86
H= 15, L= 1		
0	84	78
1	52	45
2	76	73
3	45	40
4	91	92
5	110	114
6	51	-52
7	23*	-11
8	65	-60
9	19*	11
10	76	-84
H= -15, L= 1		
0	42	41
1	140	-140
2	92	-89
3	71	-71
4	89	91
5	57	54
6	35	29
7	26*	-13
8	24*	15
9	22*	1
10	20*	-11
11	44	-31
H= 15, L= 2		
1	106	-103
2	25*	30
3	24*	18
4	54	-50
5	23*	-8
6	21*	-5
7	66	-63
8	60	54
H= -15, L= 2		
1	41	30
2	29*	-7
3	32	-22
4	28*	-16
5	119	-119
6	42	-31
7	46	-42
8	23*	-25
9	26	-20
10	20	16
11	50	51
H= 15, L= 3		
0	88	-84
1	33	-37
2	25	-21
3	19*	-12
4	74	-71
5	22	18
6	71	72
H= -15, L= 3		
0	79	81
1	78	-74
2	122	-117
3	27*	6
4	26	-25
5	33	-35
6	44	-47
7	42	48
8	21*	7
9	18*	10
10	55	55
H= -15, L= 4		
1	68	67
2	28	22
3	38	-37
4	23*	1
5	45	47
6	22	-21
7	33	32
8	19	-22
H= -15, L= 5		
0	94	93
1	35	32
2	42	41
3	18*	-17
4	20	21
5	21	20
H= 16, L= 0		
0	99	97
1	25*	15
2	40	40
3	24*	15
4	23*	1
5	22*	9
6	21*	-8
7	54	53
8	35	-29
H= 16, L= 1		
1	29	-20
2	88	-83
3	30	-33
4	40	36
5	26	30
6	46	-42
7	68	70
H= -16, L= 1		
1	25*	-2
2	45	-41
3	24*	15
4	26	-21
5	63	64
6	21*	-5
7	40	-34
8	48	48
H= 16, L= 2		
0	19	19
1	51	53
2	34	29
3	34	-34
4	45	-49
H= -16, L= 2		
0	88	-88
1	120	125
2	39	43
3	24*	17
4	31	-24
5	45	-49
6	53	56
7	19*	11
8	16*	-16
H= -16, L= 3		
1	25	24
2	32	-36
3	79	-76
4	61	57
5	48	-39
6	43	49
7	43	-43
H= -16, L= 4		
0	90	-82
1	75	74
2	24	24
3	17*	3
4	21	14
5	42	40
H= 17, L= 0		
1	114	-111
2	17*	0
3	69	-68
4	28	-28
H= -17, L= 1		
0	83	-83
1	37	-35
2	106	-109
3	17*	-13
4	16*	-10
5	42	47
H= -17, L= 2		
1	73	-70
2	50	58
3	101	101
4	15*	-8
H= -17, L= 3		
0	121	119
1	60	-70

Table 4. *Agreement summary*

2904 observed reflexions ($1{\cdot}4 \le |F_o| \le 143{\cdot}8$)
$R = 0{\cdot}043$

Category	Limits		Number
1	$\lvert\Delta F\rvert \le 1{\cdot}0\lvert F_{th}\rvert$, or	$\lvert\Delta F\rvert/\lvert F_o\rvert \le 0{\cdot}10$	2898
2	$1{\cdot}0\lvert F_{th}\rvert < \lvert\Delta F\rvert \le 2{\cdot}0\lvert F_{th}\rvert$, or	$0{\cdot}10 < \lvert\Delta F\rvert/\lvert F_o\rvert \le 0{\cdot}15$	4
3	$2{\cdot}0\lvert F_{th}\rvert < \lvert\Delta F\rvert \le 3{\cdot}0\ F_{th}$, or	$0{\cdot}15 < \lvert\Delta F\rvert/\lvert F_o\rvert \le 0{\cdot}20$	1
4	$3{\cdot}0\lvert F_{th}\rvert < \lvert\Delta F\rvert$,	or $0{\cdot}20 < \lvert\Delta F\rvert/\lvert F_o\rvert \le 0{\cdot}30$	1
	801 unobserved reflexions ($\lvert F_{c_{\max}}\rvert = 4{\cdot}1$)		
1	$\lvert F_c\rvert \le 1{\cdot}0\lvert F_{th}\rvert$		767
2	$1{\cdot}0\lvert F_{th}\rvert < \lvert F_c\rvert \le 1{\cdot}5\lvert F_{th}\rvert$		34

$|F_{th}|$ = threshold amplitude = 1·3 to 3·4

tion that only a small residual electron density ($\sim 0{\cdot}14$ e.Å^{-3}) was observed on N(7)···C(14) at about 0·75 Å from N(7).

Intermolecular distances

The shortest intermolecular contacts for the different types of atom as found in this structure, and the corresponding distances as calculated from the van der Waals radii (Pauling, 1960, p.260), given in parentheses, are as follows: H···H, 2·40 (2·4); H···O, 2·49 (2·6); C···O, 3·19 (3·1); and C···C, 3·47 (3·4) Å. The nitrogen atom is involved in only two intermolecular distances below 4·0 Å, and both are to H-atoms which are at a distance of 3·48 and 3·99 Å from it. This confirms the proposal by Mottus, Schwarz & Marion (1953), that the nitrogen atom is well buried in the molecule.

Planarity of the rings

The mean plane of the benzene ring containing atom C(1), and of that containing atom C(11), referred to the orthogonal set of axes $X' = ax + cz\,.\cos\beta$, $Y' = by$, $Z' = cz\,.\sin\beta$, are

$$0{\cdot}6772X' - 0{\cdot}4862Y' - 0{\cdot}5523Z' - 2{\cdot}1388 = 0\,, \quad (1)$$

and

$$0{\cdot}7924X' - 0{\cdot}6018Y' - 0{\cdot}0999Z' - 3{\cdot}6218 = 0\,, \quad (2)$$

respectively. Each of these two rings is non-planar since $\chi^2 = 97$ and 72, respectively, and for $\nu = 3$, $P \ll 0{\cdot}1\%$. Each ring has a very slight boat form with maximum deviation from the mean plane of only $\pm 0{\cdot}013$ Å. The angle between the normals to these two planes is 27·8°.

The carbonyl group has atom C(14) about 0·06 Å above plane (1) and atom O(5) about 0·68 Å below it, and the C(14)–O(5) bond at an angle of 37·4° from that plane. This finding is different from the prediction by Mottus, Schwarz & Marion (1953), that the carbonyl is very nearly in plane (1). For the sake of completeness, it should also be mentioned that the carbonyl is at an angle of 35·0° from plane (2).

The ten-membered ring can be described as having the four atoms C(14), C(15), C(16), C(5) approximately in plane (1), the four atoms C(8), C(17), C(18), C(13) approximately in plane (2), and the two parts are linked together by the bond C(15)–C(16) on one side, and by the three bonds C(5)–C(6), C(6)–N(7), and N(7)–C(8) on the other side. The ring is severely buckled as shown in the two views of the molecule in Fig. 3 and contains a short distance across the ring of only 2·555 Å between N(7) and C(14). Both the N(7)–C(19) and C(14)–O(5) bonds are on the same side of the ring, the angle between them is 27·9°, and the distance C(19)···O(5) is 3·19 Å. These two bonds are slightly skew, but their mean plane makes exactly equal angles of 60·7° with planes (1) and (2).

Finally, as is to be expected, each of the two five-membered rings is non-planar.

The authors are indebted to Dr W. H. Barnes for suggesting the problem, and for making his original

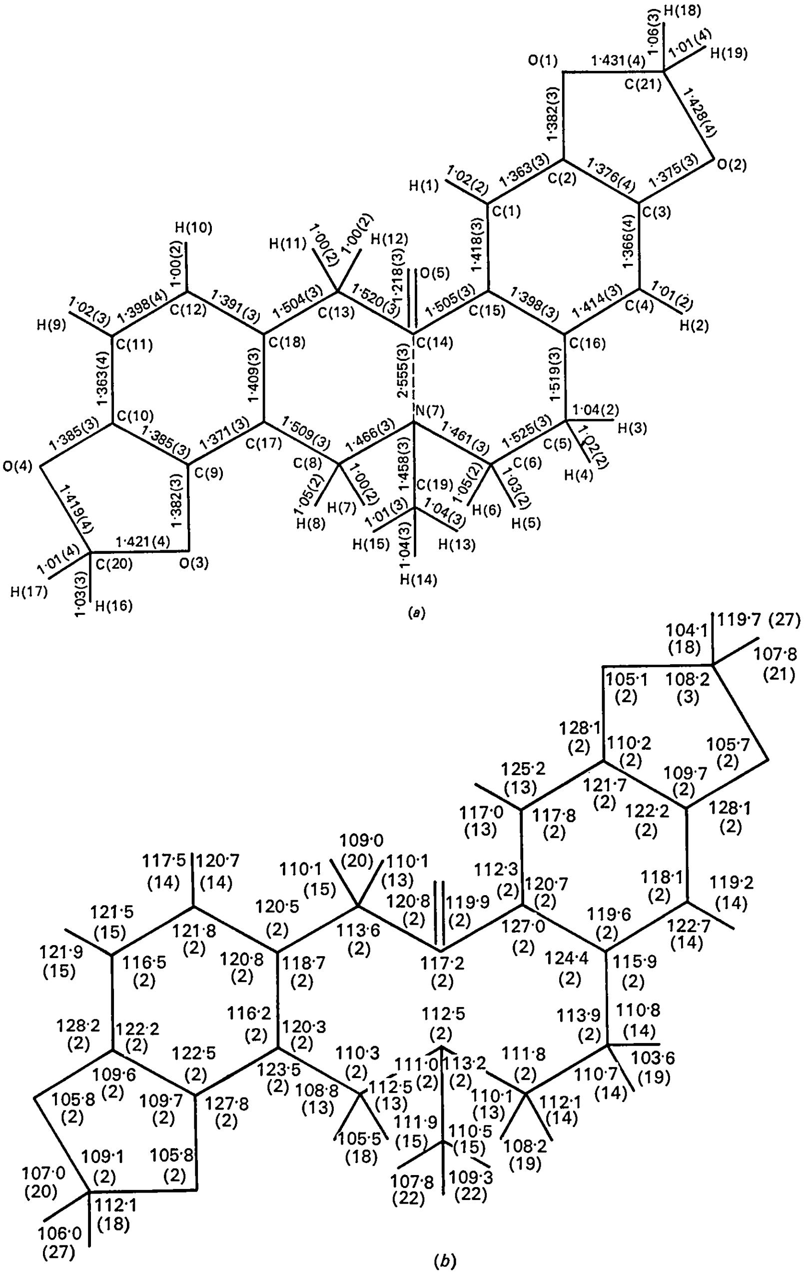

Fig. 4. Bond lengths (Å) and angles (°), and their e.s.d.'s in parentheses. The e.s.d.'s are multiplied by 10^2 for the C–H bonds, 10^3 for the other bonds, and 10 for the angles.

precession photographs available to them. All computations have been carried out with the IBM 360 system using a compatible set of programs written for that computer in FORTRAN IV by Ahmed, Hall, Pippy & Huber (1966). Grateful acknowledgement is made to Mrs M. E. Pippy of this laboratory for assistance with the computations, and to the staff of the NRC Computation Centre for their cooperation.

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The Crystal Structure of Cryptopine, $C_{21}H_{23}O_5N$

BY S. R. HALL* AND F. R. AHMED

Pure Physics Division, National Research Council of Canada, Ottawa 7, Canada

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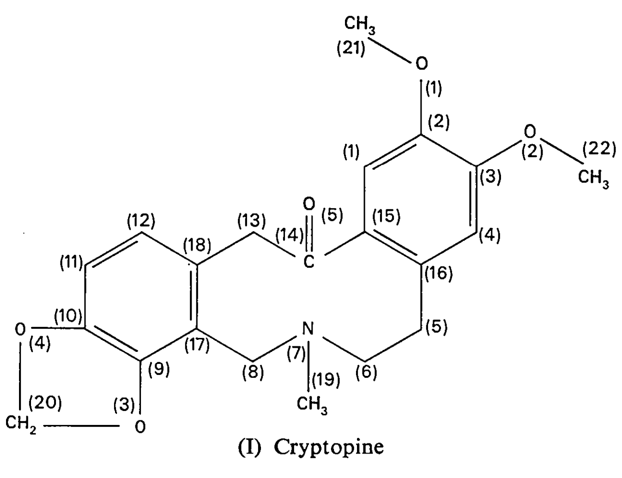
The structure of cryptopine, $C_{21}H_{23}O_5N$, has been determined by the symbolic addition procedure, and has been refined by least squares to an R index of 0·042 for 1948 observed reflexions measured with a scintillation counter. The space group is $P2_1/n$ and the cell dimensions are $a=14·438$, $b=8·702$, $c=14·369$ Å, $\beta=91°22'$. The presence of two methoxyl groups in the cryptopine molecule in place of one of the five-membered rings of the protopine molecule has resulted in significant differences in the angles at the two oxygen atoms and at four carbon atoms of the benzene ring in that part of the two molecules. The short distance between the C atom of the carbonyl group and the nitrogen atom across the ten-membered ring is 2·581 Å in cryptopine as compared with 2·555 Å in protopine. In both structures, the nitrogen atom is well buried in the molecule and has the three C–N bonds and the short C···N distance across the ten-membered ring tetrahedrally arranged around it. The carbon–oxygen double bond has ketonic character and is well off the planes of the aromatic rings.

Introduction

Cryptopine, $C_{21}H_{23}O_5N$, is the dimethyl analogue of protopine, $C_{20}H_{19}O_5N$, whose X-ray crystal structure analysis has been reported by Hall & Ahmed (1968). Reference should be made to the introduction of that paper where the purpose of the X-ray analysis of these two compounds has been discussed. The schematic formula of cryptopine is shown in (I), and the numbering of the atoms is basically the same as that adopted for protopine for ease of comparison of the two molecules.



(I) Cryptopine

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* National Research Council Postdoctorate Fellow. Present address: Department of Physics, The University of Western Australia, Nedlands, Western Australia.