This article was downloaded by:

On: 26 January 2011

Access details: Access Details: Free Access

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-

41 Mortimer Street, London W1T 3JH, UK



Nucleosides, Nucleotides and Nucleic Acids

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713597286

Solution and Solid State Structure of 2',5'-BIS-(O-Trityl)-3'-Oximinouridine

Peter Agback^a; A. Papchikhin^a; S. Neidle^b; Jyoti Chattopadhyaya^a

^a Department of Bioorganic Chemistry, Box 581 Biomedical Center, University of Uppsala, Uppsala, Sweden ^b CRC Biomolecular Structure Unit, Cancer Research Campaign, The Institute of Cancer Research, University of London, Surrey SM, NG, U.K

To cite this Article Agback, Peter, Papchikhin, A, Peter, Papchikhin, Pa

To link to this Article: DOI: 10.1080/07328319308019015 URL: http://dx.doi.org/10.1080/07328319308019015

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

SOLUTION AND SOLID STATE STRUCTURE OF 2',5'-BIS-(O-TRITYL)-3'-OXIMINOURIDINE

Peter Agback¹, A. Papchikhin¹, S. Neidle² & Jyoti Chattopadhyaya^{1*}

Department of Bioorganic Chemistry, Box 581, Biomedical Center, University of Uppsala, S-751 23 Uppsala, Sweden

²CRC Biomolecular Structure Unit, Cancer Research Campaign, The Institute of Cancer Research, University of London, Cotswold Road, Sutton, Surrey SM2 5NG, U.K

Abstract: Comparison of the solution (in CDCl₃ at 500 MHz ¹H NMR) and X-ray crystal studies of 3'-oximinouridine 1 shows in general good agreement with the high anti glycosidic angle and in the conformation about C4'-C5'. The sugar pucker (C2'-endo) is qualititatively identical in both cases. This is the first example of a conformationally sugar-rigid nucleoside in which the rigidity arises from the sp² character of an endocyclic carbon (i.e. C3'), not from the strain due to the ring fusion (see ref. 7 for conformationally strained nucleosides).

In connection with the synthesis 2',3'-dideoxy-3'-nitro uridine, we synthesized 2',5'-bis-(O-trityl)-3'-oximinouridine (1) as an intermediate. We herein report both the solid (X-ray) and the solution structure (1 H-NMR spectroscopy at 500 MHz) of oximinouridine 1. Chemical shifts of 1 and the proton-proton coupling constants (*i.e.* 3 J_{HH} and 4 J_{HH}) in deuterochloroform at -20°, 25° and 50°C are shown in Table 1 and Fig. 1. The pentofuranose ring of a ribonucleoside exists in an equilibrium of two rapidly interconverting conformers denoted by North (C3'-endo, C2'-exo) and South (C2'-endo, C3'-exo). The geometries of the North (N) and the South (S) conformers are expressed as their phase angles of pseudorotation (P_N , P_S) and their puckering amplitudes (ϕ_N , ϕ_S)¹.

Table 1. ¹ H-NMR (500 MHz) Spectral data (δ in ppm relative to TMS, J in ± 0.1 Hz)
and relative poulations (%) of Staggered C4'-C5' Rotamers $\gamma(+)$, γ (trans), and $\gamma(-)$ *.

T°C	δ1'	δ2'	δ4'	δ5'	δ5"	J _{1',2'}	J _{2',4'}	J _{4',5'}	J _{4',5"}	J _{5',5"}	x(γ(+))*
-20°C	6.09	5.37	5.03	3.74	2.93	6.8	1.1	1.7	1.7	10.3	100%
25°C											
50°C	6.07	5.26	5.0	3.71	3.12	6.7	1.5	2.4	2.1	10.3	91%

^{*} the poupulation of γ (trans), and γ (-) rotamers is negligible

The molar fractions of the N and S population, P_N , P_S , ϕ_N and ϕ_S can be calculated from the $^3J_{HH}$ coupling constants $(^3J_{1'2'}, ^3J_{2'3'}, ^3J_{3'4'})$ using suitable Karplus -Altona equation⁵.

In the case of oximinouridine 1, it is not possible to perform a full pseudorotational analysis⁵ by NMR spectroscopy due to the absence of parameters of 3'-oximino group as substituent in pseudorotational parameters in addition to the absence of ${}^3J_{2'3'}$ and ${}^3J_{3'4'}$ coupling constants. Altona *et al.* however has shown that it is possible to use equation (1) to determine the percentage of the North population (%N)² from simply ${}^3J_{1'2'}$ for qualitative determination of pouplation in the two-state North-South equilibrium:

$$%N = (7.9 - {}^{3}J_{1'2'})/6.9$$
 (1)

Using the ³J_{1'2'} coupling constants in eqn. (1), it can be seen that the pentofuranose ring in oximinouridine 1 in chloroform solution is predominantly in a South type conformation (~84 % S from -20 ° to 50 °C). This shows that the C2'-endo pucker of the pentofuranose ring observed by X-ray crystallography (vide supra) also exists in the chloroform solution. It is not however possible to calculate phase angle P and puckering amplitude φ from ³J_{1'2'} alone and therefore we are unable to compare the X-ray derived data with that of the qualitatively determined solution structure. The conformation of the pentofuranose ring does not seem to be appreciably influenced by temperature changes. This temperature independency of chemical shifts and coupling constants suggest the inflexibility of the sugar ring. Clearly, this rigidity of the pentofuranose ring arise from the sp² hybridized character of the C3'. Indeed, X-ray studies have shown that all three atoms substituted at C3' is planar explaining the rigid character of the pentofuranose ring (vide infra).

The conformation across the C4'-C5' bond (γ) could be characterised following standard methods, *i.e.* a relative distribution ("x") of various staggered rotamers population [$\gamma^+ \gtrsim$

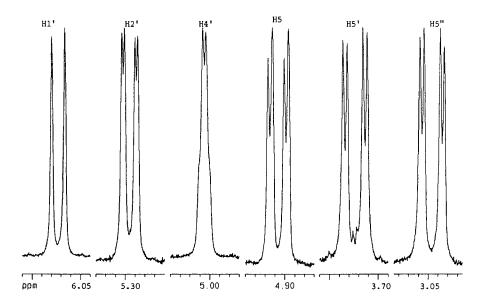


Figure 1. 1D spectrum (500 MHz ¹H) of Oximinouridine 1 showing the expansion of the region containing sugar and H5 absorptions. For J-couplings see Table 1.

 $\gamma^- \rightleftharpoons \gamma^t$] in an equilibrium can be calculated from the experimental ${}^3J_{4'5'}$ and ${}^3J_{4'5''}$ coupling constants using equations (2) and (3)³.

3
J_{4'5'} = $x(\gamma^{+})2.4 + x(\gamma^{-})10.6 + x(\gamma^{+})2.6$ (2)

$$^{3}J_{4'5''} = x(\gamma^{+})1.3 + x(\gamma^{-})3.8 + x(\gamma^{t})0.5$$
 (3)

The use of ${}^3J_{4'5'}$ and ${}^3J_{4'5''}$ coupling constants in equations (2) and (3) show that the staggered conformation across 4',5' is always γ^+ (100 % at -20 °C, 93 % at 25 °C and 92 % at 50 °C) and the temperature changes has only a marginal influence on γ^+ .

For the determination of the conformation around C1'-N1 bond (χ), it was not possible to employ reliable nOe difference spectroscopy between H1', H2' or H3' and H6 of uracil moiety because overlapping chemical shift of the H6 proton and the protons of 2'-O- and 5'-O-triphenyl groups. This made it impossible to irradiate the H6 selectively and observe relative nOe enhancements in H1', H2' or H3' in order to determine the conformation across the glycosidic bond in a straightforward manner. We therefore assessed the solution conformation around C1'-N1 bond (χ) from the vicinal 1 H, 13 C couplings (3 J_{H1'-C2} and 3 J_{H1'-C6}) using the equation of Lemieux⁴.

$$^{3}J_{H1'C6} = 6.2\cos^{2}(\phi) - 2.4\cos(\phi) + 0.1$$
 (4)

$$^{3}J_{H1'C2} = 5.0\cos^{2}(\phi + 180) - 2.1\cos(\phi + 180) + 0.1$$
 (5)

The use of experimental ${}^3J_{H1'C6} = 3.8$ Hz and ${}^3J_{H1'C2} = 1.6$ Hz in Karplus eqn. (4) and (5) allowed us to conclude that the uracil base is in the *anti* domain [$\chi = -128^{\circ}$ or -112° (*anti*), or $\chi = -157^{\circ}$ (*anti*) or -83° (high *anti*) basing on eqns (4) or (5), respectively]. The average of χ based on ${}^3J_{H1'C6}$ and ${}^3J_{H1'C2}$ is -142° (typical *anti*), and -97° (high *anti*), respectively. The glycosidic angle in oximinouridine 1 observed in the chloroform solution and in X-ray structure are thus quite qualititatively comparable (vide infra).

A careful inspection of coupling constants of the sugar protons shows a unique four bond coupling between H2'-H4' (${}^4J_{2'4'} = 1.5 \text{ Hz}$). Such effective four-bond coupling through H-C-C-C--H have been normally confined to a planar zig-zag configuration (W-path) arising from rigid systems⁶. Such rigid system for oximinouridine 1 is in fact evident from its temperature independent NMR data (-20 ° to 50 °C) and planar C3' with respect to its three substituents found in the X-ray structure (vide infra). To the best of our knowledge, this is the first example of four-bond H1', H4' coupling which did not arise through the homoallylic coupling as in 2',3'-unsaturated nucleosides⁸.

The complete X-ray structure of oximinouridine 1 is shown in Figure 2. Table 2 gives positional coordinates, and Table 3 details the important geometric characteristics of the nucleoside part of the structure and its oxime substituent. The furanose ring adopts a C2' endo pucker with a phase angle of pseudorotation P of 154° and a maximum angle of pucker τ_m of -31°. The glycoside angle, of -123.1(3)°, is in the high anti range and the conformations around C4'-C5' bond are g⁺, g⁻. The oxime group itself has a C=N bond length of 1.259(4)Å close to the norm⁹ of 1.281Å, and C-O length of 1.414(3)Å is in excellent agreement with the standard value of 1.416Å. The oxygen atom (O1) is trans with respect to C3'-C2' bond which means that the oxime is in anti conformation. The hydrogen atom attached to O1 is also trans with respect to its point of attachment (C3') on the furanose ring.

The attrachment of the oxime group to C3' has resulted in a slight shortening of the C3'-C4' bond from its average value ¹⁰ of 1.523Å. The C2'-C3'-C4' bond angle has increased by over 6°, although it is still far from a standard sp² bond angle. It is overall apparent that the oxime group has resulted in few changes to the furanose ring geometry that are of significance.

Comparison of X-ray crystal structure with the above NMR results in general shows good agreement, with the high anti glycosidic angle being found both in solution and in the

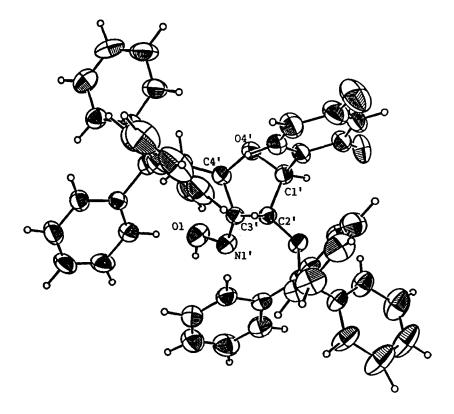


Figure 2. Crystal Structure of 2',5'-Bis-(O-trityl)-3'-oximinouridine (1).

crystal, as in the conformation about C4'-C5'. The sugar pucker (C2'-endo) is qualititatively identical in both cases.

In conclusion, this is the first example of a sugar-rigid nucleoside in which the rigidity of pentofuranose moiety comes from the inherent sp² character of an endocyclic carbon (i.e. C3') in contrast with other sugar-rigid structures (excluding the conformationally rigid aglycone-sugar fused nucleosides⁹) in which the strain originates from the fusion of a three-, four- or a five-membered ring across the v_2 torsion of the sugar ring (see for example, [3.1.0]-fused-2',3'-modified- β -D-nucleosides as 2',3'-anhydro-, 2',3'-epimino- or 2',3'-dideoxy-2',3'- α -methylene uridine)⁷.

Experimental

¹H-NMR spectra were recorded in deuterochloroform (~5 mM) using a Brucker AMX 500 spectrometer with TMS as internal standard. Single crystals were obtained from a 1:1

Table 2. Positional Parameters and Their Estimated Standard Deviations for Oximinouridine 1.

O1	Atom	х	у	Z	$B(Å^2)$
O2	<u>O1</u>		0.695	0.6650(2)	
O4		0.6741 (2)	0.9191 (1)	0.5430(1)	3.20 (4)
O4		0.3754 (3)		0.4596(1)	4.78 (5)
OS* 0.4885 (2) 0.8953 (1) 0.8409 (1) 3.04 (2) N1' 0.5940 (3) 0.7640 (2) 0.6330 (2) 3.73 (6) N1 0.4398 (3) 1.0519 (2) 0.6177 (2) 3.34 (5) N3 0.4112 (3) 1.1909 (2) 0.5692 (2) 4.41 (6) C1A 0.6099 (3) 0.8250 (2) 0.9843 (2) 3.04 (6) C1B 0.5889 (4) 0.9799 (2) 0.9722 (2) 3.49 (7) C1D 0.9045 (3) 0.8848 (2) 0.6197 (2) 3.20 (6) C1C 0.3496 (3) 0.8972 (2) 0.9819 (2) 3.26 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.25 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.27 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.27 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.88542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.20 (2) 0.5604 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.67 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.67 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.67 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.67 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.67 (7) C2C 0.2665 (4) 0.8341 (2) 1.0838 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3B 0.6775 (5) 1.0939 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3E 1.0044 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3B 0.6775 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3E 1.0044 (4) 0.7117 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 3.86 (7) C3E 1.0044 (4) 0.7117 (3) 0.7226 (3) 3.86 (7) C3E 1.0044 (4) 0.7117 (3) 0.7226 (3) 3.86 (7) C3E 1.0044 (4) 0.7117 (3) 0.7226 (3) 3.86 (7) C3E 1.0044 (4) 0.7117 (3) 0.7226 (3) 3.86 (7) C3E 1.0044 (4) 0.7118 (2) 0.6654 (2) 3.18 (6) C4C 0.0533 (4) 0.8933 (3) 1.0855 (3) 7.1 (1) C3E 1.0044 (4) 0.7118 (2) 0.6653 (3) 7.0 (1) C4E 0.0533 (4) 0.8933 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4C 0.0533 (4) 0.8933 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C5C 0.7381 (3) 0.8971 (2) 0.9439 (2) 0.996		0.4728 (4)	1.2995 (2)	0.6715 (2)	7.71 (8)
NI' 0.5940 (3) 0.7640 (2) 0.6330 (2) 3.73 (6) NI 0.4398 (3) 1.0519 (2) 0.6177 (2) 3.34 (5) NI 0.4398 (3) 1.0519 (2) 0.5692 (2) 4.41 (6) C1A 0.6099 (3) 0.8250 (2) 0.9843 (2) 3.04 (6) C1B 0.5889 (4) 0.9799 (2) 0.9722 (2) 3.49 (7) C1D 0.9045 (3) 0.8548 (2) 0.6197 (2) 3.20 (6) C1C 0.3496 (3) 0.85972 (2) 0.9819 (2) 3.26 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.25 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.25 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7844 (3) 1.0885 (3) 7.0 (1) C3E 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6693 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6993 (3) 5.14 (9) C3' 0.5315 (3) 0.8393 (3) 1.0885 (3) 7.0 (1) C3E 1.0404 (4) 1.1150 (2) 0.6993 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6693 (3) 5.14 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C3C 0.1485 (4) 0.8334 (2) 0.7226 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6690 (3) 5.20 (9) C4F 1.0004 (4) 0.7117 (3) 0.7226 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6690 (3) 5.20 (9) C4F 1.0004 (4) 0.7117 (3) 0.7226 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6690 (3) 5.20 (9) C4F 1.0006 (5) 1.1248 (2) 1.0244 (3) 6.9 (1) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.16 (9) C5C 0.1485 (4) 0.7807 (3) 0.7711 (2) 0.9459 (2) 2.99 (6) C5C 0.1485 (4) 0.7618 (2) 0.9459 (2) 3.22 (6) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.16 (9) C5F 0.7378 (3) 0.7818 (2) 0.9443 (2) 0.9476 (3) 5.9 (9) C4F 1.0090 (5) 0.9524 (3) 0.7646 (3) 5.51 (9) C5F 0.7378 (3) 0.7818 (2) 0.9746 (3) 5.9 (9) C5F 0.9860 (5) 1.1248 (2) 0.9746 (3) 5.9 (0.3341 (2)			3.78 (4)
N1 0.4398 (3) 1.0519 (2) 0.6177 (2) 3.34 (5) C1A 0.6099 (3) 0.8250 (2) 0.9843 (2) 3.04 (6) C1B 0.5889 (4) 0.9799 (2) 0.9722 (2) 3.49 (7) C1D 0.9045 (3) 0.88548 (2) 0.6197 (2) 3.20 (6) C1C 0.3496 (3) 0.8972 (2) 0.9819 (2) 3.26 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2* 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.777 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2*A 0.8379 (3) 0.9904 (2) 0.5668 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3E 1.0404 (4) 1.1150 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8352 (2) 0.6513 (2) 2.98 (6) C3D 0.9722 (4) 0.7837 (3) 1.0855 (3) 7.1 (1) C3E 1.0404 (4) 1.1150 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C4D 1.0044 (4) 1.1150 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8332 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7107 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8332 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7107 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C4D 1.0044 (4) 0.7107 (2) 0.6933 (3) 5.14 (9) C3* 0.5315 (3) 0.8393 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7107 (2) 0.6693 (3) 5.16 (9) C3* 0.5315 (3) 0.8393 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7104 (2) 0.6236 (3) 5.50 (9) C4F 1.0090 (5) 0.9524 (3) 0.8933 (3) 0.7711 (2) 4.83 (8) C3F 1.10090 (5) 0.9524 (3) 0.8933 (3) 0.7343 (2) 0.9496 (3) 4.70 (8) C5F 1.1004 (4					
N3					
C1A					
C1B					
C1D 0.9045 (3) 0.8578 (2) 0.6197 (2) 3.20 (6) C1C 0.3496 (3) 0.8972 (2) 0.9819 (2) 3.26 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1' 0.4386 (3) 0.9622 (2) 0.5978 (2) 3.21 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2E 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3B 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.66513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0652 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.8933 (4) 0.8333 (3) 1.0652 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7609 (2) 1.0298 (3) 5.50 (9) C4 0.9583 (4) 0.8933 (3) 1.0298 (3) 5.50 (9) C4 0.9583 (4) 0.8933 (3) 1.0298 (3) 5.50 (9) C4 0.9583 (4) 0.7606 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.0623 (3) 5.16 (9) C5' 0.9863 (4) 0.7104 (2) 0.0623 (3) 5.16 (9) C5' 0.9863 (4) 0.7104 (2) 0.0623 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8379 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8379 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8397 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8397 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8397 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8397 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.8397 (2) 0.9696 (3) 5.50 (9) C5' 0.3781 (3) 0.					
C1C 0.3496 (3) 0.8972 (2) 0.9819 (2) 3.26 (6) C1F 0.8939 (4) 0.9339 (2) 0.4607 (2) 3.57 (6) C1' 0.4386 (3) 0.9622 (2) 0.5978 (2) 3.21 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2' 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8342 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3B 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8315 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6694 (3) 5.8 (1) C4A 0.8075 (4) 0.7506 (5) 1.1939 (3) 1.0052 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4C 0.0533 (4) 0.8993 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4C 0.0533 (4) 0.8993 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6695 (2) 3.18 (6) C4C 0.0533 (4) 0.8993 (3) 1.0622 (3) 5.18 (9) C4F 1.0004 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3) 1.0298 (3) 5.50 (9) C4F 1.0009 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C5 0.9863 (4) 0.7104 (2) 0.6226 (3) 4.94 (8) C5F 1.1074 (5) 0.9863 (4) 0.7104 (2) 0.6226 (3) 4.94 (8) C5F 1.1074 (5) 0.9863 (4) 0.7104 (2) 0.6236 (3) 4.94 (8) C5F 1.1074 (5) 0.9863 (4) 0.7104 (2) 0.6236 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 4.70 (8) C5F 0.3781 (3) 0.8379 (2) 0.9459 (2) 2.99 (6) C5 0.9864 (4) 0.7104 (2) 0.6236 (3) 4.70 (8) C5F 0.3781 (3) 0.8379 (2) 0.9459 (2) 2.99 (6) C5 0.9486 (5) 1.1669 (2) 0.6012 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9446 (3) 5.51 (9) C5E 0.8231 (4) 1.1069 (2) 0.7118 (2) 3.88 (
C1F					
C1' 0.4386 (3) 0.9622 (2) 0.5978 (2) 3.21 (6) C1E 0.8741 (3) 1.0178 (2) 0.6047 (2) 3.12 (6) C2' 0.5889 (3) 0.9171 (2) 0.6032 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3B 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4C 0.0533 (4) 0.7509 (3) 1.0283 (3) 5.50 (9) C4 0.4590 (5) 1.2235 (2) 0.6609 (3) 4.86 (8) C4C 0.0533 (4) 0.893 (3) 1.0283 (3) 5.50 (9) C4F 1.0004 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 5.50 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 5.50 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 5.50 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 5.50 (9) C5S 0.4860 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5B 0.7721 (4) 1.0858 (2) 0.9459 (2) 2.99 (6) C5C 0.1041 (4) 0.7117 (3) 0.7226 (3) 5.51 (9) C5S 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5C 0.1041 (4) 0.7117 (3) 0.7236 (3) 5.51 (9) C5C 0.1041 (4) 0.893 (3) 0.8373 (2) 0.6609 (3) 5.50 (9) C5F 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5C 0.1041 (4) 0.9623 (3) 0.9446 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.51 (9) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.55 (9) C6G 0.4753 (4) 0.7691 (2) 0.9434 (2) 0.5755 (9) C6G 0.4753 (4) 1.0196 (2) 0.9137 (2) 4.20 (7)			, ,	, ,	
C1E					
C2' 0.5889 (3) 0.9171 (2) 0.6232 (2) 2.77 (6) C2B 0.5661 (5) 1.0219 (2) 1.0579 (3) 5.27 (9) C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3E 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8379 (5) 0.8322 (2) 0.6513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8903 (3) 1.0298 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.50 (9) C4F 1.0090 (5) 1.2235 (2) 0.6609 (3) 5.10 (9) C5'A 0.7699 (4) 0.7061 (2) 0.9963 (3) 5.10 (9) C5'A 0.7699 (4) 0.7061 (2) 0.9963 (3) 5.10 (9) C5'A 0.7699 (4) 0.7061 (2) 0.9965 (3) 5.10 (9) C5'A 0.7699 (4) 0.7061 (2) 0.99459 (2) 2.99 (6) C5 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'A 0.7699 (4) 0.7061 (2) 0.99459 (2) 2.99 (6) C5 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9860 (5) 1.1606 (2) 0.99459 (2) 0.99459 (2) 2.99 (6) C5 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.10 (9) C5'C 0.9863 (4) 0.7104 (2) 0.6236					
C2B				• ,	3.12 (6)
C2'A 0.8379 (3) 0.9304 (2) 0.5608 (2) 3.02 (6) C2D 0.9213 (3) 0.8542 (2) 0.7202 (2) 3.63 (7) C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3E 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6613 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3) 1.0298 (3) 5.50 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1218 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9459 (2) 2.99 (6) C5C 0.9863 (4) 0.7061 (2) 0.9626 (3) 5.1 (9) C5F 1.1074 (5) 0.9851 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5C 0.9863 (4) 0.7104 (2) 0.6640 (3) 5.51 (9) C5D 0.9863 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5F 1.1074 (5) 0.9851 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5C 0.1481 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5C 0.1481 (4) 1.1669 (2) 0.7043 (2) 4.94 (8) C5F 1.1074 (5) 0.9851 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0658 (2) 0.7343 (2) 4.94 (8) C5F 0.9860 (5) 1.1288 (2) 0.9412 (3) 5.71 (9) C5E 0.8231 (4) 1.1669 (2) 0.7943 (2) 4.94 (8) C5F 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6G 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C2D					
C2A 0.6496 (4) 0.8183 (2) 1.0838 (2) 3.67 (7) C2F 0.7975 (4) 0.9390 (3) 0.3776 (2) 4.91 (8) C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3E 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.044 (4) 0.7117 (3)					
C2F				, ,	
C2 0.4057 (4) 1.1076 (2) 0.5424 (2) 3.96 (7) C2E 1.0043 (4) 1.0333 (2) 0.6664 (2) 4.01 (7) C2C 0.2965 (4) 0.8341 (2) 1.0381 (2) 3.86 (7) C3A 0.7493 (4) 0.7569 (2) 1.1202 (2) 4.42 (8) C3D 0.9722 (4) 0.7837 (3) 0.7711 (2) 4.83 (8) C3F 0.8579 (5) 0.9484 (3) 0.2884 (3) 7.0 (1) C3B 0.6475 (5) 1.0939 (3) 1.0855 (3) 7.1 (1) C3E 1.0404 (4) 1.1150 (2) 0.6953 (3) 5.14 (9) C3' 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3)					
C2E					4.91 (8)
C2C	C2				3.96 (7)
C3A					4.01 (7)
C3D					
C3F			0.7569 (2)		
C3B				• /	
C3E					7.0(1)
C3' 0.5315 (3) 0.8322 (2) 0.6513 (2) 2.98 (6) C3C 0.1485 (4) 0.8363 (3) 1.0622 (3) 5.18 (9) C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3) 1.0298 (3) 5.50 (9) C4 0.4590 (5) 1.2235 (2) 0.6609 (3) 5.20 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2)		` ,			
C3C					
C4' 0.3809 (3) 0.8433 (2) 0.6895 (2) 3.18 (6) C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3) 1.0298 (3) 5.50 (9) C4 0.4590 (5) 1.2235 (2) 0.6609 (3) 5.20 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.8231 (4) 1.0858 (2) 0					2.98 (6)
C4D 1.0044 (4) 0.7117 (3) 0.7226 (3) 5.8 (1) C4A 0.8075 (4) 0.7003 (2) 1.0609 (3) 4.86 (8) C4C 0.0533 (4) 0.8993 (3) 1.0298 (3) 5.50 (9) C4 0.4590 (5) 1.2235 (2) 0.6609 (3) 5.20 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.7818 (2) 0.9746 (3) 5.9 (1) C6C 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6C 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					5.18 (9)
C4A					
C4C					
C4 0.4590 (5) 1.2235 (2) 0.6609 (3) 5.20 (9) C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2)					
C4F 1.0090 (5) 0.9524 (3) 0.2835 (3) 7.3 (1) C4E 0.9504 (5) 1.1811 (2) 0.6640 (3) 5.51 (9) C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)		• • •			
C4E					
C4B 0.7506 (5) 1.1248 (2) 1.0274 (3) 6.9 (1) C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5A 0.7699 (4) 0.7061 (2) 0.9626 (3) 4.70 (8) C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5D 0.9863 (4) 0.7104 (2) 0.6236 (3) 5.61 (9) C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5'A 0.5067 (3) 0.8971 (2) 0.9459 (2) 2.99 (6) C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					4.70 (8)
C5 0.4860 (5) 1.1605 (2) 0.7343 (2) 4.94 (8) C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					5.61 (9)
C5F 1.1074 (5) 0.9451 (3) 0.3657 (3) 7.0 (1) C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5B 0.7721 (4) 1.0858 (2) 0.9412 (3) 5.72 (9) C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5E 0.8231 (4) 1.1669 (2) 0.6012 (3) 5.16 (9) C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)		. ,			
C5' 0.3781 (3) 0.8379 (2) 0.7969 (2) 3.22 (6) C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C5C 0.1041 (4) 0.9623 (3) 0.9746 (3) 5.9 (1) C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C6F 1.0483 (4) 0.9369 (3) 0.4543 (2) 5.55 (9) C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)		* * *			
C6D 0.9389 (4) 0.7818 (2) 0.5722 (2) 4.51 (8) C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C6 0.4753 (4) 1.0799 (2) 0.7118 (2) 3.88 (7) C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)		• • •			
C6A 0.6716 (4) 0.7691 (2) 0.9243 (2) 3.85 (7) C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
C6B 0.6941 (4) 1.0116 (2) 0.9157 (2) 4.20 (7)					
COE 0.7801 (4) 1.0852 (2) 0.5717 (2) 4.00 (7)			` '	1.1	
	COE	U./861 (4)	1.0852 (2)	0.5/17 (2)	4.00 (7)

C6C	0.2510 (4)	0.9616(2)	0.9510(3)	5.09 (8)
H1	0.565 (6)	0.651 (4)	0.647 (3)	15 (2)*
H1'	0.413 (3)	0.956(2)	0.524(2)	2.2 (5)*
H2'	0.638(3)	0.944 (2)	0.684 (2)	3.8 (6)*
H2B	0.483 (4)	0.999 (3)	1.108 (3)	9 (1)*
H2D	0.896 (3)	0.907 (2)	0.753 (2)	3.4 (6)*
H2A	0.605(3)	0.855(2)	1.126 (2)	4.7 (7)*
H2F	0.689 (4)	0.941 (2)	0.376 (2)	5.7 (8)*
H2E	1.073 (3)	0.986 (2)	0.686 (2)	5.0 (8)*
H2C	0.356(3)	0.788 (2)	1.063 (2)	4.2 (7)*
Н3	0.390 (4)	1.229(2)	0.520(2)	6.6 (9)*
H3A	0.768 (4)	0.758(2)	1.188 (2)	5.6 (8)*
H3D	0.980(4)	0.781 (2)	0.847 (2)	7.0 (9)*
H3F	0.792 (4)	0.956 (3)	0.238 (2)	8(1)*
H3E	1.144 (4)	1.122 (2)	0.734 (2)	5.9 (8)*
H3C	0.121 (4)	0.793 (2)	1.102 (2)	6.5 (9)*
Н3В	0.624 (5)	1.124 (3)	1.149 (3)	13 (2)*
H4D	1.030 (4)	0.659 (3)	0.761 (3)	9(1)*
H4A	0.880(4)	0.659(2)	1.088 (2)	5.8 (8)*
H4C	-0.055 (4)	0.896(2)	1.049 (2)	7.0 (9)*
H4F	1.050 (4)	0.959(3)	0.227 (3)	9(1)*
H4E	0.978 (4)	1.238 (2)	0.683 (2)	7(1)*
H4B	0.810 (5)	1.179 (3)	1.052 (3)	11 (1)*
H4'	0.312 (3)	0.802(2)	0.660 (2)	2.9 (6)*
H5D	1.008 (4)	0.660(3)	0.580 (3)	9(1)*
H5	0.521 (4)	1.176 (2)	0.799 (2)	6.4 (9)*
H5F	1.227 (5)	0.963 (3)	0.351 (3)	10 (1)*
H5B	0.846 (4)	1.107(2)	0.900(2)	6.9 (9)*
H5E	0.754 (4)	1.212 (2)	0.572 (2)	6.7 (9)*
H5C	0.030(4)	1.011 (3)	0.949 (2)	9 (1)*
H5A	0.806(3)	0.671 (2)	0.917 (2)	5.1 (8)*
H6D	0.924(3)	0.783 (2)	0.501(2)	3.3 (6)*
Н6	0.494 (3)	1.032(2)	0.756 (2)	4.3 (7)*
H6A	0.653 (3)	0.775 (2)	0.850 (2)	4.4 (7)*
Н6В	0.713 (3)	0.978 (2)	0.858 (2)	3.1 (6)*
H6E	0.712 (3)	1.076 (2)	0.525 (2)	3.4 (6)*
H6C	0.293 (4)	1.008 (2)	0.916 (2)	7.0 (9)*
H6F	1.126 (4)	0.933 (3)	0.514 (3)	9 (1)*
H5'1	0.410(3)	0.779 (2)	0.818 (2)	5.1 (8)*
H5'2	0.270 (3)	0.855 (2)	0.814 (2)	3.3 (6)*
				(0)

^{*} Starred atoms were refined isotropically

EtOH/H₂0 mixture. Cell dimensions were obtained by least-squares refinement of Θ values from 25 reflections measured on an Enraf-Nonius CAD4 Turbo diffractometer. They are: $\underline{a} = 8.918(1)$, $\underline{b} = 15.921(2)$, $\underline{c} = 13.917(2)$ Å and $\beta = 95.80(1)^{\circ}$. Systematic absences OkO, $\underline{r} = 2N+1$, together with the subsequent successful structure analysis, confirmed the space group as P21 (No. 5). The unit cell contains two molecules of C₄₆H₄₀O₆N₄, with a calculated density of 1.23 gm cm⁻³. Intensity data were collected on the diffractometer for a crystal of approximate dimensions 0.20 x 0.10 x 0.03 mm, using graphite-monochromated Cu-K α radiation ($\lambda = 1.54051$ Å). An ω -2 Θ scan technique was

Table 3. Major geometries and conformation features of the Crystal Structures of Oximinouridine 1.

(a) B	Sond lengths (Å)						
C1'-C2' C1'-O4' C1'-N1 C2'-O2' C3'-C4'	1.530(4) 1.432(4) 1.453(4) 1.412(3) 1.504(4)		C3'-N1' N1'-O1 C4'-C5' C2'-C3' C4'-O4'	1.259(4) 1.414(3) 1.500(4) 1.511(4) 1.443(4)			
(b) B	Sond angles (°)						
C1'-O4'-C C1'-C2'-C: C1'-C2'-O: C3'-C2'-O: C2'-C3'-C: C2'-C3'-N C4'-C3'-N	3' 99. 2' 109 2' 116 4' 108 1' 123	0.0(2) 7(2) 9.6(2) 6.2(2) 8.9(2) 3.4(3) 7.1(3)	O4'-C1'-C2' O4'-C1'-N1 C2'-C1'-N1 C3'-C4'-O4' C3'-C4'-C5' O4'-C4'-C5' C3'-N1'-O1	106.5(2 105.8(2 115.3(2 104.0(2 116.7(2 108.8(2 111.2(3	2) 2) 2) 2) 2)		
(c) T	°iorsion angles (°)					
O4'-C1'-C C1'-C2'-C C4'-O4'-C O5'-C5'-C O5'-C5'-C	3'-C4' -28 1'-C2' -23 4'-C3' 52.	7(3) 3.3(3) 3.3(3) 8(3) 4.4(3)	C2'-C3'-C4' C3'-C4'-O4' O4'-C1'-N1- C3'-N1'-O1- C4'-C3'-N1'	-C1' 4.8(3) -C2 -123.1(-H1 177.8(7	3)		
Phase angle of pseudorotation (P): 154°							
	Puckering ampliker description:	itude (v _m):	-31° C2'-endo				
(d) Least-squares planes. Derivation from the planes are in Å							
*N1' *C3' *C2' *C4' *O1	*C3' -0.046(3) *C2' 0.013(3) *C4' 0.014(3)		C3' N1' O1 C2' C4'	0.0 0.0 -0.021(2) 0.040(3) 0.167(3)			

Atoms marked (*) were included in the calculation of the plane

used, with a maximum scan time per reflection of 90 sec and a maximum scan rate of 3.33° /min. Data were collected in the range $1.5 < \Theta < 65^{\circ}$, and $O \le h \le 10$, $O \le k \le 17$ and $-15 \le h \le 15$. A periodic check was kept on crystal stability and orientation; no significant decay was observed during the data collection. a total of 3240 unique reflections were measured, of which 2806 had $I > 3\sigma(I)$ and were used in the subsequent refinement.

The structure was solved by direct methods, together with tangent formula recycling procedures and difference Fourier syntheses. It was refined by full-matrix least-squares methods. The positions of all hydrogen atoms were located in a series of Fourier syntheses. Their positional and isotropic temperature factores were included in the latter stages of refinement. A weighting scheme of the form $\underline{\mathbf{w}} = 1[\sigma^2(\underline{\mathbf{F}}) + (0.04\underline{\mathbf{F}})^2]$ was used. The final least-squares cycle had an $\underline{\mathbf{R}} = 0.0284$ and $\underline{\mathbf{R}}_{\underline{\mathbf{w}}} = 0.0262$ with a maximum shift/error of <0.1. A final difference Fourier map did not have any peaks outside the values of $\pm 0.2e\text{Å}^{-3}$.

Scatteirng factors were taken from <u>International Tables for X-Ray Crystallography</u> (1974), Vol. IV). All calculations were performed with the MOIEN computer package (Delft Instruments, Holland 1990).

Acknowledgements

The authors thank the Swedish Board for Technical Development (NUTEK) and Swedish Natural Science Research Council for generous financial support. The authors also thank Wallenbergs Stifelsen, University of Uppsala and Swedish Research Council (FRN) for funds toward the purchase of a 500 MHz NMR spectrometer.

References

- (a) Altona, C.; Sundaralingam, M. J. Am. Chem. Soc. 1972, 94, 8205 (b) Altona, C.; Sundaralingam, M. J. Am. Chem. Soc. 1973, 93, 2333.
- (a) Doornbos, J.; Wreesmann, C. T. J.; van Boom, J. H.; Altona, C. Eur. J. Biochem. 1983, 131, 571 (b) de Leeuw, F. A. A. M.; Altona, C. J. Chem. Soc. Perkin Trans. II 1982, 375.
- Haasnoot, C. A. G.; de Leeuw, F. A. A. M.; de Leeuw, H. P. M.; Altona C. Recl. Trav. Chim. Pays-Bas 1979, 98, 576.
- 4. (a) Lemiex, R.U; Nagabhushan, T.J and Paul, B. JCan. J. Chem. 1972, 50, 773. (b) Davies, D. B.; Rajani, P.; Sadikot, H. J. Chem. Soc. Perkin Trans. II 1985, 279.
- Altona, C. et al. J. Comp. Chem. 1983, 4, 438 & PSEUROT: QCPE Program No. 463; Haasnoot, C.A.G.; de Leeuw, F.A.A.M.; de Leeuw, H.P.M.; Altona, C. Receuil des Trav. Chim. Pays-bas 1979, 98, 576; Haasnoot, C.A.G.; de Leeuw, F.A.A.M.; de Leeuw, H.P.M.; Altona, C. Org. Magn. Reson. 1981 15, 43;

- Haasnoot, C.A.G.; de Leeuw, F.A.A.M.; Altona, C. Tetrahedron,. 1980 36, 2783; idem, Bull. Chem. Soc. Belg. 1980 84, 125.
- 6. Jackman, L.M.; and Sternhell, S. Nuclear Magnetric Resonance Spectroscopy in Organic Chemistry, 2nd ed, Pergamon Press, 1978.
- 7. Koole, L. H., Neidle, S.; Crawford, M.R.; Krayevski, A.A.; Gurskaya, G..V.; Bochkarev, A.; Sandström, A.; Wu, J-C.; Tong, W. and Chattopadhyaya, J. J. Org Chem. 1991, 56, 6884, .
- 8. Welch, C.J.; Bazin, H. and Chattopadhyaya, J. Acta Chem. Scand., 1986, B40, 343.
- 9. Allen, F.H., Kennerd, O., Watson, D.G., Brammer, L., Orpen, A.G. and Taylor, R., J. Chem. Soc. Perkin Trans II, 1987, s1-19.
- 10. Saenger, W. Principles of Nucleic Acid Structure (1984), Springer-Verlag, Berlin.

Received 2/8/93 Accepted 4/22/93