

Structures of Four *para*-Substituted 1,1-Diphenylethylene Derivatives: 4,4'-Ethylenedibenzonitrile (I); 4,4'-Ethylenedianisole (II); *p*-(1-Phenylethylene)anisole (III) and *N,N*-Dimethyl-4-(1-*p*-Nitrophenylethylene)aniline (IV)

BY YUN YI WEI, BERNARD TINANT, JEAN-PAUL DECLERCQ AND MAURICE VAN MEERSSCHE

Laboratoire de Chimie physique et de Cristallographie, Université de Louvain, Bâtiment Lavoisier, Place Louis Pasteur, 1, B-1348 Louvain-la-Neuve, Belgium

(Received 6 June 1986; accepted 15 July 1986)

Abstract. Structures have been determined for a homogeneous series of 1,1-diphenylethylenes substituted in *para* positions by acceptor (CN, CN, I), donor (OCH₃, OCH₃, II; OCH₃, H, III) or donor [N(CH₃)₂] and acceptor (NO₂, IV) groups. (I) C₁₆H₁₀N₂, $M_r = 230.27$, monoclinic, *Cc*, $a = 10.640$ (2), $b = 19.233$ (4), $c = 7.438$ (1) Å, $\beta = 124.67$ (1)°, $V = 1251.8$ (4) Å³, $Z = 4$, $D_x = 1.22$ g cm⁻³, *Cu Kα*, $\lambda = 1.5418$ Å, $\mu = 5.83$ cm⁻¹, $F(000) = 480$, $T = 291$ K, $R = 0.033$ for 817 observed reflections. (II) C₁₆H₁₆O₂, $M_r = 240.30$, orthorhombic, *Aba2*, $a = 7.712$ (3), $b = 26.079$ (13), $c = 6.591$ (4) Å, $V = 1325.6$ (11) Å³, $Z = 4$, $D_x = 1.20$ g cm⁻³, *Mo Kα*, $\lambda = 0.71069$ Å, $\mu = 0.84$ cm⁻¹, $F(000) = 512$, $T = 291$ K, $R = 0.053$ for 311 observed reflections. (III) C₁₅H₁₄O, $M_r = 210.28$, monoclinic, *Cc*, $a = 23.088$ (3), $b = 7.828$ (1), $c = 6.667$ (1) Å, $\beta = 98.96$ (1)°, $V = 1190.2$ (3) Å³, $Z = 4$, $D_x = 1.17$ g cm⁻³, *Mo Kα*, $\lambda = 0.71069$ Å, $\mu = 0.77$ cm⁻¹, $F(000) = 448$, $T = 219$ K, $R = 0.042$ for 994 observed reflections. (IV) C₁₆H₁₆N₂O₂, $M_r = 268.32$, monoclinic, *P2₁/n*, $a = 6.597$ (1), $b = 27.813$ (8), $c = 7.793$ (1) Å, $\beta = 93.56$ (1)°, $V = 1427.1$ (5) Å³, $Z = 4$, $D_x = 1.25$ g cm⁻³, *Cu Kα*, $\lambda = 1.5418$ Å, $\mu = 6.85$ cm⁻¹, $F(000) = 568$, $T = 291$ K, $R = 0.054$ for 1420 observed reflections. In each molecule the atoms are distributed on three planes: the ethylene reference plane and the two aromatic groups. The phenyl rings are rotated in opposite directions by a mean value of 39° for I–III. For compound IV the angles between the least-squares planes of *p*-nitrophenyl and *p*-dimethylaminophenyl with the ethylenic plane are respectively 42 and 31°.

Introduction. The problem of the conformation of the phenyl rings in benzophenone and 1,1-diphenylethylene derivatives has been extensively discussed. From dipole moment measurements (Coates & Sutton, 1942), ultraviolet (Suzuki, 1960) and NMR spectra (Van der Linde, Korver, Korver, Veenland & De Boer, 1965) it has been shown that the steric hindrance between the two *ortho* hydrogen atoms prevents the

benzophenone and the 1,1-diphenylethylene molecules from being planar. A number of crystal structures of various benzophenone derivatives are known; they exhibit angles of twist of each phenyl ring in the range 20–35° (Pattabhi & Venkatesan, 1973). Surprisingly, only two structures of 1,1-diphenylethylene derivatives are reported in the literature (Casalone & Simonetta, 1971; Casalone, Gavezzoti, Mariani, Mugnoli & Simonetta, 1970). We have found it of interest to study in a systematic way the effects of the *para* substituent on the conformation of the molecule. In this paper, we report the structures of four *para*-substituted derivatives (see Fig. 1).

Experimental. The following features of data collection, structure solution and refinement are common to all four structures. For detailed information, see Table 1. Crystals obtained by slow evaporation at room temperature. Cell constants refined using 15 strong reflections in the range $5 < 2\theta < 30^\circ$. All reflections measured on a Syntex *P2₁* diffractometer; no significant variation of standard reflection intensity. No corrections for absorption or secondary extinction. Structures solved by *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Anisotropic least-squares refinement with *SHELX76* (Sheldrick,

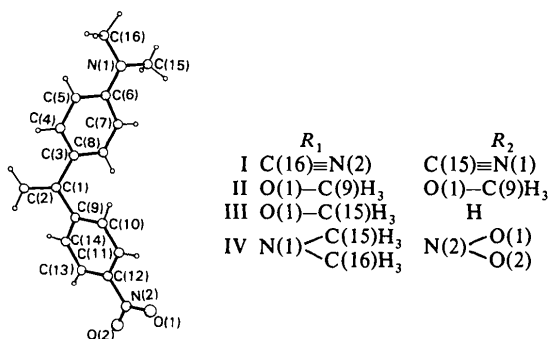


Fig. 1. View of the molecule (IV) and atom-numbering scheme of compounds I–IV.

Table 1. Details of data collection, structure solution and refinement for I-IV

	I	II	III	IV
<i>p</i> -Substituents	CN,CN	OCH ₃ ,OCH ₃	H,OCH ₃	NO ₂ ,N(CH ₃) ₂
Solvent	2-propanol; cyclohexane	ethanol	benzene	2-propanol
Crystal size (mm)	0.20 × 0.15 × 0.30	0.10 × 0.20 × 0.30	0.20 × 0.15 × 0.20	0.15 × 0.15 × 0.30
Standard reflection	22 $\bar{2}$	311	440	11 $\bar{1}$
2 θ_{\max} (°)	112	47	55	112
Number of reflections measured	817	542	1365	1860
	0 ≤ <i>h</i> ≤ 11 0 ≤ <i>k</i> ≤ 20 -7 < <i>l</i> < 7	0 ≤ <i>h</i> ≤ 8 0 ≤ <i>k</i> ≤ 28 0 ≤ <i>l</i> ≤ 7	0 ≤ <i>h</i> ≤ 29 0 ≤ <i>k</i> ≤ 10 -8 ≤ <i>l</i> ≤ 8	0 ≤ <i>h</i> ≤ 7 0 ≤ <i>k</i> ≤ 29 -8 ≤ <i>l</i> ≤ 8
Number of reflections observed <i>I</i> > 2.5σ(<i>I</i>)	782	311	994	1420
Number of H located on $\Delta\rho$ synthesis	all	5	11	all
Number of H computed	—	3	3	—
<i>B</i> _{iso} for H(Å ²)	6.27	6.25	6.49	7.21
<i>g</i>	0.0096	0.0212	0.0124	0.0226
<i>R</i>	0.033	0.053	0.042	0.054
<i>wR</i>	0.032	0.059	0.054	0.069
<i>S</i>	0.51	0.57	0.63	0.64
Number of parameters	192	98	177	181
Max. shift to e.s.d.	0.58	0.44	0.60	0.50
Max. and min. in final $\Delta\rho$ synthesis (e Å ⁻³)	+0.10, -0.17	+0.16, -0.20	+0.10, -0.20	+0.19, -0.24

1976) using *F*. Hydrogen atoms which were located in a difference Fourier synthesis have been included in the refinement process with isotropic common temperature factor; the other H atoms have been computed (C—H = 1.08 Å, H—C—H = 109.5°). Weighting scheme $w = 1/[\sigma^2(F) + gF^2]$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Atomic coordinates and equivalent isotropic temperature factors are listed in Table 2, and selected structural parameters are given in Table 3.*

Discussion. The bond lengths and angles observed agree within the standard deviations with those reported for 1,1-di-*p*-tolylethylene (V) (Casalone *et al.*, 1970) and for 1,1-bis(*p*-nitrophenyl)ethylene (VI) (Casalone & Simonetta, 1971). The values of the C=C distance range from 1.327 (5) to 1.334 (4) Å with a mean of 1.332 (2) Å as compared with 1.338 (5) and 1.326 (6) Å in V and VI. As has also been observed in V and VI, the bond angle C_(ar)—C_(eth)—C_(ar) is slightly less than 120° in the four molecules with a mean value of 119.1 (1)°.

Independent of the existence of molecular crystallographic twofold symmetry — only observed in II — the conformations of the six 1,1-diphenylethylene molecules are similar: both aromatic rings are rotated in opposite directions with respect to the ethylenic plane: C(1),

C(2), C(3), C(9). The intramolecular contacts between the ethylenic and the closest *ortho* hydrogens of the phenyl groups range from 2.2 (1) to 2.5 (1) Å while the distance between the two closest *ortho* phenyl carbons C(8) and C(10) is relatively constant: 3.21 (1) to 3.28 (1) Å. For compounds I, II, III we observe the same angle between the normals to the mean planes of each of the two aromatic rings and the normal to the ethylenic plane. Including VI the values of this angle range from 37 to 42° with an average of 39°. This is greater than the values of 20–35° generally observed in benzophenone derivatives (Van der Velden & Noordik, 1979; Pattabhi & Venkatesan, 1973). A more precise comparison is given by the structure of 4,4'-dimethoxybenzophenone (Norment & Karle, 1962) which is identically *p*-substituted as II. In this benzophenone derivative the aromatic rings are inclined at 25 and 35° to the carbonyl plane while in II each of the aromatic groups are twisted by 37° from the ethylenic bond plane. The greater twist of 1,1-diphenylethylene is the consequence of the steric hindrance between the ethylenic and the *ortho* hydrogen atoms which does not exist in benzophenone derivatives. For IV and V the angles between the normals to each aromatic group and to the ethylenic reference plane are significantly different. The considerable difference between the twist angle values of 37 and 50° observed in 1,1-di-*p*-tolylethylene (V) result from packing interactions; an earlier minimization energy calculation taking packing energy into account indicated that the preferred conformation would have both benzene rings inclined at ~35° to the ethylene plane (Casalone & Gavezzotti, 1971). In addition to packing interactions, mesomeric effects between the polar *para* substituents and the

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43252 (30 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

ethylene bond may be taken into account to explain the difference between the twist angles of 31 and 42° observed in IV. These values indicate a better conjugation with the C=C bond for the electron donor *p*-dimethylamino substituent than for the electron-

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic temperature factors (\AA^2) for I–IV

$$B_{eq} = \frac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
I				
C(1)	3066	-1855 (1)	6344	4.56 (4)
C(2)	2198 (5)	-1980 (2)	7076 (7)	6.25 (6)
C(3)	3643 (4)	-1144 (1)	6439 (6)	4.30 (4)
C(4)	2745 (4)	-561 (1)	6042 (6)	4.95 (5)
C(5)	3318 (4)	100 (1)	6302 (5)	4.81 (5)
C(6)	4809 (4)	191 (1)	6930 (5)	4.32 (4)
C(7)	5713 (4)	-385 (1)	7271 (6)	4.78 (5)
C(8)	5125 (4)	-1044 (1)	7005 (6)	4.73 (5)
C(9)	3472 (4)	-2426 (1)	5415 (6)	4.51 (4)
C(10)	3422 (5)	-2331 (1)	3529 (6)	5.45 (5)
C(11)	3700 (5)	-2863 (1)	2576 (7)	5.83 (6)
C(12)	4075 (4)	-3515 (1)	3542 (6)	5.16 (5)
C(13)	4168 (4)	-3623 (1)	5457 (6)	5.60 (5)
C(14)	3867 (4)	-3087 (2)	6369 (6)	5.40 (5)
C(15)	4325 (4)	-4087 (2)	2494 (7)	6.01 (6)
C(16)	5425 (4)	882 (1)	7231 (5)	5.11 (5)
N(1)	4493 (5)	-4532 (2)	1664 (8)	8.15 (7)
N(2)	5886 (5)	1430 (1)	7476 (6)	7.12 (6)
II				
C(1)	10000	0	3958	3.78 (25)
C(2)	10000	0	5955 (29)	4.93 (28)
C(3)	10075 (13)	488 (3)	2792 (24)	3.18 (15)
C(4)	9114 (12)	566 (3)	1030 (22)	3.64 (15)
C(5)	9064 (12)	1035 (3)	76 (22)	3.55 (15)
C(6)	10015 (16)	1448 (3)	839 (22)	3.95 (17)
C(7)	10930 (16)	1379 (3)	2582 (26)	4.56 (20)
C(8)	11041 (16)	916 (3)	3586 (26)	4.30 (19)
C(9)	9135 (18)	2013 (4)	-1804 (27)	7.00 (28)
O(1)	10086 (10)	1924 (2)	-12 (23)	5.50 (14)
III				
C(1)	1998 (3)	2500 (4)	7398 (8)	4.16 (6)
C(2)	1994	2473 (7)	5406	5.75 (8)
C(3)	1445 (3)	2430 (4)	8239 (7)	3.61 (5)
C(4)	965 (3)	1479 (5)	7296 (9)	4.77 (7)
C(5)	439 (3)	1500 (5)	8002 (9)	4.88 (7)
C(6)	361 (3)	2477 (5)	9672 (9)	4.52 (6)
C(7)	834 (3)	3417 (4)	10661 (8)	4.16 (6)
C(8)	1366 (3)	3366 (4)	9955 (8)	3.89 (5)
C(9)	2567 (3)	2597 (4)	8805 (7)	3.78 (5)
C(10)	2662 (3)	1611 (5)	10586 (8)	4.28 (6)
C(11)	3198 (3)	1596 (6)	11798 (9)	5.18 (7)
C(12)	3655 (3)	2557 (6)	11290 (11)	5.63 (8)
C(13)	3569 (3)	3569 (6)	9601 (10)	5.92 (9)
C(14)	3032 (3)	3585 (5)	8365 (9)	4.98 (7)
C(15)	-277 (3)	3473 (8)	11915 (12)	7.38 (11)
O(1)	-179 (3)	2426 (4)	10269 (8)	6.17 (6)
IV				
C(1)	6184 (4)	2425 (1)	7466 (4)	4.35 (5)
C(2)	4163 (5)	2397 (2)	7432 (5)	6.25 (8)
C(3)	7243 (4)	2895 (1)	7533 (3)	3.96 (5)
C(4)	6428 (4)	3298 (1)	8285 (4)	4.85 (6)
C(5)	7336 (4)	3744 (1)	8217 (4)	5.01 (6)
C(6)	9147 (4)	3815 (1)	7404 (3)	4.33 (5)
C(7)	9957 (4)	3406 (1)	6647 (4)	4.21 (5)
C(8)	9046 (4)	2961 (1)	6731 (3)	4.04 (5)
C(9)	7403 (4)	1974 (1)	7426 (3)	3.88 (5)
C(10)	9164 (4)	1917 (1)	8487 (3)	4.09 (5)
C(11)	10239 (4)	1493 (1)	8513 (4)	4.44 (5)
C(12)	9560 (5)	1125 (1)	7458 (4)	4.70 (5)
C(13)	7836 (5)	1168 (1)	6385 (4)	5.44 (7)
C(14)	6765 (5)	1593 (1)	6375 (4)	5.23 (6)
C(15)	11801 (7)	4323 (2)	6330 (7)	7.30 (9)
C(16)	8990 (9)	4686 (2)	7798 (7)	8.11 (11)
N(1)	10087 (4)	4255 (1)	7363 (4)	5.69 (6)
N(2)	10744 (6)	678 (1)	7468 (5)	6.65 (7)
O(1)	12258 (7)	647 (1)	8378 (6)	12.77 (10)
O(2)	10198 (5)	364 (1)	6483 (5)	10.16 (8)

withdrawing *p*-nitro group. However, it is impossible to conclude that conjugation is the cause of the observed difference in the twist angles because we cannot distinguish between packing and substituent effects. A view of the packing of the molecule of IV in the crystal is shown in Fig. 2. There are no unusually short intermolecular contacts in any of the four structures I–IV except N(2)···H(2') ($x + 0.5$, $y + 0.5$, z) = 2.44 (4) Å in I and O(1)···H(12) ($x - 0.5$, $0.5 - y$, $z - 0.5$) = 2.58 (6) Å in III.

The authors thank SPPS Belgium for financial support. They are grateful to Dr H. Allaine from the Laboratory of Organic Chemistry (Professor H. G. Viehe) who supplied the crystals.

Table 3. Selected structural parameters

	I	II	III	IV
Bond lengths (Å)				
C(2)–C(1)	1.333 (4)	1.32 (2)	1.327 (5)	1.334 (4)
C(3)–C(1)	1.485 (4)	1.49 (1)	1.473 (5)	1.480 (4)
C(9)–C(1)	1.486 (4)	—	1.493 (5)	1.492 (4)
mean C–C in phenyl I*	1.386 (4)	1.39 (1)	1.388 (5)	1.390 (4)
mean C–C in phenyl II*	1.382 (4)	—	1.381 (6)	1.380 (4)
C(16)–C(6)	1.442 (4)	—	—	—
C(16)–N(2)	1.131 (4)	—	—	—
C(15)–C(12)	1.458 (5)	—	—	—
C(15)–N(1)	1.127 (4)	—	—	—
O(1)–C(6)	—	1.36 (1)	1.368 (5)	—
O(1)–C(9)	—	1.41 (1)	—	—
O(1)–C(15)	—	—	1.416 (6)	—
N(1)–C(6)	—	—	—	1.374 (4)
N(1)–C(15)	—	—	—	1.440 (5)
N(1)–C(16)	—	—	—	1.450 (5)
N(2)–C(12)	—	—	—	1.468 (4)
N(2)–O(1)	—	—	—	1.192 (5)
N(2)–O(2)	—	—	—	1.203 (4)
Valence angles (°)				
C(3)–C(1)–C(2)	120.6 (3)	121.1 (5)	120.6 (4)	121.5 (3)
C(9)–C(1)–C(2)	120.6 (3)	—	119.9 (4)	119.2 (3)
C(9)–C(1)–C(3)	118.8 (2)	117.8 (5)	119.6 (3)	119.3 (2)
C(1)–C(3)–C(4)	121.1 (1)	122.4 (7)	122.4 (3)	122.2 (2)
C(1)–C(3)–C(8)	120.4 (2)	119.7 (9)	121.6 (3)	121.1 (2)
C(1)–C(9)–C(10)	121.3 (2)	—	120.6 (3)	120.9 (2)
C(1)–C(9)–C(14)	121.2 (3)	—	121.9 (3)	120.7 (2)
C(6)–C(16)–N(2)	178.5 (3)	—	—	—
C(12)–C(15)–N(1)	178.9 (3)	—	—	—
C(6)–O(1)–C(9)	—	118.3 (8)	—	—
C(6)–O(1)–C(15)	—	—	118.1 (3)	—
C(6)–N(1)–C(15)	—	—	—	120.0 (3)
C(6)–N(1)–C(16)	—	—	—	119.8 (3)
O(1)–N(2)–C(12)	—	—	—	119.4 (3)
O(2)–N(2)–C(12)	—	—	—	118.2 (3)
Torsion angles (°) ($\sigma = 1^\circ$)				
C(2)–C(1)–C(3)–C(4)	-38	-140	35	28
C(2)–C(1)–C(3)–C(8)	140	34	-143	-147
C(2)–C(1)–C(9)–C(10)	137	—	-139	-137
C(2)–C(1)–C(9)–C(14)	-41	—	38	40
C(5)–C(6)–O(1)–C(9)	—	0	—	—
C(7)–C(6)–O(1)–C(15)	—	—	4	—
C(7)–C(6)–N(1)–C(15)	—	—	—	9
C(5)–C(6)–N(1)–C(16)	—	—	—	-15
C(11)–C(12)–N(2)–O(1)	—	—	—	0
C(13)–C(12)–N(2)–O(2)	—	—	—	2
Angles between normals to planes (°) ($\sigma = 1^\circ$)*				
A/C	39	37	37	31
B/C	42	—	40	42
A/B	72	—	69	66

* A, B and C are respectively the mean planes through C(3), C(4), C(5), C(6), C(7), C(8) (phenyl I), C(9), C(10), C(11), C(12), C(13), C(14) (phenyl II) and C(1), C(2), C(3), C(9) (ethylenic bond).

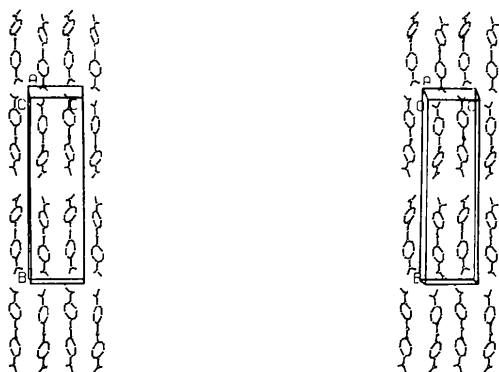


Fig. 2. View of molecular packing in the crystal of IV. (Program PLUTO, Motherwell & Clegg, 1978.)

References

CASALONE, G. & GAVEZZOTTI, A. (1971). *Rend. Ist. Lomb. Sci. Lett. A*, **105**, 824–833.

- CASALONE, G., GAVEZZOTTI, A., MARIANI, C., MUGNOLI, A. & SIMONETTA, M. (1970). *Acta Cryst.* **B26**, 1–8.
- CASALONE, G. & SIMONETTA, M. (1971). *J. Chem. Soc. B*, pp. 1180–1183.
- COATES, G. E. & SUTTON, L. E. (1942). *J. Chem. Soc.* pp. 567–570.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press (Present distributor D. Reidel, Dordrecht.)
- MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.
- MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.
- NORMENT, H. G. & KARLE, I. (1962). *Acta Cryst.* **15**, 873–878.
- PATTABHI, V. & VENKATESAN, K. (1973). *J. Cryst. Mol. Struct.* **3**, 25–35.
- SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
- SUZUKI, H. (1960). *Bull. Chem. Soc. Jpn.* **33**, 619–628.
- VAN DER LINDE, R., KORVER, O., KORVER, P. K., VEENLAND, J. V. & DE BOER, T. J. (1965). *Spectrochim. Acta*, **21**, 1893–1898.
- VAN DER VELDEN, G. P. & NOORDIK, J. H. (1979). *J. Cryst. Mol. Struct.* **9**, 283–294.

Acta Cryst. (1987). **C43**, 89–92

Structure of 3-Methylcytidinium Nitrate

BY MARIUSZ JASKÓLSKI

Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, ul. Grunwaldzka 6, 60–780 Poznań, Poland

AND MACIEJ WIEWIÓROWSKI

Institute of Bioorganic Chemistry, Polish Academy of Sciences, ul. Noskowskiego 12/14, 61–704 Poznań, Poland

(Received 7 April 1986; accepted 15 July 1986)

Abstract. $C_{10}H_{16}N_3O_5^+ \cdot NO_3^-$, $M_r = 320.3$, orthorhombic, $P2_12_12_1$, $a = 10.276$ (2), $b = 6.6950$ (6), $c = 20.244$ (2) Å, $V = 1392.8$ (2) Å³, $Z = 4$, $D_x = 1.53$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.088$ mm⁻¹, $F(000) = 672$, $T = 290$ K, $R = 0.042$ for 1015 observed reflexions. The dimensions and conformation [glycosidic torsion angle $\chi = 50.7$ (4)°, pseudorotation parameters $P = 168.1$ (7) and $\tau_m = 37.0$ (5)°, side-chain orientation $\gamma = 53.6$ (4)°] of the present 3-methylcytidinium cation are similar to those in 3-methylcytidinium chloride. The pyrimidine system shows slight but significant deviations from planarity and is overlapped by the NO_3^- anion. There is a three-dimensional network of weak H bonds in which all available proton donors are utilized and the acceptors are the nitrate O atoms and O(3') and O(5') on the ribose. O(5') is H-bonded to C(6) through a

weak intramolecular C(6)—H(6)···O(5') link [3.279 (6) Å].

Introduction. The present work is part of a series of investigations into the factors influencing dimensions and molecular interactions of nucleosides. In our previous papers we have studied the effects of base modification and protonation in both cytidine (Jaskólski, Krzyżosiak, Sierzputowska-Gracz & Wiewiórowski, 1981; Krzyżosiak, Jaskólski, Sierzputowska-Gracz & Wiewiórowski, 1982; Kozerski, Sierzputowska-Gracz, Krzyżosiak, Bratek-Wiewiórowska, Jaskólski & Wiewiórowski, 1984) and adenosine (Jaskólski, 1982*a,b*, 1984*a*) series. Our recent interest is concentrated on *N*-methylated nucleoside cations (Jaskólski & Alejska, 1985) and on the influence of different counter-anions on the conforma-