$C_{18}H_{20}O_4$

| | | | |
|---|---|---|---|
| O(3)—C(5) | 1.359 (5) | C(10)—C(11) | 1.533 (7) |
| O(3)—C(8) | 1.412 (6) | C(10)—C(12) | 1.507 (6) |
| O(4)—C(15) | 1.374 (5) | C(12)—C(13) | 1.372 (7) |
| O(4)—C(18) | 1.412 (6) | C(12)—C(17) | 1.403 (6) |
| C(2)—C(3) | 1.371 (6) | C(13)—C(14) | 1.400 (7) |
| C(2)—C(7) | 1.374 (7) | C(14)—C(15) | 1.366 (7) |
| C(3)—C(4) | 1.388 (6) | C(15)—C(16) | 1.381 (6) |
| C(4)—C(5) | 1.400 (6) | C(16)—C(17) | 1.386 (6) |
| C(1)—O(1)—C(7) | 104.5 (4) | O(1)—C(7)—C(6) | 127.5 (4) |
| C(1)—O(2)—C(2) | 105.0 (4) | C(2)—C(7)—C(6) | 122.6 (4) |
| C(5)—O(3)—C(8) | 119.9 (4) | O(3)—C(8)—C(9) | 109.4 (4) |
| C(15)—O(4)—C(18) | 117.1 (4) | C(4)—C(10)—C(11) | 113.8 (4) |
| O(1)—C(1)—O(2) | 109.0 (4) | C(4)—C(10)—C(12) | 112.4 (4) |
| O(2)—C(2)—C(3) | 129.1 (5) | C(11)—C(10)—C(12) | 111.8 (4) |
| O(2)—C(2)—C(7) | 109.6 (4) | C(10)—C(12)—C(13) | 121.6 (4) |
| C(3)—C(2)—C(7) | 121.1 (4) | C(10)—C(12)—C(17) | 121.0 (4) |
| C(2)—C(3)—C(4) | 118.6 (4) | C(13)—C(12)—C(17) | 117.3 (5) |
| C(3)—C(4)—C(5) | 119.6 (4) | C(12)—C(13)—C(14) | 121.9 (5) |
| C(3)—C(4)—C(10) | 121.6 (4) | C(13)—C(14)—C(15) | 120.0 (5) |
| C(5)—C(4)—C(10) | 118.8 (4) | O(4)—C(15)—C(14) | 124.6 (5) |
| O(3)—C(5)—C(4) | 115.3 (4) | O(4)—C(15)—C(16) | 115.7 (4) |
| O(3)—C(5)—C(6) | 122.9 (4) | C(14)—C(15)—C(16) | 119.7 (5) |
| C(4)—C(5)—C(6) | 121.8 (4) | C(15)—C(16)—C(17) | 120.2 (4) |
| C(5)—C(6)—C(7) | 116.2 (4) | C(12)—C(17)—C(16) | 121.0 (5) |
| O(1)—C(7)—C(2) | 109.9 (4) | | |

The title compound has one chiral centre but crystallized in an achiral space group as both enantiomers crystallized together. The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods using *MITHRIL* (Gilmore, 1984). H atoms were placed using optimum bonding geometry and were included in $F_c$. The H-atom displacement parameters and positions were not refined. Non-H atoms were refined anisotropically. The function minimized was $\Sigma w(|F_o| - |F_c|)^2$. Anomalous-dispersion effects were included in $F_c$ (Ibers & Hamilton, 1964). All calculations were performed using *TEXSAN* (Molecular Structure Corporation, 1985).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and torsion angles have been deposited with the IUCr (Reference: BR1059). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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# (Ozaphyrin)(TCNQ)$_{1/2}$

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## Abstract

Slow diffusion of an acetonitrile solution of tetracyanoquinodimethane (TCNQ) into a chloroform solution of the macrocycle ozaphyrin affords the title compound, 4,9,14,19-tetrapropyl-25-oxa-26,27,28,29-tetraazahexacyclo[20.2.1.1$^{2,5}$.1$^{8,11}$.1$^{12,15}$.1$^{18,21}$]nonacosa-2(26),3,5,7,9,11,13,15(28),16,18,20,22,24-tridecaene tetracyanoquinodimethane (2/1), $C_{36}H_{40}N_4O$.$0.5C_{12}H_4N_4$. The compound was characterized by a single-crystal X-ray structure determination. The packing consists of interspersed planar ozaphyrin and TCNQ molecules [mean deviations from least-squares planes, 0.041 (4) and 0.022 (4) Å, respectively]. The TCNQ molecule, which lies on an inversion center, is above one side of the ozaphyrin ring at a distance of about 3.3 Å.

## Comment

Porphyrins and related macrocycles have been widely used as donors in molecular conductors (Hoffman & Ibers, 1983; Marks, 1985) and some charge-transfer complexes (Kirner, Reed & Scheidt, 1977; Pace, Ulman & Ibers, 1982; Sidorov, 1975). The tetracyanoquinodimethane (TCNQ) molecule has been used in many organic conductors (Underhill, 1974). Here we report the structure of the 1:0.5 complex formed between the expanded macrocycle ozaphyrin and TCNQ. Ozaphyrin was synthesized as described previously (Miller, Johnson, Becker & Ibers, 1993). Crystals of the title compound (I) were obtained from slow diffusion of an acetonitrile solution of TCNQ into a chloroform solution of ozaphyrin.



(I)
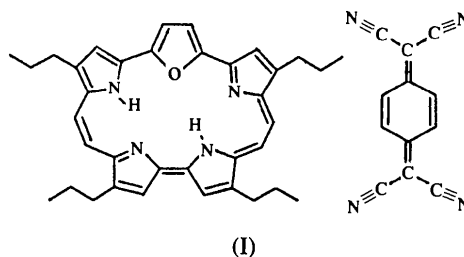
The structure consists of layers of staggered planar ozaphyrin molecules (Fig. 1a) with planar TCNQ molecules (Fig. 1b) interspersed between them. The mean deviations from the least-squares planes for non-H atoms of the ozaphyrin and TCNQ molecules are 0.041 (4) and 0.022 (4) Å, respectively. The TCNQ molecule lies over one of the two carbon bridges and two pyrrole rings of the ozaphyrin macrocycle. A stereoview of the packing in the unit cell is shown in Fig. 2. The least-squares planes of the two molecules are canted about 1.5° to each other and are about 3.3 Å apart. The closest H-atom contact is between a pyrrole H atom of ozaphyrin and an N atom of TCNQ [H(20)···N(1′) 2.399 (4) Å]. The closest non-H-atom interaction is C(1′)···N(2) with a distance of 3.280 (4) Å. The bond distances and angles within the ozaphyrin molecule of the present structure do not differ significantly from those found earlier (Miller, Johnson, Becker & Ibers, 1993), nor do the bond distances and angles of the TCNQ molecule differ signifcantly from those of the neutral molecule (Long, Sparks & Trueblood, 1965). The structural results indicate that the title compound is not a charge-transfer complex but a combination of the neutral molecules. Spectroscopic evidence, including near-IR, IR and UV–visible, is consistent with this conclusion (Pace, Ulman & Ibers, 1982).
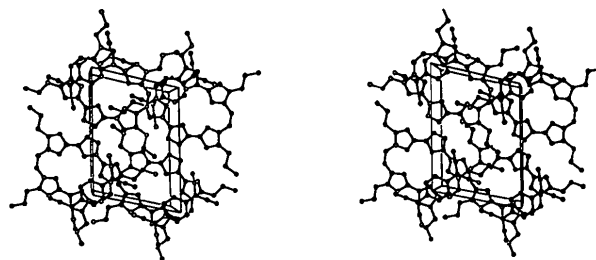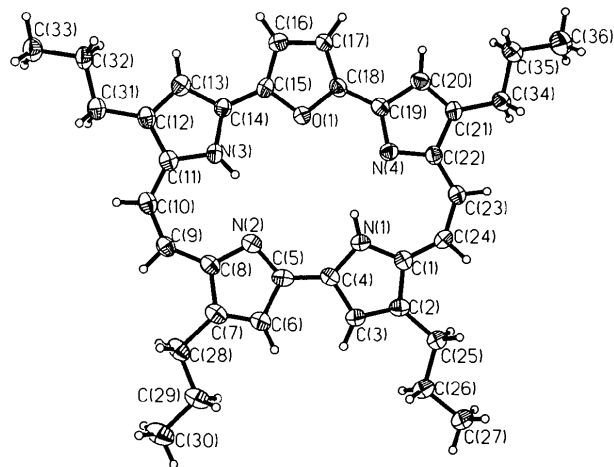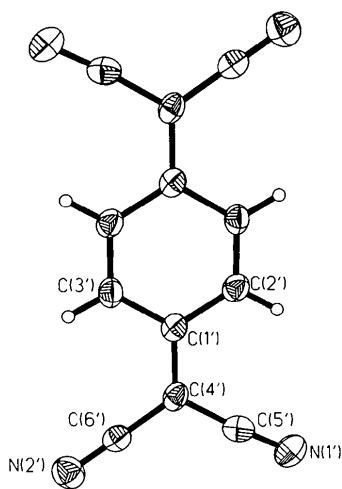


Fig. 2. Stereoview of the unit cell of (ozaphyrin)(TCNQ)$_{1/2}$ as viewed along the [001] direction.

## Experimental

### Crystal data
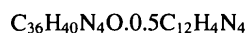
| | |
|---|---|
| $C_{36}H_{40}N_4O.0.5C_{12}H_4N_4$ | Cu $K\alpha$ radiation |
| $M_r = 646.82$ | $\lambda = 1.5418$ Å |
| Triclinic | Cell parameters from 47 |
| $P\bar{1}$ | reflections |
| $a = 10.104$ (2) Å | $\theta = 3.37–43.21°$ |
| $b = 13.479$ (3) Å | $\mu = 0.591$ mm$^{-1}$ |
| $c = 13.835$ (3) Å | $T = 113$ (2) K |
| $\alpha = 92.679$ (10)° | Flat block |
| $\beta = 108.491$ (10)° | $0.36 \times 0.12 \times 0.06$ mm |
| $\gamma = 101.262$ (10)° | Purple |
| $V = 1740.5$ (6) Å$^3$ | |
| $Z = 2$ | |
| $D_x = 1.234$ Mg m$^{-3}$ | |

### Data collection

| | |
|---|---|
| Picker diffractometer | $R_{int} = 0.0217$ |
| $\theta–2\theta$ scans | $\theta_{max} = 54.00°$ |
| Absorption correction: | $h = -5 \rightarrow 10$ |
| analytical | $k = -14 \rightarrow 13$ |
| $T_{min} = 0.919$, $T_{max} =$ | $l = -14 \rightarrow 13$ |
| 0.968 | 6 standard reflections |
| 5036 measured reflections | monitored every 100 |
| 4223 independent reflections | reflections |
| 2990 observed reflections | intensity variation: none |
| $[I > 2\sigma(I)]$ | |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $(\Delta/\sigma)_{max} = 0.118$ |
| $R(F) = 0.0487$ | $\Delta\rho_{max} = 0.535$ e Å$^{-3}$ |
| $wR(F^2) = 0.122$ | $\Delta\rho_{min} = -0.197$ e Å$^{-3}$ |
| $S = 1.64$ | Atomic scattering factors |
| 4223 reflections | from International Tables |
| 443 parameters | for Crystallography (1992, |
| H atoms riding | Vol. C, Tables 4.2.6.8 and |
| $w = 1/[\sigma^2(F_o^2) + (0.04F_o^2)^2]$ | 6.1.1.4) |



(a)



(b)

Fig. 1. The labeling scheme and thermal ellipsoids (50% probability) for (a) ozaphyrin and (b) TCNQ.

$\mathrm{C_{36}H_{40}N_4O.0.5C_{12}H_4N_4}$

## Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å$^2$)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| O(1) | 0.0826 (2) | 0.7167 (2) | 0.6886 (2) | 0.0314 (6) |
| N(1) | 0.4300 (3) | 0.9532 (2) | 0.8411 (2) | 0.0302 (7) |
| N(2) | 0.1193 (3) | 1.0163 (2) | 0.7799 (2) | 0.0309 (7) |
| N(3) | −0.1104 (3) | 0.8478 (2) | 0.6741 (2) | 0.0310 (7) |
| N(4) | 0.3827 (3) | 0.7419 (2) | 0.7787 (2) | 0.0304 (7) |
| C(1) | 0.5767 (3) | 0.9661 (2) | 0.8842 (2) | 0.0285 (8) |
| C(2) | 0.6322 (3) | 1.0696 (2) | 0.9284 (2) | 0.0298 (8) |
| C(3) | 0.5209 (3) | 1.1150 (2) | 0.9116 (2) | 0.0313 (8) |
| C(4) | 0.3911 (3) | 1.0429 (2) | 0.8562 (2) | 0.0294 (8) |
| C(5) | 0.2578 (4) | 1.0722 (2) | 0.8280 (2) | 0.0318 (9) |
| C(6) | 0.2558 (4) | 1.1774 (2) | 0.8522 (2) | 0.0349 (9) |
| C(7) | 0.1197 (4) | 1.1860 (2) | 0.8206 (2) | 0.0337 (9) |
| C(8) | 0.0330 (4) | 1.0849 (2) | 0.7755 (2) | 0.0299 (8) |
| C(9) | −0.1161 (3) | 1.0696 (2) | 0.7368 (2) | 0.0317 (8) |
| C(10) | −0.2284 (4) | 0.9884 (3) | 0.6879 (2) | 0.0339 (9) |
| C(11) | −0.2292 (3) | 0.8874 (2) | 0.6574 (2) | 0.0310 (8) |
| C(12) | −0.3511 (3) | 0.8097 (3) | 0.6044 (2) | 0.0327 (8) |
| C(13) | −0.3005 (3) | 0.7243 (3) | 0.5900 (2) | 0.0348 (9) |
| C(14) | −0.1519 (3) | 0.7474 (2) | 0.6335 (2) | 0.0288 (8) |
| C(15) | −0.0599 (3) | 0.6815 (2) | 0.6388 (2) | 0.0303 (8) |
| C(16) | −0.0855 (4) | 0.5796 (2) | 0.6023 (3) | 0.0354 (9) |
| C(17) | 0.0442 (3) | 0.5516 (2) | 0.6322 (2) | 0.0317 (8) |
| C(18) | 0.1467 (3) | 0.6359 (2) | 0.6853 (3) | 0.0308 (8) |
| C(19) | 0.2953 (3) | 0.6520 (2) | 0.7315 (2) | 0.0301 (8) |
| C(20) | 0.3739 (4) | 0.5730 (2) | 0.7316 (3) | 0.0353 (9) |
| C(21) | 0.5126 (4) | 0.6159 (2) | 0.7792 (3) | 0.0324 (8) |
| C(22) | 0.5170 (3) | 0.7228 (2) | 0.8086 (2) | 0.0299 (8) |
| C(23) | 0.6399 (3) | 0.7940 (2) | 0.8580 (3) | 0.0357 (9) |
| C(24) | 0.6632 (4) | 0.8980 (2) | 0.8898 (3) | 0.0358 (9) |
| C(25) | 0.7879 (3) | 1.1169 (2) | 0.9847 (3) | 0.0346 (9) |
| C(26) | 0.8187 (3) | 1.2278 (2) | 1.0279 (3) | 0.0402 (9) |
| C(27) | 0.9766 (3) | 1.2707 (3) | 1.0832 (3) | 0.0437 (10) |
| C(28) | 0.0658 (4) | 1.2822 (2) | 0.8277 (3) | 0.0401 (9) |
| C(29) | 0.1858 (4) | 1.3738 (2) | 0.8873 (3) | 0.0469 (10) |
| C(30) | 0.1302 (4) | 1.4675 (3) | 0.9037 (3) | 0.0563 (11) |
| C(31) | −0.5046 (3) | 0.8190 (3) | 0.5707 (3) | 0.0345 (9) |
| C(32) | −0.6073 (3) | 0.7231 (2) | 0.5089 (3) | 0.0369 (9) |
| C(33) | −0.7605 (3) | 0.7356 (3) | 0.4717 (3) | 0.0435 (10) |
| C(34) | 0.6376 (3) | 0.5673 (2) | 0.7966 (3) | 0.0387 (9) |
| C(35) | 0.5988 (4) | 0.4541 (3) | 0.7581 (3) | 0.0564 (12) |
| C(36) | 0.7281 (4) | 0.4068 (3) | 0.7800 (3) | 0.0637 (12) |
| N(1') | 0.7956 (3) | 0.6656 (2) | 0.3667 (2) | 0.0431 (8) |
| N(2') | 0.5029 (3) | 0.8769 (2) | 0.3390 (2) | 0.0412 (8) |
| C(1') | 0.8775 (3) | 0.9229 (2) | 0.4462 (2) | 0.0272 (8) |
| C(2') | 1.0174 (3) | 0.9021 (2) | 0.4807 (2) | 0.0300 (8) |
| C(3') | 0.8651 (3) | 1.0254 (2) | 0.4677 (2) | 0.0300 (8) |
| C(4') | 0.7580 (3) | 0.8472 (2) | 0.3956 (2) | 0.0294 (8) |
| C(5') | 0.7743 (3) | 0.7452 (3) | 0.3776 (3) | 0.0332 (8) |
| C(6') | 0.6167 (4) | 0.8636 (2) | 0.3630 (2) | 0.0288 (8) |

## Table 2. *Selected geometric parameters* (Å, °)

| | | | |
|---|---|---|---|
| O(1)—C(15) | 1.358 (4) | C(15)—C(16) | 1.386 (4) |
| O(1)—C(18) | 1.379 (4) | C(16)—C(17) | 1.376 (4) |
| N(1)—C(4) | 1.369 (4) | C(17)—C(18) | 1.372 (4) |
| N(1)—C(1) | 1.383 (4) | C(18)—C(19) | 1.400 (4) |
| N(2)—C(8) | 1.379 (4) | C(19)—C(20) | 1.447 (4) |
| N(2)—C(5) | 1.386 (4) | C(20)—C(21) | 1.340 (4) |
| N(3)—C(11) | 1.365 (4) | C(21)—C(22) | 1.467 (4) |
| N(3)—C(14) | 1.372 (4) | C(21)—C(34) | 1.493 (4) |
| N(4)—C(19) | 1.348 (4) | C(22)—C(23) | 1.366 (4) |
| N(4)—C(22) | 1.367 (4) | C(23)—C(24) | 1.401 (4) |
| C(1)—C(24) | 1.374 (4) | C(25)—C(26) | 1.518 (4) |
| C(1)—C(2) | 1.426 (4) | C(26)—C(27) | 1.513 (4) |
| C(2)—C(3) | 1.345 (4) | C(28)—C(29) | 1.536 (5) |
| C(2)—C(25) | 1.507 (4) | C(29)—C(30) | 1.514 (5) |
| C(3)—C(4) | 1.430 (4) | C(31)—C(32) | 1.513 (4) |
| C(4)—C(5) | 1.418 (4) | C(32)—C(33) | 1.515 (4) |
| C(5)—C(6) | 1.447 (4) | C(34)—C(35) | 1.525 (4) |
| C(6)—C(7) | 1.335 (4) | C(35)—C(36) | 1.516 (5) |
| C(7)—C(8) | 1.457 (4) | N(1')—C(5') | 1.147 (4) |
| C(7)—C(28) | 1.512 (4) | N(2')—C(6') | 1.144 (4) |
| C(8)—C(9) | 1.399 (4) | C(1')—C(4') | 1.380 (4) |
| C(9)—C(10) | 1.379 (4) | C(1')—C(2') | 1.429 (4) |
| C(10)—C(11) | 1.404 (4) | C(1')—C(3') | 1.438 (4) |
| C(11)—C(12) | 1.416 (4) | C(2')—C(3'$^i$) | 1.349 (4) |
| C(12)—C(13) | 1.378 (4) | C(3')—C(2'$^i$) | 1.349 (4) |
| C(12)—C(31) | 1.503 (4) | C(4')—C(6') | 1.420 (5) |
| C(13)—C(14) | 1.394 (4) | C(4')—C(5') | 1.437 (5) |
| C(14)—C(15) | 1.394 (4) | | |
| C(15)—O(1)—C(18) | 106.9 (2) | O(1)—C(15)—C(14) | 119.1 (3) |
| C(4)—N(1)—C(1) | 109.9 (3) | C(16)—C(15)—C(14) | 131.7 (3) |
| C(8)—N(2)—C(5) | 105.3 (3) | C(17)—C(16)—C(15) | 107.2 (3) |
| C(11)—N(3)—C(14) | 109.0 (3) | C(18)—C(17)—C(16) | 107.5 (3) |
| C(19)—N(4)—C(22) | 104.6 (3) | C(17)—C(18)—O(1) | 109.1 (3) |
| C(24)—C(1)—N(1) | 130.8 (3) | C(17)—C(18)—C(19) | 132.3 (3) |
| C(24)—C(1)—C(2) | 122.2 (3) | O(1)—C(18)—C(19) | 118.6 (3) |
| N(1)—C(1)—C(2) | 107.0 (3) | N(4)—C(19)—C(18) | 124.9 (3) |
| C(3)—C(2)—C(1) | 107.5 (3) | N(4)—C(19)—C(20) | 111.9 (3) |
| C(3)—C(2)—C(25) | 127.4 (3) | C(18)—C(19)—C(20) | 123.2 (3) |
| C(1)—C(2)—C(25) | 125.1 (3) | C(21)—C(20)—C(19) | 107.0 (3) |
| C(2)—C(3)—C(4) | 109.6 (3) | C(20)—C(21)—C(22) | 105.3 (3) |
| N(1)—C(4)—C(5) | 133.3 (3) | C(20)—C(21)—C(34) | 127.9 (3) |
| N(1)—C(4)—C(3) | 106.0 (3) | C(22)—C(21)—C(34) | 126.8 (3) |
| C(5)—C(4)—C(3) | 120.6 (3) | C(23)—C(22)—N(4) | 124.6 (3) |
| N(2)—C(5)—C(4) | 131.3 (3) | C(23)—C(22)—C(21) | 124.1 (3) |
| N(2)—C(5)—C(6) | 109.8 (3) | N(4)—C(22)—C(21) | 111.2 (3) |
| C(4)—C(5)—C(6) | 118.9 (3) | C(22)—C(23)—C(24) | 131.4 (3) |
| C(7)—C(6)—C(5) | 108.0 (3) | C(1)—C(24)—C(23) | 134.8 (3) |
| C(6)—C(7)—C(8) | 106.6 (3) | C(2)—C(25)—C(26) | 114.9 (3) |
| C(6)—C(7)—C(28) | 126.9 (3) | C(27)—C(26)—C(25) | 112.2 (3) |
| C(8)—C(7)—C(28) | 126.6 (3) | C(7)—C(28)—C(29) | 112.7 (3) |
| N(2)—C(8)—C(9) | 129.9 (3) | C(30)—C(29)—C(28) | 112.7 (3) |
| N(2)—C(8)—C(7) | 110.3 (3) | C(12)—C(31)—C(32) | 112.8 (3) |
| C(9)—C(8)—C(7) | 119.8 (3) | C(33)—C(32)—C(31) | 112.0 (3) |
| C(10)—C(9)—C(8) | 135.7 (3) | C(21)—C(34)—C(35) | 114.6 (3) |
| C(9)—C(10)—C(11) | 130.7 (3) | C(36)—C(35)—C(34) | 113.0 (3) |
| N(3)—C(11)—C(10) | 125.1 (3) | C(4')—C(1')—C(2') | 121.5 (3) |
| N(3)—C(11)—C(12) | 108.4 (3) | C(4')—C(1')—C(3') | 120.9 (3) |
| C(10)—C(11)—C(12) | 126.5 (3) | C(2')—C(1')—C(3') | 117.6 (3) |
| C(13)—C(12)—C(11) | 106.1 (3) | C(3'$^i$)—C(2')—C(1') | 122.3 (3) |
| C(13)—C(12)—C(31) | 127.2 (3) | C(2'$^i$)—C(3')—C(1') | 120.1 (3) |
| C(11)—C(12)—C(31) | 126.7 (3) | C(1')—C(4')—C(6') | 123.4 (3) |
| C(12)—C(13)—C(14) | 109.1 (3) | C(1')—C(4')—C(5') | 119.3 (3) |
| N(3)—C(14)—C(13) | 107.4 (3) | C(6')—C(4')—C(5') | 117.2 (3) |
| N(3)—C(14)—C(15) | 125.2 (3) | N(1')—C(5')—C(4') | 175.9 (4) |
| C(13)—C(14)—C(15) | 127.4 (3) | N(2')—C(6')—C(4') | 178.5 (4) |
| O(1)—C(15)—C(16) | 109.2 (3) | | |

Symmetry code: (i) $2 - x, 2 - y, 1 - z$.

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# Structure and Conformation of 5-Hydroxymethyl-2'-deoxycytidine, C10H15N3O5

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## Abstract

The deoxyribose ring in the title compound adopts a C(3')-*endo* envelope conformation ($^3E$), with the glycosyl linkage *anti* [$\chi = 195.8\,(1)°$]. The pseudorotational parameters are $P = 10.2\,(2)°$ and $\tau_m = 32.1\,(2)°$. The exocyclic side chain at C(5') has the $t$ conformation [$\gamma = 174.6\,(2)°$]. The hydroxymethyl group side chain at C(5) is on the opposite side of the pyrimidine plane as is O(4') of the furanose ring.

## Comment

Oxopyrimidines are novel constituents of the DNA of certain lytic bacteriophages (Kallen, Simon & Mamur, 1962; Roscoe & Tucker, 1964; Witmer & Wiatr, 1985). The title compound, 5-hydroxymethyl-2'-deoxycytidine (HMdCyd) (I), was synthesized and its molecular conformation was determined.



(I)
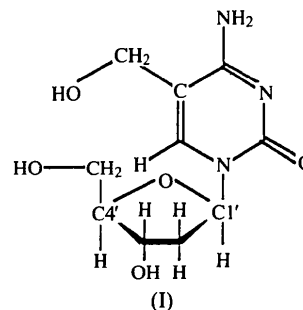
The bond lengths and angles for HMdCyd are in the range reported for 2'-deoxycytidine nucleosides (Young & Wilson, 1975; Kashino, Negishi & Hayatsu, 1988; Low, Tollin, Howie & Wilson, 1988; Silverton, Quinn, Haugwitz & Todaro, 1988; Jia, Tourigny, Stuart, Delbaere & Gupta, 1990a,b; De Winter, Blaton, Peeters, De Ranter, Van Aerschot & Herdewijn, 1991). The glycosidic bond has the *anti* conformation and the glycosidic torsion angle C(2)—N(1)—C(1')—O(4') is $\chi = 195.8\,(1)°$. The exocyclic 5'-CH2OH side chain has the $t$ conformation [$\gamma = 174.6\,(2)°$]. Although, the $g^+$ conformation is the most common found in cytidine and deoxycytidine compounds, the $t$ conformation has been reported for 5-methyl-2'-deoxycytidine (Sato, 1988) and 5-methoxymethyl-$N^4$-methyl-2'-deoxycytidine (Jia *et al.*, 1990b). The HMdCyd molecule adopts a C(3')-*endo* envelope conformation. The displacement of the C(3') atom from the mean plane through the other four ring atoms is 0.502 (3) Å in (I). The values calculated for the two pseudorotational parameters (Altona & Sundaralingam, 1972) of the furanose ring torsion angles are
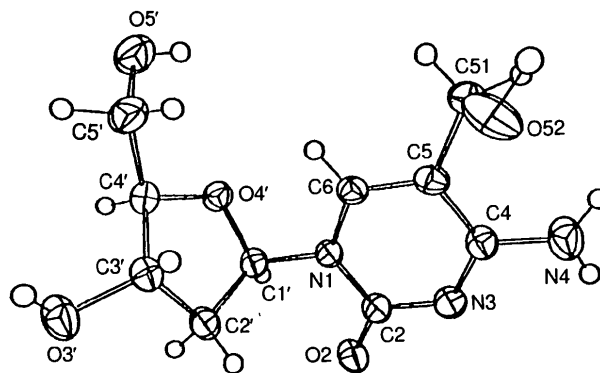


Fig. 1. A perspective view (*ORTEP*II; Johnson, 1976) of HMdCyd. Thermal ellipsoids are drawn at the 50% probability level.