Tableau 4. *Distances interatomiques* (Å) *dans l'environnement du fer*

2× Fe–O(*E*11)	1,999 (4)
2× Fe–O(*E*13)	1,974 (4)
2× Fe–O(*E*)	2,007 (3)

données, pour lesquelles $|F_o| > 10$, amènent le facteur R à une valeur de 0,043.*

Le Tableau 2 donne les coordonnées cristallographiques et les facteurs thermiques isotropes. Le Tableau 3 rassemble les longueurs et directions des axes des ellipsoïdes de vibration thermique.

Discussion. La Fig. 1 représente la projection de la structure sur le plan *ac*.

Les atomes de fer occupent des sites octaédriques (Tableau 4) et assurent, dans les trois directions de l'espace, la cohésion entre les différents groupements P_3O_{10}.

Les distances et les angles de liaison (Tableau 5) trouvés ici pour les anions P_3O_{10} sont comparables à ceux rencontrés dans d'autres structures de tripolyphosphates.

Tableau 5. *Distances interatomiques* (Å) *et principaux angles* (°) *de liaison dans l'anion* P_3O_{10}

P(1)	O(*E*11)	O(*E*12)	O(*E*13)	O(*L*)
O(*E*11)	1,518 (3)	2,533 (5)	2,483 (5)	2,539 (4)
O(*E*12)	113,6 (2)	1,509 (4)	2,519 (6)	2,462 (5)
O(*E*13)	111,0 (2)	114,0 (2)	1,494 (4)	2,463 (5)
O(*L*)	108,4 (2)	104,2 (2)	104,9 (2)	1,611 (3)
P(2)	**O(*E*)**	**O(*E'*)**	**O(*L*)**	**O(*L'*)**
O(*E*)	1,495 (3)	2,548 (7)	2,530 (5)	2,454 (4)
O(*E'*)	116,9 (2)	1,495 (3)	2,454 (4)	2,530 (5)
O(*L*)	110,7 (2)	105,9 (2)	1,580 (4)	2,528 (7)
O(*L'*)	105,9 (2)	110,7 (2)	106,3 (2)	1,580 (4)

La molécule d'eau O(*W*) ne possède que deux proches voisins qui sont les atomes d'oxygène O(*E*12), distants de O(*W*) de 2,87 Å.

Il faut signaler que les atomes d'oxygène O(*E*12) ne possèdent pas d'autres proches voisins cations hormis le phosphore.

* Les listes des facteurs de structure et des facteurs d'agitation thermique anisotrope ont été déposées au dépôt d'archives de la British Library Lending Division (Supplementary Publication No. SUP 32455: 9 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, Angleterre.

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1′-(3-Cyano-3,3-diphenylpropyl)(1,4′-bipiperidine)-4′-carboxamide Dihydrate: Piritramide

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Abstract. $C_{27}H_{34}N_4O.2H_2O$, monoclinic, $P2_1/c$; $a = 14{\cdot}967\,(5)$, $b = 12{\cdot}967\,(5)$, $c = 13{\cdot}837\,(5)$ Å $\beta = 93{\cdot}17\,(5)°$; $D_m = 1{\cdot}16$, $D_c = 1{\cdot}15$ g cm^{-3}, $Z = 4$. The molecular packing is essentially a result of hydrogen bonding.

Introduction. The present study was undertaken as part of an investigation of the structure–activity relationship in narcotic analgesics. The title compound, commercially known as Dipidolor®, is a potent analgesic which shows anti-diarrhoeal properties.

Colourless prismatic crystals were obtained by evaporation of a solution in ethanol. The space group was determined from rotation and Weissenberg photographs. The cell dimensions and intensities were measured on a CAD-4 automatic diffractometer. The experimental conditions are given in Table 1.

The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). The fifth set obtained from the tangent formula contained the whole structure. Full-matrix least-squares refinement was performed with the X-RAY 72 system (Stewart, Kruger, Ammon,

Dickinson & Hall, 1972). Refinement with anisotropic temperature factors for the O, N and C atoms, and with isotropic temperature factors for H, converged at $R = 0.049$ (for observed reflexions). The final positional parameters are given in Table 2.*

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32410 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Experimental conditions*

Source: Cu $K\bar{\alpha}$, $\lambda = 1.54178$ Å
Scan: ω–2θ
Graphite monochromator
Confidence level: 2.5σ with $\sigma^2(I) = S + B + (0.035)^2$, S being the scan and B the background count
$\Delta\theta = 0.7 + 0.3 \text{ tg } \theta$
$\theta_{min} = 2.0°$; $\theta_{max} = 70.0°$
Aperture: $2.5 + 0.5 \text{ tg } \theta$
$t_{max} = 120$ s
Total number of independent reflexions: 4687
Number observed: 2256

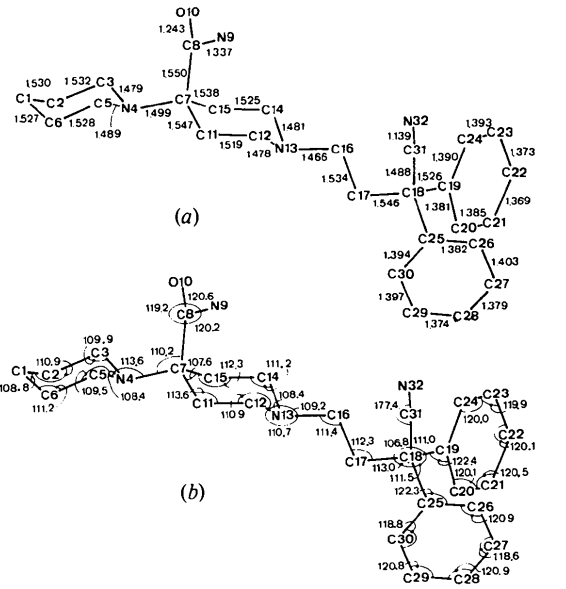

Fig. 1. Molecular structure and numbering scheme with (*a*) bond lengths (Å) and (*b*) angles (°). The maximum e.s.d.'s for the lengths are 0.015 Å, and 0.7° for the angles.

Table 2. *Final positional parameters* ($\times 10^4$) *with standard deviations in parentheses*

	x	*y*	*z*		*x*	*y*	*z*
C(1)	8208 (3)	2852 (5)	4768 (4)	H(21)	8095 (64)	3455 (82)	6201 (74)
C(2)	8051 (3)	2709 (5)	5843 (4)	H(22)	8569 (46)	2199 (57)	6158 (52)
C(3)	7133 (3)	2227 (4)	5980 (3)	H(31)	7035 (40)	2162 (50)	6765 (47)
N(4)	6421 (2)	2898 (3)	5542 (2)	H(32)	7091 (93)	1470 (95)	5659 (99)
C(5)	6533 (3)	2955 (4)	4481 (3)	H(51)	6505 (90)	2197 (95)	4166 (93)
C(6)	7429 (3)	3464 (5)	4298 (4)	H(52)	5995 (51)	3438 (65)	4144 (58)
C(7)	5499 (2)	2600 (3)	5810 (2)	H(61)	7514 (38)	3499 (47)	3527 (43)
C(8)	5272 (2)	1497 (3)	5442 (3)	H(62)	7445 (46)	4239 (55)	4603 (51)
N(9)	5324 (2)	698 (3)	6053 (2)	H(91)	5464 (43)	863 (51)	6825 (48)
O(10)	5070 (2)	1361 (2)	4567 (2)	H(92)	5116 (39)	−128 (51)	5761 (43)
C(11)	5452 (2)	2714 (3)	6919 (3)	H(111)	5848 (38)	2098 (46)	7270 (43)
C(12)	4508 (3)	2645 (3)	7263 (3)	H(112)	5733 (44)	3458 (54)	7137 (49)
N(13)	3923 (2)	3433 (3)	6784 (2)	H(121)	4234 (43)	1885 (55)	7089 (50)
C(14)	2893 (3)	3247 (3)	5727 (3)	H(122)	4524 (43)	2765 (52)	8042 (48)
C(15)	4819 (3)	3357 (3)	5331 (3)	H(141)	3649 (37)	2465 (45)	5584 (42)
C(16)	3013 (3)	3369 (4)	7123 (3)	H(142)	3441 (37)	3799 (49)	5366 (43)
C(17)	2971 (3)	2781 (4)	8159 (3)	H(151)	4770 (48)	3213 (57)	4555 (54)
C(18)	2052 (3)	3585 (3)	8581 (3)	H(152)	5058 (99)	4142 (95)	5467 (96)
C(19)	1319 (3)	4003 (4)	7877 (3)	H(161)	2562 (42)	3812 (51)	6647 (47)
C(20)	806 (4)	3371 (5)	7265 (5)	H(162)	2807 (44)	2559 (58)	7114 (51)
C(21)	204 (5)	3796 (8)	6580 (6)	H(171)	3487 (39)	3394 (47)	8620 (44)
C(22)	89 (5)	4842 (9)	6524 (6)	H(172)	3108 (48)	4606 (58)	8153 (54)
C(23)	602 (5)	5483 (6)	7118 (4)	H(201)	896 (44)	2524 (59)	7298 (53)
C(24)	1220 (3)	5066 (5)	7801 (4)	H(211)	9746 (66)	3345 (80)	6092 (74)
C(25)	1981 (3)	4041 (4)	9610 (3)	H(221)	9637 (88)	5202 (95)	6007 (99)
C(26)	2716 (3)	4417 (4)	10147 (3)	H(231)	549 (61)	6369 (78)	7085 (73)
C(27)	2632 (4)	4807 (4)	11083 (4)	H(241)	1614 (68)	5581 (80)	8303 (76)
C(28)	1798 (5)	4808 (5)	11460 (4)	H(261)	3366 (70)	4416 (84)	9831 (80)
C(29)	1064 (4)	4429 (6)	10935 (4)	H(271)	3216 (93)	5100 (95)	11509 (97)
C(30)	1142 (4)	4042 (5)	10001 (4)	H(281)	1726 (80)	5099 (97)	12186 (91)
C(31)	1966 (3)	2449 (5)	8699 (4)	H(291)	392 (94)	4454 (90)	11248 (87)
N(32)	1929 (3)	1580 (4)	8811 (4)	H(301)	564 (77)	3738 (96)	9586 (86)
O(33)	4720 (4)	5419 (4)	6923 (3)	H(331)	4393 (42)	4896 (53)	6916 (47)
O(34)	6527 (4)	4981 (5)	6405 (5)	H(332)	5298 (43)	5257 (52)	6834 (48)
H(11)	8825 (92)	3269 (99)	4694 (98)	H(341)	6934 (49)	5360 (60)	6356 (54)
H(12)	8238 (69)	2101 (87)	4426 (77)	H(342)	6602 (49)	4453 (60)	6069 (54)

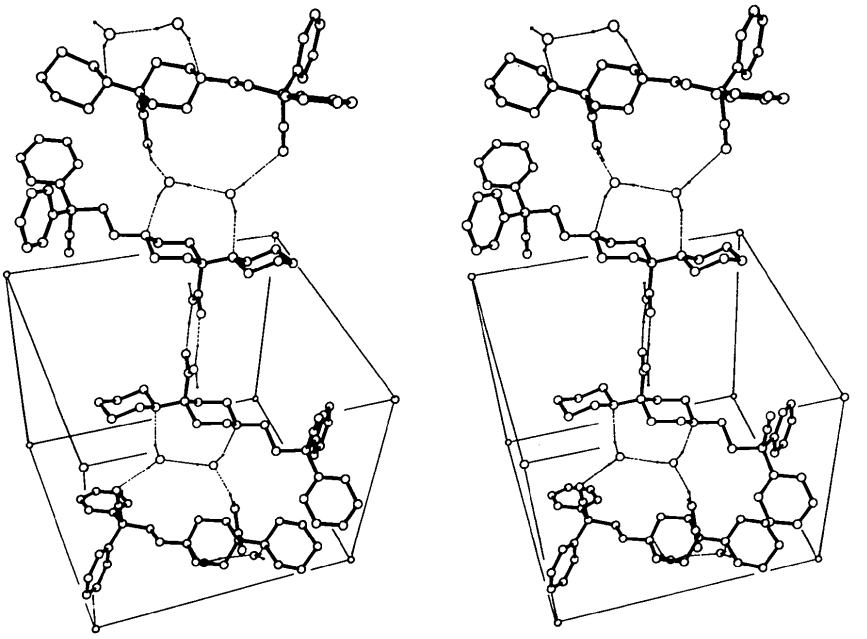

Fig. 2. Stereoscopic view of the molecular packing (Johnson, 1965). The hydrogen bonds are indicated by dotted lines.

Table 3. *Torsion angles*

C(3)–N(4)–C(7)–C(8)	−61·86°
C(5)–N(4)–C(7)–C(8)	62·33
N(4)–C(7)–C(8)–O(10)	−76·29
N(4)–C(7)–C(8)–N(9)	101·36
C(12)–N(13)–C(16)–C(17)	73·04
C(14)–N(13)–C(16)–C(17)	−167·68
N(13)–C(16)–C(17)–C(18)	−172·21
C(16)–C(17)–C(18)–C(31)	67·23
C(16)–C(17)–C(18)–C(19)	−52·74
C(16)–C(17)–C(18)–C(25)	−177·31

Discussion. The atomic numbering, bond distances and angles are given in Fig. 1. The main torsion angles required to describe the structure are listed in Table 3.

Fig. 2 shows that the molecular packing is essentially due to hydrogen bonds which arise between the following atoms:
N(4)[x,y,z]–O(34)[x,y,z]: 2·947 Å; N(4)···H(342)–O(34): 159·24°; N(32)[$x, \frac{1}{2}-y, \frac{1}{2}+z$]–O(34)[$\bar{x},\bar{y},\bar{z}$]: 3·126 Å; O(34)–H(341)···N(32): 176·06°; N(13)[x,y,z]–O(33)[x,y,z]: 2·831 Å; N(13)···H(331)–O(33): 162·95°; O(33)[x,y,z]–O(34)[x,y,z]: 2·892 Å; O(34)···H(332)–O(33): 170·10°; N(9)[x,y,z]–O(10)[$\bar{x},\bar{y},\bar{z}$]: 2·885 Å; N(9)–H(92)···O(10): 172·58°; N(9)[$x, \frac{1}{2}-y, \frac{1}{2}+z$]–O(33)[$\bar{x},\bar{y},\bar{z}$]: 2·827 Å; N(9)–H(91)···O(33): 145·42°.

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