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References

- CRAWSHAW, T. H. (1982). PhD. thesis, Univ. of Sheffield, pp. 105.
- CRAWSHAW, T. H., LAIDLER, D. A., METCALFE, J. C., PETTMAN, R. B., STODDART, J. F. & WOLSTENHOLME, J. B. (1982). *The Proceedings of the 26th OHOLO Biological Conference on Biomimetic Chemistry and Transition State Analogues as Approaches to Understanding Enzyme Catalysis*, edited by B. S. GREEN, Y. ASHANI & D. CHIPMAN, pp. 49–65. Amsterdam: Elsevier.
- GOLDBERG, I. (1984). *Inclusion Compounds*. Vol. 2. *Structural Aspects of Inclusion Compounds formed by Organic Host Lattices*, edited by J. L. ATWOOD, J. E. D. DAVIES & D. D. MACNICOL, pp. 261–335. London: Academic Press.
- GOLDBERG, I. & REZMOVITZ, H. (1978). *Acta Cryst.* **B34**, 2894–2896.
- GOODWIN, J. C., HODGE, J. E. & WEISLEDER, D. (1980). *Carbohydr. Res.* **79**, 133–141.
- GROOTENHUIS, P. D. J., VAN STAVEREN, C. J., DEN HERTOEG, H. J., REINHOUDT, D. N., BOS, M., UITERWIJK, J. W. H. M., KRUISE, L. & HARKEMA, S. (1984). *J. Chem. Soc. Chem. Commun.* pp. 1412–1413.
- International Tables for X-ray Crystallography*. (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
- MAVERICK, E., GROSSENBACHER, L. & TRUEBLOOD, K. N. (1979). *Acta Cryst.* **B35**, 2233–2237.
- METCALFE, J. C., STODDART, J. F., JONES, G., CRAWSHAW, T. H., GAVUZZO, E. & WILLIAMS, D. J. (1981). *J. Chem. Soc. Chem. Commun.* pp. 432–434.
- METCALFE, J. C., STODDART, J. F., JONES, G., CRAWSHAW, T. H., QUICK, A. & WILLIAMS, D. J. (1981). *J. Chem. Soc. Chem. Commun.* pp. 430–432.
- MONTGOMERY, R. & WIGGINS, L. F. (1948). *J. Chem. Soc.* pp. 2204–2208.
- NEWKOME, G. R., FRONCZEK, F. R. & KOHLI, D. K. (1981). *Acta Cryst.* **B37**, 2114–2117.
- NEWKOME, G. R., MAJESTIC, V. K. & FRONCZEK, F. R. (1981). *Tetrahedron Lett.* **22**, 3035–3038.
- SHAHRIARI-ZAVAREH, H., STODDART, J. F., WILLIAMS, M. K., ALLWOOD, B. L. & WILLIAMS, D. J. (1985). *J. Inclusion Phenom.* **3**, 355–377.
- SHELDRIK, G. M. (1983). *SHELXTL*, revision 4.0, January 1983. *An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data*. Univ. of Göttingen.
- STAVEREN, C. J. VAN, DEN HERTOEG, H. J., REINHOUDT, D. N., UITERWIJK, J. W. H. M., KRUISE, L. & HARKEMA, S. (1984). *J. Chem. Soc. Chem. Commun.* pp. 1409–1411.
- STODDART, J. F. (1979). *Chem. Soc. Rev.* **8**, 85–142.
- STODDART, J. F. (1981). *Progress in Macrocyclic Chemistry*, edited by R. M. IZATT & J. J. CHRISTENSEN, Vol. 2, pp. 173–250. New York: Wiley-Interscience.

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Structure Analysis of Minaprine Analogs: 3-Morpholinoethylamino-6-phenyl-4-pyridazinecarboxamide Monohydrate (I) and Butyl 3-Phenethylamino-6-phenyl-4-pyridazinecarboxylate (II)

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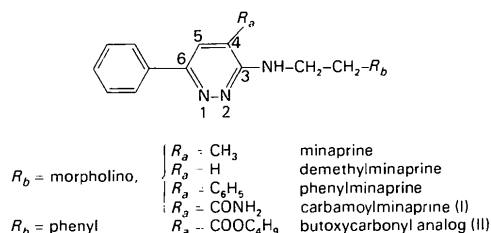
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Abstract. (I): $C_{17}H_{21}N_5O_2 \cdot H_2O$, $M_r = 345.4$, orthorhombic, $Pccn$, $a = 7.576$ (1), $b = 29.759$ (3), $c = 31.324$ (4) Å, $V = 7062.5$ Å³, $Z = 16$ (two molecules in the asymmetric unit), $D_x = 1.30$ Mg m⁻³, $\lambda(Cu K\alpha) = 1.54178$ Å, $\mu = 6.66$ mm⁻¹, $F(000) = 2944$, $T = 293$ K, $R = 0.04$ for 1362 observed reflections. Two cocrystallized water molecules participate in an extensive network of hydrogen bonds. (II): $C_{23}H_{25}N_3O_2$, $M_r = 375.2$, triclinic, $P\bar{1}$, $a = 13.969$ (2), $b = 9.763$ (3), $c = 8.469$ (4) Å, $\alpha = 115.17$ (3), $\beta = 88.57$ (2), $\gamma = 99.88$ (2)°, $V = 1028.2$ Å³, $Z = 2$, $D_x = 1.21$ Mg m⁻³, $\lambda(Mo K\alpha) = 0.71069$ Å, $\mu = 0.45$ mm⁻¹, $F(000) = 400$, $T = 293$ K, $R = 0.04$ for

1517 observed reflections. The structures studied are characterized by an intramolecular hydrogen bond between the carbonyl O and exocyclic N atoms. In both compounds, this particular N participates in an electronic delocalization specific to the aminopyridazine ring, conferring upon it sp^2 hybridization.

Introduction. This study is part of a more general investigation into conformational and electronic properties of analogs of minaprine (commercial name: Cantor – Clin Midy, France), a potent antidepressant drug (Wermuth, 1985). As the 4-demethyl analog appeared inactive, various substituents were fixed on position 4 in

order to ascertain repercussions on the molecular structure and psychopharmacological profile. The 4-carbamoyl (I) and 4-butoxycarbonyl (II) analogs, here described, were investigated because of the electroattractive character of these substituents.



Experimental. (a) Compound (I): suitable crystals obtained by the slow evaporation of a methanol/ethyl acetate solution at 293 K. Pale-yellow plate-like crystal $0.35 \times 0.08 \times 0.03$ mm for all X-ray measurements. Enraf–Nonius CAD-4 diffractometer. Lattice parameters from least-squares refinement of 17 medium-angle reflections. Lorentz and polarization corrections, no correction for absorption. No intensity variation of standard reflection. $4 \leq 2\theta \leq 130^\circ$, $(\sin\theta/\lambda)_{\max} = 0.59 \text{ \AA}^{-1}$. 6007 unique reflections measured, $0 \leq h \leq 8$, $0 \leq k \leq 35$, $0 \leq l \leq 36$, 1362 observed [$I \geq 2.5\sigma(I)$]. Direct methods [MULTAN80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980)]. All 48 non-H atoms and two O from water molecules found in the best FOM E map. Full-matrix least-squares refinement on F using SHELX76 (Sheldrick, 1976). 28 H atoms from difference Fourier map, other 18 calculated. Anisotropic temperature factors for all non-H atoms and isotropic ones for H atoms (constrained to those of the carrier atoms). $R = 0.038$, $wR = 0.043$, $S = 1.8$, $w = 1/[\sigma^2(F) + 0.001F^2]$, $(\Delta/\sigma)_{\max} = -2.093$ [z parameter of C(117)], max. and min. heights in final difference Fourier synthesis: 0.16 and -0.19 e \AA^{-3} . Atomic scattering factors from SHELX76. (b) Compound (II): crystallized from ethanol at 368 K. Colorless transparent plate-like crystal $0.33 \times 0.14 \times 0.25$ mm for all X-ray measurements. Enraf–Nonius CAD-4 diffractometer. Lattice parameters from least-squares refinement of 18 medium-angle reflections. Lorentz and polarization corrections, no correction for absorption. No intensity variation of standard reflection. $4 \leq 2\theta \leq 52^\circ$, $(\sin\theta/\lambda)_{\max} = 0.62 \text{ \AA}^{-1}$. 4030 independent reflections measured, $-7 \leq h \leq 17$, $-12 \leq k \leq 12$, $0 \leq l \leq 10$, $R_{\text{int}} = 0.01$, 1517 observed [$I \geq 2.5\sigma(I)$]. Direct methods (SHELX76). 18 H atoms from difference Fourier map, others calculated. Full-matrix least-squares anisotropic refinement on F (H atoms isotropic). $R = 0.044$, $wR = 0.050$, $S = 0.45$, $w = 1/[\sigma^2(F) + 0.001F^2]$, $(\Delta/\sigma)_{\max} = 0.7$ [x parameter of C(1)], max. and min. heights in final difference Fourier synthesis: 0.15 and -0.14 e \AA^{-3} . Atomic scattering

factors from SHELX76. For both analogs, XRAY76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) used for structural analysis.

Discussion. Atomic parameters are given in Table 1,* atomic numbering, bond lengths and angles in Fig. 1.

Both compounds are characterized by an intramolecular hydrogen bond between exocyclic N(9) and carbonyl O(24) atoms, as represented in Table 2.

The deviations from the pyridazine mean plane given for atoms C(22), O(24), N(9) and H(9) (Table 2) indicate their quasi coplanarity with the pyridazine ring. In compound (I), the observed N...O [$r_2 = 2.642$ (9) Å for molecule '10' and 2.649 (7) Å for molecule '100'] and H...O distances [$r_1 = 1.830$ (6) Å for '10' and 1.818 (3) Å for '100'] are significantly shorter than those of compound (II) [$r_2 = 2.722$ (4) and $r_1 = 2.004$ (3) Å] and than the mean value resulting from a statistical analysis of 152 intramolecular N—H...O=C hydrogen bonds [$r_2 = 2.755$ (12) and $r_1 = 1.988$ (13) Å respectively] (Taylor, Kennard & Versichel, 1984). We think that the shorter intramolecular hydrogen bonding observed in the 4-carbamoyl analog results not only from a stronger electrostatic $\text{N}^{\delta+} \dots \text{O}^{\delta-}$ interaction but also from more important crystal-packing constraints. Indeed, for this analog, crystal cohesion is achieved *via* a very dense network of intermolecular hydrogen bonds from the two water molecules (Table 3), whereas for compound (II), the cohesion is only characterized by van der Waals contacts.

In both analogs, the shortened N(9)—C(10) bond length [1.345 (9), 1.355 (9) and 1.339 (3) Å for molecules '10' and '100' of derivative (I) and for compound (II) respectively], as well as the C(8)—N(9)—C(10)—C(11) torsion angle [179.2 (7), 173.1 (6) and 176.4 (3)°] and the sum of bond angles around N(9) (360.0 , 360.0 and 359.9°) indicate sp^2 character for the N(9) atom, as previously observed for the 4-demethyl and 4-phenyl analogs (Michel, Gustin, Evrard & Durant, 1982a,b) (Table 4, deposited).

The bond-length modifications observed for compound (I), referring to unsubstituted pyridazine (Almenningen, Bjornsen, Ottersen, Seip & Strand, 1977), are comparable to those reported for other analogs (Table 5, deposited) and can be explained by the resonance scheme specific to the aminopyridazine moieties (Michel *et al.*, 1982a,b). For compound (II), similar bond-length variations are observed but are less pronounced.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and main torsion angles, Tables 4 and 5 and stereoviews of the crystal packing have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42528 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Final atomic coordinates ($\times 10^4$) and B_{eq} values with e.s.d.'s in parentheses, (a) for the two molecules ('10' and '100') in the asymmetric unit of compound (I), (b) for compound (II)

$$B_{eq} = 8\pi^2 U_{eq} \text{ and } U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j.$$

	x	y	z	$B_{eq}(\text{\AA}^2)$
(a) Compound (I)				
Molecule '10'				
O(1)	2683 (9)	623 (2)	-133 (2)	7.28 (2)
C(2)	1396 (13)	476 (3)	175 (3)	6.85 (4)
C(3)	1429 (9)	758 (2)	569 (3)	4.76 (3)
N(4)	1077 (8)	1233 (2)	458 (2)	4.02 (2)
C(5)	2377 (10)	1381 (2)	132 (2)	4.27 (2)
C(6)	2320 (12)	1074 (2)	-245 (2)	5.43 (3)
C(7)	1120 (11)	1504 (2)	849 (2)	4.76 (2)
C(8)	638 (11)	1995 (2)	773 (2)	4.48 (2)
N(9)	412 (8)	2216 (2)	1179 (2)	4.26 (2)
C(10)	-140 (10)	2645 (2)	1202 (2)	3.60 (2)
C(11)	-390 (9)	2866 (2)	1601 (2)	3.54 (2)
C(12)	-868 (10)	3305 (2)	1583 (2)	3.79 (2)
C(13)	-1130 (10)	3517 (2)	1187 (2)	3.53 (2)
N(14)	-948 (8)	3288 (2)	827 (2)	3.79 (2)
N(15)	-432 (8)	2853 (2)	826 (2)	3.86 (2)
C(16)	-1625 (9)	4001 (2)	1152 (2)	3.63 (2)
C(17)	-2293 (12)	4242 (2)	1499 (2)	5.46 (3)
C(18)	-2772 (12)	4694 (3)	1455 (3)	6.37 (3)
C(19)	-2550 (12)	4904 (2)	1078 (3)	6.03 (3)
C(20)	-1879 (11)	4680 (2)	732 (3)	5.68 (3)
C(21)	-1434 (10)	4225 (2)	769 (2)	4.54 (3)
C(22)	-61 (12)	2621 (2)	2017 (2)	5.17 (3)
N(23)	-572 (9)	2831 (2)	2366 (2)	5.41 (2)
O(24)	582 (9)	2239 (2)	2021 (2)	8.51 (2)
Molecule '100'				
O(101)	2100 (9)	518 (2)	2176 (2)	9.34 (3)
C(102)	880 (13)	405 (3)	2494 (3)	7.99 (4)
C(103)	1088 (11)	671 (2)	2897 (2)	5.71 (3)
N(104)	959 (8)	1153 (2)	2799 (2)	3.84 (2)
C(105)	2249 (10)	1273 (2)	2473 (2)	4.80 (2)
C(106)	1948 (13)	983 (3)	2083 (2)	7.12 (3)
C(107)	1147 (10)	1415 (2)	3185 (2)	4.69 (2)
C(108)	711 (10)	1901 (2)	3143 (2)	4.62 (2)
N(109)	608 (8)	2098 (2)	3570 (2)	4.56 (2)
C(110)	9 (9)	2519 (2)	3649 (2)	3.60 (2)
C(111)	-243 (9)	2677 (2)	4075 (2)	3.47 (2)
C(112)	-812 (10)	3107 (2)	4111 (2)	4.00 (2)
C(113)	-1139 (9)	3372 (2)	3745 (2)	3.73 (2)
N(114)	-889 (8)	3208 (2)	3360 (2)	4.09 (2)
N(115)	-321 (8)	2783 (2)	3306 (2)	4.38 (2)
C(116)	-1750 (10)	3846 (2)	3780 (2)	3.71 (2)
C(117)	-2891 (11)	3971 (2)	4115 (2)	5.03 (2)
C(118)	-3480 (11)	4410 (3)	4138 (2)	5.95 (3)
C(119)	-2972 (12)	4725 (2)	3831 (3)	5.93 (3)
C(120)	-1877 (11)	4600 (2)	3506 (3)	5.35 (3)
C(121)	-1253 (10)	4164 (2)	3477 (2)	4.81 (2)
C(122)	132 (10)	2382 (2)	4452 (2)	4.31 (2)
N(123)	-335 (8)	2538 (2)	4837 (1)	4.61 (2)
O(124)	843 (8)	2014 (2)	4410 (1)	7.04 (2)
O(99)	-2065 (5)	3439 (1)	5047 (1)	5.16 (1)
O(55)	2338 (6)	8660 (1)	2446 (1)	7.10 (1)

(b) Compound (II)				
C(1)	9273 (3)	10896 (9)	7214 (9)	13.16 (3)
C(2)	8938 (5)	9945 (6)	7992 (9)	12.94 (3)
C(3)	7998 (4)	9783 (5)	8454 (6)	9.13 (2)
C(4)	7363 (3)	10580 (4)	8142 (4)	6.62 (1)
C(5)	7692 (3)	11547 (4)	7353 (5)	8.33 (2)
C(6)	8645 (5)	11692 (6)	6894 (6)	11.99 (2)
C(7)	6316 (3)	10388 (4)	8603 (5)	8.01 (1)
C(8)	5613 (2)	9470 (4)	7013 (5)	7.05 (1)
N(9)	5872 (2)	7958 (3)	6026 (3)	5.92 (1)
C(10)	5380 (2)	6881 (3)	4568 (4)	5.18 (1)
C(11)	5688 (2)	5450 (3)	3585 (4)	5.14 (1)
C(12)	5107 (2)	4423 (3)	2159 (4)	5.40 (1)
C(13)	4259 (2)	4783 (3)	1715 (4)	5.20 (1)
N(14)	4021 (2)	6172 (3)	2663 (4)	6.05 (1)
N(15)	4570 (2)	7205 (3)	4079 (4)	6.02 (1)
C(16)	3590 (2)	3704 (3)	223 (4)	5.50 (1)
C(17)	3854 (2)	2391 (4)	-1062 (4)	6.32 (1)
C(18)	3222 (3)	1388 (4)	-2465 (5)	7.17 (1)
C(19)	2316 (3)	1684 (5)	-2627 (5)	8.35 (2)
C(20)	2041 (3)	2996 (5)	-1360 (6)	9.18 (2)
C(21)	2662 (3)	3986 (5)	41 (5)	7.95 (1)

Table 1 (cont.)

	x	y	z	$B_{eq}(\text{\AA}^2)$
C(22)	6593 (2)	5103 (4)	4095 (5)	5.74 (1)
O(23)	6735 (2)	3682 (3)	3001 (3)	7.12 (1)
O(24)	7129 (2)	5954 (3)	5336 (3)	7.40 (1)
C(25)	7590 (3)	3195 (4)	3401 (5)	7.94 (1)
C(26)	8487 (3)	3780 (5)	2645 (5)	8.43 (2)
C(27)	9360 (3)	3161 (5)	2852 (6)	10.26 (2)
C(28)	10242 (4)	3733 (6)	2116 (8)	13.67 (3)

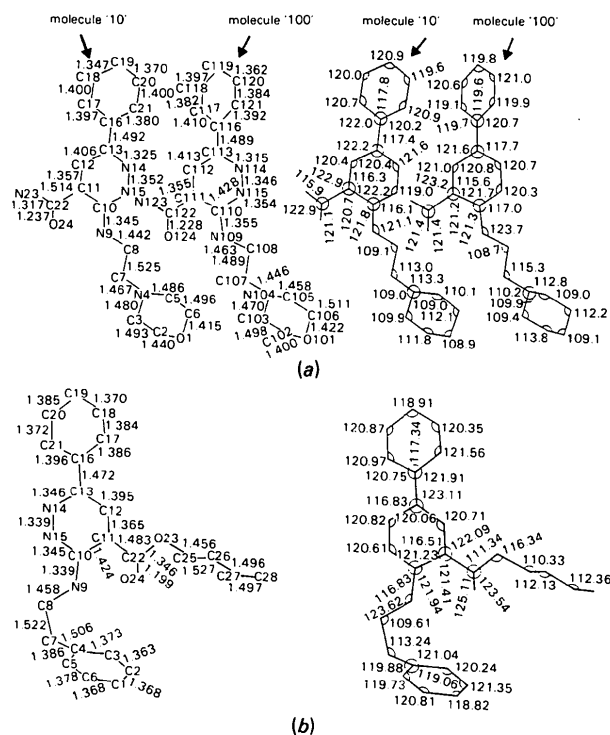
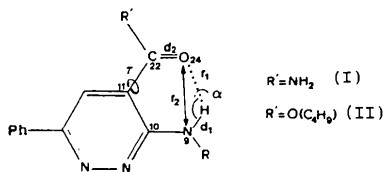


Fig. 1. Atom numbering, bond lengths (\AA) and angles ($^\circ$) for (a) the two molecules ('10' and '100') per asymmetric unit of compound (I) [maximum e.s.d.'s are 0.009 \AA and 0.6 $^\circ$ (except for the morpholino and phenyl rings whose e.s.d.'s vary between 0.009 and 0.013 \AA and 0.5 and 0.7 $^\circ$)] and (b) compound (II) [maximum e.s.d.'s are 0.006 \AA and 0.3 $^\circ$ (except for the morpholino ring whose e.s.d.'s vary between 0.006 and 0.012 \AA and 0.4 and 0.6 $^\circ$)]. [Distances not shown for (a): molecule '10': C(10)–C(11) 1.425, C(10)–N(15) 1.349 \AA ; for molecule '100': C(122)–N(123) 1.340, C(111)–C(122) 1.499 \AA . Angle not shown for (a): molecule '100': C(111)–C(122)–N(123) 117.1 $^\circ$.]

The C(13)–C(16) distance between the pyridazine and phenyl rings [1.492 (9) \AA for molecule '10', 1.489 (9) \AA for molecule '100' of compound (I), and 1.472 (4) \AA for compound (II)] corresponds to the mean value for a single bond between sp^2 C atoms and, as suggested by Hargreaves & Rizvi (1962) for biphenyl, seems to indicate lack of conjugation between two rings. This observation is supported by the non-critical value of the dihedral angle C(12)–C(13)–C(16)–C(17): -16.7 (11), -34.7 (10) $^\circ$ for molecules '10' and '100' of compound (I), -14.1 (6) $^\circ$ for compound (II).

Table 2. Selected parameters of the intramolecular hydrogen bond observed in the 4-carbamoyl and 4-butoxycarbonyl analogs



	Compound (I)		Compound (II)
	'10'	'100'	
d_1 (Å)	1.098 (6)	1.112 (6)	0.980 (3)
d_2 (Å)	1.237 (9)	1.228 (9)	1.200 (4)
r_1 (Å)	1.830 (6)	1.818 (3)	2.004 (3)
r_2 (Å)	2.642 (9)	2.649 (7)	2.722 (4)
α (°)	127.1 (4)	127.7 (4)	128.3 (1)
τ (°)	6.6 (12)	7.9 (11)	0.4 (6)
Deviations (Å) from the mean plane of the pyridazine ring			
C(22)	0.008	0.006	0.025
O(24)	0.145	0.162	0.020
N(9)	0.063	0.026	-0.057
H(9)	0.091	0.172	-0.097
E.s.d.'s (Å)	0.013	0.002	0.010

Table 3. Intermolecular hydrogen-bond distances (Å) and angles (°) for compound (I)

N...H—O	N...O	H—O	N...H	\angle N...H—O
N(4')...H(992)—O(99 ^{II})	2.877 (7)	1.176 (4)	1.734 (6)	162.5 (3)
N(14')...H(991)—O(99 ^{III})	2.905 (7)	0.954 (4)	2.087 (6)	142.8 (3)
N(104')...H(552)—O(55')	2.903 (8)	1.083 (4)	1.849 (6)	163.0 (2)
N—H...N	N...N	N—H	H...N	\angle N—H...N
N(23')—H(232)...N(115')	2.954 (9)	1.088 (6)	2.026 (6)	141.3 (4)
N—H...O	N...O	N—H	H...O	\angle N—H...O
N(23')—H(231)...O(55 ^b)	2.868 (7)	1.067 (6)	1.872 (3)	153.7 (4)
N(123')—H(123)...O(99')	3.047 (6)	1.089 (6)	1.984 (3)	167.7 (2)
Symmetry code: (i) x, y, z ; (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x - \frac{1}{2}, y, z - \frac{1}{2}$; (iv) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x - \frac{1}{2}, -y + 1, -z + \frac{1}{2}$.				

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Structure of a Tricyclo[4.3.0.0^{3,7}]nonane Derivative

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Abstract. 4-(5,8-Diacetyl-6,7-dihydroxy-3-methyltricyclo[4.3.0.0^{3,7}]non-1-yl)-2-butanone, C₁₈H₂₆O₅, $M_r = 322.40$, monoclinic, $P2_1/c$, $a = 13.762$ (2), $b = 10.507$ (2), $c = 12.110$ (1) Å, $\beta = 97.338$ (8)°, $V =$

The morpholino ring of analog (I) is in the chair form and the methylene groups 7 and 8 are in the *anti* position [N(4)—C(7)—C(8)—N(9): 170.0 (6) and 168.4 (6)° respectively]. In the 4-butoxycarbonyl derivative, these groups are in the +synclinal conformation [N(4)—C(7)—C(8)—N(9): 57.7 (5)°].

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References

- ALMENNINGEN, A., BJORNSEN, G., OTTERSEN, T., SEIP, R. & STRAND, T. G. (1977). *Acta Chem. Scand. Ser. A*, **31**, 63–68.
- HARGREAVES, A. & RIZVI, S. H. (1962). *Acta Cryst.* **15**, 365–373.
- 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*. Univ. of York, England, and Louvain-la-Neuve, Belgium.
- MICHEL, A., GUSTIN, R., EVRARD, G. & DURANT, F. (1982a). *Bull. Soc. Chim. Belg.* **91**(1), 49–55.
- MICHEL, A., GUSTIN, R., EVRARD, G. & DURANT, F. (1982b). *Bull. Soc. Chim. Belg.* **91**(2), 123–129.
- SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
- STEWART, J. M., MACHIN, P. A., DICKINSON, C. W., AMMON, H. L., HECK, H. & FLACK, H. (1976). The XRAY76 System. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.
- TAYLOR, R., KENNARD, O. & VERSICHEL, W. (1984). *Acta Cryst.* **B40**, 280–288.
- WERMUTH, C. G. (1985). *Recherches en Série Pyridazinique – Potentialité Pharmacologique et Thérapeutique des Amino-3 Pyridazines*. In *Actualités de Chimie Thérapeutique*, 12th Ser., pp. 3–35. Société de Chimie Thérapeutique.

1736.7 (4) Å³, $Z = 4$, $D_x = 1.233$ Mg m⁻³, Cu $K\alpha$, $\lambda = 1.5418$ Å, $\mu = 0.69$ mm⁻¹, $F(000) = 696$, $T = 293$ K, $R = 0.050$ for 2761 unique reflections. It has been confirmed that the compound formed by Michael