Bye, E., Schweizer, B. & Dunitz, J. D. (1982). *J. Am. Chem. Soc.* **104**, 5893–5898.
Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.
Ruban, G. & Zabel, V. (1976). *Cryst. Struct. Commun.* **6**, 671–677.
Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
Spek, A. L. (1982). The *EUCLID* package. In *Computational Crystallography*, edited by D. Sayre, p. 528. Oxford: Clarendon Press.

Acta Cryst. (1987). C**43**, 1235–1236

Structure of Diazapolycyclic Compounds. X. 1,4-Dimethyl-1,4-dihydrobenzo[*g*]pyridazino[1,2-*b*]phthalazine-6,13-dione

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Abstract. $C_{18}H_{16}N_2O_2$, M_r=292·3, monoclinic, $P2_1/m$, a = 9·8193 (4), b = 13·4046 (6), c = 5·6336 (1) Å, β = 105·083 (2)°, U = 715·97 (5) Å^3, Z = 2, D_x = 1·355 Mg m^{-3}, graphite-monochromatized Cu $K\alpha$ radiation, λ = 1·5418 Å, μ = 0·682 mm^{-1}, $F(000)$ = 308, T = 293 K, R = 0·057 for 829 observed reflexions [$I > 3\sigma(I)$]. The pyridazine ring displays a boat conformation with the methyl groups in pseudoaxial positions. The bond angles around the N atoms sum to 360·0 (2)° confirming the sp^2 hybridization. The diazoquinone also has a boat conformation, less puckered than the pyridazine one.

Experimental. Yellow crystal, 0·47 × 0·17 × 0·05 mm, used for data collection and determination of lattice constants (Cu $K\alpha$, 63 reflexions, $2 < \theta < 45°$). Philips PW 1100 diffractometer, Cu $K\alpha$, graphite monochromator, bisecting geometry, $\omega/2\theta$ scan mode, 1278 unique reflexions up to θ = 65°, in the *hkl* range −12,12; 0,16; 0,7. Two standard reflexions monitored every 90 minutes, no decay observed. The structure was solved in space group $P2_1$ by means of the *ORIENT* program (*DIRDIF* system, Beurskens *et al.*, 1984) using a three-ring-system model taken from *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain & Woolfson, 1980). Isotropic and anisotropic refinements were carried out in both space groups, $P2_1/m$ and $P2_1$, showing high correlation-matrix elements and unreasonable molecular geometry for the latter. H atoms, from difference synthesis, included isotropically in last cycles of refinement. Empirical weights so as to give no trends in $\langle w\Delta^2\rangle$ versus $\langle |F_o| \rangle$ and $\langle (\sin\theta)/\lambda \rangle$. $R(F)$ = 0·057, wR = 0·070, S = 1·01. Max. and average Δ/σ = 0·23 and 0·03. Final $\Delta\rho$ = ±0·20 e Å^{-3}. No extinction correction. Computing with *XRAY76* (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Scattering factors from *International Tables for X-ray Crystallography* (1974). Final atomic coordinates for the non-H atoms and the geometrical parameters are given in Tables 1 and 2,* according to the numbering scheme given in Fig. 1.

Related literature. 1-Methylated compound (Apreda, Foces-Foces, Cano & García-Blanco, 1978), unmethylated and 1,4-diphenyl compounds (Apreda, Foces-Foces, Cano & García-Blanco, 1982). The conformation of the pyridazine ring is shown in Fig. 2 for comparison.

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Table 1. *Final atomic coordinates and equivalent isotropic thermal parameters*

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*a_ia_j\cos(\mathbf{a}_i.\mathbf{a}_j).$$

	x	y	z	$U_{\rm eq}$(Å^2 × 10^4)
C(1)	−0·0224 (3)	0·1418 (2)	−0·4847 (5)	476 (10)
C(2)	−0·0623 (3)	0·2012 (2)	−0·7147 (5)	529 (10)
C(10)	0·5633 (4)	0·1977 (5)	0·9260 (8)	1190 (28)
C(11)	0·4878 (4)	0·1452 (6)	0·7310 (8)	962 (23)
C(11a)	0·4064 (3)	0·1972 (3)	0·5174 (5)	707 (12)
C(12)	0·3263 (3)	0·1459 (3)	0·3122 (6)	649 (13)
C(12a)	0·2471 (3)	0·1973 (2)	0·1128 (5)	498 (9)
C(13)	0·1596 (3)	0·1426 (2)	−0·0978 (5)	516 (10)
N(14)	0·0739 (2)	0·1974 (2)	−0·2805 (4)	461 (8)
O(16)	0·1588 (2)	0·0507 (2)	−0·1096 (4)	702 (9)
C(17)	−0·1513 (4)	0·1051 (3)	−0·4058 (7)	607 (12)

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* 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 43668 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2. *Bond distances* (Å), *bond angles* (°) *and torsion angles* (°)

C(1)–C(2)	1·484 (4)	C(12a)–C(12)	1·374 (4)
C(1)–N(14)	1·485 (3)	C(12a)–C(6a)	1·412 (5)
C(1)–C(17)	1·528 (5)	C(12)–C(11a)	1·398 (5)
C(2)–C(3)	1·309 (4)	C(11a)–C(7a)	1·416 (6)
N(14)–N(5)	1·410 (3)	C(11a)–C(11)	1·440 (6)
N(14)–C(13)	1·363 (3)	C(11)–C(10)	1·352 (7)
C(13)–O(16)	1·234 (4)	C(10)–C(9)	1·403 (9)
C(13)–C(12a)	1·467 (4)		

C(2)–C(1)–N(14)	112·2 (2)	C(13)–C(12a)–C(6a)	120·0 (2)
C(2)–C(1)–C(17)	112·1 (3)	C(13)–C(12a)–C(12)	119·9 (3)
C(17)–C(1)–N(14)	110·2 (2)	C(12)–C(12a)–C(6a)	120·1 (3)
C(1)–C(2)–C(3)	122·5 (3)	C(12a)–C(12)–C(11a)	120·5 (4)
C(1)–N(14)–N(5)	120·1 (2)	C(12)–C(11a)–C(11)	121·6 (4)
C(1)–N(14)–C(13)	117·3 (2)	C(12)–C(11a)–C(7a)	119·5 (3)
C(13)–N(14)–N(5)	122·6 (2)	C(7a)–C(11a)–C(11a)	119·0 (3)
O(16)–C(13)–N(14)	120·2 (3)	C(11a)–C(11)–C(10)	119·7 (5)
C(12a)–C(13)–N(14)	117·3 (3)	C(11)–C(10)–C(9)	121·4 (4)
O(16)–C(13)–C(12a)	122·5 (3)		

C(3)–C(2)–C(1)–N(14)	−25·7 (4)	N(5)–N(14)–C(13)–C(12a)	4·3 (4)
C(2)–C(1)–N(14)–N(5)	25·0 (3)	N(14)–C(13)–C(12a)–C(6a)	−4·1 (4)

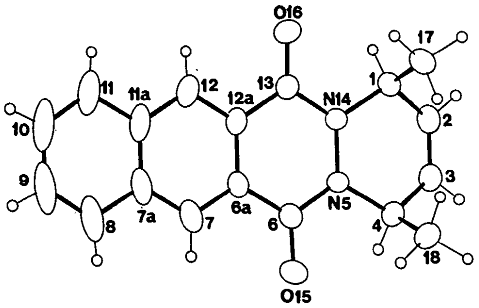

Fig. 1. *ORTEP* drawing (Johnson, 1965) showing the whole numbering scheme for comparison with the related literature.

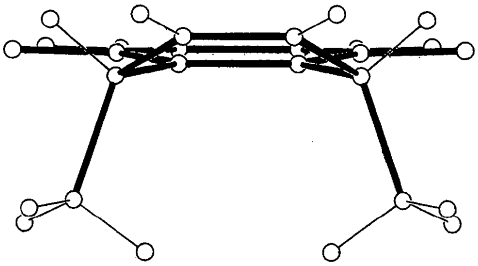

Fig. 2. Frontal view of the molecule along the plane of the benzene rings.

References

Apreda, M. C., Foces-Foces, C., Cano, F. H. & García-Blanco, S. (1978). *Acta Cryst.* B**34**, 2666–2669.

Apreda, M. C., Foces-Foces, C., Cano, F. H. & García-Blanco, S. (1982). *Acta Cryst.* B**38**, 2834–2838.

Beurskens, P. T., Bosman, W. P., Doesburg, H. M., Gould, R. O., van den Hark, Th. E. M., Prick, P. A. J., Noordik, J. H., Beurskens, G., Parthasarathi, V., Bruins Slot, H. J., Haltiwanger, R. C. & Smits, J. M. M. (1984). *DIRDIF* System. Crystallography Laboratory, Toernooiveld, Nijmegen, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Stewart, J. M., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). The *XRAY*76 system. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.