$\Delta_{\alpha 1\alpha 2})°$, scan rate a function of count rate (8° min^{-1} minimum, 30° min^{-1} maximum), 3448 reflections measured, 3131 unique, $R_{int} = 0{\cdot}018$, 2421 observed with $F_o > 3\sigma(F_o)$. Structure solved by direct methods. The least-squares refinement used program *SHELXTL* (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00023$, isotropic secondary-extinction value, $p = 0{\cdot}0026$ (5), in $F_c^* = F_c/[1{\cdot}0 + 0{\cdot}002(p)F_o^2/\sin 2\theta]^{0.25}$. 344 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, isotropic temperature factors for H, benzene-ring H atoms included using riding model, C—H = 0·96 Å, C—C—H = 120·0°, $1{\cdot}1U_{eq}$(C). $(\Delta/\sigma)_{max} = -0{\cdot}008$, $R = 0{\cdot}056$, $wR = 0{\cdot}057$, $S = 1{\cdot}512$. Final difference Fourier map excursions 0·40 and −0·23 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).† Atom numbering for Tables 1 and 2 (atom parameters, bond distances and bond angles) follows that shown in Fig. 1. The hydrogen-bond parameters are: H(18)···O(28)′ = 1·98 (3), N(18)···O(28)′ = 2·808 (5) Å, and N—H···O = 168·9 (1·8)°.

Related literature. The title compound and a closely related pentaazabicyclo[3.2.2]nonane are products of a benzoylhydrazine/formaldehyde/orthoformate condensation reaction which proceeds through the intermediate compound 1,3,5-tribenzamido-1,3,5-hexahydrotriazine. For the structure of the pentaazabicyclo[3.2.2]-nonane see George (1987). For the structure of the hexahydrotriazine see George & Gilardi (1987).

† Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43455 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

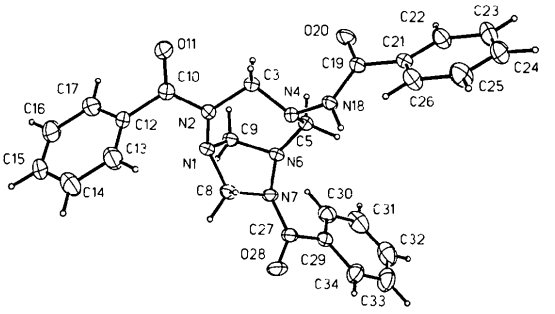

Fig. 1. Thermal-ellipsoid plot of 4-benzamido-2,7-dibenzoyl-1,2,4,6,7-pentaazabicyclo[4.2.1]nonane, drawn at 20% probability level.

This work was supported by the Office of Naval Research, ONR contract No. N0001484WR24060.

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Acta Cryst. (1987). C**43**, 1003–1005

Structure of a Substituted Hexahydrotriazine

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(*Received* 7 *April* 1986; *accepted* 23 *October* 1986)

Abstract. 1,3,5-Tribenzamido-1,3,5-hexahydrotriazine monohydrate, $C_{24}H_{24}N_6O_3.H_2O$, $M_r = 462{\cdot}51$, monoclinic, $P2_1/c$, $a = 12{\cdot}655$ (1), $b = 14{\cdot}721$ (2), $c = 13{\cdot}339$ (2) Å, $\beta = 107{\cdot}25$ (1)°, $V = 2373{\cdot}2$ (5) Å^3, $Z = 4$, $D_x = 1{\cdot}294$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 0{\cdot}709$ mm^{-1}, $F(000) = 976$, $T = 295$ K, final $R = 0{\cdot}042$, $wR = 0{\cdot}045$ for 3054 independent observed reflections. In this molecule the hexahydrotriazine ring is chair-shaped and bond distances and bond angles are normal. There are four hydrogen bonds between the water molecule and the primary molecule and its symmetry equivalents. There is an additional intermolecular hydrogen bond between an amide nitrogen and a carbonyl oxygen.

Experimental. Colorless 0·08 × 0·25 × 0·30 mm crystal, crystallized from methanol/water. Synthesized by G. Kumar and J. Boyer of the Univ. of Illinois at Chicago. Automated Nicolet *R3m* diffractometer with incident-beam graphite monochromator, $\lambda =$ 1·54178 Å (Cu $K\alpha$), 25 centered reflections within $37 \le 2\theta \le 90°$ used for determining lattice parameters.

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Data corrected for Lorentz and polarization, but not absorption effects, $(\sin\theta/\lambda)_{max} = 0.57$ Å^{-1}, range of *hkl*: $-14 \le h \le 14$, $0 \le k \le 16$, $-15 \le l \le 0$. Standards $\bar{5}0\bar{2}$, $10\bar{6}$, 060, monitored every 60 reflections with random variation 1·8% over data collection, θ–2θ mode, scan width $(1{\cdot}8 + \Delta_{\alpha1\alpha2})°$, scan rate a function of count rate (min. 6, max. 30° min^{-1}), 4156 reflections measured, 3799 unique, $R_{int} = 0{\cdot}011$, 3054 observed with $F_o > 3\sigma(F_o)$. Structure solved by direct methods. The least-squares refinement used program *SHELXTL* (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00023$, isotropic secondary-extinction value, $p = 0{\cdot}0027$ (3), in $F_c^* = F_c/[1{\cdot}0 + 0{\cdot}002(p)F_o^2/\sin 2\theta]^{0.25}$. 412 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, isotropic temperature factors for H. $(\Delta/\sigma)_{max} = -0{\cdot}006$, $R = 0{\cdot}042$, $wR = 0{\cdot}045$, $S = 1{\cdot}469$. Final difference-Fourier excursions 0·17 and −0·15 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).† Atom numbering for Tables 1, 2 and 3 (atom coordinates, bond distances and angles, details of hydrogen bonds) follows that shown in Fig. 1.

† Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43519 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atom coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

	x	*y*	*z*	U_{eq}*
N(1)	−42 (1)	2495 (1)	3183 (1)	38 (1)
C(2)	−565 (2)	3397 (1)	2924 (2)	44 (1)
N(3)	269 (1)	4084 (1)	2971 (1)	42 (1)
C(4)	962 (2)	3826 (1)	2311 (1)	43 (1)
N(5)	1388 (1)	2894 (1)	2432 (1)	40 (1)
C(6)	515 (2)	2250 (1)	2400 (1)	41 (1)
N(7)	−860 (1)	1835 (1)	3172 (1)	44 (1)
C(8)	−946 (2)	1519 (1)	4090 (1)	39 (1)
O(9)	−387 (1)	1807 (1)	4942 (1)	58 (1)
C(10)	−1804 (2)	798 (1)	4002 (2)	40 (1)
C(11)	−1666 (2)	200 (1)	4838 (2)	52 (1)
C(12)	−2436 (2)	−481 (2)	4778 (2)	64 (1)
C(13)	−3348 (2)	−564 (2)	3911 (2)	67 (1)
C(14)	−3486 (2)	29 (2)	3094 (2)	64 (1)
C(15)	−2723 (2)	707 (1)	3132 (2)	50 (1)
N(16)	891 (1)	4261 (1)	4027 (1)	40 (1)
C(17)	1366 (2)	5083 (1)	4281 (1)	38 (1)
O(18)	1276 (1)	5701 (1)	3641 (1)	60 (1)
C(19)	2046 (2)	5187 (1)	5398 (1)	39 (1)
C(20)	2912 (2)	5798 (2)	5632 (2)	64 (1)
C(21)	3588 (2)	5899 (2)	6658 (2)	76 (1)
C(22)	3398 (2)	5405 (2)	7444 (2)	69 (1)
C(23)	2524 (2)	4815 (2)	7226 (2)	62 (1)
C(24)	1848 (2)	4700 (1)	6212 (2)	49 (1)
N(25)	2305 (1)	2777 (1)	3329 (1)	44 (1)
C(26)	3290 (2)	2576 (1)	3196 (1)	40 (1)
O(27)	3422 (1)	2459 (1)	2331 (1)	60 (1)
C(28)	4229 (2)	2508 (1)	4184 (2)	42 (1)
C(29)	5107 (2)	1944 (2)	4195 (2)	61 (1)
C(30)	6001 (2)	1873 (2)	5079 (2)	73 (1)
C(31)	6044 (2)	2373 (2)	5957 (2)	64 (1)
C(32)	5175 (2)	2928 (2)	5960 (2)	62 (1)
C(33)	4270 (2)	3006 (2)	5076 (2)	54 (1)
O(*W*)	1729 (1)	2662 (1)	5290 (1)	45 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Bond lengths* (Å) *and angles* (°)

N(1)–C(2)	1·478 (3)	N(1)–C(6)	1·468 (3)
N(1)–N(7)	1·418 (2)	C(2)–N(3)	1·451 (3)
N(3)–C(4)	1·465 (3)	N(3)–N(16)	1·418 (2)
C(4)–N(5)	1·465 (3)	N(5)–C(6)	1·447 (3)
N(5)–N(25)	1·408 (2)	N(7)–C(8)	1·345 (3)
C(8)–O(9)	1·223 (2)	C(8)–C(10)	1·497 (3)
C(10)–C(11)	1·390 (3)	C(10)–C(15)	1·385 (2)
C(11)–C(12)	1·383 (3)	C(12)–C(13)	1·376 (3)
C(13)–C(14)	1·366 (4)	C(14)–C(15)	1·379 (3)
N(16)–C(17)	1·349 (2)	C(17)–O(18)	1·229 (2)
C(17)–C(19)	1·490 (2)	C(19)–C(20)	1·380 (3)
C(19)–C(24)	1·384 (3)	C(20)–C(21)	1·390 (3)
C(21)–C(22)	1·354 (4)	C(22)–C(23)	1·368 (4)
C(23)–C(24)	1·379 (3)	N(25)–C(26)	1·343 (3)
C(26)–O(27)	1·226 (3)	C(26)–C(28)	1·494 (2)
C(28)–C(29)	1·382 (3)	C(28)–C(33)	1·385 (3)
C(29)–C(30)	1·375 (3)	C(30)–C(31)	1·370 (4)
C(31)–C(32)	1·370 (4)	C(32)–C(33)	1·384 (3)

C(2)–N(1)–C(6)	109·3 (2)	C(2)–N(1)–N(7)	109·8 (1)
C(6)–N(1)–N(7)	109·1 (1)	N(1)–C(2)–N(3)	110·2 (2)
C(2)–N(3)–C(4)	110·5 (2)	C(2)–N(3)–N(16)	110·7 (2)
C(4)–N(3)–N(16)	112·9 (1)	N(3)–C(4)–N(5)	116·3 (2)
C(4)–N(5)–C(6)	111·0 (2)	C(4)–N(5)–N(25)	113·1 (1)
C(6)–N(5)–N(25)	112·0 (1)	N(1)–C(6)–N(5)	109·9 (1)
N(1)–N(7)–C(8)	118·9 (1)	N(7)–C(8)–O(9)	123·1 (2)
N(7)–C(8)–C(10)	115·2 (1)	O(9)–C(8)–C(10)	121·7 (2)
C(8)–C(10)–C(11)	118·0 (2)	C(8)–C(10)–C(15)	122·9 (2)
C(11)–C(10)–C(15)	119·0 (2)	C(10)–C(11)–C(12)	119·6 (2)
C(11)–C(12)–C(13)	120·9 (2)	C(12)–C(13)–C(14)	119·4 (2)
C(13)–C(14)–C(15)	120·6 (2)	C(10)–C(15)–C(14)	120·4 (2)
N(3)–N(16)–C(17)	119·3 (1)	N(16)–C(17)–O(18)	123·1 (2)
N(16)–C(17)–C(19)	115·2 (2)	O(18)–C(17)–C(19)	121·7 (2)
C(17)–C(19)–C(20)	118·5 (2)	C(17)–C(19)–C(24)	123·1 (2)
C(20)–C(19)–C(24)	118·4 (2)	C(19)–C(20)–C(21)	120·6 (2)
C(20)–C(21)–C(22)	120·4 (2)	C(21)–C(22)–C(23)	119·6 (2)
C(22)–C(23)–C(24)	120·9 (2)	C(19)–C(24)–C(23)	120·1 (2)
N(5)–N(25)–C(26)	118·5 (2)	N(25)–C(26)–O(27)	123·1 (2)
N(25)–C(26)–C(28)	115·2 (2)	O(27)–C(26)–C(28)	121·7 (2)
C(26)–C(28)–C(29)	118·5 (2)	C(26)–C(28)–C(33)	122·6 (2)
C(29)–C(28)–C(33)	118·9 (2)	C(28)–C(29)–C(30)	120·6 (2)
C(29)–C(30)–C(31)	120·4 (2)	C(30)–C(31)–C(32)	119·6 (2)
C(31)–C(32)–C(33)	120·6 (2)	C(28)–C(33)–C(32)	119·9 (2)

Table 3. *Hydrogen-bond parameters*

	N···O (Å)	H···O (Å)	∠N–H···O (°)
N(7)–H(7)···O(18^i)	2·856 (3)	1·99 (2)	161·2 (13)
N(16)–H(16)···O(*W*)	2·906 (4)	2·07 (2)	171·2 (12)
N(25)–H(25)···O(*W*)	2·920 (4)	2·02 (2)	171·1 (12)
	O···O (Å)	**H···O(Å)**	**∠O–H···O (°)**
O(*W*)–H(1*W*)···O(9)	2·870 (4)	1·95 (2)	173·8 (12)
O(*W*)–H(2*W*)···O(27^i)	2·929 (4)	2·13 (2)	162·6 (13)

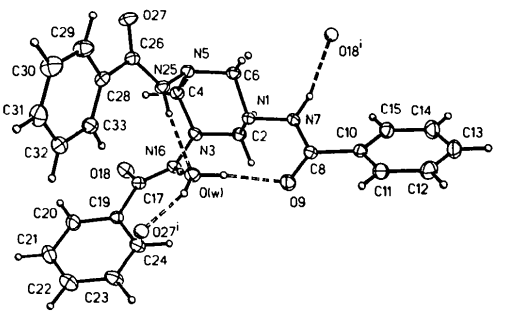

Fig. 1. Thermal-ellipsoid plot of the title compound drawn at 20% probability level. Dashed lines indicate hydrogen bonds; O(18^i) and O(27^i) are symmetry-equivalent atoms included to complete hydrogen bonds.

Related literature. For the structure of two closely related pentaazabicyclononanes formed by a condensation reaction from the title compound see George (1987) and George & Gilardi (1987).

This work was supported by the Office of Naval Research, ONR contract No. N0001484WR24060.

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Acta Cryst. (1987). C**43**, 1005–1006

Structure of (–)-Savinin

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(*Received* 28 *October* 1986; *accepted* 22 *December* 1986)

Abstract. 4-Piperonyl-3-piperonylidenetetrahydrofuran-2-one, $C_{20}H_{16}O_6$, $M_r = 352$, monoclinic, $C2/c$, $a = 14{\cdot}997\ (2)$, $b = 10{\cdot}875\ (3)$, $c = 20{\cdot}708\ (7)$ Å, $\beta = 108{\cdot}79\ (2)°$, $V = 3197\ (21)$ Å^3, $Z = 8$, $D_m = 1{\cdot}46$, $D_x = 1{\cdot}45$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 1{\cdot}0$ cm^{-1}, $F(000) = 1472$, $T = 298$ K, final $R = 0{\cdot}049$ for 1111 observed reflections. The structure contains three planar parts: two (3,4-methylenedioxy)benzyl(idene) moieties (*A* and *B*) and a tetrahydrofuran-2-one ring (*C*). The dihedral angles between the planes are *A*&*B*: 17·01 (1), *A*&*C*: 10·59 (2), *B*&*C*: 26·15 (2)°. The bond distances and angles are normal.

Table 1. *Atomic fractional coordinates and equivalent isotropic temperature factors* (Å^2)

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

	x	y	z	B_{eq}
C1	0·3679 (3)	0·8977 (4)	0·3044 (2)	3·2 (2)
C2	0·3379 (3)	0·8981 (3)	0·3624 (2)	3·6 (2)
C3	0·3214 (3)	0·7876 (4)	0·3867 (2)	3·5 (2)
C4	0·3330 (3)	0·6772 (3)	0·3570 (2)	3·7 (2)
C5	0·3621 (3)	0·6722 (4)	0·3014 (2)	4·2 (3)
C6	0·3796 (3)	0·7859 (3)	0·2756 (2)	3·6 (2)
C7	0·3831 (3)	1·0106 (3)	0·2710 (2)	3·5 (2)
C8	0·3822 (3)	1·1279 (3)	0·2890 (2)	3·1 (2)
C9	0·3924 (3)	1·2244 (4)	0·2409 (2)	3·7 (2)
O10	0·3831 (2)	1·3368 (2)	0·2673 (1)	4·6 (2)
C11	0·3620 (3)	1·3259 (4)	0·3307 (2)	4·4 (3)
C12	0·3719 (3)	1·1888 (3)	0·3519 (2)	3·1 (2)
C13	0·4547 (3)	1·1650 (4)	0·4177 (2)	3·5 (2)
C14	0·4305 (3)	1·2117 (4)	0·4794 (2)	3·4 (2)
C15	0·4534 (3)	1·3329 (4)	0·5015 (2)	3·7 (2)
C16	0·4251 (3)	1·3726 (4)	0·5542 (2)	3·4 (2)
C17	0·3770 (3)	1·3002 (4)	0·5855 (2)	3·9 (3)
C18	0·3553 (4)	1·1812 (4)	0·5661 (2)	6·1 (4)
C19	0·3822 (3)	1·1379 (4)	0·5116 (2)	4·8 (3)
O9	0·4031 (2)	1·2156 (3)	0·1863 (1)	4·9 (2)
O3	0·2932 (2)	0·7661 (2)	0·4426 (1)	5·0 (2)
O4	0·3108 (2)	0·5820 (2)	0·3929 (1)	5·2 (2)
O16	0·4400 (2)	1·4878 (2)	0·5851 (1)	5·1 (2)
O17	0·3569 (2)	1·3667 (3)	0·6364 (1)	5·8 (2)
C20	0·2740 (3)	0·6372 (4)	0·4429 (2)	5·1 (3)
C30	0·4010 (3)	1·4820 (4)	0·6392 (2)	4·9 (3)

Experimental. The compound was extracted from an acetone solution of *Calocedrus formosana* Florin.

Crystal 0·15 × 0·25 × 0·25 mm. CAD-4 diffractometer. Unit cell: 25 reflections, 2θ range 19·72 to 26·54°. D_m by flotation (*n*-hexane/CCl_4). $2\theta_{max} = 50°$.

Table 2. *Bond lengths* (Å) *and bond angles* (°) *of* $C_{20}H_{16}O_6$

C1	C2	1·411 (5)	C1	C6	1·390 (5)		
C1	C7	1·463 (5)	C2	C3	1·356 (5)		
C3	C4	1·386 (5)	C3	O3	1·374 (4)		
C4	C5	1·358 (5)	C4	O4	1·377 (4)		
C5	C6	1·404 (5)	C7	C8	1·331 (5)		
C8	C9	1·488 (5)	C8	C12	1·513 (4)		
C9	O10	1·365 (4)	C9	O9	1·195 (4)		
O10	C11	1·450 (4)	C11	C12	1·549 (5)		
C12	C13	1·541 (5)	C13	C14	1·524 (5)		
C14	C15	1·402 (5)	C14	C19	1·388 (5)		
C15	C16	1·362 (5)	C16	C17	1·364 (5)		
C16	O16	1·391 (4)	C17	C18	1·363 (5)		
C17	O17	1·389 (4)	C18	C19	1·396 (5)		
O3	C20	1·432 (4)	O4	C20	1·450 (4)		
O16	C30	1·423 (4)	O17	C30	1·410 (5)		
C2	C1	C6	119·1 (3)	C2	C1	C7	122·8 (3)
C6	C1	C7	118·0 (3)	C1	C2	C3	117·3 (3)
C2	C3	C4	122·6 (3)	C2	C3	O3	127·3 (3)
C4	C3	O3	110·1 (3)	C3	C4	C5	122·2 (3)
C3	C4	O4	108·9 (3)	C5	C4	O4	128·9 (3)
C4	C5	C6	115·9 (3)	C1	C6	C5	122·8 (3)
C1	C7	C8	130·9 (3)	C7	C8	C9	118·4 (3)
C7	C8	C12	132·3 (3)	C9	C8	C12	109·2 (3)
C8	C9	O10	108·5 (3)	C8	C9	O9	130·5 (3)
O10	C9	O9	120·9 (3)	C9	O10	C11	111·7 (2)
O10	C11	C12	107·8 (2)	C8	C12	C11	101·8 (2)
C8	C12	C13	114·2 (3)	C11	C12	C13	112·8 (3)
C12	C13	C14	110·1 (3)	C13	C14	C15	119·2 (3)
C13	C14	C19	120·9 (3)	C15	C14	C19	119·8 (3)
C14	C15	C16	116·9 (3)	C15	C16	C17	123·1 (3)
C15	C16	O16	127·4 (3)	C17	C16	O16	109·5 (3)
C16	C17	C18	121·4 (3)	C16	C17	O17	109·6 (3)
C18	C17	O17	129·0 (3)	C17	C18	C19	117·0 (3)
C14	C19	C18	121·7 (3)	C3	O3	C20	106·7 (2)
C4	O4	C20	106·8 (2)	C16	O16	C30	106·0 (2)
C17	O17	C30	106·3 (2)	O3	C20	O4	106·2 (2)
O16	C30	O17	108·3 (3)				

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