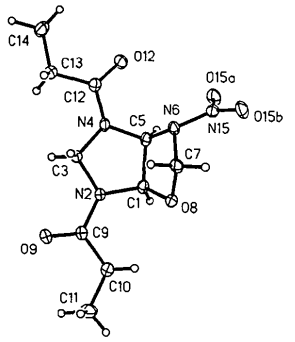

Fig. 1. A thermal ellipsoid plot of (I) with ellipsoids drawn at the 20% probability level.

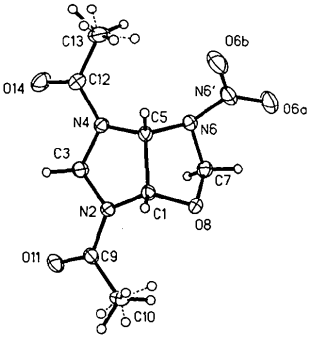

Fig. 2. A thermal ellipsoid plot of (II) with ellipsoids drawn at the 20% probability level.

(1974, Vol. IV).* Atom numbering for Tables 1 and 3 (atom coordinates) and 2 and 4 (bond distances and angles) follows that shown in Figs. 1 and 2.

Related literature. The structures of several other azabicyclo[3.3.0]octanes have been published (Boileau, Wimmer, Gilardi, Stinecipher, Gallo & Pierrot, 1988; Koppes, Chaykovsky, Adolph, Gilardi & George, 1987).

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* 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 54970 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0576]

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Structure of 2,4,6-Trinitro-8,10-dipropionyl-2,4,6,8,10-pentaazabicyclo[5.3.0]decane

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Abstract. $C_{11}H_{18}N_8O_8$, $M_r = 390.3$, orthorhombic, *Pbca*, $a = 6.552$ (2), $b = 25.794$ (6), $c = 19.412$ (5) Å, $V = 3281$ (2) Å^3, $Z = 8$, $D_x = 1.581$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54184 Å, $\mu = 1.12$ mm^{-1}, $F(000) = 1632$, $T = 295$ K, final $R = 0.054$, $wR = 0.055$ for 1481 independent observed reflections. The five-membered ring is essentially planar while the seven-membered ring has adopted a chair conformation. All three nitro groups are pyramidal with N—N to C—N—C angles of 19.8, 28.6 and 29.5°.

Experimental. A clear colorless needle 0.04 × 0.08 × 0.75 mm data crystal, recrystallized from acetone, was provided by Dr Clifford L. Coon of Livermore National Laboratory. An automated Siemens *R*3*m*/*V* diffractometer with incident beam monochromator was used for data collection. 25 centered reflections within $40.0 \le 2\theta \le 56.0°$ were used for determining lattice parameters. $(\sin\theta/\lambda)_{max} = 0.56$ Å^{-1}, range of *hkl*: $-6 \le h \le 4$, $0 \le k \le 27$, $0 \le l \le 20$. Standards 240, 082 and 006, monitored every 97 reflections, showed random variation of 2.5% over data collection: $\theta/2\theta$ scan mode, scan width $[2\theta(K\alpha_1) - 1.0]$ to $[2\theta(K\alpha_2) + 1.0]°$, ω-scan rate a function of count rate (3.0° min^{-1} minimum, 15.0° min^{-1} maximum), 4185 reflections measured, 2057 unique, $R_{int} = 1.0\%$, 1481 observed with $F_o > 3\sigma(F_o)$. Data were corrected for Lorentz and polarization effects but not for absorp-

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Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement coefficients* ($Å^2 \times 10^3$)

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

	x	y	z	U_{eq}
C(1)	−1231 (8)	1559 (2)	8926 (2)	41 (2)
N(2)	−1446 (6)	1675 (2)	9672 (2)	37 (1)
N(2′)	−3278 (8)	1864 (2)	9888 (2)	47 (2)
O(2*a*)	−3282 (6)	2136 (1)	10403 (2)	66 (2)
O(2*b*)	−4803 (6)	1747 (2)	9557 (2)	62 (1)
C(3)	395 (8)	1771 (2)	10090 (2)	41 (2)
N(4)	1174 (6)	1309 (1)	10411 (2)	43 (1)
N(4′)	405 (7)	1170 (2)	11066 (2)	54 (2)
O(4*a*)	1101 (7)	782 (2)	11328 (2)	71 (2)
O(4*b*)	−790 (7)	1471 (2)	11327 (2)	76 (2)
C(5)	1741 (8)	886 (2)	9963 (2)	42 (2)
N(6)	229 (6)	751 (1)	9452 (2)	38 (1)
N(6′)	−1540 (8)	537 (2)	9695 (2)	51 (2)
O(6*a*)	−3008 (7)	510 (2)	9305 (2)	76 (2)
O(6*b*)	−1531 (6)	374 (1)	10286 (2)	63 (1)
C(7)	−63 (8)	1052 (2)	8809 (2)	41 (2)
N(8)	1881 (6)	1202 (1)	8525 (2)	39 (1)
C(9)	1891 (8)	1745 (2)	8308 (2)	42 (2)
N(10)	−30 (6)	1941 (1)	8571 (2)	39 (1)
C(11)	3234 (9)	869 (2)	8213 (2)	44 (2)
C(12)	3025 (9)	302 (2)	8386 (2)	52 (2)
O(13)	4594 (6)	1041 (1)	7852 (2)	61 (1)
C(14)	−841 (9)	2422 (2)	8449 (2)	41 (2)
C(15)	445 (8)	2792 (2)	8045 (2)	49 (2)
O(16)	−2521 (6)	2524 (1)	8669 (2)	55 (1)
C(17)	4438 (10)	−54 (2)	7988 (3)	79 (3)
C(18)	−332 (9)	3345 (2)	8096 (2)	58 (2)

tion. The structure solution, by direct methods, and the full-matrix least-squares refinement (on F) used programs in *SHELXTL* (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ was minimized, where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0.000225$. 245 parameters were refined: atomic coordinates and anisotropic thermal parameters for all non-H atoms, H atoms included using a riding model [coordinate shifts of C applied to attached H atoms, C—H distance set to 0.96 Å, H angles idealized, U_{iso}(H) set to 1.1 U_{eq}(C) or, if methyl, 1.2 U_{eq}(C)]. $(\Delta/\sigma)_{max} = 0.01$, ratio of observations to parameters = 6.0:1, $R = 0.054$, $wR = 0.055$, $S = 1.68$ ($R = 0.077$ for all data). Final difference Fourier excursions were at 0.22 and -0.28 e $Å^{-3}$. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).* Atom numbering for Tables 1 (atom coordinates) and 2 (bond distances and angles) follows that shown in Fig. 1.

Related literature. A search of the January 1991 release of the Cambridge Structural Database (Allen, Kennard & Taylor, 1983) did not reveal any structures with an identical pentaazabicyclo[5.3.0]decane ring system.

* 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 54991 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0579]

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

C(1)—N(2)	1.486 (5)	C(1)—C(7)	1.532 (7)
C(1)—N(10)	1.437 (6)	N(2)—N(2′)	1.361 (6)
N(2)—C(3)	1.474 (6)	N(2′)—O(2*a*)	1.221 (5)
N(2′)—O(2*b*)	1.225 (6)	C(3)—N(4)	1.439 (6)
N(4)—N(4′)	1.413 (5)	N(4)—C(5)	1.444 (6)
N(4′)—O(4*a*)	1.212 (6)	N(4′)—O(4*b*)	1.213 (6)
C(5)—N(6)	1.445 (6)	N(6)—N(6′)	1.367 (6)
N(6)—C(7)	1.481 (5)	N(6′)—O(6*a*)	1.226 (6)
N(6′)—O(6*b*)	1.224 (5)	C(7)—N(8)	1.441 (6)
N(8)—C(9)	1.463 (6)	N(8)—C(11)	1.375 (6)
C(9)—N(10)	1.449 (6)	N(10)—C(14)	1.371 (6)
C(11)—C(12)	1.506 (7)	C(11)—O(13)	1.218 (6)
C(12)—C(17)	1.515 (8)	C(14)—C(15)	1.495 (7)
C(14)—O(16)	1.209 (7)	C(15)—C(18)	1.517 (7)

N(2)—C(1)—C(7)	111.3 (3)	N(2)—C(1)—N(10)	112.4 (4)
C(7)—C(1)—N(10)	103.9 (4)	C(1)—N(2)—N(2′)	117.2 (4)
C(1)—N(2)—C(3)	119.5 (4)	N(2′)—N(2)—C(3)	119.5 (3)
N(2)—N(2′)—O(2*a*)	117.4 (4)	N(2)—N(2′)—O(2*b*)	118.0 (4)
O(2*a*)—N(2′)—O(2*b*)	124.7 (5)	N(2)—C(3)—N(4)	113.0 (4)
C(3)—N(4)—N(4′)	118.3 (4)	C(3)—N(4)—C(5)	117.1 (3)
N(4′)—N(4)—C(5)	116.2 (4)	N(4)—N(4′)—O(4*a*)	116.9 (4)
N(4)—N(4′)—O(4*b*)	116.4 (4)	O(4*a*)—N(4′)—O(4*b*)	126.5 (4)
N(4)—C(5)—N(6)	114.8 (4)	C(5)—N(6)—N(6′)	116.2 (4)
C(5)—N(6)—C(7)	122.7 (4)	N(6′)—N(6)—C(7)	113.1 (4)
N(6)—N(6′)—O(6*a*)	118.4 (4)	N(6)—N(6′)—O(6*b*)	117.3 (4)
O(6*a*)—N(6′)—O(6*b*)	124.3 (5)	C(1)—C(7)—N(6)	112.8 (3)
C(1)—C(7)—N(8)	105.6 (4)	N(6)—C(7)—N(8)	110.4 (4)
C(7)—N(8)—C(9)	111.8 (4)	C(7)—N(8)—C(11)	124.8 (4)
C(9)—N(8)—C(11)	117.9 (4)	N(8)—C(9)—N(10)	103.2 (4)
C(1)—N(10)—C(9)	113.9 (4)	C(1)—N(10)—C(14)	119.4 (4)
C(9)—N(10)—C(14)	126.3 (4)	N(8)—C(11)—C(12)	116.7 (4)
N(8)—C(11)—O(13)	119.8 (4)	C(12)—C(11)—O(13)	123.4 (5)
C(11)—C(12)—C(17)	114.8 (4)	N(10)—C(14)—C(15)	116.7 (5)
N(10)—C(14)—O(16)	119.2 (4)	C(15)—C(14)—O(16)	124.0 (4)
C(14)—C(15)—C(18)	112.1 (4)		

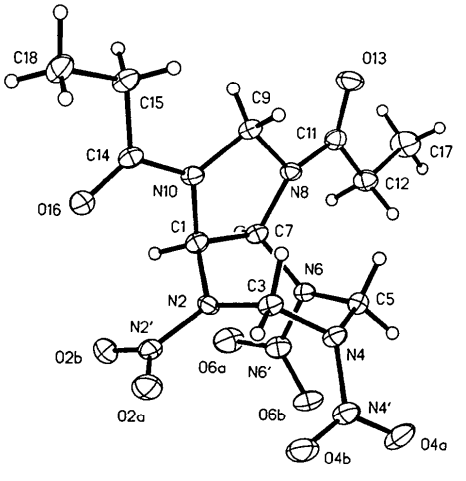

Fig. 1. A thermal ellipsoid plot of the title compound with ellipsoids drawn at the 20% probability level.

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