independent molecules with the atomic labelling scheme is shown in Fig. 1.*

Related literature. Polycyclic aromatic hydrocarbons (PAH) are the most widespread particulate genoxic environmental pollutants (Gelboin & Ts'o, 1978; Cho & Harvey, 1974). Epoxides have been proved to be the initial products of the oxidation of polycyclic aromatic hydrocarbons (Fu & von Tungeln, 1989). They subsequently metabolize to the corresponding quinones, diols or phenolic derivatives. Harvey and co-workers reported *K*-region oxidized metabolites from PAH (Goh & Harvey, 1973; Harvey, Goh & Cortez, 1975).

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[*] Lists of structure factors, anisotropic thermal parameters for non-H atoms, and atomic coordinates and thermal parameters for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55186 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0385]

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Structure of 8,10-Diacetyl-2,4,6-trinitro-2,4,6,8,10-pentaazabicyclo[5.3.0]decane

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Abstract. 2,4,6-Trinitro-2,4,6,8,10-pentaazabicyclo[5.3.0]decane-8,10-diyl dimethyl diketone, $C_9H_{14}N_8O_8$, $M_r = 362.3$, orthorhombic, $P2_12_12_1$, $a = 8.145$ (2), $b = 12.238$ (2), $c = 14.186$ (3) Å, $V = 1413.9$ (4) Å^3, $Z = 4$, $D_x = 1.702$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54184 Å, $\mu = 1.31$ mm^{-1}, $F(000) = 752$, $T = 295$ K, final $R = 0.046$, $wR = 0.053$ for 1302 independent observed reflections. The two rings in this polyamine are fused *cis* to one another, imparting a folded shape to the bicyclic system. The parameters of the five-membered ring fit a flattened envelope conformation, with one N atom lying 0.25 Å from the (±0.01 Å) plane of the other four atoms. The torsion angles of the seven-membered ring are intermediate between those of the ideal chair and twist-chair forms of cycloheptane, but are closer to a chair form. Of the five tri-substituted amine atoms, one is essentially flat, and the other four are slightly pyramidal (the angles between the exocyclic amine bonds and the adjacent CNC planes range from 16.2 to 24.0°).

Experimental. A clear colorless prism (0.08 × 0.10 × 0.10 mm) data crystal was provided by Clifford L. Coon of Lawrence Livermore National Laboratory. Data were collected on an automated Siemens *R3m/V* diffractometer with incident-beam monochromator. 25 centered reflections within $40 \le 2\theta \le 98°$ were used for determining lattice parameters. $(\sin\theta/\lambda)_{\max} = 0.588$ Å^{-1}, range of *hkl*: $0 \le h \le 9$, $0 \le k \le 12$, $0 \le l \le 16$. Three standards (301, 042, 013) monitored every 97 reflections showed linear decline of 10.0% over data collection. Data were collected using the $\theta/2\theta$-scan mode with scan width $[2\theta(K\alpha_1) - 1.4]$ to $[2\theta(K\alpha_2) + 1.4]°$ and ω-scan rate a function of count rate (minimum 3.0, maximum 12.0° min^{-1}). Of 1505 reflections measured, 1413 were unique ($R_{\rm int}$ = 2.3%), of which 1302 were observed with $F_o > 3\sigma(F_o)$. Data were corrected for Lorentz and polarization effects. No absorption correction was applied. The structure solution, by direct methods, and the full-matrix least-squares refinement used programs in *SHELXTL-Plus* (Sheldrick, 1987). The function $\sum w(|F_o| - |F_c|)^2$ was minimized, where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0.000225$. A secondary-extinction parameter $p = 0.005$ (1), in $F_c^* = F_c/[1.0 + 0.002(p)F_o^2/\sin(2\theta)]^{0.25}$. 257 parameters were refined: atom coordinates and anisotropic thermal param-

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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)	1280 (5)	1323 (3)	5238 (3)	26 (1)
N(2)	12 (5)	1174 (3)	4532 (2)	30 (1)
C(3)	− 1494 (6)	608 (4)	4782 (4)	38 (1)
N(4)	− 1312 (5)	− 568 (3)	4719 (3)	39 (1)
C(5)	− 32 (7)	− 1090 (4)	5261 (3)	37 (1)
N(6)	1616 (5)	− 716 (3)	5041 (3)	31 (1)
C(7)	2326 (6)	282 (3)	5435 (3)	26 (1)
N(8)	2446 (5)	265 (3)	6448 (2)	30 (1)
C(9)	1216 (7)	938 (4)	6911 (3)	36 (1)
N(10)	638 (4)	1635 (3)	6147 (2)	28 (1)
N(2*a*)	− 55 (5)	1942 (3)	3811 (3)	39 (1)
O(2*a*)	− 1350 (5)	2023 (3)	3378 (3)	57 (1)
O(2*b*)	1178 (5)	2462 (3)	3642 (3)	52 (1)
N(4*a*)	− 1876 (5)	− 1091 (4)	3903 (3)	46 (1)
O(4*a*)	− 1668 (5)	− 2073 (3)	3857 (3)	65 (2)
O(4*b*)	− 2624 (5)	− 537 (3)	3333 (3)	57 (1)
N(6*a*)	2563 (5)	− 1349 (3)	4450 (3)	40 (1)
O(6*a*)	3971 (4)	− 1055 (3)	4294 (3)	49 (1)
O(6*b*)	1945 (5)	− 2178 (3)	4126 (3)	59 (1)
C(8)	3811 (6)	− 29 (3)	6976 (3)	33 (1)
C(8*a*)	5252 (7)	− 472 (5)	6460 (4)	49 (2)
O(8)	3776 (5)	90 (3)	7825 (2)	49 (1)
C(10)	51 (5)	2678 (3)	6263 (3)	30 (1)
C(10*a*)	− 321 (7)	3035 (4)	7239 (3)	42 (2)
O(10)	− 99 (4)	3263 (2)	5566 (2)	38 (1)

eters for all non-H atoms; coordinates for all non-methyl H atoms; methyl H atoms, included using 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 $U_{eq}(C)$. $(\Delta/\sigma)_{max} = 0.10$, ratio of observations to parameters = 5.1:1, $R = 0.046$, $wR = 0.053$, $S = 2.0$. $R = 0.050$ for all data. Final difference Fourier excursions were 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. The four ideal (*i.e.* symmetric) conformers of cycloheptane and the continuum of relatively low-energy forms that lie between them are described by Flapper & Romers (1975). Several similar heterocycles with *N*-acetyl and *N*-nitro substituents were reported by Koppes, Chaykovsky, Adolph, Gilardi & George (1987). The structure of the 8,10-dipropionyl derivative of the title compound has also been reported (Flippen-Anderson, George & Gilardi, 1992).

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

C(1)—N(2)	1.450 (5)	C(1)—C(7)	1.558 (6)
C(1)—N(10)	1.443 (5)	N(2)—C(3)	1.453 (6)
N(2)—N(2*a*)	1.390 (5)	C(3)—N(4)	1.449 (6)
N(4)—C(5)	1.443 (6)	N(4)—N(4*a*)	1.400 (6)
C(5)—N(6)	1.453 (6)	N(6)—C(7)	1.461 (5)
N(6)—N(6*a*)	1.378 (5)	C(7)—N(8)	1.442 (5)
N(8)—C(9)	1.453 (6)	N(8)—C(8)	1.388 (6)
C(9)—N(10)	1.458 (6)	N(10)—C(10)	1.372 (5)
N(2*a*)—O(2*a*)	1.224 (6)	N(2*a*)—O(2*b*)	1.213 (6)
N(4*a*)—O(4*a*)	1.215 (6)	N(4*a*)—O(4*b*)	1.219 (6)
N(6*a*)—O(6*a*)	1.222 (6)	N(6*a*)—O(6*b*)	1.222 (5)
C(8)—C(8*a*)	1.485 (7)	C(8)—O(8)	1.212 (5)
C(10)—C(10*a*)	1.483 (7)	C(10)—O(10)	1.227 (5)

N(2)—C(1)—C(7)	114.2 (3)	N(2)—C(1)—N(10)	113.1 (3)
C(7)—C(1)—N(10)	104.7 (3)	C(1)—N(2)—C(3)	119.5 (3)
C(1)—N(2)—N(2*a*)	116.8 (3)	C(3)—N(2)—N(2*a*)	118.0 (4)
N(2)—C(3)—N(4)	111.9 (4)	C(3)—N(4)—C(5)	118.7 (4)
C(3)—N(4)—N(4*a*)	118.1 (4)	C(5)—N(4)—N(4*a*)	118.3 (4)
N(4)—C(5)—N(6)	114.5 (4)	C(5)—N(6)—C(7)	123.2 (4)
C(5)—N(6)—N(6*a*)	118.0 (3)	C(7)—N(6)—N(6*a*)	118.8 (4)
C(1)—C(7)—N(6)	113.5 (4)	C(1)—C(7)—N(8)	103.2 (3)
N(6)—C(7)—N(8)	113.3 (3)	C(7)—N(8)—C(9)	113.3 (3)
C(7)—N(8)—C(8)	126.6 (4)	C(9)—N(8)—C(8)	117.1 (3)
N(8)—C(9)—N(10)	102.6 (3)	C(1)—N(10)—C(9)	113.1 (3)
C(1)—N(10)—C(10)	118.6 (3)	C(9)—N(10)—C(10)	124.6 (4)
N(2)—N(2*a*)—O(2*a*)	117.3 (4)	N(2)—N(2*a*)—O(2*b*)	117.9 (4)
O(2*a*)—N(2*a*)—O(2*b*)	124.8 (4)	N(4)—N(4*a*)—O(4*a*)	116.8 (4)
N(4)—N(4*a*)—O(4*b*)	117.2 (4)	O(4*a*)—N(4*a*)—O(4*b*)	125.8 (5)
N(6)—N(6*a*)—O(6*a*)	118.1 (4)	N(6)—N(6*a*)—O(6*b*)	117.7 (4)
O(6*a*)—N(6*a*)—O(6*b*)	124.2 (4)	N(8)—C(8)—C(8*a*)	117.4 (4)
N(8)—C(8)—O(8)	119.0 (4)	C(8*a*)—C(8)—O(8)	123.5 (4)
N(10)—C(10)—C(10*a*)	117.2 (4)	N(10)—C(10)—O(10)	118.8 (4)
C(10*a*)—C(10)—O(10)	124.0 (4)		

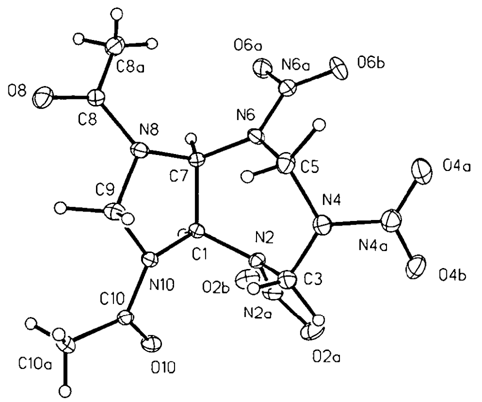

Fig. 1. A thermal ellipsoid plot showing the molecular conformation of the title compound.

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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 55173 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0608]