$C_7H_9N_7O_8$

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

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

	x	y	z	U_{eq}
C(1)	4273 (3)	−2976 (3)	6364 (3)	30 (1)
N(2)	4247 (2)	−1434 (3)	6185 (2)	31 (1)
C(3)	4953 (3)	−385 (4)	7018 (3)	36 (1)
C(4)	5389 (3)	−1164 (4)	8108 (3)	32 (1)
N(5)	4341 (2)	−2146 (3)	8205 (2)	31 (1)
C(6)	4015 (3)	−3358 (3)	7442 (2)	30 (1)
N(7)	4881 (2)	−4608 (3)	7853 (2)	30 (1)
C(8)	5839 (3)	−4798 (3)	7344 (2)	32 (1)
N(9)	5611 (2)	−3612 (3)	6577 (2)	32 (1)
N(10)	3514 (3)	−889 (3)	5186 (2)	36 (1)
O(11)	3622 (2)	424 (3)	5060 (2)	47 (1)
O(12)	2806 (2)	−1733 (3)	4514 (2)	55 (1)
N(13)	3283 (3)	−1482 (3)	8446 (2)	36 (1)
O(14)	3492 (2)	−259 (3)	8857 (2)	50 (1)
O(15)	2260 (2)	−2179 (3)	8286 (2)	50 (1)
C(16)	4566 (3)	−5599 (3)	8581 (3)	36 (1)
O(17)	3609 (2)	−5300 (3)	8854 (2)	50 (1)
C(18)	5427 (4)	−6898 (4)	8938 (4)	47 (2)
O(19)	6670 (2)	−5717 (2)	7488 (2)	43 (1)
N(20)	6089 (3)	−3775 (3)	5669 (2)	40 (1)
O(21)	5318 (2)	−3427 (3)	4793 (2)	49 (1)
O(22)	7212 (3)	−4213 (3)	5877 (2)	60 (1)

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

C(1)—N(2)	1.423 (4)	C(1)—C(6)	1.545 (5)
C(1)—N(9)	1.476 (4)	N(2)—C(3)	1.458 (4)
N(2)—N(10)	1.373 (3)	C(3)—C(4)	1.514 (5)
C(4)—N(5)	1.464 (4)	N(5)—C(6)	1.449 (4)
N(5)—N(13)	1.395 (4)	C(6)—N(7)	1.454 (4)
N(7)—C(8)	1.388 (5)	N(7)—C(16)	1.419 (4)
C(8)—N(9)	1.435 (4)	C(8)—O(19)	1.187 (4)
N(9)—N(20)	1.429 (5)	N(10)—O(11)	1.218 (4)
N(10)—O(12)	1.223 (3)	N(13)—O(14)	1.225 (4)
N(13)—O(15)	1.218 (4)	C(16)—O(17)	1.208 (5)
C(16)—C(18)	1.476 (5)	N(20)—O(21)	1.211 (3)
N(20)—O(22)	1.203 (4)		

Table 2 (cont.)

N(2)—C(1)—C(6)	111.7 (3)	N(2)—C(1)—N(9)	112.7 (2)
C(6)—C(1)—N(9)	100.4 (2)	C(1)—N(2)—C(3)	123.3 (2)
C(1)—N(2)—N(10)	119.1 (2)	C(3)—N(2)—N(10)	117.6 (2)
N(2)—C(3)—C(4)	108.3 (3)	C(3)—C(4)—N(5)	110.6 (2)
C(4)—N(5)—C(6)	115.5 (3)	C(4)—N(5)—N(13)	116.2 (2)
C(6)—N(5)—N(13)	116.7 (2)	C(1)—C(6)—N(5)	111.8 (2)
C(1)—C(6)—N(7)	103.6 (3)	N(5)—C(6)—N(7)	111.2 (2)
C(6)—N(7)—C(8)	113.4 (3)	C(6)—N(7)—C(16)	119.1 (3)
C(8)—N(7)—C(16)	126.8 (2)	N(7)—C(8)—N(9)	104.3 (2)
N(7)—C(8)—O(19)	129.3 (3)	N(9)—C(8)—O(19)	126.4 (3)
C(1)—N(9)—C(8)	111.4 (3)	C(1)—N(9)—N(20)	117.4 (2)
C(8)—N(9)—N(20)	117.7 (2)	N(2)—N(10)—O(11)	115.6 (2)
N(2)—N(10)—O(12)	118.6 (3)	O(11)—N(10)—O(12)	125.8 (3)
N(5)—N(13)—O(14)	116.4 (3)	N(5)—N(13)—O(15)	118.2 (3)
O(14)—N(13)—O(15)	125.2 (3)	N(7)—C(16)—O(17)	116.6 (3)
N(7)—C(16)—C(18)	117.7 (3)	O(17)—C(16)—C(18)	125.7 (3)
N(9)—N(20)—O(21)	115.6 (3)	N(9)—N(20)—O(22)	115.9 (3)
O(21)—N(20)—O(22)	128.5 (4)		

Related literature. The structures of two related compounds, both having the acetyl group on N(7) replaced with a fourth nitro group and one having the carbonyl O atom replaced with an acetoxy moiety, have been reported (Flippen-Anderson, George & Gilardi, 1990).

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Structures of (I) 6-Nitro-2,4-dipropionyl-8-oxa-2,4,6-triazabicyclo[3.3.0]octane and (II) 2,4-Diacetyl-6-nitro-8-oxa-2,4,6-triazabicyclo[3.3.0]octane

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Abstract. (I) $C_{10}H_{16}N_4O_5$, $M_r = 272.3$, monoclinic, $P2_1/n$, $a = 6.151$ (2), $b = 13.484$ (7), $c = 15.165$ (9) Å, $\beta = 90.94$ (5)°, $V = 1257.6$ (9) Å^3, $Z = 4$, $D_x = 1.438$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.11$ mm^{-1}, $F(000) = 576$, $T = 295$ K, final $R = 0.046$, $wR = 0.038$ for 1274 independent observed reflections. (II) $C_8H_{12}N_4O_5$, $M_r = 244.2$, monoclinic, $P2_1/c$, $a = 7.801$ (1), $b = 19.885$ (3), $c = 7.077$ (1) Å, $\beta = 91.35$ (2)°, $V = 1097.5$ (3) Å^3, $Z = 4$, $D_x = 1.478$ Mg m^{-3}, $\lambda(\text{Cu } K\alpha) = 1.54178$ Å, $\mu = 1.02$ mm^{-1}, $F(000) = 512$, $T = 295$ K, final $R = 0.039$, $wR = 0.051$ for 1718 independent observed reflections. In (I) both rings have an envelope conformation while in (II) the acetyl substituted ring is planar. The nitroamine group is pyramidal in both molecules with an N—N to C—N—C angle of 43.1 in (I) and 42.6° in (II). In (I) the carbonyl O atoms of the propionyl groups are on opposite sides of the C—N—C—N—C chain whereas in (II) the acetyl carbonyls are on the same side of the chain.

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement coefficients* (Å^2 × 10^3) *for* (I)

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

	x	y	z	U_{eq}
C(1)	1985 (5)	3068 (2)	367 (2)	40 (1)
N(2)	1069 (4)	2077 (2)	320 (2)	41 (1)
C(3)	1882 (6)	1498 (3)	−416 (3)	49 (1)
N(4)	3824 (4)	2052 (2)	−646 (2)	41 (1)
C(5)	3801 (5)	3056 (2)	−319 (2)	37 (1)
N(6)	3017 (3)	3763 (2)	−990 (2)	37 (1)
C(7)	708 (5)	3923 (2)	−834 (3)	42 (1)
O(8)	512 (3)	3825 (1)	96 (2)	44 (1)
C(9)	−662 (5)	1735 (2)	785 (2)	47 (1)
O(9)	−1495 (4)	949 (2)	586 (2)	67 (1)
C(10)	−1421 (7)	2371 (3)	1535 (3)	57 (2)
C(11)	−3535 (8)	2033 (4)	1911 (4)	65 (2)
C(12)	5458 (5)	1727 (2)	−1169 (2)	40 (1)
O(12)	6949 (4)	2278 (2)	−1363 (2)	58 (1)
C(13)	5287 (7)	670 (3)	−1490 (3)	54 (2)
C(14)	7140 (9)	350 (4)	−2045 (5)	76 (2)
N(15)	4243 (4)	4633 (2)	−1095 (2)	45 (1)
O(15a)	6130 (4)	4634 (2)	−830 (2)	59 (1)
O(15b)	3356 (4)	5306 (2)	−1500 (2)	66 (1)

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

C(1)—N(2)	1.452 (4)	C(1)—C(5)	1.540 (5)
C(1)—O(8)	1.421 (4)	N(2)—C(3)	1.457 (5)
N(2)—C(9)	1.368 (4)	C(3)—N(4)	1.456 (5)
N(4)—C(5)	1.442 (4)	N(4)—C(12)	1.362 (4)
C(5)—N(6)	1.471 (4)	N(6)—C(7)	1.460 (4)
N(6)—N(15)	1.404 (4)	C(7)—O(8)	1.424 (4)
C(9)—O(9)	1.213 (4)	C(9)—C(10)	1.504 (6)
C(10)—C(11)	1.499 (7)	C(12)—O(12)	1.220 (4)
C(12)—C(13)	1.509 (5)	C(13)—C(14)	1.492 (8)
N(15)—O(15a)	1.222 (4)	N(15)—O(15b)	1.220 (4)

N(2)—C(1)—C(5)	104.0 (3)	N(2)—C(1)—O(8)	113.7 (2)
C(5)—C(1)—O(8)	106.2 (3)	C(1)—N(2)—C(3)	113.2 (3)
C(1)—N(2)—C(9)	126.1 (3)	C(3)—N(2)—C(9)	119.7 (3)
N(2)—C(3)—N(4)	101.7 (3)	C(3)—N(4)—C(5)	112.7 (3)
C(3)—N(4)—C(12)	126.2 (3)	C(5)—N(4)—C(12)	120.9 (2)
C(1)—C(5)—N(4)	104.7 (2)	C(1)—C(5)—N(6)	103.1 (2)
N(4)—C(5)—N(6)	112.1 (3)	C(5)—N(6)—C(7)	107.0 (2)
C(5)—N(6)—N(15)	116.7 (2)	C(7)—N(6)—N(15)	114.9 (2)
N(6)—C(7)—O(8)	104.2 (2)	C(1)—O(8)—C(7)	106.8 (2)
N(2)—C(9)—O(9)	119.7 (3)	N(2)—C(9)—C(10)	116.9 (3)
O(9)—C(9)—C(10)	123.4 (3)	C(9)—C(10)—C(11)	113.4 (4)
N(4)—C(12)—O(12)	120.6 (3)	N(4)—C(12)—C(13)	116.3 (3)
O(12)—C(12)—C(13)	123.1 (3)	C(12)—C(13)—C(14)	113.9 (4)
N(6)—N(15)—O(15a)	118.2 (2)	N(6)—N(15)—O(15b)	116.2 (2)
O(15a)—N(15)—O(15b)	125.4 (3)		

Table 3. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement coefficients* (Å^2 × 10^3) *for* (II)

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

	x	y	z	U_{eq}
C(1)	3029 (2)	3674 (1)	4998 (2)	38 (1)
N(2)	2131 (2)	3432 (1)	3325 (2)	38 (1)
C(3)	294 (2)	3371 (1)	3537 (2)	46 (1)
N(4)	52 (2)	3563 (1)	5489 (2)	42 (1)
C(5)	1589 (2)	3809 (1)	6411 (2)	38 (1)
N(6)	1577 (2)	4557 (1)	6568 (2)	44 (1)
C(7)	2563 (2)	4794 (1)	4969 (3)	50 (1)
O(8)	3853 (1)	4303 (1)	4743 (2)	49 (1)
C(9)	2871 (2)	3150 (1)	1795 (2)	45 (1)
C(10)	4776 (3)	3187 (1)	1687 (3)	68 (1)
O(11)	1972 (2)	2892 (1)	556 (2)	60 (1)
C(12)	−1466 (2)	3421 (1)	6311 (3)	50 (1)
C(13)	−1652 (3)	3591 (1)	8346 (3)	71 (1)
O(14)	−2626 (2)	3173 (1)	5367 (2)	74 (1)
N(6')	2163 (2)	4810 (1)	8335 (2)	62 (1)
O(6a)	2789 (3)	5367 (1)	8340 (3)	99 (1)
O(6b)	1848 (3)	4481 (1)	9733 (2)	90 (1)

Table 4. *Bond lengths* (Å) *and bond angles* (°) *for* (II)

C(1)—N(2)	1.444 (2)	C(1)—C(5)	1.544 (2)
C(1)—O(8)	1.420 (2)	N(2)—C(3)	1.450 (2)
N(2)—C(9)	1.359 (2)	C(3)—N(4)	1.449 (2)
N(4)—C(5)	1.437 (2)	N(4)—C(12)	1.361 (2)
C(5)—N(6)	1.492 (2)	N(6)—C(7)	1.461 (2)
N(6)—N(6')	1.414 (2)	C(7)—O(8)	1.414 (2)
C(9)—C(10)	1.492 (3)	C(9)—O(11)	1.223 (2)
C(12)—C(13)	1.489 (3)	C(12)—O(14)	1.216 (2)
N(6')—O(6a)	1.211 (2)	N(6')—O(6b)	1.215 (2)

N(2)—C(1)—C(5)	104.0 (1)	N(2)—C(1)—O(8)	113.7 (1)
C(5)—C(1)—O(8)	105.5 (1)	C(1)—N(2)—C(3)	113.8 (1)
C(1)—N(2)—C(9)	125.7 (1)	C(3)—N(2)—C(9)	119.2 (1)
N(2)—C(3)—N(4)	103.2 (1)	C(3)—N(4)—C(5)	113.3 (1)
C(3)—N(4)—C(12)	119.1 (1)	C(5)—N(4)—C(12)	127.0 (1)
C(1)—C(5)—N(4)	105.0 (1)	C(1)—C(5)—N(6)	103.1 (1)
N(4)—C(5)—N(6)	111.5 (1)	C(5)—N(6)—C(7)	105.0 (1)
C(5)—N(6)—N(6')	114.7 (1)	C(7)—N(6)—N(6')	113.9 (1)
N(6)—C(7)—O(8)	104.7 (1)	C(1)—O(8)—C(7)	105.6 (1)
N(2)—C(9)—C(10)	117.5 (1)	N(2)—C(9)—O(11)	119.8 (1)
C(10)—C(9)—O(11)	122.6 (2)	N(4)—C(12)—C(13)	118.1 (2)
N(4)—C(12)—O(14)	119.5 (1)	C(13)—C(12)—O(14)	122.3 (2)
N(6)—N(6')—O(6a)	116.7 (2)	N(6)—N(6')—O(6b)	117.5 (2)
O(6a)—N(6')—O(6b)	125.4 (2)		

Experimental. Values for compound (II), whenever different, are given in parentheses. A clear colorless rod (prism) 0.10 × 0.10 × 0.45 (0.20 × 0.35 × 0.60) mm data crystal (recrystallized from ethyl acetate) was provided by Dr Clifford L. Coon of Livermore National Laboratory, California. An automated Siemens $R3m/V$ diffractometer with incident beam monochromator was used for data collection. 25 centered reflections within $20 \leq 2\theta \leq 25°$ (30 $\leq 2\theta \leq 80°$) were used for determining lattice parameters. $[\sin(\theta)/\lambda]_{max} = 0.60$ (0.59) Å^{-1}; range of hkl: $-7 \leq h \leq 7$, $0 \leq k \leq 15$, $-16 \leq l \leq 16$ ($-8 \leq h \leq 0$, $-22 \leq k \leq 19$, $-8 \leq l \leq 9$). Standards $\bar{1}11$, 031 and 004 (600, 080 and 004), monitored every 97 reflections, showed random variation of 2.5 (2.0)% 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 (6.0° min^{-1} minimum, 30.0° min^{-1} maximum), 4369 (4679) reflections measured, 2087 (1874) unique, $R_{int} = 2.9$ (1.5)%, 1274 (1718) observed with $F_o > 3\sigma(F_o)$. Data were corrected for Lorentz and polarization effects.

The structure solution, by direct methods, and the full-matrix least-squares refinement used programs in *SHELXTL*80 (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o| + g(F_o)^2]$, $g = 0.00023$. 236 (157) parameters were refined: atomic coordinates and anisotropic thermal parameters for all non-H atoms, 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) kept constant]. $(\Delta/\sigma)_{max} = 0.024$ (0.01), ratio of observations to parameters = 5.4:1 (10.9:1), $R = 0.046$ (0.039), $wR = 0.038$ (0.051), $S = 1.19$ (2.12) $[R = 0.086$ (0.042) for all data]. Final difference Fourier excursions were 0.20 and −0.21 (−0.16) e Å^{-3}. Atomic scattering factors were taken from *International Tables for X-ray Crystallography*

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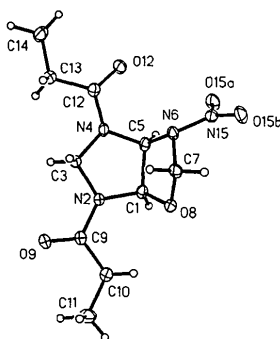

Fig. 2. A thermal ellipsoid plot of (II) with ellipsoids drawn at the 20% probability level.

(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).

* 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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Acta Cryst. (1992). C**48**, 1530–1531

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}, $\lambda(Cu\ K\alpha) = 1.54184$ 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
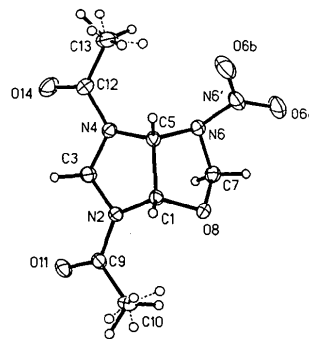
National Laboratory. An automated Siemens *R3m/V* diffractometer with incident beam monochromator was used for data collection. 25 centered reflections within $40.0 \le 2\theta \le 56.0°$ were used for determining lattice parameters. $(\sin\theta/\lambda)_{max} = 0.56$ Å^{-1}, range of *hkl*: $-6 \le h \le 4$, $0 \le k \le 27$, $0 \le l \le 20$. 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-