electron density fluctuation on final difference Fourier synthesis gave two peaks of 0·65–0·55 e Å^{-3}, respectively, at 1·1–1·2 Å from Sn, with background of ± 0·45 e Å^{-3}.

The scattering factors were taken from Cromer & Mann (1968) for Sn, O and C, and from Stewart, Davidson & Simpson (1965) for H.

The final coordinates for the non-H atoms are given in Table 1, selected bond distances and angles in Table 2.* Fig. 1 shows a thermal-ellipsoid plot with the atom numbering.

Related literature. For the preparation of some related compounds *via* a tin-mediated radical cyclization reaction, see also Fish, Kuivila & Tyminsky (1967).

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, distances and angles related to the phenyl groups, to the weighted least-squares planes and to H bonding, and a stereoview of the unit cell have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52288 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 1,3-Dinitro-1,3-diazacyclopentan-2-one

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Abstract. $C_3H_4N_4O_5$, $M_r = 176·08$, orthorhombic, $P2_12_12_1$, $a = 5·912$ (1), $b = 7·928$ (2), $c = 13·951$ (2) Å, $V = 653·9$ (2) Å^3, $Z = 4$, $D_x = 1·789$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0·16$ mm^{-1}, $F(000) = 360$, $T = 295$ K, final $R = 0·036$, $wR = 0·046$ for 653 observed reflections. Excluding H atoms the molecule is approximately planar to within ±0·27 Å. Even without the possibility of hydrogen bonding there are some very close intermolecular O···N approaches (2·91–2·96 Å).

Experimental. Colorless, 0·36 × 0·28 × 0·20 mm data crystal, synthesized and crystallized by Clifford Coon of the Lawrence Livermore Laboratory, Livermore, California. Automated Nicolet *R*3*m* diffractometer with incident-beam graphite monochromator; 25 centered reflections within $18 \le 2\theta \le 30°$ used for determining cell parameters. Data corrected for Lorentz and polarization effects, but not for absorption. $2\theta_{max} = 50°$; range of *hkl*: $-6 \le h \le 7$, $0 \le k \le 9$, $0 \le l \le 16$, standards, 400, 060, 0,0,10, monitored every 100 reflections with random variation of 2·0% over data collection, $\theta/2\theta$ mode, scan width $[2\theta(K\alpha_1) - 1·0]$ to $[2\theta(K\alpha_2) + 1·0]°$, scan rate a function of count rate (8° min^{-1} minimum, 30° min^{-1} maximum); 1366 reflections measured, 700 unique, $R_{int} = 0·015$, 653 observed $[F_o > 3\sigma(F_o)]$.

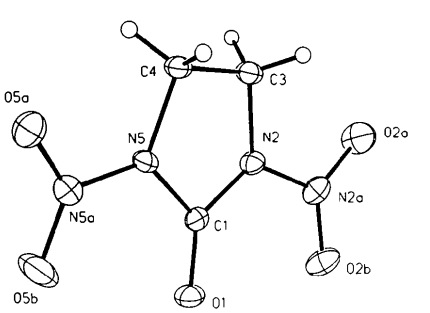

Fig. 1. Perspective drawing of the results of the X-ray study on the cyclopentane. Thermal ellipsoids are shown at the 20% probability level.

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

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	−374 (4)	1453 (3)	5791 (2)	32 (1)
O(1)	1375 (3)	1917 (2)	5471 (1)	47 (1)
N(2)	−1712 (3)	89 (3)	5508 (1)	37 (1)
N(2*a*)	−1380 (4)	−765 (3)	4660 (1)	48 (1)
O(2*a*)	−2833 (5)	−1787 (3)	4471 (2)	76 (1)
O(2*b*)	269 (4)	−458 (3)	4188 (1)	63 (1)
C(3)	−3857 (4)	−83 (3)	6017 (2)	41 (1)
C(4)	−3835 (4)	1405 (3)	6712 (2)	35 (1)
N(5)	−1592 (3)	2117 (3)	6560 (1)	37 (1)
N(5*a*)	−866 (3)	3460 (3)	7095 (2)	46 (1)
O(5*a*)	−2236 (3)	4058 (3)	7641 (1)	57 (1)
O(5*b*)	1079 (4)	3913 (3)	6996 (2)	91 (1)

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

C(1)—O(1)	1·185 (3)	C(1)—N(2)	1·396 (3)
C(1)—N(5)	1·396 (3)	N(2)—N(2*a*)	1·377 (3)
N(2)—C(3)	1·461 (3)	N(2*a*)—O(2*a*)	1·210 (3)
N(2*a*)—O(2*b*)	1·201 (3)	C(3)—C(4)	1·527 (4)
C(4)—N(5)	1·457 (3)	N(5)—N(5*a*)	1·368 (3)
N(5*a*)—O(5*a*)	1·210 (3)	N(5*a*)—O(5*b*)	1·212 (3)
O(1)—C(1)—N(2)	128·9 (2)	O(1)—C(1)—N(5)	128·5 (2)
N(2)—C(1)—N(5)	102·6 (2)	C(1)—N(2)—N(2*a*)	122·9 (2)
C(1)—N(2)—C(3)	115·3 (2)	N(2*a*)—N(2)—C(3)	119·7 (2)
N(2)—N(2*a*)—O(2*a*)	114·5 (2)	N(2)—N(2*a*)—O(2*b*)	119·2 (2)
O(2*a*)—N(2*a*)—O(2*b*)	126·3 (2)	N(2)—C(3)—C(4)	103·2 (2)
C(3)—C(4)—N(5)	102·4 (2)	C(1)—N(5)—C(4)	115·8 (2)
C(1)—N(5)—N(5*a*)	123·4 (2)	C(4)—N(5)—N(5*a*)	120·5 (2)
N(5)—N(5*a*)—O(5*a*)	116·0 (2)	N(5)—N(5*a*)—O(5*b*)	117·8 (2)
O(5*a*)—N(5*a*)—O(5*b*)	126·2 (3)		

Structure solved by direct methods. The least-squares refinement used the full-matrix program provided with the MicroVAX version of the *SHELXTL* system (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00023$, secondary isotropic extinction from $F_c^* = F_c/[1{\cdot}0 + 0{\cdot}002(p)F_o^2/\sin 2\theta]^{0{\cdot}25}$ where $p = 0{\cdot}018$ (2). There were 126 parameters refined: atom coordinates for all atoms, anisotropic temperature factors for non-H atoms and isotropic temperature factors for H atoms; $(\Delta/\sigma)_{max} = 0{\cdot}01$, $R = 0{\cdot}032$, $wR = 0{\cdot}045$, $S = 2{\cdot}09$, final difference Fourier excursions 0·27 and −0·21 e $Å^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).† Atom numbering for Tables 1 and 2, atom coordinates, bond distances and bond angles, 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 52317 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. The structure of 1,4-dinitroglycouril (DINGU) has been reported (Boileau, Wimmer, Gilardi, Stinecipher, Gallo & Pierrot, 1988).

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Structure of the Product of Addition of 7-Oxabicyclo[2.2.1]hept-5-ene-2-carbonitrile and Benzonitrile Oxide

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Abstract. 5-Phenyl-3,10-dioxa-4-azatricyclo[5.2.1.$0^{2,6}$]-dec-4-en-8-one, $C_{13}H_{11}NO_3$, $M_r = 229{\cdot}23$, orthorhombic, $Pna2_1$, $a = 5{\cdot}8737$ (4), $b = 17{\cdot}1877$ (12), $c = 10{\cdot}6692$ (10) Å, $V = 1077{\cdot}1$ (1) $Å^3$, $Z = 4$, $D_x = 1{\cdot}41$ g cm^{-3}. Mo $K\alpha$ radiation (graphite-crystal monochromator, $\lambda = 0{\cdot}71073$ Å), μ(Mo $K\alpha$) = 0·95 cm^{-1}, $F(000) = 480$, $T = 293$ K. Final conventional R factor = 0·025 for 688 unique reflections and

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