DUPONT, L., DIDEBERG, O. & DELARGE, J. (1980). *Cryst. Struct. Commun.* **9**, 1105–1110.
DUPONT, L., DIDEBERG, O., DELARGE, J., DIVE, G. & THUNUS, L. (1982). *Acta Cryst.* B**38**, 1495–1500.
DUPONT, L., DIDEBERG, O. & LAMOTTE, J. (1979). *Acta Cryst.* B**35**, 2817–2820.
DUPONT, L., LAMOTTE, J., CAMPSTEYN, H. & VERMEIRE, M. (1978). *Acta Cryst.* B**34**, 1304–1310.
DUPONT, L., LEWINSKI, K., STADNICKA, K. & DELARGE, J. (1981). *Cryst. Struct. Commun.* **10**, 925–930.
EVANS, D. G. & BOEYENS, J. C. A. (1988). *Acta Cryst.* B**44**, 663–671.
EVANS, S. V. & TROTTER, J. (1988). *Acta Cryst.* B**44**, 63–72.
HENDRICKSON, J. B. (1961). *J. Am. Chem. Soc.* **83**, 4537–4547.
HENDRICKSON, J. B. (1964). *J. Am. Chem. Soc.* **86**, 4854–4866.
HENDRICKSON, J. B. (1967). *J. Am. Chem. Soc.* **89**, 7036–7061.
NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
SHELDRICK, G. M. (1976). *SHELX76*. Programme pour la détermination des structures cristallines. Univ. de Cambridge, Angleterre.
SHELDRICK, G. M. (1986). *SHELXS86*. Programme pour la solution des structures cristallines. Univ. de Göttingen, Allemagne.

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Structure of 9-Nitro-[4]peristylane-1,5-dione

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Abstract. Decahydro-1,6:3,4-dimethano-3a-nitrocyclobuta[1,2:3,4]dicyclopentene-2,5-dione (II), $C_{12}H_{11}NO_4$, $M_r = 233{\cdot}2$, monoclinic, $P2_1/n$, $a = 13{\cdot}378\,(7)$, $b = 6{\cdot}614\,(1)$, $c = 23{\cdot}040\,(15)$ Å, $\beta = 92{\cdot}53\,(5)°$, $V = 2036{\cdot}6\,(4)$ Å^3, $Z = 8$, $D_x = 1{\cdot}521$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 9{\cdot}3$ cm^{-1}, $F(000) = 1312$, $T = 293$ K, final $R = 0{\cdot}047$, $wR = 0{\cdot}075$ for 3075 reflections with $I > 3\sigma(I)$. There are no unusually short intermolecular distances. A comparison of the molecular densities and packing coefficients of (I) [4]peristylane-1,5-dione with (II), indicates that the change in crystal density from (I) ($1{\cdot}415$ g cm^{-3}) to (II) ($1{\cdot}521$ g cm^{-3}) is the sole result of an increase in molecular density with NO_2 substitution. The packing coefficients for (I) and (II) are identical.

Introduction. Density is an important property of energetic materials, such as propellants and explosives. Characteristics such as detonation velocity and pressure are functions of density as is the quantity of material that can be packed into a limited volume. The principal determinants of crystal density are the molecular density (molecular mass/molecular volume) and the crystal packing efficiency. The volume of a molecule can be calculated by an appropriate overlap-corrected summation of atomic van der Waals radii. The crystal unit-cell volume per molecule includes contributions from both the molecular volume and the space between molecules in the crystal. Kitaigorodskii (1961) coined the term 'packing coefficient' (molecular volume/unit-cell volume) as an expression of the crystal packing efficiency. Clearly, the most dense crystals, for a series of C—H—N—O-containing molecules, will have both high molecular densities and high packing coefficients.

Ordinarily, the replacement of a low-density atom (*e.g.* H) by a high-density atom or group (*e.g.* NO_2) produces an increase in the crystal density because of an increase in the molecular density. Such a change in the crystal density, however, could be mitigated or possibly reversed if the high-density replacement group diminished the crystal packing efficiency. The influence of an additional nitro-group substitutent on the crystal densities of a series of [4]peristylane derivatives recently has been investigated by Shen & Paquette (1989), who showed that for several pairs of compounds replacement of a basal H atom by a nitro group does not lead invariably to a concomitant increase in crystal density. For example, within the four [4]peristylanes whose structures are shown below, there is the expected crystal density increase with nitro substitution from (I) to (II) ($1{\cdot}41$ to $1{\cdot}52$ g cm^{-3}), but essentially no change from (III) to (IV) ($1{\cdot}62$ to $1{\cdot}63$ g cm^{-3}). We have undertaken the determination of the crystal structures of several of the [4]peristylanes to enable a detailed study to be

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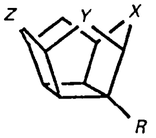
made of the crystal packing effects of basal nitro-group substitution. In this paper, we report the structure of (II).



(I) $X = Z = \mathrm{C{=}O}$, $Y = \mathrm{CH_2}$, $R = \mathrm{H}$
(II) $X = Z = \mathrm{C{=}O}$, $Y = \mathrm{CH_2}$, $R = \mathrm{NO_2}$
(III) $X - Z = \mathrm{O_2NCCNO_2}$, $Y = \mathrm{CH_2}$, $R = \mathrm{H}$
(IV) $X - Z = \mathrm{O_2NCCNO_2}$, $Y = \mathrm{CH_2}$, $R = \mathrm{NO_2}$
(V) $X = Y = Z = \mathrm{C{=}O}$, $R = \mathrm{H}$
(VI) $X = Z = \mathrm{C{=}O}$, $Y = \mathrm{C{=}C(CH_3)_2}$
(VII) $Z = \mathrm{C{=}O}$, $X = \mathrm{C(NO_2)_2}$, $Y = \mathrm{CH_2}$, $R = \mathrm{NO_2}$

Experimental. (II): 0·15 × 0·56 × 0·56 mm plate-like crystal; Enraf–Nonius CAD-4 diffractometer with incident-beam graphite monochromator; cell parameters and crystal orientation from 25 automatically centered reflections in the range $15·1 < \theta < 40·0°$; 2θ–θ scans over θ range of $1·5(1·10 + 0·14\tan\theta)°$; variable θ scan speed of $1·37$–$8·24° \min^{-1}$; each scan recorded in 96 steps with two outermost 16-step intensity blocks used for background determination; diffractometer controlled with Digital Equipment Corporation MicroVAX II computer and standard Enraf–Nonius programs (version 5.0); 10 standard reflections monitored at 1 h intervals of X-ray exposure, −0·2 to 1·7% intensity variation, 0·7% average, correction applied; ψ-scan absorption correction applied with data from nine reflections, transmission-factor range of 0·824–1·0, average 0·939; $\theta_{\max}$ of 65°, *hkl*'s selected to maintain diffractometer χ angle within 0–90° range; 4131 total data measured, 3802 unique data, 3075 data with $I > 3\sigma(I)$, $R_{\mathrm{int}} = 0·011$ for 99 pairs of data. All crystallographic calculations performed with the *TEXSAN* (Molecular Structure Corporation, 1989) program system on DEC MicroVAX II or VAXStation II computers; structure solved with the *SIR* direct-methods program (Burla, Camalli, Cascarano, Giacovazzo, Polidori, Spagna & Viterbo, 1989) incorporated in *TEXSAN*. Full-matrix least-squares refinement, $\sum[w(F_o - F_c)^2]$, $w = 1/\sigma^2(F_o)$, minimized, reflections with $I < 3\sigma(I)$ excluded from refinement, correction for secondary-isotropic extinction (Zachariasen, 1968) applied, $g = 0·146\,(5) \times 10^{-5}$; anisotropic temperature factors for C, O and N; H atoms positioned from the C-atom framework and refined with individual isotropic temperature factors, 396 total variables; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 155–175); min. and max. $\Delta\rho$ of −0·18 and 0·32 e Å^{-3}; max. Δ/σ in final least-squares cycle 0·24; R, wR and S 0·047, 0·075 and 2·39. Atomic coordinates are listed in Table 1.* The *PLOTMD* (Luo, Ammon & Gilliland, 1989) program was used to display the *ORTEP* (Johnson, 1965) drawings on a VAXStation II monitor, label the drawings and prepare print files for a Hewlett-Packard Laser-Jet II printer.

Table 1. *Fractional coordinates and equivalent isotropic temperature factors* (Å^2) *with e.s.d.'s in parentheses*

$B_{\mathrm{eq}} = (8\pi^2/3)\mathrm{trace}\mathbf{U}$.

	x	y	z	B
O1	−0·1404 (1)	0·3963 (2)	0·31701 (8)	5·06 (9)
O2	−0·2946 (1)	0·2839 (3)	0·44269 (8)	5·34 (9)
O3	0·0521 (2)	−0·2197 (4)	0·31222 (8)	6·5 (1)
O4	0·0547 (1)	−0·3143 (3)	0·4005 (1)	6·0 (1)
N	0·0177 (1)	−0·2209 (3)	0·35992 (9)	3·81 (8)
C1	−0·1322 (2)	0·2174 (3)	0·32639 (9)	3·07 (8)
C2	−0·0533 (2)	0·1287 (3)	0·3687 (1)	3·06 (8)
C3	−0·0710 (2)	0·1958 (4)	0·4313 (1)	4·0 (1)
C4	−0·1533 (2)	0·0558 (4)	0·45130 (9)	3·6 (1)
C5	−0·2561 (2)	0·1262 (3)	0·42859 (9)	3·5 (1)
C6	−0·3023 (1)	−0·0171 (3)	0·38325 (9)	3·32 (9)
C7	−0·3080 (2)	0·0836 (4)	0·3230 (1)	3·6 (1)
C8	−0·2019 (2)	0·0563 (3)	0·30062 (8)	2·97 (8)
C9	−0·0741 (1)	−0·0980 (3)	0·36841 (8)	2·71 (8)
C10	−0·1365 (2)	−0·1469 (3)	0·4211 (1)	3·29 (8)
C11	−0·2278 (2)	−0·1908 (3)	0·3788 (1)	3·28 (9)
C12	−0·1640 (2)	−0·1440 (3)	0·32601 (9)	2·91 (8)
O1′	0·0573 (1)	−0·5016 (3)	0·10703 (9)	5·3 (1)
O2′	0·3248 (1)	−0·3684 (3)	0·09189 (8)	5·17 (9)
O3′	−0·0578 (1)	0·1233 (4)	0·1849 (1)	6·1 (1)
O4′	0·0726 (2)	0·2291 (4)	0·23222 (9)	6·8 (1)
N′	0·0321 (1)	0·1307 (3)	0·19356 (8)	3·78 (8)
C1′	0·0660 (1)	−0·3208 (3)	0·1118 (1)	3·5 (1)
C2′	0·0913 (2)	−0·2156 (3)	0·1699 (1)	3·27 (9)
C3′	0·1972 (2)	−0·2638 (4)	0·1940 (1)	4·1 (1)
C4′	0·2649 (2)	−0·1232 (3)	0·1597 (1)	3·45 (9)
C5′	0·2816 (1)	−0·2108 (4)	0·1000 (1)	3·5 (1)
C6′	0·2320 (2)	−0·0856 (3)	0·0518 (1)	3·5 (1)
C7′	0·1459 (2)	−0·2001 (4)	0·0216 (1)	3·9 (1)
C8′	0·0578 (2)	−0·1719 (3)	0·0619 (1)	3·37 (9)
C9′	0·0941 (1)	0·0088 (3)	0·15477 (8)	2·69 (8)
C10′	0·2043 (1)	0·0701 (3)	0·14864 (9)	3·02 (8)
C11′	0·1838 (2)	0·0938 (3)	0·08212 (9)	3·21 (9)
C12′	0·0728 (2)	0·0373 (3)	0·08851 (9)	3·03 (8)

Discussion. Bond lengths, bond angles and selected torsion angles are given in Table 2 and *ORTEP* drawings of the two unique molecules are shown in Fig. 1. The molecular dimensions and overall structures are virtually identical. There is substantial similarity to the structures of other [4]peristylanes [*i.e.* (I), Engel, Fischer & Paquette (1984); (V) and (VI), Paquette, Shen & Engel (1989); (VII), Shen & Paquette (1989)] with sp^2-hybridized carbon at the 1,3- and/or 5-positions. The molecules have approximate C_{2v} symmetry if one ignores the nitro substituent. For the two molecules of (II), the average C_{sp^3}—C_{sp^3} distance is 1·531 (3) Å for bonds which are not part of the basal cyclobutane rings; the cyclobutane C—C average is 1·547 (3) Å. The corresponding

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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 54129 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

O1—C1	1·207 (3)	O1′—C1′	1·206 (3)
O2—C5	1·213 (3)	O2′—C5′	1·211 (3)
O3—N	1·210 (3)	O3′—N′	1·212 (3)
O4—N	1·208 (3)	O4′—N′	1·212 (3)
N—C9	1·494 (3)	N′—C9′	1·484 (3)
C1—C2	1·522 (3)	C1′—C2′	1·535 (3)
C1—C8	1·519 (3)	C1′—C8′	1·513 (3)
C2—C3	1·539 (3)	C2′—C3′	1·532 (3)
C2—C9	1·525 (3)	C2′—C9′	1·526 (3)
C3—C4	1·525 (3)	C3′—C4′	1·539 (3)
C4—C5	1·523 (3)	C4′—C5′	1·519 (3)
C4—C10	1·532 (3)	C4′—C10′	1·529 (3)
C5—C6	1·521 (3)	C5′—C6′	1·513 (3)
C6—C7	1·538 (3)	C6′—C7′	1·521 (3)
C6—C11	1·527 (3)	C6′—C11′	1·533 (3)
C7—C8	1·542 (3)	C7′—C8′	1·544 (3)
C8—C12	1·526 (3)	C8′—C12′	1·523 (3)
C9—C10	1·536 (3)	C9′—C10′	1·542 (3)
C9—C12	1·546 (3)	C9′—C12′	1·552 (3)
C10—C11	1·555 (3)	C10′—C11′	1·553 (3)
C11—C12	1·548 (3)	C11′—C12′	1·544 (3)
O3—N—O4	123·1 (2)	O3′—N′—O4′	123·5 (2)
O3—N—C9	117·6 (2)	O3′—N′—C9′	117·1 (2)
O4—N—C9	119·2 (2)	O4′—N′—C9′	119·4 (2)
O1—C1—C2	123·2 (2)	O1′—C1′—C2′	123·0 (2)
O1—C1—C8	124·6 (2)	O1′—C1′—C8′	125·0 (2)
C2—C1—C8	112·1 (2)	C2′—C1′—C8′	111·9 (2)
C1—C2—C3	111·0 (2)	C1′—C2′—C3′	112·7 (2)
C1—C2—C9	104·8 (2)	C1′—C2′—C9′	104·3 (2)
C3—C2—C9	104·6 (2)	C3′—C2′—C9′	104·7 (2)
C2—C3—C4	104·5 (2)	C2′—C3′—C4′	104·2 (2)
C3—C4—C5	111·3 (2)	C3′—C4′—C5′	110·3 (2)
C3—C4—C10	105·8 (2)	C3′—C4′—C10′	105·8 (2)
C5—C4—C10	105·1 (2)	C5′—C4′—C10′	105·4 (2)
O2—C5—C4	123·9 (2)	O2′—C5′—C4′	123·9 (2)
O2—C5—C6	123·7 (2)	O2′—C5′—C6′	123·7 (2)
C4—C5—C6	112·2 (2)	C4′—C5′—C6′	112·2 (2)
C5—C6—C7	110·6 (2)	C5′—C6′—C7′	111·2 (2)
C5—C6—C11	105·6 (2)	C5′—C6′—C11′	105·6 (2)
C7—C6—C11	105·8 (2)	C7′—C6′—C11′	105·6 (2)
C6—C7—C8	104·0 (2)	C6′—C7′—C8′	104·3 (2)
C1—C8—C7	110·2 (2)	C1′—C8′—C7′	110·3 (2)
C1—C8—C12	105·7 (2)	C1′—C8′—C12′	106·4 (2)
C7—C8—C12	105·5 (2)	C7′—C8′—C12′	105·2 (2)
N—C9—C2	112·6 (2)	N′—C9′—C2′	111·7 (2)
N—C9—C10	117·8 (2)	N′—C9′—C10′	118·3 (2)
N—C9—C12	115·6 (2)	N′—C9′—C12′	116·3 (2)
C2—C9—C10	108·0 (2)	C2′—C9′—C10′	108·1 (2)
C2—C9—C12	109·5 (2)	C2′—C9′—C12′	109·8 (2)
C10—C9—C12	91·3 (2)	C10′—C9′—C12′	90·8 (2)
C4—C10—C9	105·7 (2)	C4′—C10′—C9′	105·5 (2)
C4—C10—C11	108·7 (2)	C4′—C10′—C11′	108·6 (2)
C9—C10—C11	89·1 (2)	C9′—C10′—C11′	89·3 (2)
C6—C11—C10	108·4 (2)	C6′—C11′—C10′	108·1 (2)
C6—C11—C12	106·6 (2)	C6′—C11′—C12′	106·4 (2)
C10—C11—C12	90·6 (2)	C10′—C11′—C12′	90·6 (2)
C8—C12—C9	107·9 (2)	C8′—C12′—C9′	107·5 (2)
C8—C12—C11	106·9 (2)	C8′—C12′—C11′	106·9 (2)
C9—C12—C11	89·0 (2)	C9′—C12′—C11′	89·3 (1)
O3—N—C9—C2	−71·6 (3)	O3′—N′—C9′—C2′	−75·7 (3)
O3—N—C9—C10	161·6 (2)	O3′—N′—C9′—C10′	157·9 (2)
O3—N—C9—C12	55·2 (3)	O3′—N′—C9′—C12′	51·4 (3)
O4—N—C9—C12	107·6 (2)	O4′—N′—C9′—C2′	103·4 (3)
O4—N—C9—C10	−19·2 (3)	O4′—N′—C9′—C10′	−23·1 (3)
O4—N—C9—C12	−125·6 (2)	O4′—N′—C9′—C12′	−129·6 (2)

averages in (I) are 1·537 and 1·558 Å, respectively. The C9—C distances in (II) differ slightly from the C11—C distances and presumably reflect a C—C bond-shortening effect of the electronegative nitro group at C9. The difference in the cyclobutane lengths in (I) and (II) most probably is due to the nitro substituent in (II).

A small portion of the unit cell of (II) is shown in Fig. 2. The asymmetric unit (*i.e.* coordinates listed in Table 1) is illustrated by the lower pair of molecules. The pseudo-twofold axes of the two peristylane cages are approximately parallel to the *b* axis, the carbonyl ends point in different directions and orientations about the axes differ by approximately 90°. The positions and orientations of the molecules suggest the presence of a pseudo inversion center at approximately 0, 0, $\frac{1}{4}$; r.m.s. deviation of 0·034 Å from a rigid-body fit of the two C, N and O molecular fragments [procedure and program of Nyburg (1974)]. The C9-nitro substituents do not interfere with each other or the carbonyl groups. There are no

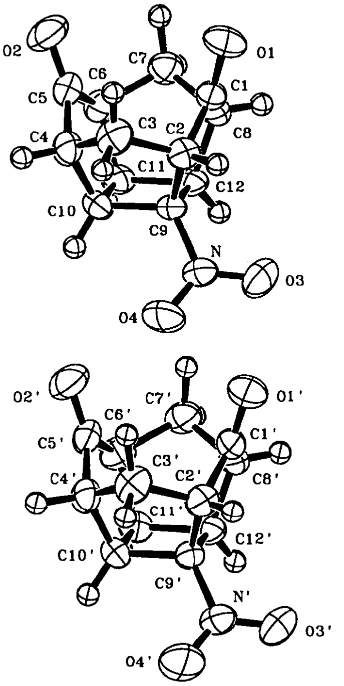

Fig. 1. *ORTEP* (Johnson, 1965) drawing of (II). The C, O and N atoms are shown as 50% ellipsoids and the H atoms are depicted as spheres with $B = 1{\cdot}5$ Å^2.

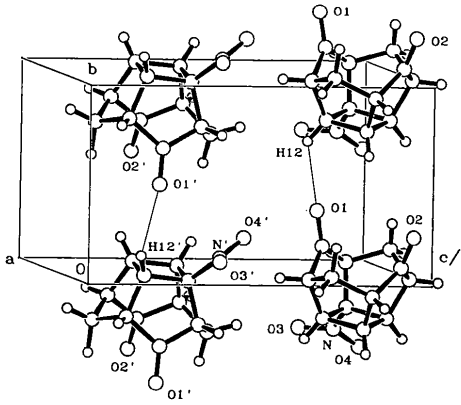

Fig. 2. Ball-and-stick *ORTEP* (Johnson, 1965) packing drawing of (II). The lower pair of molecules constitutes the asymmetric unit. The shortest intermolecular O···H distances, parallel to **b**, are indicated.

Table 3. H···O *intermolecular distances* (Å) *and symmetry operations for distances* < 2·6 Å *in* (I) *and* (II)

C—H bonds lengths adjusted to 1·10 Å.

	Distance	Symmetry operation
(II)		
O1···H12	2·27	$x, 1+y, z$
O1′···H12′	2·40	$x, -1+y, z$
O2′···H4	2·45	$\frac{1}{2}+x, -\frac{1}{2}-y, -\frac{1}{2}+z$
O1′···H6	2·45	$-\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
O2′···H2	2·47	$\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
O4′···H4′	2·54	$\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
(I)		
O1···H21	2·39	$1-x, 1-y, 1-z$

unusual intermolecular distances; a short list of distances in (I) and (II) is given in Table 3. The packing in both (I) and (II) is ordinary.

A number of density-related parameters together with the percent changes encountered from unsubstituted (I) to nitro-substituted (II) are listed in Table 4. The changes in molecular volume, the surface areas and molecular density are normal for the replacement of H in (I) by NO_2 in (II). There is little net change in the surface area available for intermolecular contacts (accessible surface area) relative to the change in molecular volume. The most interesting parameters in terms of molecular structure and crystal density are in the last three rows. One finds virtually identical percent changes in $\rho_{\rm mol}$ (molecular density) and ρ_x (crystal density from unit-cell volume) and effectively no change in packing coefficient. These data indicate that unit-cell space is utilized with the same efficiency in the crystals of (I) and (II), and that the observed increase in ρ_x is solely the result of an increase in $\rho_{\rm mol}$.

Table 4. *Comparison of several density-related parameters for* (I) *and* (II)

Parameters calculated with *SVDHA* (Zhang, 1985). All C—H lengths are normalized to 1·10 Å. van der Waals radii used are C = 1·70, H = 1·1, N = 1·55, O = 1·52 Å.

	(I)	(II)*	% change
Molecular weight	188·2	233·2	23·9
Molecular volume (Å^3)*	158·3	181·2	14·5
Molecular surface area (Å^2)	181·2	210·2	16·0
Accessible surface area (Å^2)†	71·5	82·8	15·9
Molecular density (g cm^{-3})	1·975	2·136	8·2
Crystal density from unit-cell volume (g cm^{-3})	1·415	1·521	7·5
Packing coefficient‡	0·716	0·712	~0

* Values given for (II) are averages for the two molecules.

† Surface area of a molecule that can be in contact with an external atom with a radius of 1·52 Å.

‡ Molecular volume/unit-cell volume per molecule.

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References

Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Polidori, G., Spagna, R. & Viterbo, D. (1989). *J. Appl. Cryst.* **22**, 389–393.

Engel, P., Fischer, J. W. & Paquette, L. A. (1984). *Z. Kristallogr.* **166**, 225–231.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.

Kitaigorodskii, A. I. (1961). *Organic Chemical Crystallography*, New York: Consultants Bureau.

Luo, J., Ammon, H. L. & Gilliland, G. J. (1989). *J. Appl. Cryst.* **22**, 186.

Molecular Structure Corporation (1989). *TEXSAN. TEXRAY Structure Analysis Package*. Version 5.0. MSC, 3200A Research Forest Drive, The Woodlands, TX 77381, USA.

Nyburg, S. C. (1974). *Acta Cryst.* B**30**, 251–253.

Paquette, L. A., Shen, C. & Engel, P. E. (1989). *J. Org. Chem.* **54**, 3329–3333.

Shen, C. & Paquette, L. A. (1989). *J. Org. Chem.* **54**, 3324–3328.

Zachariasen, W. H. (1968). *Acta Cryst.* A**24**, 212–216.

Zhang, D. (1985). *SVDHA*. Program to calculate molecular volume, area and accessible surface area. Unpublished.

Acta Cryst. (1991). C**47**, 2159–2164

Structure of 1,5,9-Trinitrobishomopentaprismane

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Abstract. 2,3,8-Trinitrohexacyclo[5.4.1.$0^{2,6}$.$0^{3,10}$.$0^{4,8}$.$0^{9,12}$]dodecane (IV), $C_{12}H_{11}N_3O_6$, $M_r = 293·2$, orthorhombic, $Pna2_1$, $a = 11·467$ (1), $b = 8·756$ (1), $c = 11·9339$ (8) Å, $V = 1198·2$ (4) Å^3, $D_x = 1·625$ g cm^{-3}, $Z = 4$, Cu $K\alpha$, $\lambda = 1·54178$ Å, $\mu = 11·6$ cm^{-1}, $F(000) = 608$, $T = 293$ K, final $R = 0·061$,

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