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

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

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| C(1) | 1842 (6) | 189 (4) | 9360 (3) | 66 (2) |
| N(2) | 1695 (3) | 1705 (2) | 8841 (1) | 43 (1) |
| C(3) | 670 (3) | 3134 (3) | 8896 (2) | 40 (1) |
| N(4) | 1977 (3) | 4195 (2) | 9718 (1) | 48 (1) |
| C(5) | 3186 (6) | 3661 (4) | 10778 (2) | 64 (1) |
| N(6) | 2588 (3) | 1829 (3) | 8271 (2) | 50 (1) |
| O(6*a*) | 2536 (3) | 3123 (2) | 7865 (1) | 64 (1) |
| O(6*b*) | 3398 (3) | 620 (2) | 8195 (1) | 71 (1) |
| N(7) | 2265 (3) | 5689 (2) | 9452 (1) | 49 (1) |
| O(7*b*) | 1143 (3) | 6193 (2) | 8580 (1) | 69 (1) |
| O(7*a*) | 3646 (3) | 6443 (2) | 10122 (1) | 65 (1) |
| O(8) | −743 (2) | 2668 (2) | 9125 (1) | 49 (1) |
| C(9) | −2449 (4) | 2041 (4) | 8231 (2) | 59 (1) |

$[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0.00030$. Secondary-extinction parameter $p = 0.004$ (1) in $F_c^* = F_c/[1.0 + 0.002(p)F_o^2/\sin(2\theta)]^{0.25}$. There were 159 parameters refined: atom coordinates, anisotropic thermal parameters for all non-H atoms, isotropic thermal parameters for H atoms. $(\Delta/\sigma)_{max} = 0.004$, $R = 0.044$, $wR = 0.059$, $S = 2.164$. Final difference Fourier excursions 0·19 and −0·17 e $Å^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).† Atom numbering for Tables 1 and 2, which give atom coordinates, and bond distances and angles, respectively, follows that shown in Fig. 1.

† Lists of structure factors, anisotropic thermal parameters and hydrogen coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51749 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

| | | | |
|---|---|---|---|
| C(1)–N(2) | 1·450 (4) | N(2)–C(3) | 1·467 (3) |
| N(2)–N(6) | 1·349 (4) | C(3)–N(4) | 1·444 (2) |
| C(3)–O(8) | 1·382 (4) | N(4)–C(5) | 1·441 (3) |
| N(4)–N(7) | 1·357 (3) | N(6)–O(6*a*) | 1·223 (3) |
| N(6)–O(6*b*) | 1·230 (3) | N(7)–O(7*b*) | 1·221 (2) |
| N(7)–O(7*a*) | 1·225 (2) | O(8)–C(9) | 1·443 (3) |
| Average C–H | 0·95 (6) | | |

| | | | |
|---|---|---|---|
| C(1)–N(2)–C(3) | 125·3 (3) | C(1)–N(2)–N(6) | 117·9 (3) |
| C(3)–N(2)–N(6) | 116·9 (2) | N(2)–C(3)–N(4) | 110·7 (2) |
| N(2)–C(3)–O(8) | 109·2 (2) | N(4)–C(3)–O(8) | 107·5 (2) |
| C(3)–N(4)–C(5) | 122·6 (2) | C(3)–N(4)–N(7) | 118·1 (2) |
| C(5)–N(4)–N(7) | 118·6 (2) | N(2)–N(6)–O(6*a*) | 118·3 (2) |
| N(2)–N(6)–O(6*b*) | 117·2 (2) | O(6*a*)–N(6)–O(6*b*) | 124·5 (3) |
| N(4)–N(7)–O(7*b*) | 118·7 (2) | N(4)–N(7)–O(7*a*) | 116·6 (2) |
| O(7*b*)–N(7)–O(7*a*) | 124·7 (2) | C(3)–O(8)–C(9) | 112·9 (2) |
| Average H–C–H | 108 (4) | Average *A*–*B*–H | 110 (3) |

**Related literature.** A compound with a fragment of similar connectivity with respect to the tertiary carbon is 2-chloro-5,5-dinitro-3-aza-4-oxahexene (Grigoreva, Margolis, Makarenko, Strochkina, Shchedrova, Selivanov, Melnikov & Gidaspov, 1975).

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### References

GRIGOREVA, N. V., MARGOLIS, N. V., MAKARENKO, G. V., STROCHKINA, T. K., SHCHEDROVA, V. K., SELIVANOV, V. F., MELNIKOV, V. V. & GIDASPOV, B. V. (1975). *Zh. Strukt. Chem.* **16**, 157–159.

*International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

SHELDRICK, G. M. (1980). *SHELXTL80. An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* Univ. of Göttingen, Federal Republic of Germany.

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# Structure of 1,9-Diacetyl-3,5,7-trinitro-1,3,5,7,9-pentaazanonane*

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**Abstract.** $C_8H_{16}N_8O_8$, $M_r = 352.17$, monoclinic, $P2_1$, $a = 7.243$ (2), $b = 19.986$ (4), $c = 10.692$ (2) Å, $\beta = 96.18$ (3)°, $V = 1538.7$ (6) $Å^3$, $Z = 4$, $D_x = 1.520$ g $cm^{-3}$, $\lambda$(Cu $K\alpha$) = 1·54178 Å, $\mu = 11.3$ $cm^{-1}$, $F(000) = 736$, $T = 295$ K, final $R = 0.038$, $wR = 0.045$ for 2900 independent reflections. The two molecules in the asymmetric unit each have the same chirality and an approximate twofold axis along the N–N bond of the central nitramine in the azanonane chain. The nitrogens in the chain are roughly trigonal planar in bonding geometry with the chain torsions in the two molecules all of the same sign and ranging in magnitude from −90 to −116°; this imparts a semi-regular helicity to the chains. Intermolecular

* 5,7,9-Trinitro-3,5,7,9,11-pentaazatridecane-2,12-dione.

0108-2701/89/081244-03$03.00

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

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

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| N(1) | 2366 (4) | 1369 | 2530 (3) | 47 (1) |
| C(2) | 3135 (5) | 1826 (2) | 3496 (3) | 46 (1) |
| N(3) | 3248 (4) | 2519 (2) | 3110 (3) | 40 (1) |
| C(4) | 4884 (5) | 2793 (2) | 2614 (3) | 40 (1) |
| N(5) | 5854 (3) | 3313 (2) | 3367 (2) | 36 (1) |
| C(6) | 5759 (5) | 4009 (2) | 3022 (3) | 40 (1) |
| N(7) | 7502 (4) | 4282 (2) | 2682 (3) | 45 (1) |
| C(8) | 8570 (5) | 4791 (2) | 3419 (4) | 50 (1) |
| N(9) | 8067 (5) | 5463 (2) | 3054 (3) | 49 (1) |
| C(10) | 3391 (5) | 1119 (2) | 1664 (3) | 46 (1) |
| O(11) | 4990 (4) | 1322 (2) | 1589 (3) | 61 (1) |
| C(12) | 2496 (7) | 586 (3) | 833 (5) | 66 (2) |
| N(13) | 1661 (4) | 2891 (2) | 3009 (3) | 47 (1) |
| O(14) | 215 (3) | 2599 (2) | 3163 (3) | 63 (1) |
| O(15) | 1804 (4) | 3483 (2) | 2776 (3) | 58 (1) |
| N(16) | 6805 (4) | 3150 (2) | 4482 (3) | 39 (1) |
| O(17) | 6732 (4) | 2566 (2) | 4831 (2) | 51 (1) |
| O(18) | 7660 (3) | 3600 (2) | 5064 (2) | 52 (1) |
| N(19) | 7959 (4) | 4146 (2) | 1502 (3) | 48 (1) |
| O(20) | 7048 (4) | 3712 (2) | 913 (3) | 66 (1) |
| O(21) | 9235 (4) | 4467 (2) | 1132 (3) | 62 (1) |
| C(22) | 6694 (6) | 5798 (3) | 3538 (3) | 50 (1) |
| O(23) | 5757 (4) | 5530 (2) | 4289 (3) | 66 (1) |
| C(24) | 6388 (7) | 6505 (3) | 3094 (4) | 66 (2) |
| N(1′) | 7455 (5) | 1471 (2) | −290 (3) | 53 (1) |
| C(2′) | 8381 (5) | 2089 (3) | −2 (3) | 49 (1) |
| N(3′) | 8201 (4) | 2573 (2) | −1034 (3) | 43 (1) |
| C(4′) | 9681 (5) | 2729 (2) | −1801 (3) | 41 (1) |
| N(5′) | 10603 (4) | 3361 (2) | −1514 (2) | 42 (1) |
| C(6′) | 10519 (5) | 3921 (2) | −2364 (3) | 41 (1) |
| N(7′) | 12204 (4) | 4031 (2) | −2984 (3) | 44 (1) |
| C(8′) | 13449 (5) | 4591 (2) | −2759 (3) | 49 (1) |
| N(9′) | 13170 (5) | 5119 (2) | −3686 (3) | 51 (1) |
| C(10′) | 8071 (5) | 1030 (2) | −1091 (4) | 49 (1) |
| O(11′) | 9416 (4) | 1170 (2) | −1665 (3) | 60 (1) |
| C(12′) | 7066 (6) | 380 (3) | −1249 (5) | 65 (2) |
| N(13′) | 6536 (4) | 2873 (2) | −1343 (3) | 48 (1) |
| O(14′) | 5240 (4) | 2676 (2) | −785 (3) | 67 (1) |
| O(15′) | 6440 (4) | 3299 (2) | −2160 (3) | 68 (1) |
| N(16′) | 11748 (4) | 3404 (2) | −431 (3) | 44 (1) |
| O(17′) | 11812 (4) | 2917 (2) | 272 (2) | 58 (1) |
| O(18′) | 12646 (4) | 3920 (2) | −228 (2) | 57 (1) |
| N(19′) | 12564 (4) | 3592 (2) | −3902 (3) | 47 (1) |
| O(20′) | 11631 (4) | 3085 (2) | −4030 (3) | 59 (1) |
| O(21′) | 13819 (4) | 3753 (2) | −4529 (3) | 64 (1) |
| C(22′) | 11830 (5) | 5565 (2) | −3649 (4) | 54 (1) |
| O(23′) | 10753 (4) | 5537 (2) | −2830 (4) | 81 (1) |
| C(24′) | 11687 (6) | 6105 (3) | −4633 (5) | 66 (2) |

Table 2. *Bond lengths* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bond parameters* (Å, °)

| | | | |
|---|---|---|---|
| N(1)–C(2) | 1·444 (4) | N(1)–C(10) | 1·344 (5) |
| C(2)–N(3) | 1·451 (6) | N(3)–C(4) | 1·456 (5) |
| N(3)–N(13) | 1·363 (5) | C(4)–N(5) | 1·449 (5) |
| N(5)–C(6) | 1·440 (6) | N(5)–N(16) | 1·351 (4) |
| C(6)–N(7) | 1·457 (5) | N(7)–C(8) | 1·457 (5) |
| N(7)–N(19) | 1·365 (4) | C(8)–N(9) | 1·435 (6) |
| N(9)–C(22) | 1·348 (6) | C(10)–O(11) | 1·237 (5) |
| C(10)–C(12) | 1·490 (7) | N(13)–O(14) | 1·226 (5) |
| N(13)–O(15) | 1·217 (6) | N(16)–O(17) | 1·229 (6) |
| N(16)–O(18) | 1·223 (5) | N(19)–O(20) | 1·223 (5) |
| N(19)–O(21) | 1·226 (5) | C(22)–O(23) | 1·229 (5) |
| C(22)–C(24) | 1·500 (7) | N(1′)–C(2′) | 1·424 (6) |
| N(1′)–C(10′) | 1·338 (6) | C(2′)–N(3′) | 1·463 (5) |
| N(3′)–C(4′) | 1·451 (5) | N(3′)–N(13′) | 1·355 (4) |
| C(4′)–N(5′) | 1·446 (6) | N(5′)–C(6′) | 1·439 (5) |
| N(5′)–N(16′) | 1·353 (4) | C(6′)–N(7′) | 1·466 (5) |
| N(7′)–C(8′) | 1·442 (6) | N(7′)–N(19′) | 1·362 (5) |
| C(8′)–N(9′) | 1·447 (6) | N(9′)–C(22′) | 1·322 (6) |
| C(10′)–O(11′) | 1·238 (5) | C(10′)–C(12′) | 1·489 (7) |
| N(13′)–O(14′) | 1·230 (5) | N(13′)–O(15′) | 1·217 (5) |
| N(16′)–O(17′) | 1·227 (5) | N(16′)–O(18′) | 1·225 (6) |
| N(19′)–O(20′) | 1·217 (6) | N(19′)–O(21′) | 1·229 (5) |
| C(22′)–O(23′) | 1·235 (6) | C(22′)–C(24′) | 1·502 (7) |

| | | | |
|---|---|---|---|
| C(2)–N(1)–C(10) | 121·9 (3) | N(1)–C(2)–N(3) | 115·5 (3) |
| C(2)–N(3)–C(4) | 122·3 (3) | C(2)–N(3)–N(13) | 118·0 (3) |
| C(4)–N(3)–N(13) | 118·6 (4) | N(3)–C(4)–N(5) | 115·5 (3) |
| C(4)–N(5)–C(6) | 123·0 (3) | C(4)–N(5)–N(16) | 119·3 (4) |
| C(6)–N(5)–N(16) | 117·7 (3) | N(5)–C(6)–N(7) | 114·0 (3) |
| C(6)–N(7)–C(8) | 123·4 (3) | C(6)–N(7)–N(19) | 117·3 (3) |
| C(8)–N(7)–N(19) | 118·2 (3) | N(7)–C(8)–N(9) | 113·7 (3) |
| C(8)–N(9)–C(22) | 122·4 (4) | N(1)–C(10)–O(11) | 120·9 (4) |
| N(1)–C(10)–C(12) | 116·1 (3) | O(11)–C(10)–C(12) | 123·0 (4) |
| N(3)–N(13)–O(14) | 117·1 (4) | N(3)–N(13)–O(15) | 117·2 (3) |
| O(14)–N(13)–O(15) | 125·7 (4) | N(5)–N(16)–O(17) | 117·5 (3) |
| N(5)–N(16)–O(18) | 117·0 (4) | O(17)–N(16)–O(18) | 125·5 (3) |
| N(7)–N(19)–O(20) | 116·5 (3) | N(7)–N(19)–O(21) | 117·4 (3) |
| O(20)–N(19)–O(21) | 126·1 (3) | N(9)–C(22)–O(23) | 121·1 (4) |
| N(9)–C(22)–C(24) | 115·9 (4) | O(23)–C(22)–C(24) | 123·0 (4) |
| C(2′)–N(1′)–C(10′) | 121·9 (4) | N(1′)–C(2′)–N(3′) | 114·2 (3) |
| C(2′)–N(3′)–C(4′) | 123·8 (3) | C(2′)–N(3′)–N(13′) | 118·7 (3) |
| C(4′)–N(3′)–N(13′) | 117·4 (3) | N(3′)–C(4′)–N(5′) | 114·8 (3) |
| C(4′)–N(5′)–C(6′) | 123·9 (3) | C(4′)–N(5′)–N(16′) | 117·6 (3) |
| C(6′)–N(5′)–N(16′) | 118·1 (4) | N(5′)–C(6′)–N(7′) | 114·9 (3) |
| C(6′)–N(7′)–C(8′) | 125·2 (3) | C(6′)–N(7′)–N(19′) | 117·6 (3) |
| C(8′)–N(7′)–N(19′) | 117·1 (3) | N(7′)–C(8′)–N(9′) | 114·4 (3) |
| C(8′)–N(9′)–C(22′) | 121·3 (4) | N(1′)–C(10′)–O(11′) | 120·2 (4) |
| N(1′)–C(10′)–C(12′) | 117·0 (4) | O(11′)–C(10′)–C(12′) | 122·8 (4) |
| N(3′)–N(13′)–O(14′) | 116·6 (4) | N(3′)–N(13′)–O(15′) | 117·7 (3) |
| O(14′)–N(13′)–O(15′) | 125·8 (3) | N(5′)–N(16′)–O(17′) | 116·9 (4) |
| N(5′)–N(16′)–O(18′) | 118·0 (4) | O(17′)–N(16′)–O(18′) | 125·0 (3) |
| N(7′)–N(19′)–O(20′) | 118·0 (3) | N(7′)–N(19′)–O(21′) | 115·8 (4) |
| O(20′)–N(19′)–O(21′) | 126·2 (4) | N(9′)–C(22′)–O(23′) | 120·8 (4) |
| N(9′)–C(22′)–C(24′) | 117·3 (4) | O(23′)–C(22′)–C(24′) | 121·9 (4) |

| | Molecule 1 | Molecule 2 |
|---|---|---|
| N(1)–C(2)–N(3)–C(4) | −90·8 (3) | 104·9 (3) |
| C(2)–N(3)–C(4)–N(5) | −116·0 (2) | −103·8 (3) |
| N(3)–C(4)–N(5)–C(6) | −105·7 (2) | −114·1 (2) |
| C(4)–N(5)–C(6)–N(7) | −112·4 (2) | −104·2 (2) |
| N(5)–C(6)–N(7)–C(8) | −113·2 (2) | −111·9 (3) |
| C(6)–N(7)–C(8)–N(9) | −89·6 (3) | −99·6 (3) |

| | H···O | N···O | ∠N–H···O |
|---|---|---|---|
| N(1)–H(1)···O(23′) | 2·06 (3) | 2·850 (5) | 166·7 (2·5) |
| N(1′)–H(1′)···O(11) | 2·11 (3) | 2·839 (5) | 156·6 (2·4) |
| N(9)–H(9)···O(11′) | 2·06 (4) | 2·864 (6) | 168·9 (2·6) |
| N(9′)–H(9′)···O(23) | 2·35 (4) | 3·117 (6) | 165·4 (2·6) |

hydrogen bonding occurs between the two molecules in the asymmetric unit and their symmetry equivalents at each secondary amine and acetyl oxygen.

**Experimental.** A clear colorless 0·25 × 0·15 × 0·45 mm data crystal, crystallized from methyl chloride, was provided by C. Coon of Lawrence Livermore Laboratory. Automated Nicolet $R3m$ diffractometer with incident-beam monochromator, 25 centered reflections within $40 \le 2\theta \le 65°$ used for determining lattice parameters. $[(\sin\theta)/\lambda]_{max} = 0{\cdot}61$ Å$^{-1}$, range of $hkl$: $-7 \le h \le 8$, $-24 \le k \le 0$, $-12 \le l \le 1$. Standards (203, 080, 005) monitored every 60 reflections with random variation of 1·4% over data collection, $\theta/2\theta$ mode, scan width $[2\theta(K_{\alpha 1}) - 1{\cdot}0]$ to $[2\theta(K_{\alpha 2}) + 1{\cdot}0]°$, scan rate a function of count rate (4·0° min$^{-1}$ minimum, 30·0° min$^{-1}$ maximum), 4272 reflections measured, 2982 unique, $R_{int} = 0{\cdot}027$, 2900 observed with $F_o > 3\sigma(F_o)$. Data corrected for Lorentz and polarization effects, empirical ellipsoidal absorption correction applied, max. and min. transmission 0·84 and 0·55. Structure solved by direct methods. The least-squares refinement used program *SHELXTL* (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00030$. There were 458 parameters refined: atom coordinates, anisotropic thermal parameters for all non-H atoms, H atoms included using riding model, coordinate shifts of

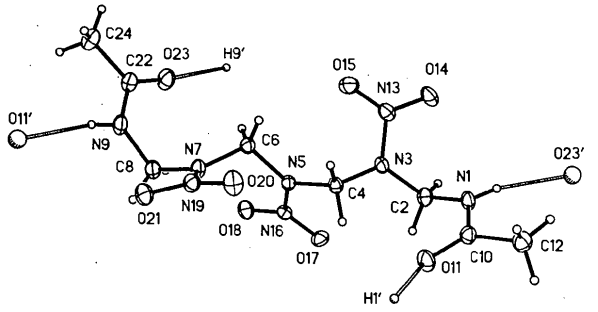


Fig. 1. Thermal ellipsoid plot of 1,9-diacetyl-3,5,7-trinitro-1,3,5,-7,9-pentaazanonane with ellipsoids drawn at the 20% probability level. Only one of the two similar molecules in the asymmetric unit is shown. The open bonds indicate hydrogen bonding to H(1'), H(9'), O(23'), and O(11') of molecule 2 or its symmetry equivalents.

C atoms applied to bonded hydrogens, C—H = 0·96 Å. $U(H) = 1{\cdot}2\,U_{eq}(C)$, amine hydrogens refined isotropically. $(\Delta/\sigma)_{max} = 0{\cdot}40$, $R = 0{\cdot}038$, $wR = 0{\cdot}045$, $S = 1{\cdot}737$. Final difference Fourier excursions 0·14 and −0·31 e Å$^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).* Atom numbering for Tables 1 and 2, which give atom coordinates, and bond distances, bond angles and selected torsion angles, respectively, follows that shown in Fig. 1; molecule 2 is numbered similarly and differentiated by the inclusion of an apostrophe.

**Related literature.** For the structure of a similar compound, 1,7-diacetyl-2,4,6-trinitro-2,4,6-triazaheptane, see Cobbledick & Small (1973*a–c*). For a similarly substituted tetraazaoxanonane, see Gilardi & George (1989).

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* Lists of structure factors, anisotropic thermal parameters and hydrogen coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51747 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

**References**

COBBLEDICK, R. E. & SMALL, R. W. (1973*a*). *Acta Cryst.* B**29**, 1659–1666.
COBBLEDICK, R. E. & SMALL, R. W. (1973*b*). *Acta Cryst.* B**29**, 2585–2592.
COBBLEDICK, R. E. & SMALL, R. W. (1973*c*). *Acta Cryst.* B**29**, 2795–2798.
GILARDI, R. & GEORGE, C. (1989). *Acta Cryst.* C**45**. Submitted.
*International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
SHELDRICK, G. M. (1980). *SHELXTL*80. *An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* Univ. of Göttingen, Federal Republic of Germany.

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# Crystal Studies of Heterocyclic Compounds Containing One Oxygen and Two Nitrogen Atoms. XIV. 4,5,6,7,8,9-Hexahydro-1-oxa-5,8-diazadibenzo[*b*,*j*]cycloundecene

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**Abstract.** $C_{16}H_{18}N_2O$, $M_r = 254{\cdot}3$, monoclinic, $P2_1/n$, $a = 5{\cdot}035\ (2)$, $b = 9{\cdot}928\ (3)$, $c = 26{\cdot}831\ (9)$ Å, $\beta = 92{\cdot}10\ (3)°$, $V = 1340{\cdot}2\ (8)$ Å$^3$, $Z = 4$, $D_x = 1{\cdot}260\ (8)$ g cm$^{-3}$, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54178$ Å, $\mu = 5{\cdot}48$ cm$^{-1}$, $F(000) = 544$. Diffractometer data at room temperature, $R = 0{\cdot}033$ for 1711 reflections with $I > 2{\cdot}5\sigma(I)$. Neglecting the oxygen and benzene C

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