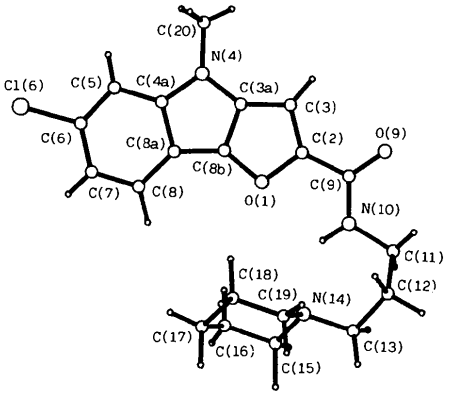

Fig. 1. Molecular structure and atomic numbering system.

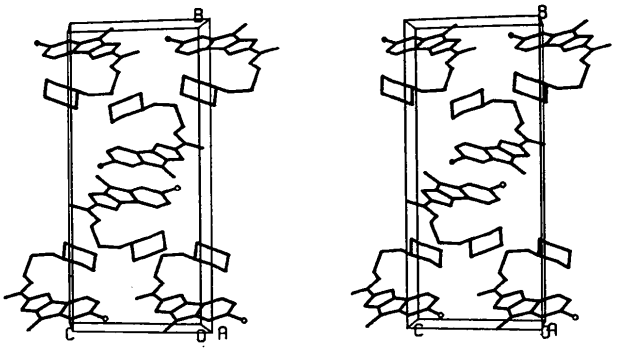

Fig. 2. Stereoscopic view along the *a* axis showing the cell packing.

$(\Delta/\sigma)_{max} = 0.36$ for non-H atoms. Final $\Delta\rho$ excursions ± 0.2 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Programs: *MULTAN*84 (Main, Germain & Woolfson, 1984) and *HBLS*V (Ashida, 1979). Calculations on a PANAFACOM U-1200 and ACOS850 at the Computing Center for Research in Agriculture, Foresty and Fishery. The final atomic parameters are given in Table 1. Bond distances and angles are listed in Table 2.* Fig. 1 shows the molecule and the numbering scheme, and Fig. 2 the packing of the molecules in the cell.

Related literature. This structure is one of a series of furo[3,2-*b*]indoles. The previous structure of the series is listed in Mizuno, Kawashima, Sota & Kitamura (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 44365 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1988). C**44**, 203–205

anti-5,16:10,15-Bis(*tert*-butylimino)-1,2,3,4,11,12,13,14-octamethyl-5,10,15,16-tetrahydrobenzo[*h*]pentaphene

BY H. PREUT, TH. HILDEBRAND AND R. P. KREHER

Fachbereich Chemie, Universität Dortmund, D-4600 *Dortmund* 50, *Postfach* 500500, *Federal Republic of Germany*

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Abstract. $C_{42}H_{50}N_2$, $M_r = 582.88$, triclinic, $P\bar{1}$, $a = 11.701$ (9), $b = 11.796$ (15), $c = 15.538$ (8) Å, $\alpha = 69.12$ (7), $\beta = 62.27$ (7), $\gamma = 67.15$ (7)°, $V = 1708$ Å^3, $Z = 2$, $D_x = 1.133$ Mg m^{-3}, $F(000) = 632$, λ(Mo $K\alpha$) $= 0.71069$ Å, $\mu = 0.06$ mm^{-1}, $T = 291$ (1) K, final $R = 0.062$ for 3466 unique observed $[F \geq 4.0\sigma(F)]$ diffractometer data and 398 variables. The constitution and configuration of the hitherto unknown Diels–Alder adduct of 2,5-di-*tert*-butyl-2,5-dihydrobenzo[*e*]-pyrrolo[3,4-*g*]isoindole with 3,4,5,6-tetramethyl-1,2-dehydrobenzene has been elucidated *via* the crystal-structure analysis. The *tert*-butyl groups of the annelated cyclic compound are in *anti* position. The perpendicular to the plane of the naphthalene ring and the direction through the position of the N atom and the central C atom of the *tert*-butyl groups are nearly parallel and therefore there is ample space at the N atoms for the free electron pairs.

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Experimental. 2,5-Di-*tert*-butyl-2,5-dihydrobenzo[*e*]-pyrrolo[3,4-*g*]isoindole reacted with 1,2-dibromo-3,4,5,6-tetramethylbenzene in the presence of a solution of methyllithium in diethyl ether at 173 K under argon in tetrahydrofuran. The reaction mixture was warmed up to room temperature for 12 h and hydrolysed with water. The substituted pentaphene was extracted with chloroform, dried with $MgSO_4$, and the chloroform was distilled. In order to grow the crystals the raw product was dissolved in chloroform and pentane vapour was diffused into the solution. Crystal size ~0·19 × 0·48 × 0·27 mm, $\omega/2\theta$ scan, scan speed 1·7–6·7°min^{-1} in θ, Nonius CAD-4 diffractometer, graphite-mono-

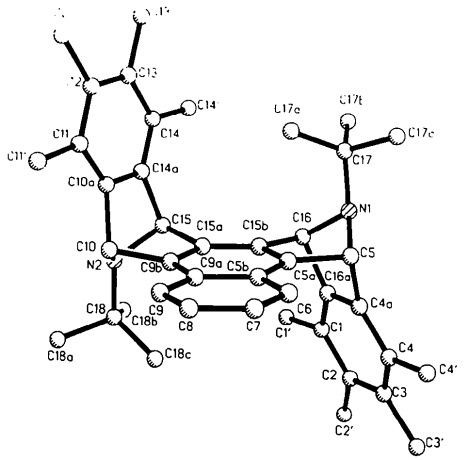

Fig. 1. General view of the molecule, showing the atom-numbering scheme.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3)

$U_{eq} = (1/6\pi^2)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
C(1)	−0·0244 (4)	0·2044 (3)	0·1930 (3)	48
C(2)	−0·0713 (4)	0·2663 (4)	0·1144 (3)	58
C(3)	−0·1353 (4)	0·3951 (4)	0·0997 (3)	58
C(4)	−0·1511 (4)	0·4675 (4)	0·1624 (3)	50
C(4a)	−0·1061 (3)	0·4050 (3)	0·2392 (2)	42
C(5)	−0·0975 (4)	0·4492 (3)	0·3162 (3)	42
C(5a)	0·0534 (3)	0·4298 (3)	0·2848 (2)	38
C(5b)	0·1345 (4)	0·5122 (3)	0·2421 (2)	40
C(6)	0·0829 (4)	0·6461 (3)	0·2208 (3)	51
C(7)	0·1671 (6)	0·7207 (4)	0·1826 (3)	67
C(8)	0·3032 (5)	0·6704 (4)	0·1629 (3)	67
C(9)	0·3584 (4)	0·5421 (4)	0·1810 (3)	57
C(9a)	0·2756 (4)	0·4600 (3)	0·2211 (2)	42
C(9b)	0·3246 (3)	0·3277 (3)	0·2436 (2)	39
C(10)	0·4633 (3)	0·2413 (3)	0·2433 (2)	41
C(10a)	0·4413 (3)	0·2044 (3)	0·3536 (2)	39
C(11)	0·4813 (3)	0·2420 (3)	0·4068 (3)	42
C(12)	0·4296 (4)	0·1985 (3)	0·5118 (3)	47
C(13)	0·3406 (3)	0·1231 (3)	0·5574 (3)	42
C(14)	0·3025 (3)	0·0852 (3)	0·5001 (2)	38
C(14a)	0·3547 (3)	0·1271 (3)	0·3988 (2)	36
C(15)	0·3285 (3)	0·1177 (3)	0·3144 (2)	37
C(15a)	0·2418 (4)	0·2498 (4)	0·2861 (3)	37
C(15b)	0·1066 (4)	0·3004 (4)	0·3057 (3)	36
C(16)	−0·0105 (4)	0·2441 (4)	0·3457 (3)	38
C(16a)	−0·0469 (4)	0·2750 (4)	0·2559 (3)	40
C(1′)	0·0516 (6)	0·0669 (5)	0·2064 (4)	60
C(2′)	−0·0492 (7)	0·1883 (6)	0·0463 (5)	92
C(3′)	−0·1888 (7)	0·4622 (7)	0·0175 (5)	92
C(4′)	−0·2149 (6)	0·6077 (5)	0·1469 (5)	72
N(1)	−0·1263 (4)	0·3385 (3)	0·4007 (3)	41
C(17)	−0·1387 (5)	0·3403 (4)	0·5003 (3)	48
C(17a)	−0·0149 (6)	0·3438 (5)	0·5088 (4)	68
C(17b)	−0·1774 (6)	0·2196 (5)	0·5706 (4)	65
C(17c)	−0·2547 (7)	0·4543 (6)	0·5321 (4)	82
N(2)	0·4627 (4)	0·1190 (3)	0·2345 (3)	42
C(18)	0·4913 (5)	0·1011 (5)	0·1361 (3)	52
C(18a)	0·6383 (6)	0·0967 (7)	0·0748 (4)	77
C(18b)	0·4720 (8)	−0·0275 (6)	0·1549 (5)	90
C(18c)	0·4082 (6)	0·2015 (6)	0·0769 (4)	72
C(11′)	0·5746 (5)	0·3253 (5)	0·3540 (4)	63
C(12′)	0·4703 (6)	0·2364 (6)	0·5750 (4)	75
C(13′)	0·2833 (6)	0·0806 (6)	0·6694 (3)	62
C(14′)	0·2070 (5)	0·0046 (5)	0·5474 (4)	53

Table 2. *Bond distances* (Å) *and angles* (°)

C(2)–C(1)	1·416 (6)	C(11′)–C(11)	1·502 (7)
C(16a)–C(1)	1·374 (8)	C(11′)–C(11)–C(10a)	120·2 (4)
C(16a)–C(1)–C(2)	117·6 (4)	C(11′)–C(11)–C(12)	123·2 (5)
C(1′)–C(1)	1·509 (6)	C(13)–C(12)	1·401 (6)
C(1′)–C(1)–C(2)	121·8 (5)	C(13)–C(12)–C(11)	120·9 (5)
C(1′)–C(1)–C(16a)	120·5 (5)	C(12′)–C(12)	1·517 (11)
C(3)–C(2)	1·396 (6)	C(12′)–C(12)–C(11)	119·2 (4)
C(3)–C(2)–C(1)	121·3 (5)	C(12′)–C(12)–C(13)	119·9 (4)
C(2′)–C(2)	1·513 (11)	C(14)–C(13)	1·414 (7)
C(2′)–C(2)–C(1)	117·7 (4)	C(14)–C(13)–C(12)	121·0 (3)
C(2′)–C(2)–C(3)	120·9 (5)	C(13′)–C(13)	1·511 (6)
C(4)–C(3)	1·421 (8)	C(13′)–C(13)–C(12)	120·3 (5)
C(4)–C(3)–C(2)	120·0 (4)	C(13′)–C(13)–C(14)	118·7 (4)
C(3′)–C(3)	1·512 (9)	C(14a)–C(14)	1·371 (4)
C(3′)–C(3)–C(2)	122·0 (6)	C(14a)–C(14)–C(13)	117·1 (4)
C(3′)–C(3)–C(4)	117·9 (5)	C(14′)–C(14)	1·502 (8)
C(4a)–C(4)	1·378 (6)	C(14′)–C(14)–C(13)	121·9 (4)
C(4a)–C(4)–C(3)	117·6 (4)	C(14′)–C(14)–C(14a)	121·0 (5)
C(4′)–C(4)	1·508 (7)	C(14)–C(14a)–C(10a)	121·8 (5)
C(4′)–C(4)–C(3)	121·9 (5)	C(15)–C(14a)	1·527 (7)
C(4′)–C(4)–C(4a)	120·5 (5)	C(15)–C(14a)–C(10a)	105·2 (3)
C(5)–C(4a)	1·519 (7)	C(15)–C(14a)–C(14)	132·7 (4)
C(5)–C(4a)–C(4)	133·0 (4)	C(15a)–C(15)	1·532 (5)
C(16a)–C(4a)	1·399 (5)	C(15a)–C(15)–C(14a)	103·4 (3)
C(16a)–C(4a)–C(4)	122·0 (5)	N(2)–C(15)	1·483 (4)
C(16a)–C(4a)–C(5)	104·9 (4)	N(2)–C(15)–C(14a)	98·5 (4)
C(5a)–C(5)	1·541 (6)	N(2)–C(15)–C(15a)	102·9 (3)
C(5a)–C(5)–C(4a)	104·8 (4)	C(15)–C(15a)–C(9b)	105·7 (4)
N(1)–C(5)	1·500 (5)	C(15b)–C(15a)	1·378 (6)
N(1)–C(5)–C(4a)	97·6 (4)	C(15b)–C(15a)–C(9b)	119·9 (4)
N(1)–C(5)–C(5a)	103·2 (3)	C(15b)–C(15a)–C(15)	133·9 (4)
C(5b)–C(5a)	1·399 (6)	C(15a)–C(15b)–C(5a)	120·3 (5)
C(5b)–C(5a)–C(5)	133·6 (3)	C(16)–C(15b)	1·525 (8)
C(15b)–C(5a)	1·386 (5)	C(16)–C(15b)–C(5a)	105·7 (4)
C(15b)–C(5a)–C(5)	105·0 (4)	C(16)–C(15b)–C(15a)	134·0 (4)
C(15b)–C(5a)–C(5b)	121·4 (4)	C(16a)–C(16)	1·526 (8)
C(6)–C(5b)	1·429 (5)	C(16a)–C(16)–C(15b)	104·2 (3)
C(6)–C(5b)–C(5a)	123·0 (4)	N(1)–C(16)	1·495 (5)
C(9a)–C(5b)	1·437 (5)	N(1)–C(16)–C(15b)	103·0 (4)
C(9a)–C(5b)–C(5a)	118·5 (3)	N(1)–C(16)–C(16a)	98·0 (3)
C(9a)–C(5b)–C(6)	118·5 (4)	C(4a)–C(16a)–C(1)	121·3 (4)
C(7)–C(6)	1·361 (8)	C(16)–C(16a)–C(1)	133·1 (4)
C(7)–C(6)–C(5b)	119·8 (4)	C(16)–C(16a)–C(4a)	105·5 (5)
C(8)–C(7)	1·387 (8)	C(16)–N(1)–C(5)	94·4 (3)
C(8)–C(7)–C(6)	121·7 (4)	C(17)–N(1)	1·492 (8)
C(9)–C(8)	1·375 (6)	C(17)–N(1)–C(5)	119·0 (4)
C(9)–C(8)–C(7)	120·9 (5)	C(17)–N(1)–C(16)	118·3 (4)
C(9a)–C(9)	1·415 (7)	C(17a)–C(17)	1·532 (10)
C(9a)–C(9)–C(8)	119·9 (4)	C(17a)–C(17)–N(1)	117·7 (4)
C(9)–C(9a)–C(5b)	119·2 (3)	C(17b)–C(17)	1·535 (7)
C(9b)–C(9a)	1·410 (5)	C(17b)–C(17)–N(1)	105·8 (5)
C(9b)–C(9a)–C(5b)	117·7 (4)	C(17b)–C(17)–C(17a)	107·9 (5)
C(9b)–C(9a)–C(9)	123·0 (4)	C(17c)–C(17)	1·525 (7)
C(10)–C(9b)	1·545 (5)	C(17c)–C(17)–N(1)	106·3 (5)
C(10)–C(9b)–C(9a)	131·6 (4)	C(17c)–C(17)–C(17a)	109·7 (6)
C(15a)–C(9b)	1·372 (7)	C(17c)–C(17)–C(17b)	109·1 (4)
C(15a)–C(9b)–C(9a)	122·1 (3)	C(15)–N(2)–C(10)	95·2 (3)
C(15a)–C(9b)–C(10)	105·7 (3)	C(18)–N(2)	1·480 (8)
C(10a)–C(10)	1·528 (5)	C(18)–N(2)–C(10)	119·9 (3)
C(10a)–C(10)–C(9b)	102·7 (2)	C(18)–N(2)–C(15)	119·1 (5)
N(2)–C(10)	1·500 (7)	C(18a)–C(18)	1·520 (8)
N(2)–C(10)–C(9b)	102·5 (4)	C(18a)–C(18)–N(2)	106·0 (6)
N(2)–C(10)–C(10a)	97·7 (3)	C(18b)–C(18)	1·526 (10)
C(11)–C(10a)	1·372 (7)	C(18b)–C(18)–N(2)	106·2 (4)
C(11)–C(10a)–C(10)	131·7 (3)	C(18b)–C(18)–C(18a)	108·9 (5)
C(14a)–C(10a)	1·396 (6)	C(18c)–C(18)	1·535 (8)
C(14a)–C(10a)–C(10)	105·4 (4)	C(18c)–C(18)–N(2)	117·2 (4)
C(14a)–C(10a)–C(11)	122·6 (3)	C(18c)–C(18)–C(18a)	108·4 (4)
C(12)–C(11)	1·421 (5)	C(18c)–C(18)–C(18b)	109·8 (7)
C(12)–C(11)–C(10a)	116·5 (4)		

chromated Mo $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 28{\cdot}0°$ equally distributed in reciprocal space; six standard reflections recorded every 2·5 h, only random deviations; 6413 reflections measured, $1{\cdot}5 \le \theta \le 25{\cdot}0°$, $-13 \le h \le 13$, $-14 \le k \le 14$, $0 \le l \le 18$; after averaging ($R_{int} = 0{\cdot}013$): 5993 unique reflections, 3466 with $F \ge 4{\cdot}0\sigma(F)$; Lorentz–polarization correction, no absorption correction; space group $P\bar{1}$; structure solution *via* direct methods, ΔF syntheses and full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C–H 1·08 Å); refinement on F with 3466 reflections and 398 refined parameters; $w = 1{\cdot}9/[\sigma^2(F) + 0{\cdot}0005F^2]$; $S = 0{\cdot}92$, $R = 0{\cdot}062$, $wR = 0{\cdot}068$, $(\Delta/\sigma)_{max}$ 0·09; no extinction correction; largest peak in final ΔF map 0·3 (2) e Å^{-3}; complex neutral-atom scattering factors from Cromer & Mann (1968) and Cromer & Liberman (1970); programs: *SHELXS* (Sheldrick, 1986) for structure solution, *SHELX*76 (Sheldrick, 1976) for structure refinement, Enraf–Nonius *Structure Determination Package* (Frenz, 1985) for data reduction, *SHELXTL PLUS* (Sheldrick, 1987) for the plot.

The molecule and the numbering scheme are shown in Fig. 1. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are given in Table 2.

Related literature. Kreher & Hildebrand (1987).

* Lists of H-atom coordinates, anisotropic thermal parameters, structure-factor amplitudes and least-squares planes, dihedral angles and angles between a perpendicular of a plane and a direction have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44375 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of *r*-1-Isopropyl-*t*-2,*t*-3-diphenylaziridine

BY T. SKARŻYŃSKI

Blackett Laboratory, Imperial College, London SW7 2BZ, England

T. OLSZAK

Department of Crystallography, Institute of Chemistry, University of Łódź, Nowotki 18, 91-416 *Łódź, Poland*

AND R. BARTNIK AND G. MLOSTOŃ

Department of Organic Synthesis, Institute of Chemistry, University of Łódź, Narutowicza 68, 90-136 *Łódź, Poland*

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Abstract. $C_{17}H_{19}N$, $M_r = 239{\cdot}3$, monoclinic, $P2_1/n$, $a = 11{\cdot}331$ (2), $b = 14{\cdot}690$ (3), $c = 9{\cdot}402$ (2) Å, $\beta = 113{\cdot}49$ (2)°, $V = 1435{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}107$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}412$ mm^{-1}, $F(000) = 512$, $T = 293$ K, $R = 0{\cdot}049$ for 1281 observed reflexions. The aziridine ring has bond lengths C–N 1·444 (4), 1·449 (3), C–C 1·499 (5) Å and bond angles 62·4 (2)° at N and 58·6 (2), 58·9 (2)° at C. The phenyl rings are in *cis* conformation with an interplanar angle of 85·1 (1)°.

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