Acta Cryst. (1982). B**38**, 3112–3113

t-3-Methyl-*r*-2,*c*-4,*c*-5-triphenyl-1,3-oxazolidine

BY T. SKARŻYŃSKI

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

(*Received* 15 *April* 1982; *accepted* 16 *June* 1982)

Abstract. $C_{22}H_{21}NO$, monoclinic, $P2_1/a$, a = 8·880 (1), b = 12·015 (2), c = 16·557 (3) Å, β = 90·97 (1)°, $Z = 4$, $D_x = 1{\cdot}186$ Mg m^{-3}, m.p. 367–368 K, $R = 0{\cdot}044$ for 1585 reflexions with $I > 2{\cdot}5\sigma(I)$. The oxazolidine ring is in the half-chair conformation.

Introduction. The compound was synthesized by G. Mlostoń (1981) and was recrystallized from ethanol solution. Cell parameters and intensity data were measured on a CAD-4 diffractometer using Cu $K\alpha$ radiation with a graphite monochromator. Data were collected to a maximum of $\theta = 75°$. Of 4068 independent reflexions, 1585 were accepted as observed on the criterion $I > 2{\cdot}5\sigma(I)$. The intensities were not corrected for absorption. The structure was solved by direct methods using *SHELX* 76 (Sheldrick, 1976) and refined by a full-matrix least-squares procedure. Positions of all H atoms were obtained from a difference map. Positional parameters of all the atoms and the anisotropic thermal parameters of the non-hydrogen atoms and isotropic ones of the H atoms were refined. The weights were based on counting statistics. The final R was 0·044 and R_w was 0·051. The positional parameters of the atoms are listed in

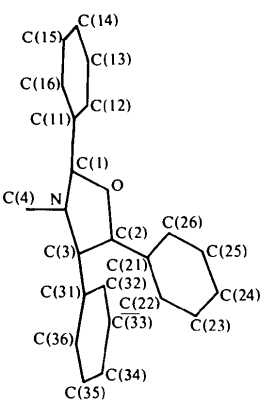

Fig. 1. The atom-numbering scheme.

Table 1. *Final fractional coordinates* (×10⁴) *and mean isotropic temperature factors* (×10³) *with e.s.d.'s in parentheses*

For non-H atoms $U_{iso} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	y	z	U_{iso} (Å²)
C(2)	2308 (3)	3283 (2)	7314 (1)	65 (1)
C(3)	3597 (3)	4155 (2)	7433 (1)	64 (2)
O	1969 (2)	2929 (1)	8111 (1)	81 (1)
N	3574 (2)	4345 (2)	8303 (1)	62 (1)
C(4)	5032 (4)	4753 (4)	8612 (2)	85 (2)
C(1)	3167 (3)	3272 (2)	8635 (1)	69 (2)
C(11)	2640 (3)	3297 (2)	9483 (1)	69 (2)
C(12)	1961 (4)	4211 (3)	9810 (2)	93 (2)
C(13)	1468 (4)	4204 (3)	10600 (2)	106 (3)
C(14)	1630 (4)	3261 (3)	11060 (2)	108 (3)
C(15)	2365 (7)	2368 (4)	10742 (2)	156 (4)
C(16)	2836 (6)	2385 (3)	9963 (2)	133 (3)
C(21)	907 (3)	3674 (2)	6888 (1)	59 (1)
C(22)	734 (4)	3496 (3)	6073 (2)	76 (2)
C(23)	−501 (4)	3880 (3)	5645 (2)	93 (3)
C(24)	−1574 (4)	4463 (3)	6028 (2)	93 (3)
C(25)	−1463 (4)	4650 (3)	6842 (3)	90 (2)
C(26)	−217 (3)	4251 (2)	7279 (2)	75 (2)
C(31)	3473 (3)	5215 (2)	6951 (1)	62 (2)
C(32)	2576 (4)	6084 (2)	7192 (2)	74 (2)
C(33)	2464 (5)	7050 (3)	6735 (2)	91 (2)
C(34)	3251 (5)	7153 (4)	6043 (2)	105 (3)
C(35)	4133 (5)	6305 (4)	5786 (2)	102 (3)
C(36)	4249 (4)	5338 (3)	6240 (2)	84 (2)
H(2)	2685 (26)	2649 (20)	7002 (12)	66 (7)
H(3)	4520 (28)	3718 (19)	7263 (13)	70 (7)
H(41)	4898 (29)	4880 (21)	9193 (18)	85 (8)
H(42)	5811 (40)	4247 (28)	8469 (19)	118 (3)
H(43)	5239 (41)	5530 (34)	8377 (21)	131 (14)
H(1)	4008 (31)	2741 (21)	8548 (13)	74 (8)
H(12)	1834 (41)	4907 (30)	9438 (21)	140 (12)
H(13)	747 (50)	4867 (34)	10839 (25)	164 (16)
H(14)	1267 (41)	3239 (27)	11607 (24)	136 (13)
H(15)	2248 (73)	1620 (53)	11145 (37)	267 (26)
H(16)	3229 (51)	1745 (35)	9700 (27)	188 (19)
H(22)	1530 (32)	3043 (23)	5795 (16)	93 (9)
H(23)	−558 (38)	3683 (27)	5029 (21)	130 (12)
H(24)	−2416 (39)	4700 (27)	5730 (20)	121 (12)
H(25)	−2166 (35)	5010 (26)	7146 (17)	102 (11)
H(26)	−115 (29)	4366 (20)	7831 (16)	78 (8)
H(32)	2024 (29)	6037 (20)	7676 (16)	80 (8)
H(33)	1777 (39)	7566 (30)	6974 (19)	115 (12)
H(34)	3317 (47)	7811 (33)	5712 (23)	145 (14)
H(35)	4678 (37)	6406 (26)	5280 (21)	114 (11)
H(36)	4766 (35)	4780 (28)	6073 (19)	107 (13)

0567-7408/82/123112-02$01.00 © 1982 International Union of Crystallography

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

O–C(1)	1·423 (3)	C(21)–C(22)	1·372 (3)
C(1)–N	1·449 (3)	C(22)–C(23)	1·376 (5)
N–C(3)	1·457 (3)	C(23)–C(24)	1·349 (5)
C(3)–C(2)	1·562 (4)	C(24)–C(25)	1·368 (6)
C(2)–O	1·423 (3)	C(25)–C(26)	1·396 (5)
N–C(4)	1·469 (4)	C(26)–C(21)	1·385 (4)
C(1)–C(11)	1·488 (4)	C(3)–C(31)	1·506 (3)
C(11)–C(12)	1·369 (4)	C(31)–C(32)	1·376 (4)
C(12)–C(13)	1·385 (5)	C(32)–C(33)	1·388 (4)
C(13)–C(14)	1·372 (5)	C(33)–C(34)	1·357 (5)
C(14)–C(15)	1·366 (6)	C(34)–C(35)	1·358 (6)
C(15)–C(16)	1·361 (6)	C(35)–C(36)	1·387 (6)
C(16)–C(11)	1·364 (4)	C(36)–C(31)	1·381 (4)
C(2)–C(21)	1·495 (4)		

O–C(1)–N	102·4 (2)	C(22)–C(21)–C(26)	118·0 (3)
C(1)–N–C(3)	104·1 (2)	C(21)–C(22)–C(23)	121·9 (3)
N–C(3)–C(2)	101·9 (2)	C(22)–C(23)–C(24)	119·7 (3)
C(3)–C(2)–O	104·4 (2)	C(23)–C(24)–C(25)	120·6 (3)
C(2)–O–C(1)	108·1 (2)	C(24)–C(25)–C(26)	119·8 (3)
O–C(1)–C(11)	109·7 (2)	C(25)–C(26)–C(21)	120·0 (3)
N–C(1)–C(11)	115·1 (2)	C(2)–C(3)–C(31)	116·9 (2)
C(1)–C(11)–C(12)	122·5 (2)	N–C(3)–C(31)	112·9 (2)
C(1)–C(11)–C(16)	119·7 (3)	C(3)–C(31)–C(32)	121·7 (2)
C(12)–C(11)–C(16)	117·8 (3)	C(3)–C(31)–C(36)	120·6 (3)
C(11)–C(12)–C(13)	121·1 (3)	C(32)–C(31)–C(36)	117·7 (3)
C(12)–C(13)–C(14)	119·8 (3)	C(31)–C(32)–C(33)	120·9 (3)
C(13)–C(14)–C(15)	118·7 (4)	C(32)–C(33)–C(34)	120·2 (3)
C(14)–C(15)–C(16)	120·7 (4)	C(33)–C(34)–C(35)	120·3 (4)
C(15)–C(16)–C(11)	121·7 (4)	C(34)–C(35)–C(36)	119·7 (3)
O–C(2)–C(21)	110·1 (2)	C(35)–C(36)–C(31)	121·2 (3)
C(3)–C(2)–C(21)	116·8 (2)	C(1)–N–C(4)	112·8 (2)
C(2)–C(21)–C(22)	119·6 (2)	C(3)–N–C(4)	111·7 (2)
C(2)–C(21)–C(26)	122·4 (2)		

Table 1, Fig. 1 shows the numbering scheme, and the bond lengths and angles are listed in Table 2.*

Discussion. The methyl group on the N atom is on the opposite side of the five-membered ring from the aromatic groups on C(1), C(2) and C(3). The angles between the best planes through the phenyl rings are: ∠ I,II = 47·8 (2), ∠ I,III = 13·2 (2) and ∠ II, III = 52·1 (2)°, where I, II and III represent the phenyl rings on C(1), C(2) and C(3) respectively. The oxazolidine system is in the half-chair conformation, with atoms N and C(1) displaced by 0·30 (2) and 0·36 (2) Å to opposite sides of the plane through C(2), C(3), and O.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38013 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

MLOSTOŃ, G. (1981). Praca doktorska. Univ. of Łódź, Poland.

SHELDRICK, G. M. (1976). *SHELX* 76. Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1982). B**38**, 3113–3115

t-3-Methyl-*r*-2,*c*-4,*t*-5-triphenyl-1,3-oxazolidine

BY T. SKARŻYŃSKI, Z. DEREWENDA AND A. M. BRZOZOWSKI

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

AND G. MLOSTOŃ

Department of Organic Chemistry, Institute of Chemistry, University of Łódź, Narutowicza 68, *Łódź, Poland*

(*Received* 15 *April* 1982; *accepted* 16 *June* 1982)

Abstract. $C_{22}H_{21}NO$, monoclinic, $P2_1/c$, $a = 22·937$ (3), $b = 19·569$ (2), $c = 7·866$ (1) Å, $\beta = 94·74$ (1)°, $Z = 8$, $D_x = 1·190$ Mg m^{-3}, m.p. 361–362 K, $R = 0·035$ for 2837 reflexions with $I > 2·5\sigma(I)$. There are two molecules in the asymmetric unit. The oxazolidine rings are in the half-chair conformation.

Introduction. The title compound has been synthesized in the reaction of azomethine ylide with benzaldehyde (Mlostoń, 1981). Colourless, elongated crystals suitable for X-ray investigation were obtained from ethanol solution. Lattice parameters and intensities of reflexions were measured on a CAD-4 diffractometer with Cu $K\alpha$ radiation. 5218 independent reflexions with $2\theta > 140°$ were collected; of these, 2837 which had $I > 2·5\sigma(I)$ were considered as observed. Intensity data were not corrected for absorption or extinction.

The E maps obtained by direct methods contained only a few peaks, which could be recognized as a fragment of the molecule. Positions of all non-hydrogen atoms were found by a partial-structure method by the use of *SHELX* 76 (Sheldrick, 1976) on the basis of a fragment consisting of seven atoms. Positions of H atoms bound to phenyl C atoms were calculated from the molecular geometry. Other H atoms were located on a difference Fourier map. The positional and thermal parameters were refined by a full-matrix least-squares method. Refinement with anisotropic temperature factors for the non-hydrogen atoms and isotropic temperature factors for H atoms gave a discrepancy

0567-7408/82/123113-03$01.00

© 1982 International Union of Crystallography