

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)	119.8 (3)
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:  $\angle$  I,II = 47.8 (2),  $\angle$  I,III = 13.2 (2) and  $\angle$  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.

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

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**Abstract.** C<sub>22</sub>H<sub>21</sub>NO, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 22.937 (3), *b* = 19.569 (2), *c* = 7.866 (1) Å, β = 94.74 (1)°, *Z* = 8, *D*<sub>x</sub> = 1.190 Mg m<sup>-3</sup>, m.p. 361–362 K, *R* = 0.035 for 2837 reflexions with *I* > 2.5σ(*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*α radiation. 5218 independent reflexions with 2θ > 140° were collected; of these, 2837 which had *I* > 2.5σ(*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

Table 1. Final fractional coordinates ( $\times 10^4$ ) and mean isotropic temperature factors ( $\times 10^3$ ) with e.s.d.'s in parentheses

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{iso}$ (Å <sup>2</sup> )
For non-H atoms $U_{iso} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$ .				
C(2A)	-549 (1)	1016 (1)	10066 (3)	54 (1)
C(3A)	-761 (1)	1028 (1)	8172 (3)	52 (1)
C(1A)	-55 (1)	1688 (1)	8509 (3)	55 (1)
N(A)	-211 (1)	1152 (1)	7418 (2)	55 (1)
O(A)	-75 (1)	1501 (1)	10189 (2)	70 (1)
C(4A)	-283 (1)	1352 (2)	5626 (3)	70 (1)
C(11A)	702 (1)	1752 (1)	8365 (2)	51 (1)
C(12A)	920 (1)	2294 (1)	7500 (3)	64 (1)
C(13A)	1509 (1)	2333 (1)	7278 (3)	75 (2)
C(14A)	1883 (1)	1838 (1)	7914 (3)	72 (2)
C(15A)	1676 (1)	1304 (1)	8807 (3)	66 (2)
C(16A)	1086 (1)	1252 (1)	9022 (3)	59 (1)
C(21A)	-1004 (1)	1194 (1)	11244 (3)	53 (1)
C(22A)	-1254 (1)	691 (1)	12192 (3)	66 (2)
C(23A)	-1694 (1)	855 (2)	13234 (3)	79 (2)
C(24A)	-1879 (1)	1511 (2)	13367 (3)	80 (2)
C(25A)	-1639 (1)	2009 (2)	12442 (3)	79 (2)
C(26A)	-1203 (1)	1853 (1)	11394 (3)	66 (2)
C(31A)	-1090 (1)	396 (1)	7544 (2)	52 (1)
C(32A)	-820 (1)	-158 (1)	6882 (3)	68 (2)
C(33A)	-1149 (1)	-727 (1)	6314 (4)	84 (2)
C(34A)	-1737 (1)	-740 (1)	6435 (3)	76 (2)
C(35A)	-2008 (1)	-203 (1)	7121 (3)	71 (2)
C(36A)	-1685 (1)	367 (1)	7666 (3)	60 (1)
C(2B)	5645 (1)	1061 (1)	5199 (3)	60 (1)
C(3B)	5848 (1)	1048 (1)	3380 (3)	54 (1)
C(1B)	5047 (1)	1763 (1)	3385 (3)	59 (1)
N(B)	5305 (1)	1225 (1)	2392 (2)	57 (1)
O(B)	5213 (1)	1593 (1)	5122 (2)	72 (1)
C(4B)	5383 (1)	1434 (2)	646 (3)	73 (2)
C(11B)	4396 (1)	1794 (1)	3023 (3)	53 (1)
C(12B)	4044 (1)	1285 (1)	3607 (3)	66 (1)
C(13B)	3451 (1)	1292 (1)	3192 (4)	75 (2)
C(14B)	3202 (1)	1804 (1)	2187 (3)	76 (2)
C(15B)	3539 (1)	2310 (1)	1609 (3)	78 (2)
C(16B)	4140 (1)	2312 (1)	2049 (3)	66 (1)
C(21B)	6121 (1)	1197 (1)	6570 (3)	62 (1)
C(22B)	6381 (1)	1837 (1)	6733 (4)	79 (2)
C(23B)	6833 (1)	1951 (2)	7983 (5)	109 (3)
C(24B)	7025 (2)	1427 (3)	9033 (5)	126 (3)
C(25B)	6786 (2)	805 (3)	8876 (4)	117 (3)
C(26B)	6328 (1)	681 (2)	7656 (3)	84 (2)
C(31B)	6111 (1)	382 (1)	2893 (3)	55 (1)
C(32B)	6700 (1)	261 (1)	3263 (3)	62 (1)
C(33B)	6956 (1)	-345 (1)	2828 (3)	74 (2)
C(34B)	6627 (1)	-837 (2)	1985 (4)	89 (2)
C(35B)	6046 (1)	-728 (1)	1600 (5)	105 (2)
C(36B)	5783 (1)	-128 (1)	2070 (4)	85 (2)
H(2A)	-388 (8)	578 (9)	10399 (23)	54 (6)
H(3A)	-1016 (8)	1433 (9)	7990 (23)	49 (5)
H(1A)	-131 (8)	2154 (9)	8196 (22)	50 (5)
H(41A)	79 (12)	1525 (11)	5213 (31)	96 (8)
H(42A)	-564 (13)	1760 (14)	5461 (37)	119 (11)
H(43A)	-436 (11)	933 (13)	4951 (36)	96 (8)
H(12A)	643 (9)	2636 (11)	7125 (27)	76 (7)
H(13A)	1651 (9)	2660 (11)	6677 (27)	68 (7)
H(14A)	2324 (12)	1842 (12)	7783 (32)	101 (8)
H(15A)	1922 (10)	944 (12)	9213 (33)	89 (8)
H(16A)	955 (8)	896 (10)	9687 (27)	62 (6)
H(22A)	-1094 (9)	247 (12)	12202 (29)	72 (7)
H(23A)	-1827 (9)	521 (11)	13881 (29)	72 (7)

Table 1 (cont.)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{iso}$ (Å <sup>2</sup> )
H(24A)	-2202 (12)	1616 (12)	14142 (33)	87 (8)
H(25A)	-1786 (10)	2503 (14)	12460 (31)	97 (9)
H(26A)	-1033 (10)	2274 (12)	10763 (30)	93 (8)
H(32A)	-415 (10)	-124 (11)	6735 (30)	86 (8)
H(33A)	-944 (12)	-1089 (14)	5930 (39)	109 (10)
H(34A)	-1952 (11)	-1148 (13)	5957 (35)	95 (8)
H(35A)	-2430 (12)	-209 (14)	7285 (35)	112 (9)
H(36A)	-1872 (9)	741 (10)	8065 (28)	69 (7)
H(2B)	5454 (9)	584 (10)	5424 (26)	66 (6)
H(3B)	6150 (8)	1438 (9)	3258 (23)	52 (5)
H(1B)	4769 (9)	-2193 (11)	6779 (26)	67 (7)
H(41B)	4987 (12)	-1589 (12)	9925 (33)	102 (9)
H(42B)	5503 (12)	1006 (14)	-89 (37)	106 (9)
H(43B)	5663 (13)	1792 (14)	586 (36)	107 (10)
H(12B)	5790 (9)	-924 (11)	5644 (29)	73 (7)
H(13B)	6795 (10)	-953 (12)	6434 (29)	79 (7)
H(14B)	7225 (13)	-1789 (13)	8150 (34)	107 (9)
H(15B)	6628 (11)	-2684 (13)	9109 (34)	104 (9)
H(16B)	4415 (9)	2690 (12)	1630 (28)	82 (7)
H(22B)	6233 (11)	2192 (13)	5937 (34)	97 (9)
H(23B)	7024 (15)	2468 (18)	7943 (43)	148 (13)
H(24B)	7314 (15)	1474 (16)	9822 (46)	125 (12)
H(25B)	6942 (15)	418 (18)	9658 (46)	149 (14)
H(26B)	6107 (13)	234 (16)	7492 (39)	121 (12)
H(32B)	6943 (11)	624 (12)	3829 (34)	93 (8)
H(33B)	2625 (10)	413 (12)	6940 (30)	80 (7)
H(34B)	3197 (13)	1275 (15)	8293 (39)	125 (11)
H(35B)	5813 (14)	-1064 (15)	1001 (42)	127 (11)
H(36B)	4656 (12)	69 (13)	8157 (32)	103 (9)

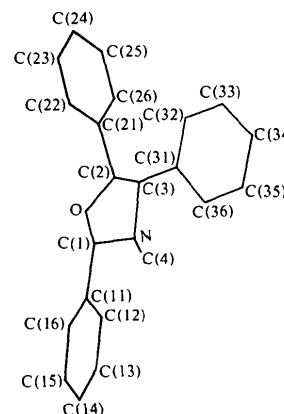


Fig. 1. The atom-numbering scheme.

index  $R = 0.035$  and  $R_w = 0.040$ . A weighting scheme of the form  $w = 1/[\sigma^2(F) + pF^2]$  was employed during refinement with the  $p$  values recalculated after each cycle. Final positional parameters are listed in Table 1 and bond lengths and angles in Table 2. Fig. 1 shows our numbering scheme.\*

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38012 (15 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 angles (°)

	Molecule <i>A</i>	Molecule <i>B</i>		Molecule <i>A</i>	Molecule <i>B</i>
O—C(1)	1.426 (3)	1.427 (3)	C(2)—O—C(1)	108.7 (1)	109.7 (2)
C(1)—N	1.457 (3)	1.465 (3)	O—C(1)—C(11)	112.0 (2)	111.9 (2)
N—C(3)	1.458 (3)	1.454 (2)	N—C(1)—C(11)	112.6 (2)	111.7 (2)
C(3)—C(2)	1.529 (3)	1.542 (3)	C(1)—C(11)—C(12)	120.1 (2)	120.4 (2)
C(2)—O	1.441 (3)	1.435 (3)	C(1)—C(11)—C(16)	120.8 (2)	120.6 (2)
N—C(4)	1.459 (3)	1.458 (3)	C(12)—C(11)—C(16)	119.0 (2)	118.9 (2)
C(1)—C(11)	1.504 (3)	1.499 (3)	C(11)—C(12)—C(13)	120.3 (2)	120.5 (2)
C(11)—C(12)	1.376 (3)	1.384 (3)	C(12)—C(13)—C(14)	120.6 (2)	120.1 (2)
C(12)—C(13)	1.378 (3)	1.372 (3)	C(13)—C(14)—C(15)	119.9 (2)	120.2 (2)
C(13)—C(14)	1.361 (3)	1.372 (4)	C(14)—C(15)—C(16)	120.2 (2)	119.9 (2)
C(14)—C(15)	1.367 (4)	1.359 (4)	C(15)—C(16)—C(11)	120.0 (2)	120.4 (2)
C(15)—C(16)	1.383 (3)	1.393 (3)	O—C(2)—C(21)	111.5 (2)	111.3 (2)
C(16)—C(11)	1.387 (3)	1.372 (3)	C(3)—C(2)—C(21)	114.7 (2)	114.4 (2)
C(2)—C(21)	1.493 (3)	1.495 (3)	C(2)—C(21)—C(22)	120.6 (2)	120.6 (2)
C(21)—C(22)	1.388 (3)	1.390 (4)	C(2)—C(21)—C(26)	121.8 (2)	120.7 (2)
C(22)—C(23)	1.389 (4)	1.387 (4)	C(22)—C(21)—C(26)	117.6 (2)	118.7 (2)
C(23)—C(24)	1.359 (5)	1.367 (7)	C(21)—C(22)—C(23)	120.5 (3)	120.0 (3)
C(24)—C(25)	1.361 (4)	1.337 (8)	C(22)—C(23)—C(24)	120.7 (3)	119.4 (4)
C(25)—C(26)	1.381 (4)	1.383 (5)	C(23)—C(24)—C(25)	119.5 (3)	121.3 (4)
C(26)—C(21)	1.376 (3)	1.381 (4)	C(24)—C(25)—C(26)	120.4 (3)	120.4 (4)
C(3)—C(31)	1.511 (3)	1.499 (3)	C(25)—C(26)—C(21)	121.4 (2)	120.2 (3)
C(31)—C(32)	1.371 (3)	1.379 (3)	C(2)—C(3)—C(31)	114.6 (2)	114.2 (2)
C(32)—C(33)	1.399 (4)	1.378 (4)	N—C(3)—C(31)	115.4 (2)	114.5 (2)
C(33)—C(34)	1.359 (4)	1.359 (4)	C(3)—C(31)—C(32)	122.8 (2)	122.2 (2)
C(34)—C(35)	1.355 (4)	1.359 (4)	C(3)—C(31)—C(36)	118.8 (2)	120.3 (2)
C(35)—C(36)	1.386 (3)	1.385 (4)	C(32)—C(31)—C(36)	118.3 (2)	117.6 (2)
C(36)—C(31)	1.377 (3)	1.380 (3)	C(31)—C(32)—C(33)	120.1 (2)	120.3 (2)
			C(32)—C(33)—C(34)	120.3 (3)	121.1 (3)
			C(33)—C(34)—C(35)	120.2 (2)	119.4 (3)
O—C(1)—N	104.6 (2)	104.8 (2)	C(34)—C(35)—C(36)	119.7 (2)	120.0 (2)
C(1)—N—C(3)	102.4 (2)	104.6 (2)	C(35)—C(36)—C(31)	121.3 (2)	121.7 (2)
N—C(3)—C(2)	100.5 (2)	100.4 (2)	C(1)—N—C(4)	112.6 (2)	112.7 (2)
C(3)—C(2)—O	103.5 (2)	103.5 (2)	C(3)—N—C(4)	113.9 (2)	113.9 (2)

**Discussion.** The asymmetric unit contains an enantiomeric pair of molecules. The molecules of each pair are related by approximate glide-plane symmetry with translation along *c*. Equivalent interatomic distances and angles are generally equal within experimental error. Only two angles differ significantly: C(1)—O—C(2) is 108.7 (1)° in molecule *A* and 109.7 (2)° in *B*, and C(1)—N—C(3) is 102.4 (2)° in *A* and 104.6 (2)° in *B*. The angles between planes fitted by least squares to the phenyl rings are as follows: ∠I, II = 38.8 (1)° in *A* [35.1 (1)° in *B*], ∠I, III = 54.8 (1)° in *A* [57.0 (1)° in *B*] and ∠II, III = 47.6 (1)° in *A* [50.5 (1)° in *B*], where I, II and III represent the phenyl rings bonded to C(1), C(2) and C(3) respectively. The geometries of the oxazolidine rings of the two molecules are also some-

what different. The two rings are of the half-chair type. In molecule *A* atoms N and C(3) are 0.43 (2) and 0.25 (2) Å from the plane defined by atoms C(1), O, C(2), while in molecule *B* the equivalent distances are 0.27 (2) and 0.37 (2) Å. These differences indicate a significant flexibility of the oxazolidine system.

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