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

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Abstract. $C_{23}H_{23}NO$, orthorhombic, *Pcab*, $a = 7{\cdot}641\ (2)$, $b = 17{\cdot}324\ (2)$, $c = 29{\cdot}042\ (6)$ Å, $Z = 8$, $D_x = 1{\cdot}14$ Mg m^{-3}, m.p. 324–325 K, $R = 0{\cdot}044$ for 1781 reflexions with $I > 2{\cdot}5\sigma(I)$. The central oxazolidine ring is in the half-chair conformation.

Introduction. The title compound was synthesized by G. Mlostoń (1981) and was recrystallized from ethanol. The unit-cell parameters and intensities were measured at room temperature on a CAD-4 diffractometer using Cu $K\alpha$ radiation. 3018 independent reflexions with θ values below 75° were measured; of these, 1781 were considered as observed by the criterion $I > 2{\cdot}5\sigma(I)$. No absorption corrections were applied.

The E map showed the positions of only six non-hydrogen atoms. The remaining non-hydrogen atoms were located by application of the partial-structure procedure using *SHELX* 76 (Sheldrick, 1976). The refinement was carried out by the full-matrix least-squares method. Most of the H-atom positions were located on a difference Fourier map and the rest were calculated from the geometry of the molecule. Isotropic temperature factors were used for the H atoms and anisotropic values for non-H atoms. A weighting scheme of the form $w = 1/[\sigma^2(F) + pF^2]$ was employed with the p equal to 0·002. The final R index was 0·044 and R_w was 0·052.

The atom parameters are listed in Table 1, the bond lengths and angles are given in Table 2, and Fig. 1 shows the numbering of the atoms.*

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38018 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

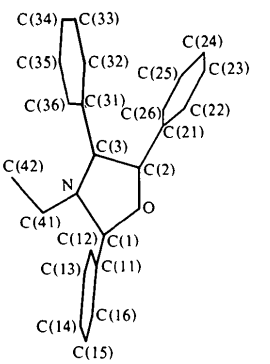

Fig. 1. The atom-numbering scheme.

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Table 1. *Final fractional coordinates* ($\times 10^4$) *and mean isotropic temperature factors* ($\times 10^3$) *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} (Å^2)
C(3)	9898 (3)	4563 (1)	1448 (1)	62 (1)
C(2)	8552 (4)	5214 (1)	1567 (1)	66 (2)
C(31)	9509 (3)	4108 (1)	1018 (1)	66 (2)
C(32)	10170 (5)	4346 (2)	600 (1)	100 (3)
C(33)	9825 (8)	3945 (4)	206 (1)	141 (4)
C(34)	8779 (9)	3302 (3)	220 (2)	151 (5)
C(35)	8130 (8)	3052 (2)	627 (2)	128 (3)
C(36)	8502 (5)	3456 (2)	1028 (1)	87 (2)
C(21)	7352 (4)	5481 (2)	1192 (1)	84 (2)
C(22)	7697 (8)	6194 (3)	989 (2)	132 (4)
C(23)	6621 (14)	6428 (6)	627 (2)	202 (7)
C(24)	5299 (12)	5973 (7)	473 (2)	248 (10)
C(25)	4948 (8)	5273 (7)	686 (2)	201 (6)
C(26)	5984 (6)	5049 (3)	1044 (1)	116 (3)
O	7582 (2)	4899 (1)	1943 (1)	64 (1)
N	9883 (2)	4092 (1)	1863 (1)	60 (1)
C(41)	11618 (4)	3846 (2)	2026 (1)	74 (2)
C(42)	12438 (5)	3271 (2)	1704 (1)	86 (2)
C(1)	8876 (3)	4513 (1)	2209 (1)	60 (1)
C(11)	8032 (3)	3991 (1)	2556 (1)	58 (1)
C(12)	6649 (4)	3514 (1)	2434 (1)	70 (2)
C(13)	5916 (4)	3019 (2)	2750 (1)	80 (2)
C(14)	6562 (4)	2991 (2)	3193 (1)	83 (2)
C(15)	7906 (4)	3465 (2)	3320 (1)	81 (2)
C(16)	8634 (4)	3965 (1)	3003 (1)	71 (2)
H(411)	12408 (38)	4287 (15)	2064 (9)	97 (9)
H(412)	11441 (33)	3556 (13)	2350 (9)	77 (7)
H(421)	11602 (47)	2862 (19)	1634 (11)	127 (12)
H(422)	12721 (37)	3501 (16)	1387 (10)	98 (10)
H(423)	13476 (45)	3020 (16)	1850 (10)	106 (10)
H(1)	9589 (31)	4906 (12)	2376 (7)	64 (6)
H(12)	6249 (31)	3534 (13)	2111 (9)	76 (7)
H(13)	4993 (40)	2695 (16)	2661 (9)	101 (10)
H(14)	5991 (39)	2674 (17)	3420 (9)	104 (10)
H(15)	8372 (42)	3449 (16)	3622 (10)	98 (9)
H(16)	9551 (36)	4291 (14)	3098 (8)	86 (8)
H(3)	11046 (35)	4840 (14)	1405 (8)	80 (7)
H(2)	9228 (28)	5676 (13)	1691 (7)	68 (7)
H(32)	11047 (50)	4815 (21)	639 (13)	133 (14)
H(33)	10269 (52)	4152 (21)	−104 (15)	137 (13)
H(34)	8677 (56)	3084 (22)	−45 (15)	147 (15)
H(35)	7397 (69)	2598 (30)	682 (14)	179 (20)
H(36)	8028 (40)	3299 (16)	1339 (10)	90 (9)
H(22)	8513 (108)	6455 (46)	1075 (24)	298 (45)
H(23)	7359 (95)	6913 (33)	469 (23)	277 (32)
H(24)	4791 (92)	6274 (34)	250 (23)	201 (25)
H(25)	4110 (125)	5183 (44)	452 (30)	318 (43)
H(26)	5811 (52)	4587 (20)	1178 (11)	84 (14)

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

O–C(1)	1·423 (3)	C(2)–C(21)	1·497 (4)
C(1)–N	1·461 (3)	C(21)–C(22)	1·394 (6)
N–C(3)	1·456 (3)	C(22)–C(23)	1·397 (10)
C(3)–C(2)	1·565 (3)	C(23)–C(24)	1·357 (14)
C(2)–O	1·427 (3)	C(24)–C(25)	1·387 (15)
N–C(41)	1·471 (3)	C(25)–C(26)	1·363 (8)
C(41)–C(42)	1·504 (5)	C(26)–C(21)	1·355 (6)
C(1)–C(11)	1·498 (3)	C(3)–C(31)	1·507 (3)
C(11)–C(12)	1·388 (3)	C(31)–C(32)	1·377 (4)
C(12)–C(13)	1·375 (4)	C(32)–C(33)	1·365 (6)
C(13)–C(14)	1·378 (5)	C(33)–C(34)	1·371 (9)
C(14)–C(15)	1·366 (4)	C(34)–C(35)	1·353 (7)
C(15)–C(16)	1·380 (4)	C(35)–C(36)	1·388 (5)
C(16)–C(11)	1·380 (3)	C(36)–C(31)	1·367 (4)

O–C(1)–N	103·1 (2)	C(22)–C(21)–C(26)	120·1 (4)
C(1)–N–C(3)	107·1 (2)	C(21)–C(22)–C(23)	117·7 (6)
N–C(3)–C(2)	102·4 (2)	C(22)–C(23)–C(24)	121·1 (8)
C(3)–C(2)–O	103·6 (2)	C(23)–C(24)–C(25)	120·4 (7)
C(2)–O–C(1)	103·5 (2)	C(24)–C(25)–C(26)	118·5 (7)
O–C(1)–C(11)	110·5 (2)	C(25)–C(26)–C(21)	122·2 (6)
N–C(1)–C(11)	112·8 (2)	C(2)–C(3)–C(31)	115·6 (2)
C(1)–C(11)–C(12)	121·1 (2)	N–C(3)–C(31)	113·0 (2)
C(1)–C(11)–C(16)	120·6 (2)	C(3)–C(31)–C(32)	120·0 (2)
C(12)–C(11)–C(16)	118·3 (2)	C(3)–C(31)–C(36)	121·7 (2)
C(11)–C(12)–C(13)	120·8 (3)	C(32)–C(31)–C(36)	118·3 (3)
C(12)–C(13)–C(14)	119·9 (3)	C(31)–C(32)–C(33)	121·0 (4)
C(13)–C(14)–C(15)	120·0 (3)	C(32)–C(33)–C(34)	120·1 (4)
C(14)–C(15)–C(16)	120·1 (3)	C(33)–C(34)–C(35)	119·9 (5)
C(15)–C(16)–C(11)	120·9 (3)	C(34)–C(35)–C(36)	119·8 (4)
O–C(2)–C(21)	110·8 (2)	C(35)–C(36)–C(31)	120·9 (3)
C(3)–C(2)–C(21)	117·6 (2)	C(3)–N–C(41)	115·0 (2)
C(2)–C(21)–C(22)	117·7 (3)	C(1)–N–C(41)	113·4 (2)
C(2)–C(21)–C(26)	122·2 (3)	N–C(41)–C(42)	111·5 (2)

Discussion. All three phenyl rings are in the *trans* configuration with respect to the ethyl group bonded to N. The angles between planes fitted by least squares to the phenyl rings are as follows: ∠I, II = 26·5 (2), ∠I, III = 26·9 (2) and ∠II, III = 48·6 (3)°, where I, II and III represent the phenyl groups on C(1), C(2) and C(3) respectively. The conformation of the oxazolidine ring is of the half-chair type with atoms O and C(1) 0·35 (2) and 0·28 (2) Å from the plane defined by atoms C(2), C(3) and N. High values of the temperature factors of the atoms, especially those forming the phenyl rings, result from the diffraction data being collected at a temperature close to the melting point.

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