pital, 1975; dihedral angle 53°). A value of 1.51 Å was assigned to C(1')—C(3) in licoricone.

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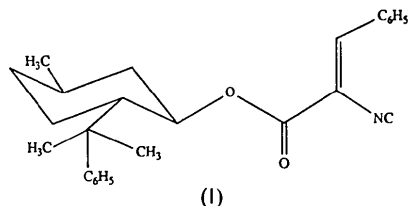

Structure of a Cinnamic Acid Derivative

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Abstract. (1R,2S,5R)-5-Methyl-2-(1-methyl-1-phenylethyl)cyclohexyl (Z)-2-isocyano-3-phenylpropenoate, $C_{26}H_{29}NO_2$, $M_r = 387.5$, orthorhombic, $P2_12_12_1$, $a = 9.777$ (1), $b = 10.211$ (1), $c = 22.585$ (2) Å, $V = 2254.7$ (3) Å^3, $Z = 4$, $D_x = 1.142$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0.7107$ Å, $\mu = 0.07$ mm^{-1}, $F(000) = 832$, $T = 293$ K, final $R = 0.043$ for 1982 unique observed reflections. The isocyano group is *syn* to the carbonyl O atom and *cis* to the phenyl group, which is rotated by 29° from the plane of the adjacent conjugated π system. One side of the C=C double bond is shielded by the second phenyl ring (distance approximately 3.5 Å).

Experimental. Crystals of (I) obtained from methanol at 243 K were yellow rectangular prisms, 0.2 × 0.5 × 0.8 mm. A Stoe four-circle diffractometer was

(I)

used for data collection with monochromated Mo $K\alpha$ radiation. Lattice parameters were measured by centring 60 reflections with $20 < 2\theta < 25°$. Data were collected with the profile-fitting method (Clegg, 1981); 4274 measured intensities, $2\theta_{max} = 50°$ ($-11 \leq h \leq 11$, $0 \leq k \leq 12$, $0 \leq l \leq 26$). Three standard reflections measured every 100 reflections showed no

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

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

	x	y	z	U_{eq}
O(1)	3382 (2)	−1310 (2)	7135 (1)	51 (1)
C(2)	3155 (2)	−2319 (3)	7491 (1)	50 (1)
C(3)	3894 (3)	−2187 (3)	8062 (1)	54 (1)
C(4)	4781 (3)	−1242 (3)	8191 (1)	59 (1)
O(21)	2450 (2)	−3242 (2)	7376 (1)	73 (1)
N(31)	3640 (2)	−3230 (2)	8444 (1)	67 (1)
C(32)	3385 (4)	−4115 (4)	8741 (1)	98 (1)
C(41)	5634 (3)	−1055 (3)	8721 (1)	60 (1)
C(42)	6849 (3)	−380 (3)	8656 (1)	70 (1)
C(43)	7738 (4)	−206 (3)	9128 (1)	86 (1)
C(44)	7406 (4)	−690 (3)	9671 (1)	94 (1)
C(45)	6195 (4)	−1342 (4)	9751 (1)	101 (1)
C(46)	5298 (3)	−1535 (4)	9279 (1)	85 (1)
C(1')	2782 (2)	−1344 (2)	6538 (1)	47 (1)
C(2')	3913 (2)	−1782 (3)	6124 (1)	52 (1)
C(3')	3469 (3)	−1761 (3)	5477 (1)	58 (1)
C(3'')	4629 (3)	−2228 (4)	5076 (1)	85 (1)
C(4')	2985 (3)	−391 (3)	5329 (1)	65 (1)
C(5')	1836 (2)	58 (2)	5733 (1)	58 (1)
C(6')	2221 (2)	12 (2)	6395 (1)	44 (1)
C(7')	1013 (2)	453 (2)	6811 (1)	47 (1)
C(8')	343 (3)	1717 (3)	6571 (1)	61 (1)
C(9')	−112 (2)	−591 (3)	6837 (1)	63 (1)
C(71')	1548 (2)	789 (2)	7432 (1)	47 (1)
C(72')	2529 (3)	1758 (2)	7503 (1)	58 (1)
C(73')	3017 (3)	2127 (3)	8047 (1)	71 (1)
C(74')	2552 (3)	1524 (4)	8551 (1)	81 (1)
C(75')	1581 (3)	561 (3)	8497 (1)	78 (1)
C(76')	1079 (3)	201 (3)	7947 (1)	62 (1)

significant intensity variation. Intensities were corrected for Lorentz and polarization factors, but not for absorption. 2262 unique reflections were collected ($R_{int} = 0.021$) of which 1982 with $|F| > 3\sigma(F)$ were treated as observed. The structure was solved by direct methods. All H atoms were located by difference synthesis and refined with fixed individual displacement parameters [$U(H) = 1.2U_{eq}(C)$] using a riding model with C—H = 0.96 Å. Anisotropic

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

O(1)—C(2)	1.325 (3)	O(1)—C(1')	1.473 (2)
C(2)—C(3)	1.485 (3)	C(2)—O(21)	1.196 (3)
C(3)—C(4)	1.330 (4)	C(3)—N(31)	1.393 (3)
C(4)—C(41)	1.472 (3)	N(31)—C(32)	1.153 (4)
C(41)—C(42)	1.381 (4)	C(41)—C(46)	1.392 (4)
C(42)—C(43)	1.386 (4)	C(43)—C(44)	1.362 (4)
C(44)—C(45)	1.370 (5)	C(45)—C(46)	1.395 (4)
C(1')—C(2')	1.515 (3)	C(1')—C(6')	1.523 (3)
C(2')—C(3')	1.523 (3)	C(3')—C(3'')	1.529 (4)
C(3')—C(4')	1.514 (4)	C(4')—C(5')	1.519 (3)
C(5')—C(6')	1.543 (3)	C(6')—C(7')	1.575 (3)
C(7')—C(8')	1.546 (3)	C(7')—C(9')	1.532 (3)
C(7')—C(71')	1.534 (3)	C(71')—C(72')	1.388 (3)
C(71')—C(76')	1.387 (3)	C(72')—C(73')	1.372 (4)
C(73')—C(74')	1.371 (4)	C(74')—C(75')	1.372 (5)
C(75')—C(76')	1.386 (4)		

C(2)—O(1)—C(1')	118.1 (2)	O(1)—C(2)—C(3)	112.0 (2)
O(1)—C(2)—O(21)	125.3 (2)	C(3)—C(2)—O(21)	122.7 (2)
C(2)—C(3)—C(4)	125.0 (2)	C(2)—C(3)—N(31)	112.5 (2)
C(4)—C(3)—N(31)	122.4 (2)	C(3)—C(4)—C(41)	129.9 (2)
C(3)—N(31)—C(32)	176.7 (3)	C(4)—C(41)—C(42)	117.8 (2)
C(4)—C(41)—C(46)	123.9 (2)	C(42)—C(41)—C(46)	118.4 (2)
C(41)—C(42)—C(43)	121.5 (2)	C(42)—C(43)—C(44)	119.7 (3)
C(43)—C(44)—C(45)	120.1 (3)	C(44)—C(45)—C(46)	120.8 (3)
C(41)—C(46)—C(45)	119.6 (3)	O(1)—C(1')—C(2')	106.4 (2)
O(1)—C(1')—C(6')	108.4 (2)	C(2')—C(1')—C(6')	113.6 (2)
C(1')—C(2')—C(3')	112.3 (2)	C(2')—C(3')—C(3'')	110.6 (2)
C(2')—C(3')—C(4')	108.3 (2)	C(3'')—C(3')—C(4')	112.9 (2)
C(3')—C(4')—C(5')	112.1 (2)	C(4')—C(5')—C(6')	113.2 (2)
C(1')—C(6')—C(5')	108.6 (2)	C(1')—C(6')—C(7')	113.8 (2)
C(5')—C(6')—C(7')	112.7 (2)	C(6')—C(7')—C(8')	110.3 (2)
C(6')—C(7')—C(9')	111.2 (2)	C(8')—C(7')—C(9')	106.8 (2)
C(6')—C(7')—C(71')	110.7 (2)	C(8')—C(7')—C(71')	106.1 (2)
C(9')—C(7')—C(71')	111.5 (2)	C(7')—C(71')—C(72')	120.1 (2)
C(7')—C(71')—C(76')	123.8 (2)	C(72')—C(71')—C(76')	116.1 (2)
C(71')—C(72')—C(73')	122.6 (2)	C(72')—C(73')—C(74')	120.4 (3)
C(73')—C(74')—C(75')	118.5 (3)	C(74')—C(75')—C(76')	121.0 (3)
C(71')—C(76')—C(75')	121.3 (2)		

C(1')—O(1)—C(2)—C(3)	176.4 (2)	C(2)—C(3)—C(4)—C(41)	−175.7 (3)
O(1)—C(2)—C(3)—C(4)	−5.9 (4)	N(31)—C(3)—C(4)—C(41)	−0.7 (4)
O(21)—C(2)—C(3)—N(31)	−1.5 (3)	C(3)—C(4)—C(41)—C(46)	−26.6 (5)

blocked-cascade refinement (on F) of 263 parameters with *SHELXTL* (Sheldrick, 1983) converged at $R = 0.043$, $wR = 0.047$ $[w^{-1} = \sigma^2(F) + 0.0005F^2]$, $S = 1.34$, $(\Delta/\sigma)_{max} = 0.02$ in the last cycle; $-0.11 < \Delta\rho < 0.12$ e Å^{-3} in the final difference map. Scattering factors were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV).
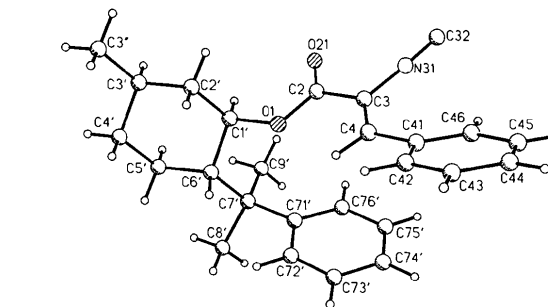

Fig. 1. Perspective view with the atom numbering.

Final atomic parameters are listed in Table 1,* bond lengths and angles, as well as selected torsion angles, in Table 2. Fig. 1 shows the molecular conformation.

Related literature. The title compound is an educt for the diastereoselective 1,4-addition of organocopper reagents (Oppolzer & Löher, 1981) because one face of the double bond is shielded.

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Structures of Two Acylpyridinium Salts and One Simple Pyridinium Salt

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Abstract. N-Phenoxycarbonyl-4-dimethylaminopyridinium chloride (I), $C_{14}H_{15}N_2O_2^+.Cl^-$, $M_r = 278.7$, monoclinic, $P2_1/c$, $a = 17.397$ (4), $b = 5.865$ (2), $c = 13.482$ (5) Å, $\beta = 104.26$ (2)°, $V = 1333.2$ Å^3, $Z = 4$, $D_x = 1.389$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 2.83$ cm^{-1}, $F(000) = 584$, $T = 198$ K,

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