

Fig. 1. A view of the (2,2'-bipyrimidine)Cr(CO)<sub>4</sub> and 2,2'-bipyrimidine complex molecules.

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## Structure of $\alpha$ -*trans*-Cinnamic Acid

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**Abstract.** 3-Phenyl-2-propenoic-acid, C<sub>9</sub>H<sub>8</sub>O<sub>2</sub>,  $M_r = 148.2$ , monoclinic,  $P2_1/n$ ,  $a = 5.582$  (2),  $b = 17.671$  (4),  $c = 7.735$  (2) Å,  $\beta = 96.49$  (2)°,  $V = 758.0$  (3) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.298$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 0.46$  cm<sup>-1</sup>,  $F(000) = 312$ ,  $T = 193$  (1) K, final  $R = 0.041$  for 1724 unique reflections. The molecule is planar with a slight decrease of the C–C single bonds [C(1)–C(2) = 1.469 (2), C(3)–C(4) = 1.467 (2) Å] and an increase of the C=C double bond [C(2)–C(3) = 1.334 (2) Å] as a result of conjugation. The structural units are dimers formed by the hydrogen bonding of carboxyl groups across centres of symmetry, the O...O distance being 2.634 (2) Å.

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**Experimental.** Cinnamic acid was recrystallized from ethanol. A crystal of size 0.2 × 0.3 × 0.3 mm was used for diffraction measurement. Unit-cell parameters were obtained from a least-squares refinement of 25 reflections. Nicolet R3m/V diffractometer, equipped with an LT-1 low temperature device, and graphite-monochromated radiation. The intensities of 1982 reflections were measured in the 2 $\theta$  range 4–45°, with the  $\theta/2\theta$  scan mode. Index ranges 0 <  $h$  < 7, 0 <  $k$  < 22, –10 <  $l$  < 10. Three intensity control reflections were monitored every 60 reflections of data collected; no crystal decay was observed. 1724 unique reflections ( $R_{\text{int}} = 0.026$ ) of which 1503 were considered observed, the criterion  $F_o > 4\sigma(F_o)$ , were used in the refinement. Lorentz–polarization and empirical absorption corrections ( $\psi$  scans) were applied. The structure was

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )

	x	y	z	$U_{eq}^*$
O(1)	2627 (2)	4506 (1)	5822 (1)	40 (1)
O(2)	-507 (2)	4930 (1)	7112 (1)	39 (1)
C(1)	1514 (2)	4615 (1)	7177 (2)	30 (1)
C(2)	2694 (2)	4348 (1)	8859 (2)	30 (1)
C(3)	4795 (2)	3981 (1)	9006 (2)	29 (1)
C(4)	6095 (2)	3684 (1)	10618 (2)	28 (1)
C(5)	8204 (2)	3263 (1)	10531 (2)	33 (1)
C(6)	9469 (2)	2970 (1)	12032 (2)	38 (1)
C(7)	8669 (3)	3097 (1)	13633 (2)	41 (1)
C(8)	6587 (3)	3513 (1)	13737 (2)	41 (1)
C(9)	5306 (2)	3804 (1)	12244 (2)	33 (1)
H(10)	1638 (51)	4724 (15)	4669 (43)	128 (10) ( $U_{iso}$ )

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

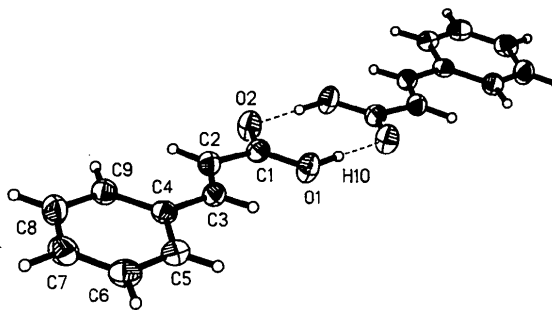


Fig. 1. The atom numbering.

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

O(1)—C(1)	1.292 (2)	O(1)—C(1)—C(2)	117.5 (1)
O(2)—C(1)	1.254 (2)	O(1)—C(1)—O(2)	123.1 (1)
C(1)—C(2)	1.469 (2)	C(1)—C(2)—C(3)	122.3 (1)
C(2)—C(3)	1.334 (2)	O(2)—C(1)—C(2)	119.4 (1)
C(3)—C(4)	1.467 (2)	C(2)—C(3)—C(4)	126.3 (1)
C(4)—C(5)	1.401 (2)	C(3)—C(4)—C(5)	119.2 (1)
C(5)—C(6)	1.389 (2)	C(3)—C(4)—C(9)	122.4 (1)
C(6)—C(7)	1.381 (2)	C(4)—C(9)—C(8)	120.6 (1)
C(7)—C(8)	1.386 (2)	C(4)—C(5)—C(6)	120.6 (1)
C(8)—C(9)	1.387 (2)	C(5)—C(4)—C(9)	118.4 (1)
C(4)—C(9)	1.395 (2)	C(5)—C(6)—C(7)	120.2 (1)
O(1)—O(2)	2.634 (2)	C(6)—C(7)—C(8)	119.8 (1)
		C(7)—C(8)—C(9)	120.4 (1)

solved by a routine application of *SHELXTL-Plus* (Sheldrick, 1987). All H atoms found from a difference synthesis. Full-matrix least-squares [using  $w(F_o - F_c)^2$ ] anisotropic refinement of the positions of non-H atoms and isotropic refinement of H atoms gave a final  $R = 0.0412$  [ $wR = 0.0540$ ;  $w^{-1} = \sigma^2(F) + 0.0002F^2$ ]. The model was refined to convergence:  $\Delta/\sigma = 0.004$ . Data to parameter ratio 11.4:1.

The final difference map was essentially featureless:  $0.24 \text{ e \AA}^{-3}$  (max),  $-0.19 \text{ e \AA}^{-3}$  (min). Scattering fac-

tors from *International Tables for X-ray Crystallography* (1974).

Final atomic coordinates are given in Table 1, and bond lengths and angles in Table 2. The atom-numbering scheme is shown in Fig. 1.\*

**Related literature.** Lattice constants at room temperature and 90 K (Ladell, McDonald & Schmidt, 1956). Magnetic anisotropies and susceptibilities (Lonsdale, 1939; Lasheen, 1964).

\* Lists of structure factors, anisotropic thermal parameters and atomic parameters for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51390 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## $\alpha$ -Cyano-*N,N*-diisopropyl- $\alpha$ -(3-methoxy-6-methylphenyl)acetamide

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**Abstract.**  $C_{17}H_{24}N_2O_2$ ,  $M_r = 288.4$ , orthorhombic, *Pbca*,  $a = 8.032$  (3),  $b = 17.076$  (7),  $c = 24.83$  (1)  $\text{\AA}$ ,  $V = 3405$  (1)  $\text{\AA}^3$ ,  $Z = 8$ ,  $D_x = 1.12 \text{ g cm}^{-3}$ ,  $\lambda(\text{Mo K}\alpha)$

$= 0.71073 \text{ \AA}$ ,  $\mu = 0.69 \text{ cm}^{-1}$ ,  $F(000) = 1248$ ,  $T = 295 \text{ K}$ , final  $R = 0.056$  for 1308 observed reflections. The phenyl, amide and nitrile groups and the H atoms are arranged in a distorted tetrahedron with respect to the  $\alpha$ -C atom. The X-ray structure reveals the de-

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