

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)
$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	U_{eq}
S1	0.0071 (2)	0.11537 (12)	0.83844 (15)	0.0722 (7)
O1	0.5435 (6)	-0.1254 (4)	0.9104 (4)	0.103 (2)
O2	-0.0652 (5)	0.0744 (3)	0.9061 (4)	0.088 (2)
O3	-0.0706 (5)	0.1248 (3)	0.7360 (4)	0.095 (2)
N1	0.1655 (5)	0.0622 (3)	0.8404 (4)	0.066 (2)
C2	0.2116 (7)	-0.0041 (4)	0.9004 (5)	0.060 (2)
C3	0.3488 (6)	-0.0317 (4)	0.8876 (5)	0.063 (2)
C4	0.3945 (7)	0.0231 (4)	0.8181 (5)	0.059 (2)
C5	0.5259 (8)	0.0276 (5)	0.7797 (6)	0.077 (2)
C6	0.5327 (9)	0.0866 (6)	0.7123 (6)	0.094 (3)
C7	0.4121 (10)	0.1410 (5)	0.6782 (6)	0.093 (3)
C8	0.2850 (8)	0.1373 (5)	0.7179 (5)	0.078 (2)
C9	0.2780 (7)	0.0770 (4)	0.7874 (5)	0.064 (2)
C10	0.4234 (8)	-0.1061 (4)	0.9316 (5)	0.069 (2)
C11	0.3458 (8)	-0.1571 (5)	0.9945 (6)	0.084 (2)
C12	0.4302 (9)	-0.2304 (5)	1.0398 (6)	0.089 (2)
C13	0.3462 (10)	-0.2770 (5)	1.1059 (7)	0.101 (3)
C14	0.4346 (13)	-0.3473 (7)	1.1594 (10)	0.149 (4)
C15	0.3520 (13)	-0.3886 (8)	1.2279 (10)	0.173 (6)
C16	0.0742 (7)	0.2090 (4)	0.8845 (5)	0.062 (2)
C17	0.0553 (9)	0.2752 (5)	0.8218 (6)	0.083 (2)
C18	0.1144 (10)	0.3489 (5)	0.8573 (7)	0.095 (3)
C19	0.1883 (9)	0.3593 (5)	0.9569 (7)	0.084 (2)
C20	0.2033 (9)	0.2913 (6)	1.0183 (6)	0.084 (2)
C21	0.1464 (8)	0.2179 (5)	0.9833 (6)	0.075 (2)
C22	0.2508 (12)	0.4394 (6)	0.9931 (7)	0.124 (3)

Table 2. Selected geometric parameters (\AA , $^\circ$)

S1—O2	1.422 (5)	C3—C4	1.445 (9)
S1—O3	1.428 (5)	C3—C10	1.466 (9)
S1—N1	1.669 (5)	C4—C9	1.368 (8)
S1—C16	1.733 (7)	C4—C5	1.401 (9)
O1—C10	1.223 (7)	C5—C6	1.358 (11)
N1—C2	1.379 (8)	C6—C7	1.405 (11)
N1—C9	1.396 (8)	C7—C8	1.376 (10)
C2—C3	1.364 (8)	C8—C9	1.393 (9)
C2—N1—C9	107.3 (5)	C6—C5—C4	117.9 (7)
C2—N1—S1	124.7 (4)	C5—C6—C7	122.6 (7)
C9—N1—S1	128.0 (5)	C8—C7—C6	119.0 (8)
C3—C2—N1	110.4 (6)	C7—C8—C9	118.4 (7)
C2—C3—C4	106.0 (6)	C4—C9—C8	121.9 (6)
C9—C4—C5	120.0 (7)	C4—C9—N1	108.6 (6)
C9—C4—C3	107.6 (5)	C8—C9—N1	129.4 (6)
C5—C4—C3	132.4 (7)		

Data collection: *MSCIAFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSCIAFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*. Literature survey: *CSSR* (1984).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1004). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Beddoes, R. L., Dalton, L., Joule, J. A., Mills, O. S., Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans. 2*, pp. 787–797.
- CSSR* (1984). *Crystal Structure Search and Retrieval Instruction Manual*. SERC Daresbury Laboratory, Warrington, England.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
- Molecular Structure Corporation (1988). *MSCIAFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
- Sheldrick, G. M. (1990). *Acta Cryst. A* **46**, 467–473.
- Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
- Surcouf, E., Mornon, J. P. & Malgrange, C. (1978). *Acta Cryst. B* **34**, 2169–2172.

Acta Cryst. (1996). **C52**, 2609–2612

3,4,6,7,9,10-Hexahydro-3,3,6,6-tetramethyl-1,8(2H,5H)-dioxo-10-phenyl-9-acridinyl-methyl Acetate

K. GUNASEKARAN,^a D. VELMURUGAN,^{a*} P. MURUGAN,^b V. T. RAMAKRISHNAN,^b K. PANNEERSELVAM^c AND M. SORIANO-GARCÍA^c

^aDepartment of Crystallography and Biophysics,† University of Madras, Madras 600 025, India, ^bDepartment of Organic Chemistry, School of Chemistry, University of Madras, Madras 600 025, India, and ^cInstituto de Química, UNAM Circuito Exterior ed Universitaria, México DF 04510, México

(Received 8 January 1996; accepted 15 May 1996)

Abstract

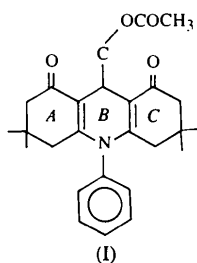
The conformation of the title compound, $\text{C}_{26}\text{H}_{31}\text{NO}_4$, is folded. The substituents are in a *cis* orientation, even though they are bulky, which helps stacking interactions.

Comment

Acridine compounds are well known DNA intercalating agents (Neidle, 1979) and are involved in mutagenesis (Brenner, Barnett, Crick & Orgel, 1961; Orgel, 1965). In acridinediones, the electron delocalization along a stretch of nine non-H atoms results in fluorescence and laser activity (Selladurai, Subramanian & Ramakrishnan, 1990). The effectiveness of lasing can be controlled by the substituents at the N atom and at the C atom opposite the N atom of the acridine chromophore. With this in mind, the structure of 9-acetoxymethyl-

† DCB contribution No. 872.

3,4,6,7,9,10-hexahydro-3,3,6,6-tetramethyl-10-phenyl-1,8(2*H*,5*H*)-acridinedione, (I), was determined.



The C6=O6 and C4=O4 bonds in (I) are longer than the C17=O18 bond. The angles around atom N10 sum to 359.5(2)° which is indicative of *sp*² hybridization (Hempel, Hull, Ledochowska & Dauter, 1979). The phenyl ring at the N atom is nearly perpendicular to the central moiety (N10, C10, C4a, C5, C6a, C9a) making an angle of 91.0(1)° with it. The atoms of the acetoxy substituent at C5 are coplanar and make an angle of 96.3(1)° with the piperidine ring. The acridine moiety is folded about the line passing through atoms C5 and N10, and the dihedral angle between the two halves (C1, C2, C3, C4, C4a, C10, N10, C5 and N10, C5, C9a, C6a, C6, C7, C8, C9) is 15°, as observed previously in acridinium compounds (George, Clark & Stewart, 1986). Rings A and C adopt half-chair conformations as shown by the torsion angles reported in Table 2 (Sivaraman, 1994). The central piperidine ring adopts a near boat conformation in which atoms C10, C9a, C6a and C4a are coplanar, with atom N10 slightly above [0.097(2) Å] and atom C5 very much

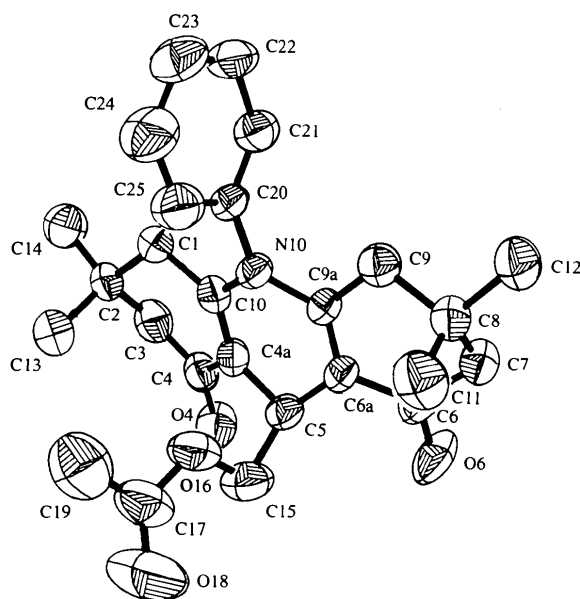


Fig. 1. An ORTEPII (Johnson, 1976) diagram of the title molecule with the atom-numbering scheme and 50% probability displacement ellipsoids.

above [0.212(3) Å] this plane, and with the substituents including C15 and C20 occupying equatorial positions (ΔC_2 is 1.6470 for C15 and 0.2500 for C20). The inability of the phenyl ring to resonate with the piperidine moiety can be seen in the fact that the N10—C20 bond is longer than the N10—C10 and N10—C9a bonds.

Both the substituents at C5 and N10 are *cis* with respect to the plane of the acridine moiety. This type of substitution helps stacking which occurs between inversion-related molecules. This type of stacking pattern is observed in most of the DNA intercalating agents such as 9-amino acridine (Talacki, Carrell & Glusker, 1974).

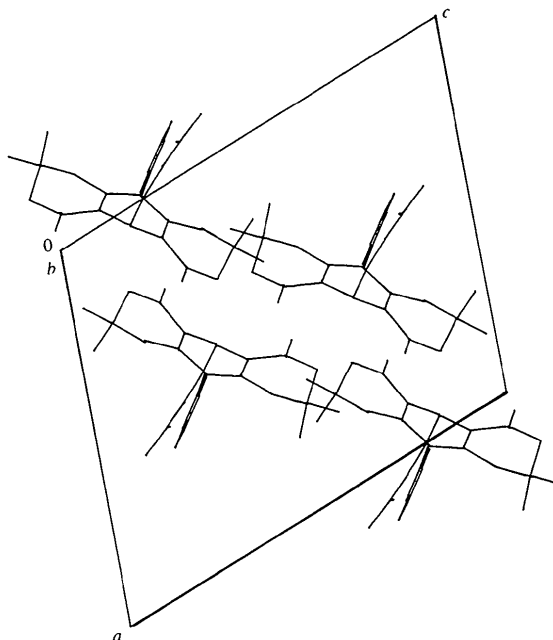


Fig. 2. Packing of the molecules down the *c* axis.

Experimental

Crystal data

C₂₆H₃₁NO₄

M_r = 421.52

Monoclinic

*P*2₁/*n*

a = 13.616(1) Å

b = 11.977(2) Å

c = 15.804(1) Å

β = 111.09(2)°

V = 2404.7 Å³

Z = 4

D_x = 1.164 Mg m⁻³

D_m = 1.159 Mg m⁻³

D_m measured by flotation

Cu *K*α radiation

λ = 1.54184 Å

Cell parameters from 21 reflections

θ = 14–22°

μ = 0.623 mm⁻¹

T = 293 K

Cube

0.36 × 0.34 × 0.31 mm

Pale yellow

Data collection

Enraf–Nonius CAD-4

diffractometer

$\omega/2\theta$ scans

2633 observed reflections

[*I* > 2σ(*I*)]

*R*_{int} = 0.041

Absorption correction: empirical *via* ψ scans (North, Phillips & Mathews, 1968)
 $T_{\min} = 0.638$, $T_{\max} = 0.790$
 4268 measured reflections
 3177 independent reflections

$\theta_{\max} = 66.4^\circ$
 $h = -1 \rightarrow 14$
 $k = -1 \rightarrow 12$
 $l = -17 \rightarrow 16$
 3 standard reflections monitored every 200 reflections
 frequency: 120 min
 intensity decay: <1.3%

Refinement

Refinement on F^2
 $R(F) = 0.0516$
 $wR(F^2) = 0.134$
 $S = 0.903$
 3175 reflections
 405 parameters
 $w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 1.3581P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.563$

$\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL93* (Sheldrick, 1993)
 Extinction coefficient: 0.0075 (9)
 Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C)

C3—C4	1.511 (5)	C10—N10	1.406 (4)
C4—O4	1.237 (3)	N10—C20	1.453 (3)
C4—C4a	1.459 (5)	C15—O16	1.449 (4)
C4a—C10	1.355 (4)	O16—C17	1.334 (4)
C4a—C5	1.506 (5)	C17—O18	1.192 (5)
C5—C6a	1.512 (5)	C17—C19	1.482 (7)
C5—C15	1.530 (5)	C20—C25	1.377 (5)
C6—O6	1.237 (3)	C20—C21	1.388 (4)
C6—C6a	1.461 (4)	C21—C23	1.397 (4)
C6—C7	1.506 (5)	C22—C23	1.372 (6)
C6a—C9a	1.356 (4)	C22—C24	1.376 (6)
C7—C8	1.523 (4)	C24—C25	1.382 (5)
C10—C1—C2	113.2 (3)	C7—C8—C9	108.7 (2)
C3—C2—C13	109.7 (3)	C11—C8—C9	110.5 (3)
C3—C2—C14	110.1 (3)	C12—C8—C9	108.5 (3)
C13—C2—C14	108.8 (3)	C9a—C9—C8	113.4 (3)
C3—C2—C1	108.3 (2)	C6a—C9a—N10	120.0 (2)
C13—C2—C1	110.8 (3)	C6a—C9a—C9	122.8 (2)
C14—C2—C1	109.2 (3)	N10—C9a—C9	117.2 (3)
C4—C3—C2	112.7 (3)	C4a—C10—N10	120.0 (2)
O4—C4—C4a	120.9 (3)	C4a—C10—C1	123.0 (3)
O4—C4—C3	121.4 (3)	N10—C10—C1	117.0 (3)
C4a—C4—C3	117.7 (3)	C10—N10—C9a	119.9 (3)
C10—C4a—C4	120.3 (3)	C10—N10—C20	120.0 (2)
C10—C4a—C5	121.7 (2)	C9a—N10—C20	119.6 (2)
C4—C4a—C5	117.9 (3)	O16—C15—C5	108.2 (2)
C4a—C5—C6a	109.4 (3)	C17—O16—C15	117.9 (3)
C4a—C5—C15	111.9 (2)	O18—C17—O16	122.5 (5)
C6a—C5—C15	112.8 (3)	O18—C17—C19	125.2 (5)
O6—C6—C6a	120.0 (3)	O16—C17—C19	112.2 (4)
O6—C6—C7	121.4 (3)	C25—C20—C21	121.3 (3)
C6a—C6—C7	118.5 (3)	C25—C20—N10	118.8 (3)
C9a—C6a—C6	120.1 (3)	C21—C20—N10	120.0 (2)
C9a—C6a—C5	121.7 (2)	C20—C21—C23	118.5 (3)
C6—C6a—C5	118.1 (3)	C23—C22—C24	120.8 (3)
C6—C7—C8	113.6 (2)	C22—C23—C21	120.1 (3)
C7—C8—C11	110.1 (3)	C22—C24—C25	120.0 (4)
C7—C8—C12	110.0 (3)	C20—C25—C24	119.3 (3)
C11—C8—C12	109.1 (3)		
C2—C1—C10—C4a	17.8 (3)	C6a—C6—C7—C8	29.7 (3)
C2—C3—C4—C4a	-34.6 (3)	C5—C6a—C9a—N10	-7.5 (3)
C4—C4a—C10—N10	-170.7 (2)	C8—C9—C9a—C6a	-18.2 (3)
C10—C4a—C5—C15	98.6 (3)	C6a—C9a—N10—C20	174.4 (2)
C5—C4a—C10—N10	9.5 (3)	C4a—C10—N10—C20	-175.4 (2)
C15—C5—C6a—C9a	-99.0 (3)		

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
C1	0.3416 (2)	-0.0729 (2)	0.1569 (2)	0.054 (6)
C2	0.2501 (2)	-0.0075 (2)	0.0882 (2)	0.056 (6)
C3	0.1972 (2)	0.0614 (2)	0.1407 (2)	0.065 (7)
C4	0.2730 (2)	0.1381 (2)	0.2094 (2)	0.056 (6)
O4	0.2446 (2)	0.2300 (2)	0.2281 (1)	0.075 (6)
C4a	0.3806 (2)	0.0989 (2)	0.2552 (1)	0.049 (6)
C5	0.4556 (2)	0.1736 (2)	0.3259 (2)	0.056 (6)
C6	0.5851 (2)	0.1438 (2)	0.4872 (2)	0.058 (6)
O6	0.5532 (2)	0.2320 (2)	0.5090 (1)	0.090 (7)
C6a	0.5393 (2)	0.1031 (2)	0.3939 (2)	0.051 (6)
C7	0.6665 (2)	0.0729 (2)	0.5560 (2)	0.061 (7)
C8	0.7311 (2)	0.0014 (2)	0.5155 (2)	0.055 (6)
C9	0.6552 (2)	-0.0669 (2)	0.4364 (2)	0.056 (6)
C9a	0.5671 (2)	0.0017 (2)	0.3717 (1)	0.047 (6)
C10	0.4111 (2)	-0.0017 (2)	0.2340 (1)	0.046 (6)
N10	0.50960 (14)	-0.0462 (2)	0.2871 (1)	0.049 (5)
C11	0.8012 (3)	0.0754 (3)	0.4825 (3)	0.083 (9)
C12	0.8006 (3)	-0.0802 (3)	0.5874 (2)	0.079 (9)
C13	0.2905 (3)	0.0699 (3)	0.0304 (2)	0.074 (8)
C14	0.1709 (3)	-0.0904 (3)	0.0252 (2)	0.083 (9)
C15	0.5018 (3)	0.2646 (2)	0.2833 (2)	0.074 (8)
O16	0.5476 (2)	0.2114 (2)	0.2239 (1)	0.078 (7)
C17	0.5812 (3)	0.2766 (3)	0.1715 (3)	0.091 (1)
O18	0.5831 (3)	0.3759 (2)	0.1775 (3)	0.154 (1)
C19	0.6164 (6)	0.2114 (6)	0.1079 (5)	0.131 (2)
C20	0.5457 (2)	-0.1499 (2)	0.2604 (1)	0.049 (6)
C21	0.5182 (2)	-0.2513 (2)	0.2881 (2)	0.056 (6)
C22	0.6146 (3)	-0.3443 (3)	0.2082 (2)	0.090 (1)
C23	0.5541 (2)	-0.3495 (2)	0.2612 (2)	0.071 (8)
C24	0.6409 (3)	-0.2431 (3)	0.1810 (3)	0.099 (1)
C25	0.6073 (3)	-0.1450 (2)	0.2080 (2)	0.075 (8)

Table 2. Selected geometric parameters (\AA , $^\circ$)

C1—C10	1.509 (4)	C8—C11	1.526 (5)
C1—C2	1.539 (5)	C8—C12	1.539 (5)
C2—C3	1.523 (5)	C8—C9	1.540 (5)
C2—C13	1.535 (4)	C9—C9a	1.509 (5)
C2—C14	1.539 (5)	C9a—N10	1.407 (4)

The three H atoms at C19 were fixed geometrically and refined isotropically for one cycle. The remaining H atoms were obtained from difference Fourier syntheses and refined isotropically.

Data collection: *SDP* (Frenz, 1978). Cell refinement: *SDP*. Data reduction: *SDP*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

KG and DV thank the University Grants Commission for providing the funding (SRF and Career award, respectively).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the IUCr (Reference: DE1036). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Brenner, S., Barnett, L., Crick, F. H. C. & Orgel, A. (1961). *J. Mol. Biol.* **3**, 121–124.

- Frenz, B. A. (1978). *The Enraf-Nonius CAD-4 SDP - a Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution. Computing in Crystallography*, edited by H. Schenk, R. Olthof-Hazekamp, H. van Koningsveld & G. C. Bassi, pp. 64–71. Delft University Press.
- George, R., Clark, G. & Stewart, M. (1986). *Acta Cryst.* **C42**, 628–630.
- Hempel, A., Hull, S. E., Ledochowska, M. B. & Dauter, Z. (1979). *Acta Cryst.* **B35**, 474–476.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO. Program for Plotting Molecular and Crystal Structures*. University of Cambridge, England.
- Nardelli, M. (1983). *Comput. Chem.* **7**, 95–98.
- Neidle, S. (1979). *Prog. Med. Chem.* **16**, 151–221.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Orgel, L. E. (1965). *Adv. Enzymol.* **27**, 289–293.
- Selladurai, S., Subramanian, K. & Ramakrishnan, V. T. (1990). *J. Crystallogr. Spectrosc. Res.* **20**, 227–232.
- Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures*. University of Göttingen, Germany.
- Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
- Sivaraman, J. (1994). PhD thesis, Anna University, Madras, India.
- Talacki, R., Carrell, H. L. & Glusker, J. P. (1974). *Acta Cryst.* **B30**, 1044–1047.

served in functionally unelaborated acids. In most cases, however, the ketone does not participate and typical mutually hydrogen-bonded carboxylic acid dimers result. Less frequently, intermolecular carboxyl-to-ketone hydrogen bonds repeat along one cell axis to yield a catemer. A third, rare, arrangement has an internal hydrogen bond and one instance is known of acid-to-ketone dimerization (Abell, Trent & Morris, 1991). We have previously referenced and discussed numerous examples of these various hydrogen-bonding patterns (Thompson, Lalancette & Vanderhoff, 1992; Coté, Thompson & Lalancette, 1996).

Previous reports of internal hydrogen bonding in solid β -oxo acids have involved the oxo functions of vinylogous esters or amides rather than of genuine ketones. We recently reported the first instance of an intramolecularly hydrogen-bonded true β -keto acid, 2-carboxy-4,5-benzotropone (Thompson, Lalancette & Coté, 1996). In that case, the coplanarity of ketone and carboxyl required for internal hydrogen bonding was favored by unsaturation α,β to both the ketone and acid, plus a cyclic system holding the ketone and vinyl groups coplanar. We now report a closely analogous case which has the α,β -unsaturation without the coplanarity constraints of the ring.

Acta Cryst. (1996). **C52**, 2612–2614

(*E*)-2-Acetylcinnamic Acid: Hydrogen-Bonding Pattern of an α,β -Unsaturated β' -Keto Acid

MARIE L. COTÉ,^a HUGH W. THOMPSON,^a ROGER A. LALANCETTE*^a AND JOHN A. WILLIAMS IV^b

^aCarl A. Olson Memorial Laboratories, Department of Chemistry, Rutgers University, Newark, NJ 07102, USA, and ^bEssex County Community College, Newark, NJ 07102, USA. E-mail: lalancette@hades.rutgers.edu

(Received 28 February 1996; accepted 7 May 1996)

Abstract

The title compound, (*E*)-2-acetyl-3-phenylpropenoic acid, C₁₁H₁₀O₃, adopts a conformation incorporating a planar *trans*-cinnamic acid, with the α -acetyl group rotated orthogonal to it. Pairs of molecules of identical conformational chirality form carboxyl dimers across C_2 axes, and the acid group displays disorder. There is a 2.64 Å ketone-O...methyl-H close contact between centrosymmetrically related dimer units.

Comment

Keto carboxylic acids offer opportunities for variation on the standard pattern of dimeric hydrogen bonding ob-

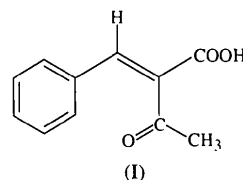


Fig. 1 shows the title compound, (I), in the chiral conformation it adopts and with its atom-numbering scheme. The cinnamic acid portion of (I) is very nearly planar, as is the case in cinnamic acid itself (Bryan & Freyberg, 1975; Wierda, Feng & Barron, 1989), with a dihedral angle between the aromatic ring and the carboxyl group of 7.5 (2)°. The acetyl group is

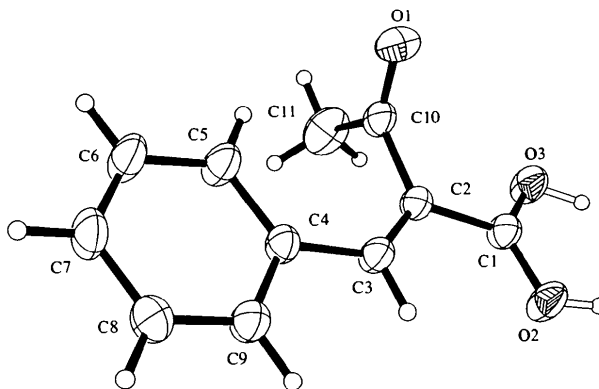


Fig. 1. Compound (I) with its numbering scheme. Ellipsoids are at the 40% probability level. The half-occupancy carboxyl-H atoms are shown with clear bonds.