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Note added in proof. After this article was accepted for publication, a work reporting the structure of fluorene at 295 K (Belsky, Zavodnik & Vozzhennikov, 1984) was brought to our attention. The bond lengths and angles reported therein are in very good agreement with those given for the present study, with the exception that Belsky *et al.* give the C(6)–C(6^l) bond length as 1.491 (8) Å. While the 0.019 (9) Å difference in this bond length is of questionable significance, it may also be a direct consequence of slightly different conformations of the fluorene molecule at 159 and 295 K.

A major point of disagreement in the interpretations of these structures concerns the planarity of the fluorene molecule: Belsky *et al.* report that the molecule is planar at room temperature, whereas we have determined that only the asymmetric unit is planar at 295 K, as well as at 159 K. The values of χ^2 calculated for each of the planes in question are presented in Table 3. Since $\chi^2_{0.01,10}$ is less than the calculated value at each temperature, the departures from planarity of the C atoms in the fluorene molecule are statistically significant at the 99% confidence level. However, the planarity of the asymmetric unit at each temperature is clearly evident from Table 3, and we therefore conclude that the molecule is 'V' shaped at both 159 and 295 K. The angle between the two planes in the molecule is

Table 3. χ^2 values for some least-squares planes in the fluorene molecule; ν represents the number of degrees of freedom

Plane	ν	χ^2 (calc.)			
		Present work	Belsky <i>et al.</i>	$\chi^2_{0.01,\nu}$	$\chi^2_{0.5,\nu}$
Molecule	10	280	24.7	23.21	9.34
Asymmetric unit	4	2.4	2.2	13.28	2.37

0.77 (20)° calculated from the data obtained at room temperature, in contrast to the value of 1.28 (4)° given above for the molecule at low temperature. Owing to the lower precision of the results at 295 K, the significance of the small difference between these two angles is again questionable. However, a decrease in the C(6)–C(6^l) bond length is consistent with an increase in the dihedral angle of the fluorene molecule at lower temperature.

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The Structure of Benzyl *N*-(*tert*-Butoxycarbonyl)oxamate, C₁₄H₁₇NO₅

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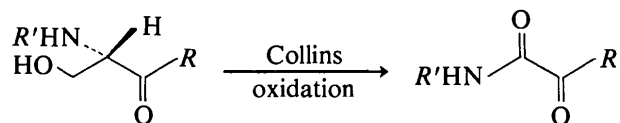
Abstract. $M_r = 279.3$, monoclinic, $P2_1/c$, $a = 11.089$ (2), $b = 13.751$ (2), $c = 10.145$ (2) Å, $\beta = 111.0$ (4)°, $V = 1444.2$ Å³, $D_m = 1.23$, $D_x = 1.284$ Mg m⁻³, $Z = 4$, $\lambda(\text{Cu K}\alpha) = 1.54178$ Å, $\mu = 0.78$ mm⁻¹, $F(000) = 592$, $T = 295$ K, $R = 0.040$ for 2227 observed reflections. The formation of this compound corroborates the Collins reaction which, by oxidation of *N*-butoxycarbonyl- and *N*-benzyloxy-carbonylserine amides and esters, yields the corresponding diamides and amide esters of oxalic acid. The

molecule is basically an amide ester of oxalic acid. The ester is a nearly planar benzyl group inclined by about 43 (1)° to the plane of the carboxylic group of atoms. The distance, 1.533 (2) Å, separating the carboxylic and the amide groups is unusually long for a C(sp²)–C(sp²) type bond. This, however, is consistent with the fact that the carboxylic plane is 90 (1)° to the amide group. The latter is coplanar with the terminal butoxycarbonyl group. A dimer is formed by hydrogen bonding of the amide groups of two adjacent molecules.

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Introduction. A recent report by Stachulski (1982) commented on the paucity of information pertaining to the oxidation of the hydroxyl group of serine, and described an intriguing oxidation of ester derivatives of serine and threonine to the corresponding oxamates. The structure of the proposed product was corroborated by a synthesis from benzyl carbamate and methyl oxalyl chloride.



- (1) $R=\text{OCH}_2\text{Ph}$; $R'=\text{Boc}$ (3) $R=\text{OCH}_2\text{Ph}$; $R'=\text{Boc}$
 (2) $R=\text{NHC}_6\text{H}_4\text{OMe}-p$; $R'=\text{Boc}$ (4) $R=\text{NHC}_6\text{H}_4\text{OMe}-p$; $R'=\text{Boc}$

We wish to report on concurrent studies in our laboratory which support these results and extend this unusual oxidation to amides as well. Thus, treatment of *N*-butoxycarbonylserine benzyl ester (Guttmann & Boissonas, 1958) (1) (1.7 mmol) with chromium trioxide in pyridine in 25 ml dichloromethane (Collins, Hess & Frank, 1968) gave, after column chromatography, a crystalline product (68%); m.p. 371–372 K; $[\alpha]_D^{22} = 0^\circ$ ($c = 1\%$, CHCl_3); IR 1800, 1740 cm^{-1} ; $M^+ + 1$, which was assigned structure (3). Definitive confirmation was secured by single-crystal X-ray analysis.

Experimental. Recrystallization from an ether/hexane mixture, crystal size 0.15 × 0.40 × 0.50 mm, unit-cell dimensions from 25 θ values, $10 < \theta < 20^\circ$, Nonius CAD-4 diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, density by flotation in ZnCl_2 aqueous solution, ω -2 θ scan mode up to $\theta = 70.0^\circ$ ($0 \leq h \leq 13$, $0 \leq k \leq 16$, $-12 \leq l \leq 11$), orientation monitored every 100 reflections, intensity checked every hour with three standard reflections (largest intensity fluctuation 1.4%). 2741 reflections measured, 2227 with $I \geq 1.90\sigma(I)$ used in structure determination and refinement. Lp correction, no absorption correction, direct methods (*MULTAN*)* anisotropic block-diagonal least-squares refinement based on F . H atoms from difference Fourier syntheses, refined isotropically. Final $R = 0.040$, $R_w = 0.042$, for 2227 reflections, weights based on counting statistics, $S = 1.36$. Maximum $(\Delta/\sigma) = 0.90$, mean $(\Delta/\sigma) = 0.20$, electron density fluctuation on the final difference Fourier synthesis -0.40 , $+0.25 \text{ e } \text{\AA}^{-3}$. Scattering factors for O, N, and C from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965).

* The programs used in this work are modified versions of *NRC-2*, data reduction, *NRC-10*, bond distances and angles, *NRC-22*, mean planes (Ahmed, Hall, Pippy & Huber, 1973); *FORDAP*, Fourier and Patterson maps (A. Zalkin); *NUCLS*, least-squares refinement (Doedens & Ibers, 1967); *MULTAN*, multisolution program (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); *ORTEP*, stereoviews (Johnson, 1965).

Table 1. *Final atomic coordinates for $\text{C}_{14}\text{H}_{17}\text{NO}_5$ ($\times 10^4$ for O, N and C atoms, $\times 10^3$ for H atoms), U_{eq} (\AA^2 , $\times 10^4$ for O, N and C) and U_{iso} (\AA^2 , $\times 10^3$ for H atoms)*

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}/U_{\text{iso}}$
O(1)	3474 (1)	2274 (1)	8347 (1)	456 (5)
O(2)	4158 (1)	−912 (1)	8850 (1)	495 (5)
O(3)	2390 (1)	−727 (1)	5784 (1)	422 (5)
O(4)	1237 (1)	−714 (1)	7215 (1)	542 (6)
O(5)	1984 (1)	1347 (1)	6695 (1)	550 (6)
N(1)	3707 (1)	682 (1)	8463 (2)	421 (6)
C(1)	1649 (2)	−1246 (1)	3365 (2)	413 (7)
C(2)	820 (2)	−956 (2)	2037 (2)	547 (9)
C(3)	1151 (3)	−1087 (2)	868 (2)	664 (11)
C(4)	2318 (3)	−1496 (2)	996 (3)	704 (12)
C(5)	3151 (3)	−1797 (2)	2304 (3)	664 (11)
C(6)	2822 (2)	−1677 (2)	3485 (2)	525 (9)
C(7)	1258 (2)	−1095 (2)	4617 (2)	472 (7)
C(8)	2202 (2)	−570 (1)	6974 (2)	383 (7)
C(9)	3457 (2)	−272 (1)	8158 (2)	378 (7)
C(10)	2941 (2)	1457 (1)	7719 (2)	409 (7)
C(11)	2852 (2)	3240 (1)	7839 (2)	465 (8)
C(12)	2787 (3)	3415 (2)	6352 (3)	694 (12)
C(13)	3789 (3)	3925 (2)	8873 (3)	793 (12)
C(14)	1539 (2)	3269 (2)	7979 (3)	624 (10)
H(N)	437 (2)	81 (2)	920 (2)	59 (6)
H(2)	−6 (2)	−62 (2)	198 (2)	83 (8)
H(3)	52 (2)	−86 (2)	−7 (3)	96 (9)
H(4)	256 (2)	−160 (2)	17 (3)	90 (8)
H(5)	392 (2)	−209 (2)	241 (3)	94 (9)
H(6)	339 (2)	−188 (2)	440 (2)	67 (7)
H(7)	100 (2)	−173 (2)	506 (2)	76 (7)
H(72)	57 (2)	−60 (2)	444 (2)	74 (7)
H(121)	355 (3)	330 (2)	636 (3)	98 (9)
H(122)	209 (3)	299 (2)	575 (3)	113 (10)
H(123)	252 (3)	411 (2)	616 (3)	101 (9)
H(131)	379 (3)	376 (2)	980 (3)	98 (9)
H(132)	460 (3)	387 (2)	874 (3)	98 (9)
H(133)	350 (2)	458 (2)	865 (3)	89 (8)
H(141)	151 (3)	315 (2)	891 (3)	98 (9)
H(142)	118 (2)	391 (2)	772 (2)	74 (7)
H(143)	98 (2)	279 (2)	731 (3)	91 (9)

Discussion. The final fractional coordinates and equivalent U_{iso} values are listed in Table 1.* The atomic numbering and molecular conformation are shown in Fig. 1. The bond distances, bond angles and torsion angles of interest are given in Table 2. The atoms in the phenyl ring are nearly coplanar, the bond distances and angles are normal. The endocyclic angle at C(1), the substituted atom, shows the usual narrowing with a value of $118.6(2)^\circ$. The nearly planar phenyl ring is inclined with respect to the O(3), O(4), C(8), C(9) group of atoms, the torsion angles C(2)–C(1)–C(7)–O(3) and C(6)–C(1)–C(7)–O(3) having values of $-137.1(3)$ and $43.3(3)^\circ$ respectively. Of the three C=O bonds, C(8)–O(4) and C(10)–O(5) are 1.197 (3) and 1.200 (3) Å respectively while C(9)–O(2) has a length of 1.217 (2) Å. The latter C=O distance, which belongs to an amide group, is shorter than usual. For an amide group, one normally finds a C=O distance of the order of 1.235 Å (Brisson & Brisse, 1982). This

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39540 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

observation coupled with the near planarity of the O(2), O(5), N(1), C(9), C(10) group of atoms indicates a more delocalized π -electron system than is usually observed with amides. Another interesting feature of this molecule is the orientation of the two planar groups of atoms O(2), N(1), C(8), C(9) and O(3), O(4), C(8), C(9). Their relative orientation is measured by N(1)–C(9)–C(8)–O(3) = 97.2 (3)° and O(2)–C(9)–C(8)–O(4) = 86.6 (3)°. Here, there is no π -electron delocalization across the two groups of atoms. This is further confirmed by the very long C(sp²)–C(sp²) bond, 1.533 (3) Å, between C(8) and C(9). Two molecules are associated into dimers through hydrogen bonding across a center of symmetry of the unit cell: N(1)···O(2') = 2.918 (2), N(1)–H(N) = 0.85 (2), H(N)···O(2') = 2.07 (2) Å, angle N(1)–H(N)···O(2') = 169 (2)°.

Application of the oxidation reaction to *N*²-butoxycarbonyl-*N*¹-(*p*-methoxyphenyl)serinamide (2), m.p. 381–384 K; [α]_D^{22°C} = –82.8° (*c* = 1%, CHCl₃), gave the corresponding diamide derivative (4), [α]_D = 0°; IR 1800 cm^{–1}; *M*⁺ + 1. Other oxidations by variations in the *N*-protecting group (*N*-Cbz), or the amide group (2,4-dimethoxybenzyl), gave similar results and led to crystalline products in each case. A variety of other well known oxidation methods such as pyridinium chlorochromate, with (Herscovici & Antonakis, 1980) or without (Corey & Suggs, 1975) molecular sieves, oxalyl chloride–Me₂SO (Mancuso, Huang & Swern, 1978), pyridine–SO₃ in Me₂SO (Parikh & Doering, 1975), (diethylaminopropyl)ethylcarbodiimide hydrochloride (Hanessian & Lavallée, 1977, 1981), CrO₃–pyridine/acetic anhydride, and NBS oxidation (Saigo, Morikawa & Mukaiyama, 1976) of the tri-*n*-butyltin ether of *N*-substituted serine amides, were either unsatisfactory or proceeded very inefficiently. Similar observations were reported by Stachulski

Table 2. Bond distances (Å), angles (°) and torsion angles (°) for C₁₄H₁₇NO₅

C(1)–C(2)	1.390 (3)	C(1)–C(2)–C(3)	120.7 (2)
C(2)–C(3)	1.373 (3)	C(2)–C(3)–C(4)	120.4 (3)
C(3)–C(4)	1.374 (4)	C(3)–C(4)–C(5)	119.7 (3)
C(4)–C(5)	1.381 (4)	C(4)–C(5)–C(6)	120.3 (3)
C(5)–C(6)	1.381 (4)	C(5)–C(6)–C(11)	120.2 (2)
C(6)–C(11)	1.395 (3)	C(6)–C(11)–C(2)	118.6 (2)
C(1)–C(7)	1.496 (3)	C(2)–C(1)–C(7)	119.4 (2)
C(7)–O(3)	1.472 (2)	C(6)–C(11)–C(7)	122.0 (2)
O(3)–C(8)	1.315 (2)	C(1)–C(7)–O(3)	107.9 (2)
C(8)–O(4)	1.197 (3)	C(7)–O(3)–C(8)	115.2 (2)
C(8)–C(9)	1.533 (3)	O(3)–C(8)–O(4)	127.4 (2)
C(9)–O(2)	1.217 (2)	O(3)–C(8)–C(9)	111.5 (2)
C(9)–N(1)	1.353 (3)	C(9)–C(8)–O(4)	120.8 (2)
N(1)–H(N)	0.85 (2)	C(8)–C(9)–O(2)	118.1 (2)
N(1)–C(10)	1.402 (3)	C(8)–C(9)–N(1)	119.5 (2)
C(10)–O(5)	1.200 (3)	N(1)–C(9)–O(2)	122.3 (2)
C(10)–O(1)	1.322 (2)	C(9)–N(1)–C(10)	125.4 (2)
O(1)–C(11)	1.500 (3)	N(1)–C(10)–O(5)	123.2 (2)
C(11)–C(12)	1.504 (3)	N(1)–C(10)–O(1)	107.9 (2)
C(11)–C(13)	1.513 (4)	O(1)–C(10)–O(5)	128.9 (2)
C(11)–C(14)	1.514 (4)	C(10)–O(1)–C(11)	121.0 (2)
		O(1)–C(11)–C(12)	109.7 (2)
		O(1)–C(11)–C(13)	101.3 (2)
		O(1)–C(11)–C(14)	109.3 (2)
		C(12)–C(11)–C(13)	111.7 (2)
		C(12)–C(11)–C(14)	112.8 (2)
		C(13)–C(11)–C(14)	111.3 (2)
C(2)–C(1)–C(7)–O(3)	–137.1 (3)	O(2)–C(9)–N(1)–C(10)	–179.7 (3)
C(6)–C(11)–C(7)–O(3)	43.3 (3)	C(8)–C(9)–N(1)–C(10)	–4.3 (3)
C(1)–C(7)–O(3)–C(8)	–179.1 (3)	C(9)–N(1)–C(10)–O(1)	178.4 (3)
C(7)–O(3)–C(8)–C(9)	175.3 (3)	C(9)–N(1)–C(10)–O(5)	–1.9 (3)
C(7)–O(3)–C(8)–O(4)	1.9 (3)	N(1)–C(10)–O(1)–C(11)	–177.4 (3)
O(3)–C(8)–C(9)–N(1)	97.2 (3)	O(5)–C(10)–O(1)–C(11)	3.0 (3)
O(3)–C(8)–C(9)–O(2)	–87.2 (3)	C(10)–O(1)–C(11)–C(12)	–62.5 (3)
O(4)–C(8)–C(9)–N(1)	–88.9 (3)	C(10)–O(1)–C(11)–C(13)	179.4 (3)
O(4)–C(8)–C(9)–O(2)	86.6 (3)	C(10)–O(1)–C(11)–C(14)	61.8 (3)

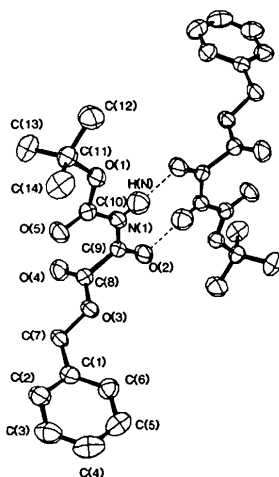


Fig. 1. Atomic numbering and dimer formation through hydrogen bonding.

(1982). While the mechanism of the reaction remains open to discussion and subject to reasonable hypotheses (Stachulski, 1982; Pianacatelli, Scettri & D'Auria, 1977) the generality of the oxidative degradation and applications to serine-containing natural products are evident.

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Structure and Conformation of 6-(4-Nitrobenzyl)thioinosine, C₁₇H₁₇N₅O₆S, a Potent Inhibitor of Nucleoside Transport

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Abstract. $M_r = 419.4$, monoclinic, $P2_1$, $a = 14.718$ (1), $b = 8.678$ (1), $c = 7.269$ (1) Å, $\beta = 93.55$ (1)°, $V = 926.6$ (3) Å³, $Z = 2$, $D_m = 1.49$, $D_x = 1.503$ g cm⁻³, $\lambda(\text{Cu K}\alpha) = 1.5418$ Å, $\mu = 19.3$ cm⁻¹, $F(000) = 436$, $T = 294$ K; $R = 0.042$ for 2205 observed reflections. The 6-substituent is distal to the imidazole ring; the nucleoside has the *syn* conformation [$\chi_{\text{CN}} = -127.9$ (4)°] with an intramolecular O(5')–H(O5')...N(3) hydrogen bond; the ribose has the C(2')-*endo* (²*E*) pucker with the following pseudorotational parameters: $P = 158.9$ (3)° and $\tau_m = 38.0$ (2)°; the conformation across C(4')–C(5') is *g*⁺ [*i.e.* C(3')–C(4')–C(5')–O(5') is 53.5 (5)°]. It is suggested that the preferred conformations across the S–C(*sp*³) and C(*sp*³)–C(*sp*²) bridges which link the purine moiety to the substituent on the 6-position of purine are important among the determinants of the nucleoside-transport inhibitory activity.

Introduction. The passage of nucleoside molecules across the plasma membrane of animal cells is mediated by nucleoside-specific transport elements of the membrane. This transport is reversible, non-concentrative, and of broad specificity in that physiological nucleo-

sides and a diverse array of nucleoside analogs are accepted as substrates by transporter elements of a single type (for reviews see Plagemann & Wohlheuter, 1980; Paterson, Kolassa & Cass, 1981; Paterson, Jakobs, Harley, Cass & Robins, 1983). Nucleoside transport in many cell types, but not in all, is powerfully inhibited by 6-(4-nitrobenzyl)thioinosine (NBMPR) and various related compounds. Various cell types in which nucleoside transport is NBMPR-sensitive possess surface sites at which NBMPR is bound with high affinity (K_d 0.1–1 nM) (Paterson *et al.*, 1981; Paterson, Jakobs, Harley, Cass & Robins, 1983; Paterson, Jakobs, Harley, Fu, Robins & Cass, 1983). NBMPR occupancy of these sites, which appear to be located on the nucleoside-transporter protein(s) (Jarvis, Janmohamed & Young, 1983), correlates with blockade of transporter function (Cass, Gaudette & Paterson, 1974). The possibility that NBMPR binding sites may be distinct from the transporter sites at which nucleoside molecules interact during the permeation process has been discussed recently (Koren, Paterson & Cass, 1983; Jarvis *et al.*, 1983). The existence of NBMPR-insensitive nucleoside-transport mechanisms has been recognized recently (Belt, 1984; Paterson, Jakobs, Harley, Fu, Robins & Cass, 1983), but their characterization is yet at an early stage.

Various NBMPR congeners have been evaluated for their ability to inhibit a transport-dependent aspect of cellular nucleoside metabolism (Paul, Chen & Paterson,

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