substituent dihedral angles of 68·2 (II), 69·9 (V*a*) and 64·8° (V*b*) have been observed. Favourable non-bonding interactions between the *ortho* substituent and the anthracene must be stabilizing this conformation (Heldt, 1983), although in (V) some intermolecular interactions also play an important role.

All bond lengths, bond angles and torsion angles in the acetoxy groups are within one standard deviation of the average values calculated from a sample of 102 acetoxy groups bonded to aromatic six-membered carbon rings (Roszak, 1986).

The acetoxy group bonded to the anthracene is almost perpendicular to it [dihedral angle 89·2 (1)°]. A similar conformation is observed in (V) (89·7 and 86·3° for the two molecules in the asymmetric unit). The OAc bonded to the phenyl ring forms a dihedral angle of 81·3 (1)° with it, resembling the conformation observed for (II).

Fig. 3 illustrates the packing of the title compound in the unit cell. The arrangement of the methyl H atoms in relation to the plane of the OAc group is shown in Fig. 4. It resembles the conformation found for methyl H atoms in the rhombohedral form of acetamide [neutron study at 23 K: Jeffrey, Ruble, McMullan, DeFrees, Binkley & Pople (1980)].

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Structure of 1-Nitro-7*H*-benzo[*h,i*]chrysen-7-one

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Abstract. $C_{21}H_{11}NO_3$, $M_r = 325{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 16{\cdot}407$ (4), $b = 11{\cdot}909$ (4), $c = 7{\cdot}407$ (2) Å, $V = 1447{\cdot}3$ (7) Å^3, $Z = 4$, $D_m = 1{\cdot}46$, $D_x = 1{\cdot}493$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 10{\cdot}9$ mm^{-1}, $F(000) = 672$, $T = 298$ K. Final $R = 0{\cdot}059$ for 1220 independent reflections. The molecule is greatly distorted from a planar structure owing to the overcrowding around the nitro and carbonyl groups. The mean planes of the two naphthalene moieties make an angle of 25·7 (2)°. The NO_2 group rotates around the C—N bond from a coplanar conformation. The torsion angle O—N—C—C is 45·7 (3)°.

Introduction. Nitration of ketones of condensed polycyclic aromatic compounds gives various nitro derivatives. It is often difficult, however, to assign the

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positions of the nitro groups by chemical or theoretical procedures. On the other hand, it is of interest to compare the structure of the nitro derivative with that of the original ketone, since the bulky NO_2 group is expected to affect the conformation of the parent molecule. The present work reports the structure of the title compound which was provided by the nitration of 7*H*-benzo[*h,i*]chrysen-7-one (8,9-BzBT).

Experimental. Golden-yellow plate-like crystals from chlorobenzene solution; D_m by flotation in $ZnCl_2$ solution; systematic absences: *h*00, $h = 2n+1$, 0*k*0, $k = 2n+1$, 00*l*, $l = 2n+1$; crystal dimensions 0·65 × 0·50 × 0·10 mm; Rigaku AFC-6 diffractometer; graphite monochromator; cell parameters refined by least-squares method on the basis of 25 independent 2θ values; $18 < 2\theta < 23°$, intensity measurement performed up to $2\theta = 55°$; range of *hkl* 0 to 21, 0 to 14 and 0 to 9; ω–2θ scan, scan speed 2° min^{-1} (2θ), scan width $(1{\cdot}2 + 0{\cdot}35\tan\theta)°$; background 5 s before and after each scan; three standard reflections monitored every 100 reflections, no significant variation in intensities; 2001 independent reflections measured, 1220 with $|F_o| > 3\sigma(|F_o|)$ considered observed and used for structure determination; corrections for Lorentz and polarization, absorption ignored; direct methods (*MULTAN*78: Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and subsequent difference Fourier calculation; block-diagonal least squares (*HBLS*: Ohashi, 1975) with anisotropic thermal parameters for all non-H atoms; H atoms derived geometrically (C—H 1·08 Å) and refined; $\sum w(|F_o| - |F_c|)^2$ minimized with $w = [\sigma^2(F_o) + (0{\cdot}03F)^2]^{-1}$; max. (Δ/σ) 0·5; final $R = 0{\cdot}059$; $wR = 0{\cdot}072$; $S = 2{\cdot}2$. $\Delta\rho$ excursions in final difference map 0·3 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); calculation carried out on HITAC M-280 computer at the Computer Center of the University of Tokyo.

Discussion. The final atomic parameters for non-H atoms are given in Table 1.* A projection of the structure along the *c* axis is shown in Fig. 1. There are no unusually short contacts between the molecules. A perspective drawing of the molecule with the numbering scheme is shown in Fig. 2. The NO_2 group is attached to the C(1) atom. Bond distances and angles are listed in Table 2. The molecular structure is greatly distorted from a planar conformation owing to the overcrowding around the nitro and carbonyl groups. The mean planes

Table 1. *Final atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters,* B_{eq}(Å^2) (× 10)

$$B_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
C(1)	594 (3)	4254 (4)	3743 (7)	36 (1)
C(2)	691 (3)	3088 (4)	3614 (8)	43 (1)
C(3)	1431 (3)	2653 (4)	3976 (9)	48 (2)
C(4)	2901 (3)	2911 (4)	4583 (8)	45 (1)
C(5)	3559 (3)	3623 (5)	4776 (8)	46 (2)
C(6)	3439 (3)	4784 (5)	4709 (8)	42 (1)
C(7)	2563 (3)	6473 (4)	4392 (8)	37 (1)
C(8)	1646 (3)	8052 (4)	5458 (7)	34 (1)
C(9)	860 (3)	8405 (4)	6080 (7)	36 (1)
C(10)	210 (3)	7649 (4)	5978 (8)	41 (1)
C(11)	320 (3)	6582 (4)	5351 (8)	36 (1)
C(12)	1078 (3)	6191 (4)	4740 (7)	32 (1)
C(13)	1185 (3)	4996 (4)	4239 (8)	36 (1)
C(14)	1994 (3)	4529 (4)	4416 (7)	34 (1)
C(15)	2116 (3)	3352 (4)	4341 (8)	38 (1)
C(16)	2665 (3)	5245 (4)	4546 (7)	35 (1)
C(17)	1751 (3)	6924 (4)	4864 (7)	33 (1)
C(18)	2312 (3)	8822 (4)	5692 (9)	47 (2)
C(19)	2171 (3)	9865 (4)	6415 (9)	46 (2)
C(20)	1381 (3)	10219 (4)	6920 (8)	46 (2)
C(21)	756 (3)	9499 (4)	6737 (8)	42 (1)
N	−231 (2)	4640 (3)	3180 (6)	42 (1)
O(1)	3133 (2)	7063 (3)	3904 (6)	53 (1)
O(2)	−825 (2)	4116 (3)	3700 (7)	66 (1)
O(3)	−271 (2)	5431 (3)	2109 (6)	55 (1)

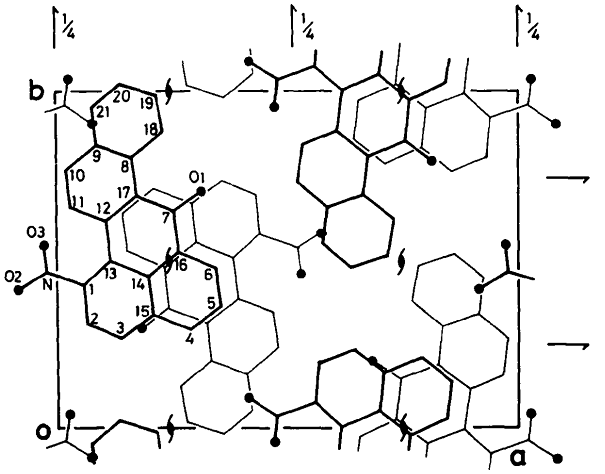

Fig. 1. A projection of the crystal structure along the *c* axis and the numbering scheme.

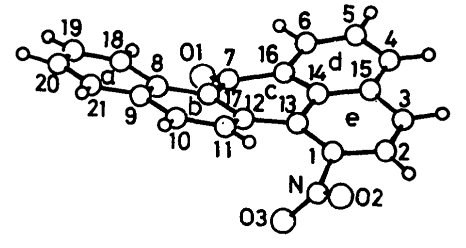

Fig. 2. A perspective drawing of the molecule.

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* Lists of structure factors, anisotropic thermal parameters for non-H atoms, positional and thermal parameters for H atoms and results of least-squares-planes calculations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43334 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and angles* (°) *with their estimated standard deviations*

C(1)—C(2)	1·401 (8)	C(9)—C(10)	1·398 (8)
C(1)—C(13)	1·362 (8)	C(9)—C(21)	1·401 (8)
C(1)—N	1·490 (7)	C(10)—C(11)	1·365 (8)
C(2)—C(3)	1·346 (9)	C(11)—C(12)	1·403 (7)
C(3)—C(15)	1·425 (9)	C(12)—C(13)	1·481 (7)
C(4)—C(5)	1·381 (8)	C(12)—C(17)	1·411 (7)
C(4)—C(15)	1·402 (8)	C(13)—C(14)	1·445 (8)
C(5)—C(6)	1·397 (8)	C(14)—C(15)	1·418 (7)
C(6)—C(16)	1·388 (8)	C(14)—C(16)	1·396 (7)
C(7)—C(16)	1·477 (8)	C(18)—C(19)	1·373 (10)
C(7)—C(17)	1·477 (8)	C(19)—C(20)	1·414 (9)
C(7)—O(1)	1·225 (7)	C(20)—C(21)	1·343 (9)
C(8)—C(9)	1·433 (8)	N—O(2)	1·219 (7)
C(8)—C(17)	1·424 (7)	N—O(3)	1·233 (6)
C(8)—C(18)	1·437 (9)		
C(2)—C(1)—C(13)	125·5 (6)	C(1)—C(13)—C(12)	127·4 (5)
C(2)—C(1)—N	112·9 (5)	C(1)—C(13)—C(14)	115·3 (5)
C(13)—C(1)—N	121·5 (5)	C(12)—C(13)—C(14)	117·1 (5)
C(1)—C(2)—C(3)	118·0 (6)	C(13)—C(14)—C(15)	120·5 (5)
C(2)—C(3)—C(15)	121·6 (6)	C(13)—C(14)—C(16)	119·8 (5)
C(5)—C(4)—C(15)	120·1 (6)	C(15)—C(14)—C(16)	119·6 (5)
C(4)—C(5)—C(6)	119·6 (6)	C(3)—C(15)—C(4)	122·0 (6)
C(5)—C(6)—C(16)	121·6 (6)	C(3)—C(15)—C(14)	118·3 (6)
C(16)—C(7)—C(17)	116·4 (5)	C(4)—C(15)—C(14)	119·7 (5)
C(16)—C(7)—O(1)	120·3 (6)	C(6)—C(16)—C(7)	120·2 (5)
C(17)—C(7)—O(1)	123·3 (6)	C(6)—C(16)—C(14)	119·1 (5)
C(9)—C(8)—C(17)	119·1 (5)	C(7)—C(16)—C(14)	120·6 (5)
C(9)—C(8)—C(18)	117·3 (6)	C(7)—C(17)—C(8)	121·7 (5)
C(17)—C(8)—C(18)	123·1 (6)	C(7)—C(17)—C(12)	117·7 (5)
C(8)—C(9)—C(10)	118·7 (5)	C(8)—C(17)—C(12)	120·6 (5)
C(8)—C(9)—C(21)	119·6 (5)	C(8)—C(18)—C(19)	119·8 (6)
C(10)—C(9)—C(21)	121·7 (6)	C(18)—C(19)—C(20)	121·8 (7)
C(9)—C(10)—C(11)	121·2 (6)	C(19)—C(20)—C(21)	118·9 (6)
C(10)—C(11)—C(12)	122·4 (6)	C(9)—C(21)—C(20)	122·4 (6)
C(11)—C(12)—C(13)	120·3 (5)	C(1)—N—O(2)	118·7 (5)
C(11)—C(12)—C(17)	117·9 (5)	C(1)—N—O(3)	117·6 (5)
C(13)—C(12)—C(17)	121·3 (5)	O(2)—N—O(3)	123·5 (5)

of the two naphthalene moieties [(*a,b*) and (*d,e*) rings in Fig. 2] make an angle of 25·7 (2)°. The central *c* ring shows the quinonoid structure. The steric repulsion is also relieved by an enlargement of the C(1)—C(13)—C(12) angle [127·4 (5)°]. Moreover, the C—NO_2 and C=O bonds are bent from the mean planes of the *e* and *c* rings, respectively. The twisting angle of C(1)—N and C(12)—C(11) around the line of C(1)···C(12) and that of C(7)—O(1) and C(8)—C(18) around C(7)···C(8) become 30·0 (6) and 23·5 (5)°, respectively. The N···H(11) distance is 2·33 (5) Å, which is significantly shorter than the sum of van der Waals radii. The NO_2 group rotates around the C(1)—N bond from the coplanar conformation. The torsion angle O(3)—N—C(1)—C(13) is 45·7 (3)°. The O(3)···H(11) distance becomes 2·51 (5) Å. Although the original 8,9-BzBT molecule without the NO_2 group also deviates from a planar conformation, the degree of deviation is smaller than in the present nitro compound (Fujisawa, Sato & Saito, 1981). The twisting angle of O—C(7)···C(8)—C(18) is 6 (1)°. This indicates that the distortion of the present molecule is caused mainly by the steric repulsion of the NO_2 group.

It is interesting to consider why the NO_2 group is substituted on the C(1) atom in spite of the large steric repulsion. The reaction mechanism will be discussed in detail elsewhere.

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Structure of 5-Tritylamino-1,4-dihydronaphthalene

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Abstract. $C_{29}H_{25}N$, $M_r = 387·53$, monoclinic, $C2/c$, $a = 14·214$ (5), $b = 13·691$ (4), $c = 22·095$ (7) Å, $\beta = 97·97$ (3)°, $V = 4258·11$ Å^3, $Z = 8$, $D_x = 1·209$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ(Mo $K\alpha$) = 0·35 mm^{-1}, $F(000) = 1648$, $T = 253$ K, final $R = 0·073$, $wR = 0·044$ for 1342 [$I > 3\sigma(I)$] independent reflections. The dihydro ring has a flattened, slightly distorted boat conformation. There are no unusual bond distances or angles.

Introduction. An investigation into the possible factors determining the regioselectivity observed in the cycloaddition reactions of vinylnitrosonium ions with various 5-substituted 1,4-dihydronaphthalenes (Holzapfel, Koekemoer & Van Dyk, 1985) required, amongst others, information on the conformation and puckering amplitude of the dihydro ring in these compounds. NMR conformational analysis of 1,4-dihydro-1-naphthoic acid (based on the ratios of $^5J_{cis}/^5J_{trans}$ for the

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