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[4-(1-Hydroxyethyl)-5-phenanthryl]methyl Acetate

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Abstract. $C_{19}H_{18}O_3$, $M_r = 294.33$, monoclinic, $P2_1/c$, $a = 7.7157$ (10), $b = 27.019$ (3), $c = 7.6219$ (10) Å, $\beta = 107.473$ (10)°, $V = 1515.6$ (7) Å^3, $Z = 4$, $D_x = 1.290$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 0.09$ mm^{-1}, $F(000) = 624$, $T = 293$ K, $R = 0.057$ for 2038 reflections. The bulky substituents cause the aromatic ring system to be helical, with a torsion angle C(4)—C(4a)—C(4b)—C(5) of −32° (standard phenanthrene numbering). Atoms C(4) and C(5), bearing the substituents, deviate furthest from the mean aromatic plane (±0.40 Å). The central ring is the most deformed, with a maximum torsion angle of −23° about C(4a)—C(4b). The molecules are linked in pairs by hydrogen bonds from the OH group to the carbonyl O atom, with O···O 2.99 Å.

Experimental. A colourless prism 0.8 × 0.3 × 0.15 mm was mounted in a glass capillary. Using a Stoe–Siemens four-circle diffractometer, 4364 intensities (ω scans) were registered to $2\theta_{max} = 50°$, with monochromated Mo $K\alpha$ radiation. Of 2647 unique reflections ($R_{int} = 0.016$, index ranges h −8 to 8, k 0 to 32, l 0 to 9) 2039 [$F > 4\sigma(F)$] were considered observed. The cell constants were refined from $\pm\omega$ angles of 56 reflections in the 2θ range 20–22°. Three check reflections showed no significant intensity variation. No absorption correction was applied.

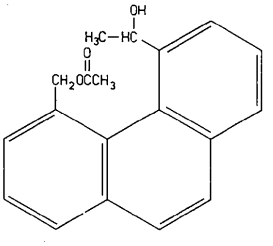

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement parameters* (Å^2 × 10^3)

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

	x	y	z	U_{eq}
C(1)	417 (3)	6515 (1)	966 (3)	62 (1)
C(2)	292 (3)	6170 (1)	−364 (3)	65 (1)
C(3)	1851 (3)	6012 (1)	−736 (3)	53 (1)
C(4)	3569 (3)	6165 (1)	304 (3)	40 (1)
C(4a)	3739 (3)	6471 (1)	1859 (3)	39 (1)
C(4b)	5459 (3)	6611 (1)	3221 (3)	42 (1)
C(5)	7036 (3)	6310 (1)	3749 (3)	44 (1)
C(6)	8639 (3)	6507 (1)	4878 (3)	61 (1)
C(7)	8713 (5)	6977 (1)	5606 (3)	76 (1)
C(8)	7160 (5)	7245 (1)	5327 (3)	70 (1)
C(8a)	5505 (4)	7064 (1)	4188 (3)	54 (1)
C(9)	3833 (5)	7302 (1)	4155 (3)	64 (1)
C(10)	2237 (4)	7098 (1)	3262 (3)	64 (1)
C(10a)	2113 (3)	6685 (1)	2058 (3)	49 (1)
C(41)	5126 (3)	6058 (1)	−483 (3)	45 (1)
C(42)	4837 (4)	6325 (1)	−2295 (3)	62 (1)
O(4)	5433 (3)	5544 (1)	−656 (3)	69 (1)
C(51)	6999 (3)	5762 (1)	3405 (3)	50 (1)
O(52)	7549 (2)	5538 (1)	5227 (2)	61 (1)
C(52)	7716 (3)	5057 (1)	5319 (3)	59 (1)
O(53)	7482 (4)	4808 (1)	3967 (3)	124 (1)
C(53)	8262 (4)	4863 (1)	7224 (3)	74 (1)

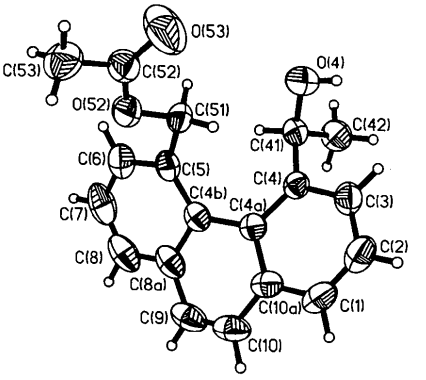

Fig. 1. The molecule of the title compound in the crystal. Thermal ellipsoids are drawn at the 50% level. H-atom radii are arbitrary.

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

C(1)—C(2)	1.360 (4)	C(1)—C(10a)	1.400 (3)
C(2)—C(3)	1.383 (3)	C(3)—C(4)	1.387 (3)
C(4)—C(4a)	1.418 (3)	C(4)—C(41)	1.523 (3)
C(4a)—C(4b)	1.467 (3)	C(4a)—C(10a)	1.430 (3)
C(4b)—C(5)	1.417 (3)	C(4b)—C(8a)	1.425 (3)
C(5)—C(6)	1.383 (3)	C(5)—C(51)	1.502 (3)
C(6)—C(7)	1.381 (4)	C(7)—C(8)	1.361 (4)
C(8)—C(8a)	1.399 (4)	C(8a)—C(9)	1.435 (4)
C(9)—C(10)	1.335 (4)	C(10)—C(10a)	1.430 (3)
C(41)—C(42)	1.514 (3)	C(41)—O(4)	1.422 (3)
C(51)—O(52)	1.457 (2)	O(52)—C(52)	1.304 (3)
C(52)—O(53)	1.199 (3)	C(52)—C(53)	1.481 (3)
C(10a)—C(1)—C(2)	120.8 (2)	C(3)—C(2)—C(1)	119.5 (2)
C(4)—C(3)—C(2)	122.1 (2)	C(4a)—C(4)—C(3)	119.0 (2)
C(41)—C(4)—C(3)	116.7 (2)	C(41)—C(4)—C(4a)	123.6 (2)
C(4b)—C(4a)—C(4)	125.4 (2)	C(10a)—C(4a)—C(4)	117.4 (2)
C(10a)—C(4a)—C(4b)	117.2 (2)	C(5)—C(4b)—C(4a)	124.8 (2)
C(8a)—C(4b)—C(4a)	117.7 (2)	C(8a)—C(4b)—C(5)	117.4 (2)
C(6)—C(5)—C(4b)	119.2 (2)	C(51)—C(5)—C(4b)	123.1 (2)
C(51)—C(5)—C(6)	117.0 (2)	C(7)—C(6)—C(5)	121.6 (3)
C(8)—C(7)—C(6)	119.9 (3)	C(8a)—C(8)—C(7)	120.5 (3)
C(8)—C(8a)—C(4b)	119.9 (3)	C(9)—C(8a)—C(4b)	119.6 (2)
C(9)—C(8a)—C(8)	120.1 (3)	C(10)—C(9)—C(8a)	120.7 (2)
C(10a)—C(10)—C(9)	121.6 (3)	C(4a)—C(10a)—C(1)	119.9 (2)
C(10)—C(10a)—C(1)	120.5 (2)	C(10)—C(10a)—C(4a)	119.5 (2)
C(42)—C(41)—C(4)	110.6 (2)	O(4)—C(41)—C(4)	113.3 (2)
O(4)—C(41)—C(42)	111.3 (2)	O(52)—C(51)—C(5)	105.1 (2)
C(52)—O(52)—C(51)	117.5 (2)	O(53)—C(52)—O(52)	121.8 (2)
C(53)—C(52)—O(52)	113.6 (2)	C(53)—C(52)—O(53)	124.6 (3)

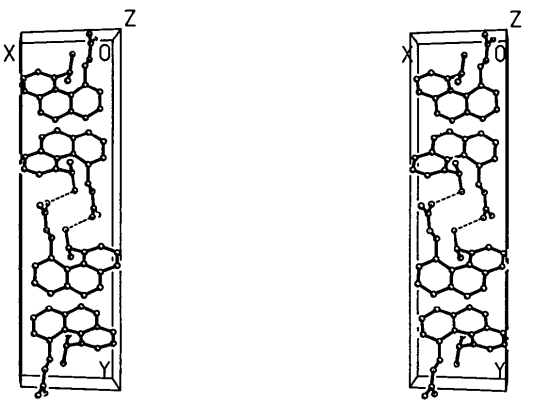

Fig. 2. Stereographic packing dragram (without H atoms) along the *z* axis. Hydrogen bonds are indicated by dashed lines.

The structure was solved by direct methods and subjected to anisotropic full-matrix least-squares refinement on *F*. H atoms were included using a riding model. The weighting scheme was $w^{-1} = \sigma^2(F) + 0.0002F^2$; final $R = 0.057$, $wR = 0.059$, for 209 parameters; $S = 2.4$; maximum $\Delta/\sigma = 0.001$, maximum $\Delta\rho = 0.28$, minimum $\Delta\rho = -0.26$ e Å^{-3}. Atomic scattering factors and f', f'' values were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The program system used was *SHELXTL-Plus* (Sheldrick, 1989). Final atom coordinates are given in Table 1,* with derived bond lengths and angles in Table 2. Fig. 1 shows the atomic labelling scheme and Fig. 2 shows the crystal packing.

Related literature. Similar helical ring systems are described by Schrumpf & Jones (1988) and Jones & Schrumpf (1988).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55328 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0105]

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9,10-Dihydrophenanthrene-4,5-dimethanol

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Abstract. $C_{16}H_{16}O_2$, $M_r = 240.29$, orthorhombic, $P2_12_12$, $a = 15.6464$ (12), $b = 23.027$ (3), $c = 6.9320$ (8) Å, $V = 2497.5$ (7) Å^3, $Z = 8$, $D_x = 1.278$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 0.08$ mm^{-1}, $F(000) = 1024$, $T = 293$ K, $R = 0.076$ for 3362 reflections. The two independent molecules are essentially identical except for the orientation of one hydroxyl group O(4); however, they display opposite

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