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1-Phenyl-3-(pyren-1-yl)prop-2-en-1-one

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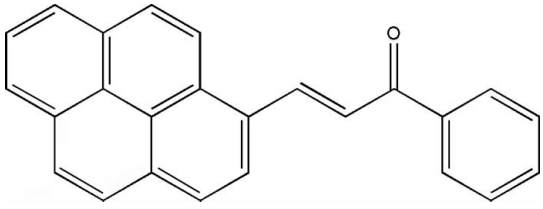
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 6.4.

The title compound, $C_{25}H_{16}O$, was prepared by the condensation reaction of pyrene-1-carbaldehyde and acetophenone in ethanol solution at room temperature. The phenyl ring forms a dihedral angle of 39.10 (11)° with the pyrene ring system. In the crystal structure, adjacent pyrene ring systems are linked by aromatic π–π stacking interactions, with a perpendicular interplanar distance of 3.267 (6) Å and a centroid–centroid offset of 2.946 (7) Å.

Related literature

For related literature, see: Ansari *et al.* (2005); Nielsen *et al.* (2005); Pattanaik *et al.* (2002); Strack (1997).



Experimental

Crystal data

$C_{25}H_{16}O$
M_r = 332.38
Monoclinic, $P2_1$
a = 4.6739 (15) Å
b = 22.535 (7) Å
c = 8.250 (3) Å
β = 106.45 (2)°
V = 833.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.12 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.981, T_{max} = 0.991
3489 measured reflections
1512 independent reflections
914 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.00
1512 reflections
235 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2180).

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supplementary materials

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1-Phenyl-3-(pyren-1-yl)prop-2-en-1-one

Y. Wang, Z. Wang, T. Liang, H. Fu and J. Yao

Comment

Chalcone derivatives have always been of interest in the field of inorganic, organic and physical chemists and biology (Strack, 1997) due to their importance in many organic synthetic pathways, biochemical processes and enzymatic mechanisms (Ansari *et al.*, 2005; Pattanaik *et al.*, 2002; Nielsen *et al.*, 2005). In this paper, we report the crystal structure of the title compound, which was obtained by the condensation reaction of pyrene-1-carbaldehyde and acetophenone in ethanol solution at room temperature.

In the title compound, the pyrene ring is substantially planar (maximum displacement 0.011 (4) Å for C12) and forms a dihedral angle of 39.10 (11)° with the phenyl ring. In the crystal packing, adjacent pyrene rings are linked by aromatic π-π stacking interactions, with a centroid-centroid distance of 4.339 (7) Å, a perpendicular interplanar distance of 3.267 (6) Å and a centroid-centroid offset of 2.946 (7) Å.

Experimental

The title compound was prepared by the condensation reaction of pyrene-1-carbaldehyde (0.05 mol) and acetophenone (0.05 mol) in ethanol (20 ml) at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by slow evaporation of an ethanol/acetonitrile solution (1:1 *v*/*v*) at room temperature.

Refinement

All H atoms were fixed geometrically and were treated as riding on the parent C atoms, with C—H distances of 0.93 Å. U_{iso}(H) = 1.2 U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged in the final refinement.

Figures

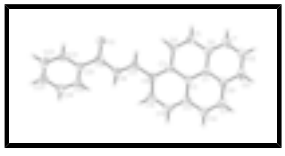


Fig. 1. The molecular structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

1-Phenyl-3-(pyren-1-yl)prop-2-en-1-one

Crystal data

$C_{25}H_{16}O$	F_{000} = 348
M_r = 332.38	D_x = 1.324 Mg m^{-3}

Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 824 reflections
$a = 4.6739\ (15)$ Å	$\theta = 2.6–25.7°$
$b = 22.535\ (7)$ Å	$\mu = 0.08$ mm^{-1}
$c = 8.250\ (3)$ Å	$T = 294\ (2)$ K
$\beta = 106.45\ (2)°$	Block, yellow
$V = 833.4\ (5)$ Å^3	0.24 × 0.22 × 0.12 mm
$Z = 2$	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	1512 independent reflections
Radiation source: fine-focus sealed tube	914 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 294(2)$ K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.7°$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -5\rightarrow5$
$T_{min} = 0.981$, $T_{max} = 0.991$	$k = -26\rightarrow14$
3489 measured reflections	$l = -9\rightarrow9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.098$	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
1512 reflections	$\Delta\rho_{max} = 0.11$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.12$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.0978 (8)	0.06540 (14)	0.3854 (4)	0.0865 (10)
C1	0.2634 (8)	0.31864 (18)	0.6348 (5)	0.0474 (10)
C2	0.4014 (8)	0.30397 (17)	0.5070 (5)	0.0456 (10)
C3	0.5149 (8)	0.24553 (17)	0.4986 (5)	0.0437 (9)
C4	0.4779 (8)	0.20312 (18)	0.6221 (5)	0.0532 (11)
H4	0.5470	0.1646	0.6191	0.064*
C5	0.3463 (9)	0.21795 (19)	0.7411 (5)	0.0558 (11)
H5	0.3277	0.1892	0.8184	0.067*
C6	0.2339 (8)	0.27586 (18)	0.7539 (5)	0.0507 (10)
C7	0.0951 (9)	0.2918 (2)	0.8760 (6)	0.0676 (12)
H7	0.0754	0.2637	0.9547	0.081*
C8	−0.0129 (11)	0.3477 (2)	0.8831 (6)	0.0781 (15)
H8	−0.1058	0.3572	0.9656	0.094*
C9	0.0158 (9)	0.3905 (2)	0.7673 (6)	0.0706 (14)
H9	−0.0569	0.4286	0.7736	0.085*
C10	0.1518 (9)	0.37699 (19)	0.6421 (5)	0.0561 (11)
C11	0.1810 (9)	0.4196 (2)	0.5191 (6)	0.0657 (13)
H11	0.1079	0.4578	0.5231	0.079*
C12	0.3107 (9)	0.40594 (19)	0.3987 (6)	0.0619 (12)
H12	0.3263	0.4347	0.3208	0.074*
C13	0.4260 (8)	0.34749 (15)	0.3881 (5)	0.0481 (10)
C14	0.5642 (9)	0.33242 (19)	0.2671 (5)	0.0555 (11)
H14	0.5841	0.3610	0.1897	0.067*
C15	0.6733 (9)	0.27656 (17)	0.2572 (5)	0.0542 (11)
H15	0.7622	0.2680	0.1723	0.065*
C16	0.6540 (8)	0.23186 (16)	0.3724 (5)	0.0460 (10)
C17	0.7838 (9)	0.17355 (17)	0.3629 (5)	0.0527 (10)
H17	0.7879	0.1477	0.4513	0.063*
C18	0.8963 (9)	0.15305 (17)	0.2438 (5)	0.0585 (11)
H18	0.8827	0.1765	0.1491	0.070*
C19	1.0416 (9)	0.09496 (19)	0.2545 (6)	0.0561 (11)
C20	1.1212 (8)	0.07115 (16)	0.1054 (5)	0.0486 (9)
C21	1.3317 (9)	0.0265 (2)	0.1272 (5)	0.0617 (11)
H21	1.4290	0.0135	0.2357	0.074*
C22	1.3998 (10)	0.00115 (19)	−0.0091 (7)	0.0751 (14)
H22	1.5397	−0.0293	0.0076	0.090*
C23	1.2618 (11)	0.0207 (2)	−0.1689 (6)	0.0732 (13)
H23	1.3094	0.0040	−0.2611	0.088*
C24	1.0536 (11)	0.0648 (2)	−0.1928 (5)	0.0740 (13)
H24	0.9581	0.0777	−0.3018	0.089*
C25	0.9834 (11)	0.09030 (18)	−0.0569 (5)	0.0632 (13)
H25	0.8426	0.1206	−0.0747	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.123 (3)	0.079 (2)	0.0604 (19)	0.027 (2)	0.0325 (18)	0.0182 (18)
C1	0.035 (2)	0.059 (3)	0.043 (2)	−0.0053 (19)	0.0029 (18)	−0.007 (2)
C2	0.038 (2)	0.055 (3)	0.042 (2)	−0.0131 (19)	0.0081 (19)	−0.0036 (19)
C3	0.037 (2)	0.054 (3)	0.037 (2)	−0.0056 (19)	0.0062 (18)	0.0029 (19)
C4	0.057 (3)	0.056 (3)	0.048 (2)	−0.004 (2)	0.017 (2)	0.004 (2)
C5	0.056 (3)	0.065 (3)	0.047 (3)	−0.009 (2)	0.015 (2)	0.007 (2)
C6	0.042 (2)	0.068 (3)	0.041 (2)	−0.007 (2)	0.0105 (19)	−0.003 (2)
C7	0.056 (3)	0.093 (4)	0.054 (3)	−0.003 (3)	0.016 (2)	−0.006 (2)
C8	0.068 (3)	0.107 (5)	0.064 (3)	−0.001 (3)	0.026 (3)	−0.018 (3)
C9	0.054 (3)	0.085 (4)	0.069 (3)	0.001 (2)	0.011 (3)	−0.029 (3)
C10	0.045 (2)	0.065 (3)	0.054 (3)	−0.005 (2)	0.008 (2)	−0.016 (2)
C11	0.056 (3)	0.054 (3)	0.078 (3)	0.004 (2)	0.005 (3)	−0.002 (2)
C12	0.060 (3)	0.051 (3)	0.072 (3)	−0.003 (2)	0.014 (3)	0.008 (2)
C13	0.041 (2)	0.051 (3)	0.050 (2)	−0.0058 (19)	0.009 (2)	0.003 (2)
C14	0.061 (3)	0.056 (3)	0.051 (3)	−0.006 (2)	0.019 (2)	0.015 (2)
C15	0.059 (3)	0.061 (3)	0.045 (2)	−0.007 (2)	0.018 (2)	−0.001 (2)
C16	0.047 (2)	0.047 (3)	0.044 (2)	−0.009 (2)	0.012 (2)	0.000 (2)
C17	0.058 (2)	0.055 (3)	0.046 (2)	−0.004 (2)	0.015 (2)	−0.001 (2)
C18	0.077 (3)	0.053 (3)	0.049 (2)	0.004 (2)	0.022 (2)	0.006 (2)
C19	0.058 (3)	0.056 (3)	0.053 (3)	0.000 (2)	0.013 (2)	0.004 (2)
C20	0.057 (2)	0.041 (2)	0.050 (2)	−0.005 (2)	0.0174 (19)	−0.0035 (19)
C21	0.065 (3)	0.057 (2)	0.058 (3)	−0.002 (2)	0.009 (2)	0.001 (2)
C22	0.073 (3)	0.062 (3)	0.091 (4)	0.007 (3)	0.026 (3)	−0.015 (3)
C23	0.082 (4)	0.074 (3)	0.070 (3)	0.000 (3)	0.031 (3)	−0.011 (3)
C24	0.099 (4)	0.069 (3)	0.054 (3)	0.017 (3)	0.023 (3)	0.001 (2)
C25	0.086 (3)	0.052 (3)	0.051 (3)	0.017 (2)	0.020 (3)	0.003 (2)

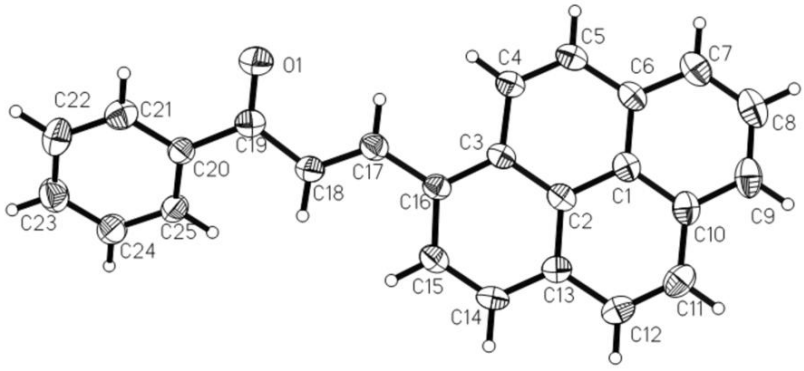
Geometric parameters (Å, °)

O1—C19	1.232 (5)	C12—H12	0.9300
C1—C6	1.411 (5)	C13—C14	1.377 (5)
C1—C2	1.422 (4)	C14—C15	1.369 (5)
C1—C10	1.422 (6)	C14—H14	0.9300
C2—C13	1.414 (5)	C15—C16	1.405 (5)
C2—C3	1.429 (5)	C15—H15	0.9300
C3—C16	1.409 (5)	C16—C17	1.459 (5)
C3—C4	1.443 (5)	C17—C18	1.322 (5)
C4—C5	1.340 (5)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.466 (5)
C5—C6	1.422 (5)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.483 (5)
C6—C7	1.391 (5)	C20—C25	1.380 (5)
C7—C8	1.364 (6)	C20—C21	1.382 (5)
C7—H7	0.9300	C21—C22	1.377 (5)
C8—C9	1.390 (6)	C21—H21	0.9300

C8—H8	0.9300	C22—C23	1.366 (6)
C9—C10	1.392 (5)	C22—H22	0.9300
C9—H9	0.9300	C23—C24	1.365 (6)
C10—C11	1.431 (6)	C23—H23	0.9300
C11—C12	1.338 (6)	C24—C25	1.381 (5)
C11—H11	0.9300	C24—H24	0.9300
C12—C13	1.435 (5)	C25—H25	0.9300
C6—C1—C2	120.8 (3)	C2—C13—C12	119.2 (4)
C6—C1—C10	119.5 (4)	C15—C14—C13	121.9 (4)
C2—C1—C10	119.7 (4)	C15—C14—H14	119.0
C13—C2—C1	119.7 (3)	C13—C14—H14	119.0
C13—C2—C3	120.1 (3)	C14—C15—C16	121.5 (4)
C1—C2—C3	120.2 (3)	C14—C15—H15	119.2
C16—C3—C2	119.5 (3)	C16—C15—H15	119.2
C16—C3—C4	123.3 (4)	C15—C16—C3	118.3 (4)
C2—C3—C4	117.1 (3)	C15—C16—C17	120.1 (3)
C5—C4—C3	121.6 (4)	C3—C16—C17	121.5 (3)
C5—C4—H4	119.2	C18—C17—C16	127.9 (4)
C3—C4—H4	119.2	C18—C17—H17	116.1
C4—C5—C6	122.6 (4)	C16—C17—H17	116.1
C4—C5—H5	118.7	C17—C18—C19	122.8 (4)
C6—C5—H5	118.7	C17—C18—H18	118.6
C7—C6—C1	119.0 (4)	C19—C18—H18	118.6
C7—C6—C5	123.3 (4)	O1—C19—C18	121.1 (4)
C1—C6—C5	117.7 (3)	O1—C19—C20	119.3 (4)
C8—C7—C6	121.6 (5)	C18—C19—C20	119.6 (4)
C8—C7—H7	119.2	C25—C20—C21	118.2 (3)
C6—C7—H7	119.2	C25—C20—C19	122.3 (3)
C7—C8—C9	120.1 (4)	C21—C20—C19	119.5 (4)
C7—C8—H8	119.9	C22—C21—C20	121.1 (4)
C9—C8—H8	119.9	C22—C21—H21	119.4
C8—C9—C10	120.8 (4)	C20—C21—H21	119.4
C8—C9—H9	119.6	C23—C22—C21	119.9 (4)
C10—C9—H9	119.6	C23—C22—H22	120.0
C9—C10—C1	118.9 (4)	C21—C22—H22	120.0
C9—C10—C11	122.4 (4)	C24—C23—C22	119.7 (4)
C1—C10—C11	118.7 (4)	C24—C23—H23	120.1
C12—C11—C10	121.7 (4)	C22—C23—H23	120.1
C12—C11—H11	119.1	C23—C24—C25	120.6 (4)
C10—C11—H11	119.1	C23—C24—H24	119.7
C11—C12—C13	120.9 (4)	C25—C24—H24	119.7
C11—C12—H12	119.6	C20—C25—C24	120.3 (4)
C13—C12—H12	119.6	C20—C25—H25	119.8
C14—C13—C2	118.6 (4)	C24—C25—H25	119.8
C14—C13—C12	122.1 (4)		
C6—C1—C2—C13	179.5 (4)	C3—C2—C13—C14	−0.9 (5)
C10—C1—C2—C13	−0.1 (5)	C1—C2—C13—C12	0.0 (5)
C6—C1—C2—C3	−0.6 (5)	C3—C2—C13—C12	−180.0 (3)

C10—C1—C2—C3	179.9 (4)	C11—C12—C13—C14	−179.1 (4)
C13—C2—C3—C16	0.7 (5)	C11—C12—C13—C2	0.0 (6)
C1—C2—C3—C16	−179.3 (3)	C2—C13—C14—C15	1.0 (6)
C13—C2—C3—C4	−179.0 (4)	C12—C13—C14—C15	−179.8 (4)
C1—C2—C3—C4	1.0 (4)	C13—C14—C15—C16	−1.1 (6)
C16—C3—C4—C5	179.5 (3)	C14—C15—C16—C3	0.8 (6)
C2—C3—C4—C5	−0.8 (5)	C14—C15—C16—C17	−177.4 (4)
C3—C4—C5—C6	0.2 (6)	C2—C3—C16—C15	−0.7 (5)
C2—C1—C6—C7	−179.4 (3)	C4—C3—C16—C15	179.0 (3)
C10—C1—C6—C7	0.1 (5)	C2—C3—C16—C17	177.5 (3)
C2—C1—C6—C5	−0.1 (5)	C4—C3—C16—C17	−2.8 (6)
C10—C1—C6—C5	179.5 (3)	C15—C16—C17—C18	−8.4 (6)
C4—C5—C6—C7	179.6 (4)	C3—C16—C17—C18	173.5 (4)
C4—C5—C6—C1	0.3 (6)	C16—C17—C18—C19	175.2 (4)
C1—C6—C7—C8	0.0 (6)	C17—C18—C19—O1	−8.9 (6)
C5—C6—C7—C8	−179.3 (4)	C17—C18—C19—C20	170.8 (4)
C6—C7—C8—C9	−0.4 (7)	O1—C19—C20—C25	157.8 (4)
C7—C8—C9—C10	0.6 (7)	C18—C19—C20—C25	−21.9 (6)
C8—C9—C10—C1	−0.4 (6)	O1—C19—C20—C21	−19.5 (6)
C8—C9—C10—C11	179.0 (4)	C18—C19—C20—C21	160.8 (4)
C6—C1—C10—C9	0.1 (5)	C25—C20—C21—C22	−0.9 (6)
C2—C1—C10—C9	179.6 (3)	C19—C20—C21—C22	176.5 (4)
C6—C1—C10—C11	−179.4 (3)	C20—C21—C22—C23	1.1 (7)
C2—C1—C10—C11	0.2 (5)	C21—C22—C23—C24	−0.9 (7)
C9—C10—C11—C12	−179.6 (4)	C22—C23—C24—C25	0.7 (7)
C1—C10—C11—C12	−0.2 (6)	C21—C20—C25—C24	0.7 (6)
C10—C11—C12—C13	0.1 (6)	C19—C20—C25—C24	−176.7 (4)
C1—C2—C13—C14	179.1 (3)	C23—C24—C25—C20	−0.6 (7)

Fig. 1


O1
C22
C21
C19
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C18
C17
C16
C3
C4
C5
C6
C7
C8
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C9
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C14
C12