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3-Phenylpyrrolo[2,3-*b*]tropone

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The title compound, $C_{15}H_{11}NO$, exists in the crystal in its keto form as 3-phenylpyrrolo[2,3-*b*]tropone [systematic name: 3-phenylcyclohepta[*b*]pyrrol-8(1*H*)-one] rather than in the enol form as 8-hydroxy-3-phenyl-1-azaazulene. The seven-membered ring shows pronounced bond alternation typical of tropone derivatives.

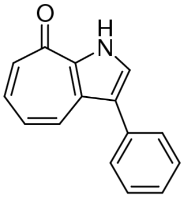
Key indicators

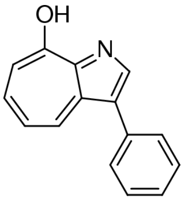
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.116
Data-to-parameter ratio = 17.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

It is known that tris(8-quinolinolido)Al^{III} is widely used for electron-transporting materials (Tang & VanSlyke, 1987). Pyrrolo[*b*]tropones (Nozoe *et al.*, 1954) are isoelectronic with 8-quinolinols, and so might have the potential to form emitting materials. However, our studies (yet unpublished) show that pyrrolo[*b*]tropones and their metal complexes do not have reasonable emitting properties. We now report the structure of 3-phenylpyrrolo[2,3-*b*]tropone, (I), to determine its major tautomer.


(I)


(I')

The pyrrolotropone moiety of molecule (I) is approximately planar; the deviations from the least-squares plane defined by C1–C9/O1/N1 do not exceed 0.1 Å. The dihedral angle between the pyrrolotropone and the phenyl substituent planes is 45.31 (5)°; this is much greater than the analogous angle formed by the phenyl and indolizine planes in 2-phenyl-6-nitroindolizine (6.1°; Tafeenko & Aslanov, 1980).

The C—C bond lengths of the seven-membered ring show bond alternation typical of tropone; the C1—O1 bond length [1.2460 (17) Å] is similar to that observed in the structure of unsubstituted tropone (1.259 Å; Barrow *et al.*, 1973). The C—C and C—N bond lengths in the pyrrole ring are close to those found in pyrrole (Goddard *et al.*, 1997). The objective location of the H1 atom bonded to N1, rather than O1, as well as the tropone-like bond-length distribution, makes assignment of the keto form, (I), rather than the enol form, (I'), unambiguous.

The pyrrole NH group participates in an intermolecular hydrogen bond [N1—H1 0.959 (17), N1···O1^{i} 2.773 (2) and H1···O1^{i} 1.968 (16) Å; symmetry code: (i) $-x, -\frac{1}{2}+y, -\frac{1}{2}-z$] of the N—H···O type. This hydrogen bond links the mol-

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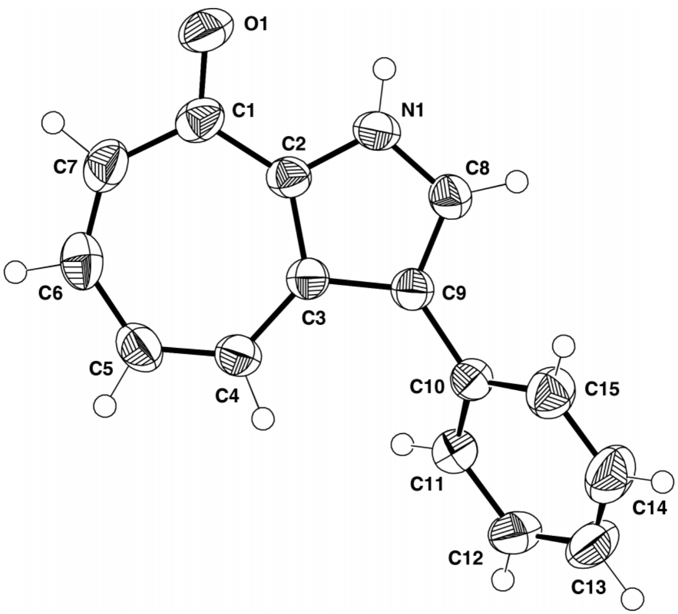

Figure 1
The molecular structure of (I) showing 50% probability displacement ellipsoids.

ecules in the crystal into infinite chains stretching along the *b* axis.

Experimental

The title compound, (I), was prepared by condensation of 2-hydrazinotropone with acetophenone accompanied by cyclization (Nozoe *et al.*, 1954). Single crystals of (I) were obtained by recrystallization from ethyl acetate.

Crystal data

$C_{15}H_{11}NO$
$M_r = 221.25$
Monoclinic, $P2_1/c$
$a = 14.2145$ (10) Å
$b = 7.7681$ (5) Å
$c = 10.3928$ (6) Å
$\beta = 101.980$ (5)°
$V = 1122.58$ (13) Å^3
$Z = 4$

$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.0$–$18.2°$
$\mu = 0.08$ mm^{-1}
$T = 296$ (2) K
Prism, pale yellow
0.47 × 0.47 × 0.43 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
ψ scan (North *et al.*, 1968)
$T_{\rm min} = 0.978$, $T_{\rm max} = 0.999$
2851 measured reflections
2700 independent reflections
1921 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.022$
$\theta_{\rm max} = 28.0°$
$h = -18 \rightarrow 18$
$k = 0 \rightarrow 10$
$l = -13 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity decay: 3.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.116$
$S = 1.03$
2700 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.2047P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.22$ e Å^{-3}

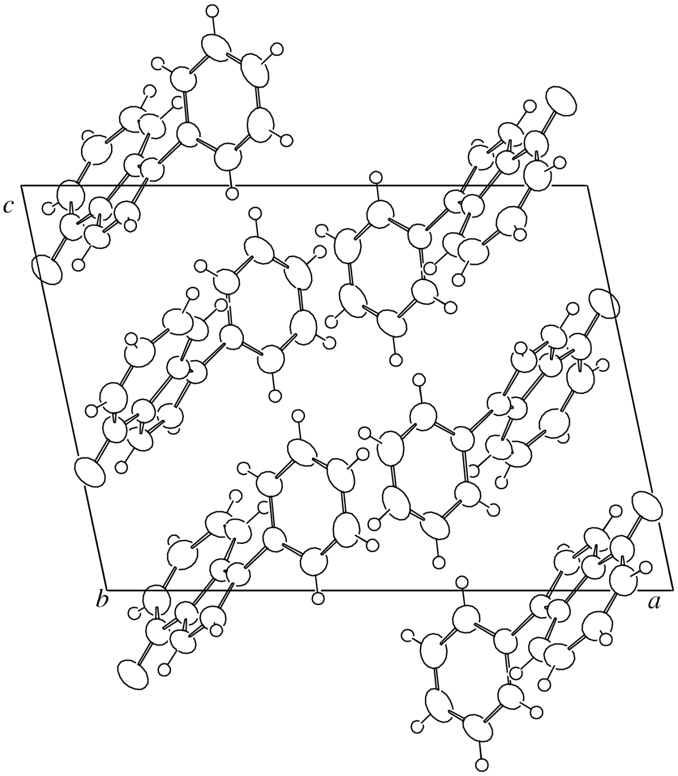

Figure 2
Packing diagram viewed down the *b* axis.

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.3591 (17)	C5—C6	1.419 (2)
N1—C8	1.3510 (18)	C6—C7	1.353 (2)
N1—H1	0.959 (17)	C8—C9	1.3712 (18)
O1—C1	1.2460 (17)	C9—C10	1.4777 (18)
C1—C2	1.4452 (19)	C10—C11	1.3948 (19)
C1—C7	1.442 (2)	C10—C15	1.394 (2)
C2—C3	1.4149 (18)	C11—C12	1.386 (2)
C3—C4	1.4199 (19)	C12—C13	1.375 (3)
C3—C9	1.4326 (19)	C13—C14	1.375 (3)
C4—C5	1.354 (2)	C14—C15	1.382 (2)
C3—C9—C10—C11	48.0 (2)	C3—C9—C10—C15	−135.37 (15)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1$^{\rm i}$	0.959 (17)	1.968 (16)	2.773 (2)	140.38 (10)

Symmetry code: (i) $-x, y-\frac{1}{2}, -\frac{1}{2}-z$.

All H atoms were included in the refinement in geometrically calculated positions in the riding model approximation with C—H set to 0.93 Å, except for the NH group H atom, which was located in the difference synthesis and for which both positional and displacement parameters were refined.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *Xtal_GX* (Hall & du Boulay, 1995); software used to prepare material for publication: *SHELXL*97.

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