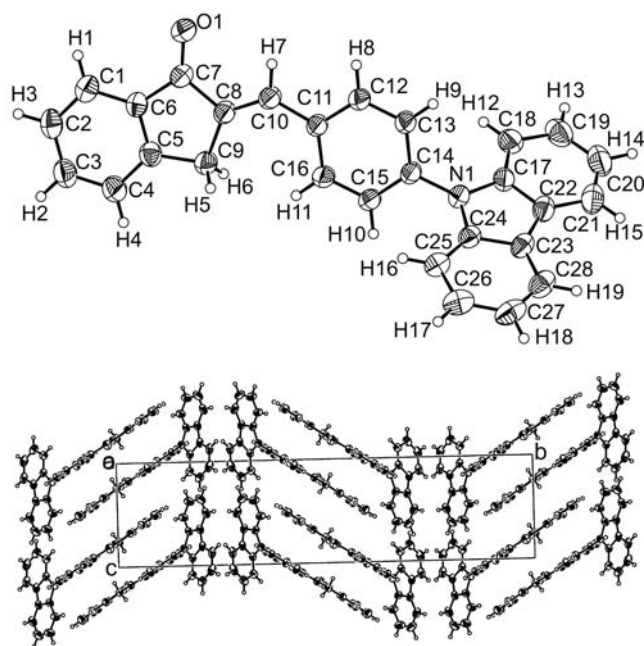


Crystal structure of 2-[4-(9*H*-carbazol-9-yl)benzylidene]-2,3-dihydroinden-1-one, C₂₈H₁₉NO

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(figure, top). The electro-withdrawing moiety (C1, C2, C3, C4, C5, C6, C7, C8 and O1) and electro-donating moiety (C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28 and N1) of the molecule consists of an almost planar aromatic system. A bridge aromatic ring is tilted by 53.8(3)° against the electro-donating moiety, whereas it has an almost planar system to electro-withdrawing moiety. The torsion angle C8, C10, C11, C12 is estimated to be 178.6(2)°. The crystal structure is built by packing molecules layer by layer with $d = 3.402(3)$ Å (figure, bottom). The packing scheme is characterized by a herring-bone arrangement [5]. A gradient angle of 114.5° is observed between the neighboring two-dimensional layers.

Table 1. Data collection and handling.

Crystal:	yellow prism, size 0.10 × 0.10 × 0.30 mm
Wavelength:	Cu K α radiation (1.54187 Å)
μ :	5.96 cm ⁻¹
Diffractometer, scan mode:	Rigaku RAXIS-RAPID, ω
$2\theta_{\max}$:	136.46°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	18287, 3674
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1746
$N(\text{param})_{\text{refined}}$:	290
Programs:	SIR92 [6]

Abstract

C₂₈H₁₉NO, monoclinic, $P12_1/a1$ (no. 14), $a = 7.7107(3)$ Å, $b = 32.422(1)$ Å, $c = 8.3715(4)$ Å, $\beta = 105.095(3)^\circ$, $V = 2020.6$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.036$, $wR_{\text{ref}}(F) = 0.071$, $T = 296$ K.

Source of material

2-(4-(9*H*-carbazol-9-yl)benzylidene)-2,3-dihydroinden-1-one was synthesized easily according to a previously described method with some modifications [1–4]. Yellow crystals of 2-(4-(9*H*-carbazol-9-yl)benzylidene)-2,3-dihydroinden-1-one suitable for X-ray diffraction measurement were grown by solvent diffusion method in which dichloromethane and n-hexane were used as a good and a poor solvent, respectively. All hydrogen atoms were positioned from the geometrical point of view and not refined.

Discussion

The crystal structure contains four symmetry-equivalent molecules per unit cell. The interatomic distances within the molecule are in the normal range. The molecular structure shows the electro-withdrawing and electro-donating moieties bridged by aromatic ring, which is defined by C11, C12, C13, C14, C15 and C16

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	−0.1909	−0.0526	1.3952	0.081
H(2)	4e	0.2691	−0.1171	1.5639	0.097
H(3)	4e	−0.0320	−0.1074	1.5497	0.091
H(4)	4e	0.4215	−0.0721	1.4301	0.092
H(5)	4e	0.3713	0.0132	1.3154	0.077
H(6)	4e	0.3161	−0.0131	1.1551	0.078
H(7)	4e	−0.0168	0.0728	1.0686	0.066
H(8)	4e	0.0498	0.1286	0.9255	0.067
H(9)	4e	0.2435	0.1692	0.8207	0.068
H(10)	4e	0.6457	0.0892	1.0047	0.075
H(11)	4e	0.4544	0.0497	1.1169	0.075
H(12)	4e	0.3202	0.1378	0.5504	0.087
H(13)	4e	0.3206	0.1628	0.2872	0.106
H(14)	4e	0.5351	0.2095	0.2551	0.119
H(15)	4e	0.7648	0.2308	0.4805	0.107
H(16)	4e	0.7692	0.1590	1.1657	0.076
H(17)	4e	1.0267	0.1996	1.2660	0.093
H(18)	4e	1.1455	0.2386	1.0871	0.105
H(19)	4e	1.0028	0.2414	0.8055	0.098

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	4e	−0.1961(2)	0.02016(5)	1.1849(2)	0.056(1)	0.075(1)	0.088(1)	0.0004(8)	0.0226(9)	0.0073(9)
N(1)	4e	0.5789(2)	0.15760(6)	0.8356(2)	0.049(1)	0.061(1)	0.059(1)	−0.0019(8)	0.0180(9)	0.0088(9)
C(1)	4e	−0.0668(3)	−0.05657(8)	1.4036(2)	0.072(2)	0.068(2)	0.063(2)	−0.013(1)	0.020(1)	−0.001(1)
C(2)	4e	0.0272(4)	−0.08891(8)	1.4934(3)	0.094(2)	0.064(2)	0.069(2)	−0.014(2)	0.024(2)	0.009(1)
C(3)	4e	0.2071(4)	−0.09448(8)	1.5024(3)	0.095(2)	0.066(2)	0.081(2)	0.004(2)	0.024(2)	0.017(1)
C(4)	4e	0.2979(3)	−0.06796(7)	1.4239(3)	0.078(2)	0.065(2)	0.087(2)	0.008(1)	0.026(2)	0.016(1)
C(5)	4e	0.2052(3)	−0.03503(7)	1.3355(2)	0.065(2)	0.052(1)	0.060(2)	−0.000(1)	0.019(1)	0.002(1)
C(6)	4e	0.0242(3)	−0.02965(7)	1.3247(2)	0.064(2)	0.050(1)	0.054(1)	−0.007(1)	0.019(1)	−0.001(1)
C(7)	4e	−0.0414(3)	0.00734(7)	1.2247(2)	0.056(1)	0.056(1)	0.058(2)	−0.004(1)	0.019(1)	−0.004(1)
C(8)	4e	0.1156(2)	0.02582(6)	1.1784(2)	0.052(1)	0.050(1)	0.060(1)	−0.001(1)	0.020(1)	0.002(1)
C(9)	4e	0.2758(3)	−0.00162(7)	1.2436(2)	0.062(2)	0.059(1)	0.073(2)	0.003(1)	0.021(1)	0.008(1)
C(10)	4e	0.1000(2)	0.06109(7)	1.0938(2)	0.049(1)	0.053(1)	0.062(2)	0.002(1)	0.017(1)	0.001(1)
C(11)	4e	0.2303(2)	0.08464(6)	1.0322(2)	0.049(1)	0.047(1)	0.057(1)	0.001(1)	0.018(1)	0.001(1)
C(12)	4e	0.1719(2)	0.12069(6)	0.9429(2)	0.046(1)	0.056(1)	0.066(2)	0.006(1)	0.019(1)	0.005(1)
C(13)	4e	0.2858(2)	0.14472(6)	0.8803(2)	0.054(1)	0.052(1)	0.065(2)	0.007(1)	0.022(1)	0.012(1)
C(14)	4e	0.4627(2)	0.13311(6)	0.9034(2)	0.049(1)	0.051(1)	0.057(1)	−0.003(1)	0.019(1)	0.003(1)
C(15)	4e	0.5243(3)	0.09737(7)	0.9904(3)	0.045(1)	0.062(1)	0.082(2)	0.005(1)	0.023(1)	0.015(1)
C(16)	4e	0.4103(2)	0.07379(7)	1.0549(3)	0.050(1)	0.057(1)	0.081(2)	0.008(1)	0.021(1)	0.018(1)
C(17)	4e	0.5456(3)	0.16946(7)	0.6697(3)	0.062(1)	0.058(1)	0.062(2)	0.009(1)	0.026(1)	0.012(1)
C(18)	4e	0.4098(3)	0.15648(8)	0.5362(3)	0.066(2)	0.090(2)	0.061(2)	0.012(1)	0.015(1)	0.010(1)
C(19)	4e	0.4103(4)	0.1715(1)	0.3821(3)	0.089(2)	0.112(2)	0.063(2)	0.033(2)	0.019(2)	0.012(2)
C(20)	4e	0.5401(5)	0.1991(1)	0.3623(4)	0.116(2)	0.100(2)	0.081(2)	0.042(2)	0.047(2)	0.032(2)
C(21)	4e	0.6759(4)	0.21191(8)	0.4947(4)	0.100(2)	0.066(2)	0.100(2)	0.020(2)	0.059(2)	0.024(2)
C(22)	4e	0.6805(3)	0.19656(7)	0.6529(3)	0.071(2)	0.051(1)	0.078(2)	0.012(1)	0.039(1)	0.010(1)
C(23)	4e	0.8009(3)	0.20165(7)	0.8151(3)	0.059(1)	0.044(1)	0.090(2)	0.002(1)	0.037(1)	−0.001(1)
C(24)	4e	0.7341(2)	0.17721(6)	0.9252(3)	0.048(1)	0.049(1)	0.068(2)	0.003(1)	0.022(1)	−0.001(1)
C(25)	4e	0.8160(3)	0.17574(7)	1.0935(3)	0.053(1)	0.065(1)	0.071(2)	0.001(1)	0.019(1)	−0.006(1)
C(26)	4e	0.9683(3)	0.19938(8)	1.1511(3)	0.064(2)	0.077(2)	0.093(2)	0.001(1)	0.018(2)	−0.023(2)
C(27)	4e	1.0385(3)	0.22329(8)	1.0436(4)	0.064(2)	0.066(2)	0.133(2)	−0.012(1)	0.035(2)	−0.028(2)
C(28)	4e	0.9558(3)	0.22475(7)	0.8777(4)	0.072(2)	0.052(1)	0.120(2)	−0.005(1)	0.048(2)	−0.005(2)

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