Crystal structure of 2-[4-(9*H*-carbazol-9-yl)benzylidene]-2,3-dihydroinden-1-one, $C_{28}H_{19}NO$

Byung-Soon Kim[I], Su-Ho Kim[II], Shinya Matsumoto[I] and Young-A Son[*,II]

[I] Yokohama National University, Graduate School of Environmental and Information Sciences, Hodogaya-ku, Yokohama 240-8501, Japan
[II] Chungnam National University, Department of Organic Materials and Textile System Engineering, Daejeon 305-764, Korea

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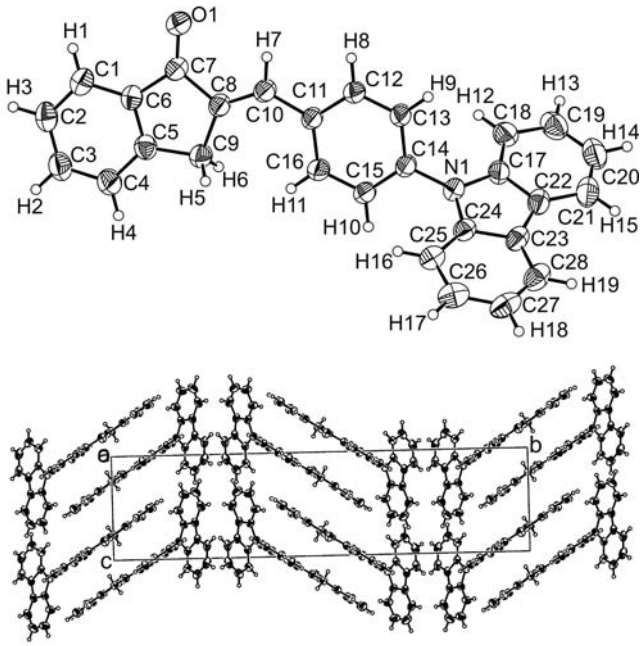

Abstract

$C_{28}H_{19}NO$, monoclinic, $P12_1/a1$ (no. 14), a = 7.7107(3) Å, b = 32.422(1) Å, c = 8.3715(4) Å, β = 105.095(3)°, V = 2020.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.036, $wR_{ref}(F)$ = 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 (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°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	18287, 3674
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1746
$N(param)_{refined}$:	290
Programs:	SIR92 [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

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

* Correspondence author (e-mail: yason@cnu.ac.kr)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	–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)	4*e*	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)	4*e*	–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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	–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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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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