Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-{4-[(*E*)-2-(9*H*-Carbazol-9-yl)ethenyl]-phenyl}ethan-1-one

Wiesław Prukała, Bogdan Marciniec and Maciej Kubicki*

Department of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland
Correspondence e-mail: mkubicki@amu.edu.pl

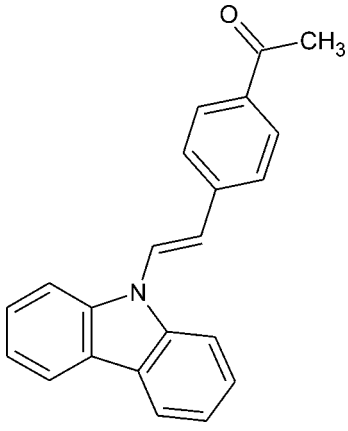
Received 24 August 2007; accepted 14 September 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.095; data-to-parameter ratio = 13.4.

In the title molecule, $C_{22}H_{17}NO$, the two approximately planar carbazole and phenyl groups make a dihedral angle of 45.34 (5)°. In the crystal structure, C—H···O hydrogen-bonded dimers are connected by additional C—H···O and C—H···π interactions into chains along the [001] direction.

Related literature

The synthesis and catalytic activities of *para*-substituted (*E*)-*N*-styrylcarbazoles have recently been described by Prukała *et al.* (2007). For related literature, see Hyun *et al.* (2006); Anni *et al.* (2004); Zhang *et al.* (2004); Marciniec *et al.* (2005).



Experimental

Crystal data

$C_{22}H_{17}NO$
M_r = 311.37
Monoclinic, $P2_1/c$
a = 8.6392 (6) Å
b = 24.6618 (17) Å
c = 8.0637 (7) Å
β = 103.665 (7)°
V = 1669.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.45 × 0.2 × 0.1 mm

Data collection

Kuma KM4 CCD diffractometer
Absorption correction: none
10180 measured reflections
2931 independent reflections
1618 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.095
S = 1.09
2931 reflections
218 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*3 is the centroid of the five-membered ring C5/C6/C11/N12/C13.

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···O23^{i}	0.99	2.57	3.554 (2)	168
C10—H10···O23^{ii}	0.96	2.69	3.632 (2)	167
C4—H4···*Cg*3^{iii}	0.96	2.91	3.555 (2)	126

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+1, -y+1, -z-1$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2134).

References

Anni, M., Manna, L., Cingolani, R., Valerini, D., Creti, A. & Lomascolo, M. (2004). *Appl. Phys. Lett.* **85**, 4169–4171.
Hyun, A.-R., Lee, J.-H., Kang, I.-N. & Park, J.-W. (2006). *Thin Solid Films*, **209**, 127–131.
Marciniec, B., Majchrzak, M., Prukała, W., Kubicki, M. & Chadyniak, D. (2005). *J. Org. Chem.* **70**, 8550–8555.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Version 1.171.29.9. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Prukała, W., Marciniec, B., Majchrzak, M. & Kubicki, M. (2007). *Tetrahedron*, **63**, 1107–1115.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1989). *XP*. Release 3.4. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhang, Q., Chen, J., Cheng, Y., Wang, L., Ma, D., Jing, X. & Wang, F. (2004). *J. Mater. Chem.* **14**, 895–900.

supplementary materials

Acta Cryst. (2007). E**63**, o4255 [**doi:10.1107/S1600536807045151**]

1-{4-[(*E*)-2-(9*H*-Carbazol-9-yl)ethenyl]phenyl}ethan-1-one

W. Prukala, B. Marciniec and M. Kubicki

Comment

Carbazole and its derivatives are very attractive compounds due to their electroactivity and luminescent properties (Hyun *et al.*., 2006). The aromatic rings in carbazole-containing compounds form relatively stable radical cations (holes) and many carbazole derivatives have sufficiently high triplet energy to host red, full-color triplet emitters (*e.g.* Anni *et al.*, 2004). Such properties make them attractive components of light-emitting diodes, and photorefractive materials (Zhang *et al.*, 2004). Very interesting are N-styryl-substituted carbazole derivatives with electron-withdrawing groups (Prukała *et al*., 2007). The title compound is a part of our studies on styryl-carbazole derivatives.

The molecule of the title compound (Fig. 1) is built of two approximately planar aromatic fragments, connected by the *trans* N—C=C—C moity (A). The maximum deviation from the mean plane of nine atoms of the carbazole moiety (B) is 0.0354 (16)Å and from the least-squares plane of the phenyl ring (C) − 0.0098 (12) Å. The overall conformation of the molecule (I) can be described by the dihedral angles between these three planar fragments: A/B: 34.26 (13)°, A/C: 11.19 (14)°, B/C: 45.34 (5)°. The molecule of (I) is significantly less twisted that the closely related methoxy-derivative (Prukała *et al.*, 2007), in which the dihedral angle between the carbazole and phenyl planes is 64.29 (4)°. The bond lengths in the central N—C=C—C fragment show the lack of the delocalization (double C=C bond 1.296 (2) Å, single C—C: 1.480 (2) Å, N—C 1.404 (2) Å).

In the crystal structure centrosymmetric dimers generated by hydrogen bond C—H···O (C21—H···O23^{i} , i = 1 − *x*, 1 − *y*, −1 − *z*) (Table 1, Fig. 2) are connected by C10···O23^{i} (i = *x*, *y*, 1 + *z*) into the chains along the direction [001]. Additional C—H···π interaction (*Cg*3 in Table 1 denotes the middlepoint of the five-membered ring C5, C6, C11, N12) also support these chains.

Experimental

Compound **I** was synthesized according to the procedure described earlier (Prukała *et al.*, 2007).

Refinement

The hydrogen atoms were located in the difference Fourier maps and refined as 'riding model'. Isotropic displacement parameters for hydrogen atoms were set at 1.2 (1.3 for methyl group) times the U_{eq} values of appropriate carrier atoms. Weak restraints to the U^{ij} components were appled due to the large values of Hirshfeld differences for some pairs of atoms.

Figures

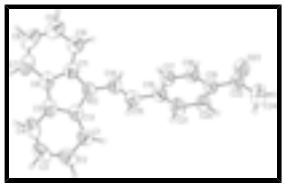


Fig. 1. The molecular structure of (I) with atom labels and the 50% probability displacement ellipsoids for non-H atoms.

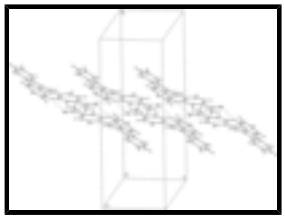


Fig. 2. The chain along [001] formed by C—H···O interactions.

1-{4-[(*E*)-2-(9*H*-Carbazol-9-yl)ethenyl]phenyl}ethan-1-one

Crystal data

$C_{22}H_{17}NO$	$F_{000} = 656$
$M_r = 311.37$	$D_x = 1.239$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3826 reflections
$a = 8.6392$ (6) Å	$\theta = 4$–23º
$b = 24.6618$ (17) Å	$\mu = 0.08$ mm^{-1}
$c = 8.0637$ (7) Å	$T = 294$ (2) K
$\beta = 103.665$ (7)º	Block, colourless
$V = 1669.4$ (2) Å^3	0.45 × 0.2 × 0.1 mm
$Z = 4$	

Data collection

KUMA KM4CCD diffractometer	1618 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.030$
Monochromator: graphite	$\theta_{max} = 25.0$º
$T = 294(2)$ K	$\theta_{min} = 2.4$º
ω–scan	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -29 \rightarrow 28$
10180 measured reflections	$l = -5 \rightarrow 9$
2931 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.095$	$w = 1/[\sigma^2(F_o^2) + (0.040P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
2931 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
218 parameters	$\Delta\rho_{min} = -0.12$ e Å^{-3}
10 restraints	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 calculating *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}
C1	0.6313 (2)	0.34028 (7)	0.3173 (2)	0.0695 (5)
H1	0.7133	0.3583	0.2679	0.083*
C2	0.6783 (3)	0.31391 (8)	0.4715 (2)	0.0869 (6)
H2	0.7972	0.3141	0.5305	0.104*
C3	0.5693 (3)	0.28726 (8)	0.5428 (3)	0.0976 (7)
H3	0.6060	0.2718	0.6455	0.117*
C4	0.4104 (3)	0.28523 (7)	0.4613 (3)	0.0883 (6)
H4	0.3244	0.2687	0.4982	0.106*
C5	0.3595 (2)	0.31135 (7)	0.3037 (2)	0.0658 (5)
C6	0.2073 (2)	0.31597 (7)	0.1820 (2)	0.0660 (5)
C7	0.0531 (3)	0.29664 (8)	0.1758 (3)	0.0868 (6)
H7	0.0483	0.2763	0.2709	0.104*
C8	−0.0687 (3)	0.31089 (10)	0.0405 (4)	0.0981 (7)
H8	−0.1770	0.2955	0.0323	0.118*
C9	−0.0414 (2)	0.34367 (9)	−0.0883 (3)	0.0935 (6)
H9	−0.1301	0.3553	−0.1824	0.112*
C10	0.1086 (2)	0.36252 (8)	−0.0885 (2)	0.0783 (5)
H10	0.1317	0.3867	−0.1733	0.094*
C11	0.2321 (2)	0.34749 (7)	0.0473 (2)	0.0623 (5)
N12	0.39291 (17)	0.36185 (6)	0.07909 (16)	0.0623 (4)
C13	0.4717 (2)	0.33970 (6)	0.2363 (2)	0.0587 (4)
C14	0.4584 (2)	0.39064 (7)	−0.0382 (2)	0.0695 (5)
H14	0.4206	0.3852	−0.1545	0.083*

C15	0.5778 (2)	0.42392 (7)	−0.0040 (2)	0.0697 (5)
H15	0.6239	0.4337	0.1187	0.084*
C16	0.6464 (2)	0.45242 (7)	−0.1315 (2)	0.0617 (4)
C17	0.60586 (19)	0.43922 (7)	−0.3039 (2)	0.0657 (5)
H17	0.5348	0.4145	−0.3568	0.079*
C18	0.67108 (19)	0.46792 (7)	−0.4199 (2)	0.0652 (5)
H18	0.6385	0.4598	−0.5410	0.078*
C19	0.77922 (19)	0.50939 (6)	−0.36486 (19)	0.0565 (4)
C20	0.8206 (2)	0.52105 (7)	−0.1916 (2)	0.0675 (5)
H20	0.9034	0.5502	−0.1474	0.081*
C21	0.7553 (2)	0.49312 (8)	−0.0779 (2)	0.0711 (5)
H21	0.7872	0.5024	0.0456	0.085*
C22	0.8457 (2)	0.53991 (7)	−0.4901 (2)	0.0637 (5)
O23	0.80691 (16)	0.52895 (6)	−0.64132 (16)	0.0937 (4)
C24	0.9629 (2)	0.58373 (8)	−0.4314 (2)	0.0944 (6)
H24A	1.0224	0.5948	−0.5177	0.123*
H24B	1.0298	0.5776	−0.3271	0.123*
H24C	0.9131	0.6124	−0.4135	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0778 (10)	0.0578 (11)	0.0715 (12)	0.0015 (10)	0.0151 (9)	0.0018 (10)
C2	0.1083 (16)	0.0629 (13)	0.0807 (14)	0.0066 (11)	0.0050 (11)	0.0055 (11)
C3	0.145 (2)	0.0728 (15)	0.0719 (13)	0.0074 (14)	0.0188 (14)	0.0206 (11)
C4	0.1262 (19)	0.0629 (13)	0.0841 (12)	−0.0049 (13)	0.0416 (14)	0.0146 (10)
C5	0.0882 (11)	0.0450 (10)	0.0725 (10)	0.0003 (10)	0.0353 (8)	−0.0001 (8)
C6	0.0784 (10)	0.0485 (10)	0.0816 (12)	−0.0028 (9)	0.0398 (8)	−0.0085 (10)
C7	0.0925 (14)	0.0673 (14)	0.1162 (16)	−0.0165 (12)	0.0555 (14)	−0.0180 (12)
C8	0.0730 (16)	0.0923 (17)	0.1363 (19)	−0.0190 (13)	0.0395 (15)	−0.0400 (16)
C9	0.0707 (12)	0.0970 (17)	0.1110 (16)	−0.0033 (11)	0.0181 (13)	−0.0277 (14)
C10	0.0752 (12)	0.0790 (14)	0.0813 (12)	−0.0003 (10)	0.0194 (11)	−0.0064 (11)
C11	0.0657 (13)	0.0575 (12)	0.0683 (12)	0.0008 (10)	0.0250 (10)	−0.0062 (9)
N12	0.0648 (10)	0.0642 (9)	0.0617 (9)	−0.0014 (8)	0.0228 (7)	0.0074 (7)
C13	0.0709 (9)	0.0476 (10)	0.0620 (11)	0.0008 (9)	0.0248 (9)	−0.0012 (9)
C14	0.0724 (12)	0.0704 (13)	0.0715 (12)	−0.0007 (10)	0.0288 (9)	0.0094 (9)
C15	0.0770 (13)	0.0717 (13)	0.0636 (11)	−0.0008 (11)	0.0226 (9)	0.0047 (9)
C16	0.0659 (11)	0.0625 (12)	0.0614 (9)	0.0104 (10)	0.0243 (8)	0.0057 (8)
C17	0.0626 (11)	0.0638 (12)	0.0714 (9)	−0.0094 (9)	0.0174 (8)	−0.0048 (8)
C18	0.0656 (11)	0.0712 (12)	0.0610 (10)	−0.0011 (8)	0.0197 (8)	−0.0023 (8)
C19	0.0590 (10)	0.0553 (10)	0.0595 (8)	0.0071 (7)	0.0228 (7)	0.0021 (7)
C20	0.0764 (12)	0.0665 (12)	0.0635 (9)	−0.0068 (10)	0.0240 (9)	−0.0034 (9)
C21	0.0856 (13)	0.0710 (13)	0.0601 (10)	−0.0057 (11)	0.0239 (10)	−0.0033 (10)
C22	0.0652 (11)	0.0652 (12)	0.0663 (12)	0.0037 (10)	0.0269 (9)	0.0039 (9)
O23	0.0997 (10)	0.1208 (12)	0.0646 (8)	−0.0205 (9)	0.0272 (7)	0.0072 (8)
C24	0.1189 (17)	0.0773 (14)	0.0996 (15)	−0.0230 (13)	0.0509 (13)	−0.0082 (12)

Geometric parameters (Å, °)

C1—C2	1.377 (2)	N12—C13	1.4003 (19)
C1—C13	1.379 (2)	N12—C14	1.404 (2)
C1—H1	0.9960	C14—C15	1.296 (2)
C2—C3	1.380 (3)	C14—H14	0.9270
C2—H2	1.0250	C15—C16	1.480 (2)
C3—C4	1.375 (3)	C15—H15	1.0050
C3—H3	0.8988	C16—C21	1.374 (2)
C4—C5	1.400 (2)	C16—C17	1.389 (2)
C4—H4	0.9550	C17—C18	1.394 (2)
C5—C13	1.404 (2)	C17—H17	0.8986
C5—C6	1.447 (2)	C18—C19	1.385 (2)
C6—C11	1.392 (2)	C18—H18	0.9705
C6—C7	1.405 (3)	C19—C20	1.388 (2)
C7—C8	1.370 (3)	C19—C22	1.480 (2)
C7—H7	0.9259	C20—C21	1.370 (2)
C8—C9	1.380 (3)	C20—H20	1.0165
C8—H8	0.9977	C21—H21	0.9949
C9—C10	1.377 (3)	C22—O23	1.2160 (17)
C9—H9	0.9857	C22—C24	1.480 (2)
C10—C11	1.387 (2)	C24—H24A	0.9954
C10—H10	0.9625	C24—H24B	0.9131
C11—N12	1.397 (2)	C24—H24C	0.8566
C2—C1—C13	118.10 (18)	C1—C13—N12	129.96 (16)
C2—C1—H1	119.1	C1—C13—C5	121.76 (16)
C13—C1—H1	122.8	N12—C13—C5	108.17 (16)
C1—C2—C3	121.1 (2)	C15—C14—N12	127.20 (17)
C1—C2—H2	117.8	C15—C14—H14	112.2
C3—C2—H2	121.1	N12—C14—H14	120.5
C4—C3—C2	121.35 (19)	C14—C15—C16	125.65 (17)
C4—C3—H3	121.3	C14—C15—H15	118.1
C2—C3—H3	117.3	C16—C15—H15	116.1
C3—C4—C5	118.74 (19)	C21—C16—C17	118.53 (16)
C3—C4—H4	128.9	C21—C16—C15	119.06 (16)
C5—C4—H4	112.3	C17—C16—C15	122.41 (17)
C4—C5—C13	118.86 (18)	C16—C17—C18	120.43 (16)
C4—C5—C6	133.78 (18)	C16—C17—H17	128.1
C13—C5—C6	107.35 (15)	C18—C17—H17	111.4
C11—C6—C7	118.77 (19)	C19—C18—C17	120.55 (16)
C11—C6—C5	106.86 (16)	C19—C18—H18	119.1
C7—C6—C5	134.36 (19)	C17—C18—H18	120.3
C8—C7—C6	119.0 (2)	C18—C19—C20	117.99 (16)
C8—C7—H7	128.5	C18—C19—C22	119.85 (15)
C6—C7—H7	112.5	C20—C19—C22	122.16 (16)
C7—C8—C9	120.9 (2)	C21—C20—C19	121.37 (17)
C7—C8—H8	119.1	C21—C20—H20	119.2
C9—C8—H8	119.8	C19—C20—H20	119.4

C10—C9—C8	121.8 (2)	C20—C21—C16	121.10 (17)
C10—C9—H9	117.5	C20—C21—H21	119.6
C8—C9—H9	120.7	C16—C21—H21	119.3
C9—C10—C11	117.19 (19)	O23—C22—C24	119.25 (16)
C9—C10—H10	124.2	O23—C22—C19	120.76 (17)
C11—C10—H10	118.5	C24—C22—C19	119.98 (16)
C10—C11—C6	122.27 (18)	C22—C24—H24A	113.8
C10—C11—N12	128.52 (16)	C22—C24—H24B	114.2
C6—C11—N12	109.15 (16)	H24A—C24—H24B	111.7
C11—N12—C13	108.45 (14)	C22—C24—H24C	108.8
C11—N12—C14	123.11 (15)	H24A—C24—H24C	104.8
C13—N12—C14	128.30 (15)	H24B—C24—H24C	102.4
C13—C1—C2—C3	0.5 (3)	C14—N12—C13—C1	0.3 (3)
C1—C2—C3—C4	1.2 (3)	C11—N12—C13—C5	−0.09 (17)
C2—C3—C4—C5	−0.6 (3)	C14—N12—C13—C5	−175.95 (15)
C3—C4—C5—C13	−1.4 (3)	C4—C5—C13—C1	3.1 (2)
C3—C4—C5—C6	177.36 (19)	C6—C5—C13—C1	−175.97 (15)
C4—C5—C6—C11	−179.82 (18)	C4—C5—C13—N12	179.72 (14)
C13—C5—C6—C11	−0.93 (18)	C6—C5—C13—N12	0.63 (17)
C4—C5—C6—C7	0.7 (3)	C11—N12—C14—C15	149.70 (17)
C13—C5—C6—C7	179.63 (18)	C13—N12—C14—C15	−35.0 (3)
C11—C6—C7—C8	−2.1 (3)	N12—C14—C15—C16	178.21 (15)
C5—C6—C7—C8	177.26 (19)	C14—C15—C16—C21	169.39 (17)
C6—C7—C8—C9	0.0 (3)	C14—C15—C16—C17	−11.2 (3)
C7—C8—C9—C10	1.3 (3)	C21—C16—C17—C18	−1.9 (2)
C8—C9—C10—C11	−0.4 (3)	C15—C16—C17—C18	178.69 (15)
C9—C10—C11—C6	−1.8 (3)	C16—C17—C18—C19	1.1 (2)
C9—C10—C11—N12	−178.59 (16)	C17—C18—C19—C20	0.3 (2)
C7—C6—C11—C10	3.1 (2)	C17—C18—C19—C22	−179.22 (15)
C5—C6—C11—C10	−176.48 (16)	C18—C19—C20—C21	−0.9 (2)
C7—C6—C11—N12	−179.57 (14)	C22—C19—C20—C21	178.63 (15)
C5—C6—C11—N12	0.88 (18)	C19—C20—C21—C16	0.1 (3)
C10—C11—N12—C13	176.65 (17)	C17—C16—C21—C20	1.4 (3)
C6—C11—N12—C13	−0.51 (17)	C15—C16—C21—C20	−179.23 (16)
C10—C11—N12—C14	−7.2 (3)	C18—C19—C22—O23	−0.2 (2)
C6—C11—N12—C14	175.62 (14)	C20—C19—C22—O23	−179.72 (17)
C2—C1—C13—N12	−178.40 (16)	C18—C19—C22—C24	−179.18 (16)
C2—C1—C13—C5	−2.6 (2)	C20—C19—C22—C24	1.3 (2)
C11—N12—C13—C1	176.13 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O23^{i}	0.99	2.57	3.554 (2)	168
C10—H10···O23^{ii}	0.96	2.69	3.632 (2)	167
C4—H4···Cg3^{iii}	0.96	2.91	3.555 (2)	126

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*+1, −*y*+1, −*z*−1; (iii) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

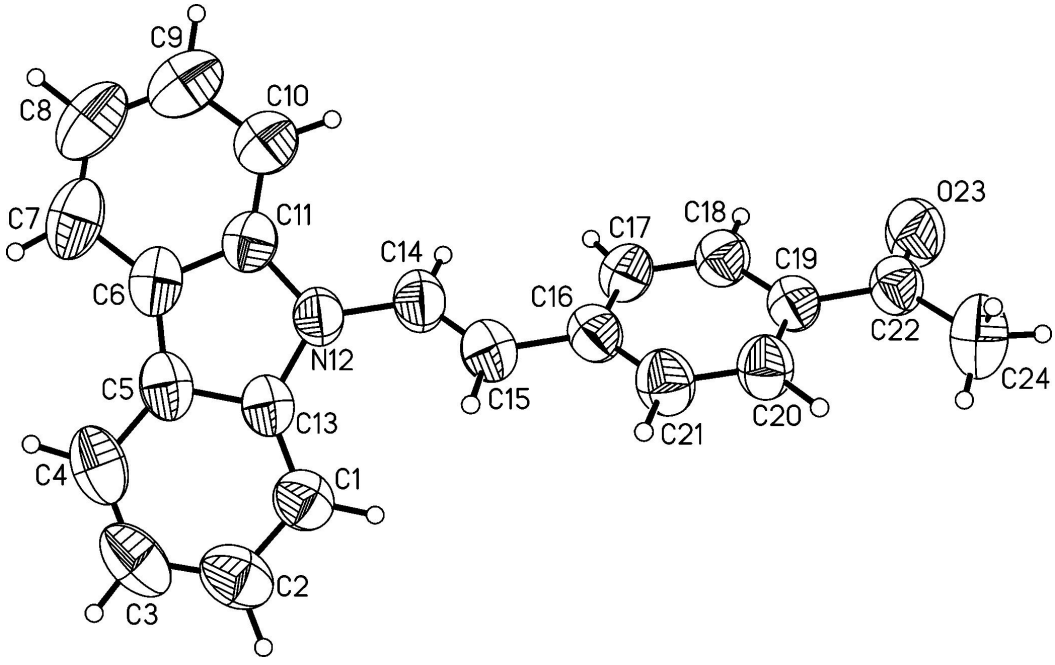

C9
C10
C8
C7
C11
C14
C6
C16
C17
C18
O23
C19
C22
N12
C15
C24
C5
C13
C20
C21
C4
C1
C2
C3

Fig. 2