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trans-4-[2-(1,3-Benzoxazol-2-yl)-ethenyl]benzaldehyde

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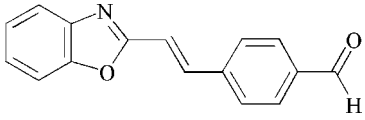
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.193; data-to-parameter ratio = 12.5.

The title molecule, $C_{16}H_{11}NO_2$, is planar with an r.m.s. deviation of 0.0362 (4) Å. The benzene ring and benzoxazole ring system adopt a *trans* configuration with respect to the central double bond.

Related literature

For related literature, see: Denk *et al.* (1990); Helmchen & Denk (2002); Huang *et al.* (2003); Zhang *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{11}NO_2$
M_r = 249.26
Triclinic, $P\overline{1}$
a = 6.509 (2) Å
b = 7.404 (3) Å
c = 14.005 (5) Å
α = 79.885 (6)°
β = 80.766 (6)°
γ = 68.565 (7)°
V = 615.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.993
3147 measured reflections
2147 independent reflections
1248 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.193
S = 1.18
2147 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: AT2332).

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supplementary materials

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trans-4-[2-(1,3-Benzoxazol-2-yl)ethenyl]benzaldehyde

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Comment

Recently, a number of organic two-photon induced fluorescent (TPIF) materials have beeen widely investigated because of their various applications, especially in TPIF microscopy (Denk *et al.*, 1990; Helmchen *et al.*, 2002; Zhang *et al.*, 2002). Among the design strategies for TPIF materials, it is reported that introducing a heteroatom into a molecular structure is an efficient way to obtain excellent TPIF molecules because π-deficient and π-excesive heterocycles may act as efficent acceptor and donor moieties, respectively. The title compound, namely tran-2-(*p*-formylstyryl)benzexazole, consists of atypical A-π-A' structure, where the heterocyclic, styryl and formyl groups are employed as A, π-conjugated and A' moieties, repectively. Here, we present the crystal structure of the title compound, (I).

The molecule of (I) contains a benzexazole ring and a benzene ring which they bounded through a C═C double bond to each other. The terminal benzene ring and benzexazole ring adopt a *trans* configuration with respect to the central double bond. The whole molecule assumes a planar structure, with an r.m.s deviation of 0.0362 (4) Å. As atom C6 is a bridged atom in benzexazole ring, it has a distorted trigonal geometry, with the C1—C6—N1 [108.9 (3) °] and C5—C6—N1 [131.3 (3) °] angles deviating significantly from ideal sp^2 value of 120°. The similar result is also observed for the other bridged C1 atom. As a result of the π-π conjugation, the C7—C8 [1.442 (4) Å] and C9—C10 [1.461 (4) Å] bonds are significantly shorter than the ideal single bonds.

Experimental

The title compound was prepared according to the literature's report (Huang *et al.*, 2003). Single crystals suitable for X-ray analysis were obtained by slow evaporation at 298 K of a mixture solution of dichloromethane and ethyl acetate in volume of 1:5.

Refinement

All H atoms were positioned geometrically and refined using a riding model. Constrained distances: 0.93Å for Csp^2—H. U_{iso}(H) values were fixed at 1.2U_{eq}(C).

Figures

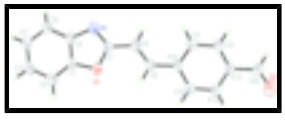

Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

trans-4-[2-(1,3-Benzoxazol-2-yl)ethenyl]benzaldehyde

Crystal data

$C_{16}H_{11}NO_2$	$Z = 2$
$M_r = 249.26$	$F_{000} = 260$
Triclinic, $P\overline{1}$	$D_x = 1.346$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.509$ (2) Å	Cell parameters from 943 reflections
$b = 7.404$ (3) Å	$\theta = 3.0$–26.0º
$c = 14.005$ (5) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 79.885$ (6)º	$T = 294$ (2) K
$\beta = 80.766$ (6)º	Plate, colourless
$\gamma = 68.565$ (7)º	0.22 × 0.20 × 0.08 mm
$V = 615.1$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2147 independent reflections
Radiation source: fine-focus sealed tube	1248 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 294$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 7$
$T_{min} = 0.981$, $T_{max} = 0.993$	$k = -8 \rightarrow 7$
3147 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.193$	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.2468P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.18$	$(\Delta/\sigma)_{max} = 0.001$
2147 reflections	$\Delta\rho_{max} = 0.69$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.0390 (4)	0.7576 (4)	0.18636 (16)	0.0614 (7)
O2	−0.5701 (6)	0.8461 (5)	−0.3828 (2)	0.1154 (12)
N1	0.4016 (5)	0.6624 (4)	0.13459 (19)	0.0626 (8)
C1	0.1516 (5)	0.7422 (5)	0.2649 (2)	0.0531 (9)
C2	0.0685 (7)	0.7789 (7)	0.3581 (3)	0.0821 (13)
H2	−0.0829	0.8178	0.3780	0.098*
C3	0.2213 (7)	0.7550 (6)	0.4211 (3)	0.0776 (12)
H3	0.1714	0.7775	0.4855	0.093*
C4	0.4451 (7)	0.6987 (6)	0.3918 (3)	0.0671 (11)
H4	0.5434	0.6837	0.4365	0.080*
C5	0.5254 (6)	0.6646 (6)	0.2974 (3)	0.0656 (10)
H5	0.6765	0.6277	0.2771	0.079*
C6	0.3727 (5)	0.6870 (5)	0.2331 (2)	0.0503 (8)
C7	0.2032 (6)	0.7049 (5)	0.1118 (2)	0.0515 (8)
C8	0.1403 (6)	0.7046 (5)	0.0177 (2)	0.0570 (9)
H8	0.2536	0.6616	−0.0316	0.068*
C9	−0.0657 (6)	0.7607 (5)	−0.0037 (2)	0.0542 (9)
H9	−0.1763	0.7984	0.0474	0.065*
C10	−0.1412 (5)	0.7706 (4)	−0.0978 (2)	0.0463 (8)
C11	0.0027 (6)	0.7232 (6)	−0.1820 (2)	0.0635 (10)
H11	0.1551	0.6820	−0.1794	0.076*
C12	−0.0774 (6)	0.7366 (6)	−0.2684 (2)	0.0683 (11)
H12	0.0220	0.7048	−0.3237	0.082*
C13	−0.3023 (6)	0.7960 (5)	−0.2757 (2)	0.0527 (9)
C14	−0.4468 (6)	0.8462 (6)	−0.1935 (2)	0.0677 (11)
H14	−0.5991	0.8896	−0.1969	0.081*
C15	−0.3668 (6)	0.8325 (6)	−0.1066 (2)	0.0657 (10)
H15	−0.4671	0.8657	−0.0517	0.079*
C16	−0.3789 (7)	0.8041 (6)	−0.3703 (3)	0.0742 (12)
H16	−0.2727	0.7748	−0.4237	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0536 (14)	0.0881 (18)	0.0465 (14)	−0.0250 (12)	−0.0114 (11)	−0.0122 (12)
O2	0.107 (3)	0.162 (3)	0.088 (2)	−0.043 (2)	−0.032 (2)	−0.031 (2)
N1	0.0557 (19)	0.088 (2)	0.0449 (18)	−0.0203 (15)	−0.0109 (13)	−0.0166 (15)
C1	0.052 (2)	0.069 (2)	0.0400 (18)	−0.0195 (17)	−0.0139 (15)	−0.0052 (16)
C2	0.065 (3)	0.134 (4)	0.050 (2)	−0.037 (2)	0.0000 (19)	−0.019 (2)
C3	0.090 (3)	0.111 (3)	0.036 (2)	−0.039 (3)	−0.0101 (19)	−0.010 (2)
C4	0.076 (3)	0.079 (3)	0.051 (2)	−0.027 (2)	−0.0269 (19)	−0.0050 (19)
C5	0.055 (2)	0.085 (3)	0.056 (2)	−0.0169 (19)	−0.0191 (17)	−0.0127 (19)
C6	0.060 (2)	0.057 (2)	0.0340 (17)	−0.0181 (16)	−0.0107 (15)	−0.0060 (14)
C7	0.060 (2)	0.059 (2)	0.0375 (18)	−0.0216 (17)	−0.0071 (16)	−0.0062 (15)
C8	0.066 (2)	0.069 (2)	0.0406 (19)	−0.0252 (18)	−0.0082 (16)	−0.0112 (16)
C9	0.061 (2)	0.062 (2)	0.0416 (19)	−0.0204 (17)	−0.0119 (16)	−0.0080 (15)
C10	0.052 (2)	0.050 (2)	0.0389 (18)	−0.0187 (15)	−0.0114 (14)	−0.0033 (14)
C11	0.050 (2)	0.091 (3)	0.048 (2)	−0.0175 (18)	−0.0104 (16)	−0.0151 (18)
C12	0.063 (2)	0.103 (3)	0.0386 (19)	−0.022 (2)	−0.0054 (16)	−0.0207 (19)
C13	0.060 (2)	0.065 (2)	0.0383 (18)	−0.0244 (17)	−0.0130 (15)	−0.0088 (15)
C14	0.053 (2)	0.104 (3)	0.052 (2)	−0.031 (2)	−0.0103 (17)	−0.012 (2)
C15	0.058 (2)	0.099 (3)	0.043 (2)	−0.029 (2)	−0.0031 (16)	−0.0176 (19)
C16	0.063 (3)	0.096 (3)	0.069 (3)	−0.025 (2)	−0.026 (2)	−0.016 (2)

Geometric parameters (Å, °)

O1—C7	1.365 (4)	C8—C9	1.318 (5)
O1—C1	1.383 (4)	C8—H8	0.9300
O2—C16	1.202 (4)	C9—C10	1.461 (4)
N1—C7	1.292 (4)	C9—H9	0.9300
N1—C6	1.397 (4)	C10—C15	1.389 (5)
C1—C2	1.365 (5)	C10—C11	1.393 (4)
C1—C6	1.365 (4)	C11—C12	1.367 (5)
C2—C3	1.377 (5)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.381 (5)
C3—C4	1.375 (5)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.377 (5)
C4—C5	1.372 (5)	C13—C16	1.473 (5)
C4—H4	0.9300	C14—C15	1.373 (5)
C5—C6	1.393 (4)	C14—H14	0.9300
C5—H5	0.9300	C15—H15	0.9300
C7—C8	1.442 (4)	C16—H16	0.9300
C7—O1—C1	104.0 (2)	C7—C8—H8	117.5
C7—N1—C6	104.7 (3)	C8—C9—C10	127.8 (3)
C2—C1—C6	123.2 (3)	C8—C9—H9	116.1
C2—C1—O1	129.0 (3)	C10—C9—H9	116.1
C6—C1—O1	107.7 (3)	C15—C10—C11	116.9 (3)
C1—C2—C3	116.3 (4)	C15—C10—C9	119.8 (3)

C1—C2—H2	121.8	C11—C10—C9	123.3 (3)
C3—C2—H2	121.8	C12—C11—C10	120.8 (3)
C4—C3—C2	122.0 (3)	C12—C11—H11	119.6
C4—C3—H3	119.0	C10—C11—H11	119.6
C2—C3—H3	119.0	C11—C12—C13	121.7 (3)
C5—C4—C3	120.8 (3)	C11—C12—H12	119.2
C5—C4—H4	119.6	C13—C12—H12	119.2
C3—C4—H4	119.6	C14—C13—C12	118.3 (3)
C4—C5—C6	117.8 (3)	C14—C13—C16	122.5 (3)
C4—C5—H5	121.1	C12—C13—C16	119.3 (3)
C6—C5—H5	121.1	C15—C14—C13	120.2 (3)
C1—C6—C5	119.8 (3)	C15—C14—H14	119.9
C1—C6—N1	108.9 (3)	C13—C14—H14	119.9
C5—C6—N1	131.3 (3)	C14—C15—C10	122.2 (3)
N1—C7—O1	114.7 (3)	C14—C15—H15	118.9
N1—C7—C8	127.1 (3)	C10—C15—H15	118.9
O1—C7—C8	118.2 (3)	O2—C16—C13	124.1 (4)
C9—C8—C7	124.9 (3)	O2—C16—H16	118.0
C9—C8—H8	117.5	C13—C16—H16	118.0
C7—O1—C1—C2	179.6 (4)	C1—O1—C7—C8	179.7 (3)
C7—O1—C1—C6	1.5 (3)	N1—C7—C8—C9	−175.6 (3)
C6—C1—C2—C3	−0.8 (6)	O1—C7—C8—C9	3.5 (5)
O1—C1—C2—C3	−178.6 (4)	C7—C8—C9—C10	177.7 (3)
C1—C2—C3—C4	0.5 (6)	C8—C9—C10—C15	179.5 (3)
C2—C3—C4—C5	0.2 (6)	C8—C9—C10—C11	−1.4 (5)
C3—C4—C5—C6	−0.6 (6)	C15—C10—C11—C12	−0.4 (5)
C2—C1—C6—C5	0.4 (6)	C9—C10—C11—C12	−179.5 (3)
O1—C1—C6—C5	178.6 (3)	C10—C11—C12—C13	−0.4 (6)
C2—C1—C6—N1	−179.7 (4)	C11—C12—C13—C14	1.3 (6)
O1—C1—C6—N1	−1.5 (4)	C11—C12—C13—C16	−178.9 (4)
C4—C5—C6—C1	0.3 (5)	C12—C13—C14—C15	−1.5 (6)
C4—C5—C6—N1	−179.6 (3)	C16—C13—C14—C15	178.7 (4)
C7—N1—C6—C1	0.8 (4)	C13—C14—C15—C10	0.7 (6)
C7—N1—C6—C5	−179.3 (4)	C11—C10—C15—C14	0.3 (5)
C6—N1—C7—O1	0.2 (4)	C9—C10—C15—C14	179.4 (3)
C6—N1—C7—C8	179.3 (3)	C14—C13—C16—O2	−3.4 (7)
C1—O1—C7—N1	−1.1 (4)	C12—C13—C16—O2	176.8 (4)

Fig. 1