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(*Z*)-3-*o*-Tolyl-3-(*p*-tolyloxy)acrylonitrile

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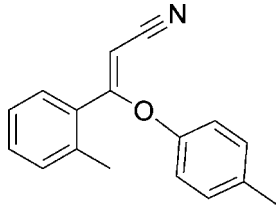
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 7.4.

The title compound, $C_{17}H_{15}NO$, exists in a Z conformation. The dihedral angle between the O-bonded benzene ring and the vinyl plane is 80.97 (18)° while the dihedral angle between the rings is 80.06 (10)°. In the crystal structure, no classical hydrogen bonds occur.

Related literature

For general background to acrylonitrile compounds and their biological, medical and pharmacological properties, see: Boedec *et al.* (2008); Napolitano *et al.* (2001); Reggio *et al.* (1998).



Experimental

Crystal data

$C_{17}H_{15}NO$ M_r = 249.30
Tetragonal, $P4_1$
a = 9.8731 (6) Å
c = 14.2455 (17) Å
V = 1388.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.40 × 0.37 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.971, T_{max} = 0.975
2539 measured reflections
1277 independent reflections
1028 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.03
1277 reflections
172 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2361).

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supplementary materials

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(*Z*)-3-*o*-Tolyl-3-(*p*-tolyloxy)acrylonitrile

Li Zhou, Chuan-Hu Wang and Mi Zhou

Comment

Acrylonitrile compounds have been widely found in dyes, agrochemicals, pharmaceutically active compounds, materials and natural products. Recent studies indicate that acrylonitrile compounds have broad range of biological, medical and pharmacological properties (Boedec *et al.*, 2008; Napolitano *et al.*, 2001; Reggio *et al.*, 1998).

As part of our interest in these materials, we report here the crystal structure of the title compound $C_{17}H_{15}NO$. The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between phenol ring and vinyl plane is 80.97 (18)°. The any hydrogen bonds in crystal structure are not found.

Experimental

For the preparation of the title compound, under nitrogen atmosphere, a sealable reaction tube equipped with a magnetic stirrer bar was charged with (*Z*)-1-(2-bromo-1-(*p*-tolyloxy)vinyl)-2-methylbenzene (1.0 mmol), $K_4Fe(CN)_6$ (0.20 mmol), Pd(O*Ac*)2 (0.01 mmol), P*Ph*$_3$ (0.02 mmol) and *DMF* (2.0 ml). Then the reaction vessel placed in an oil bath at 393 K for 12 h and it was cooled to room temperature and diluted with ethyl acetate, washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel to afford the product. Single crystals suitable for X-ray diffraction were prepared by slow evaporation of a solution of the title compound in dichloromethane at room temperature for three days.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93Å (for aryl H) and U_{iso}(H) = 1.2U_{eq}(C); C—H = 0.96Å (for methyl H) and U_{iso}(H) = 1.5U_{eq}(C) .

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

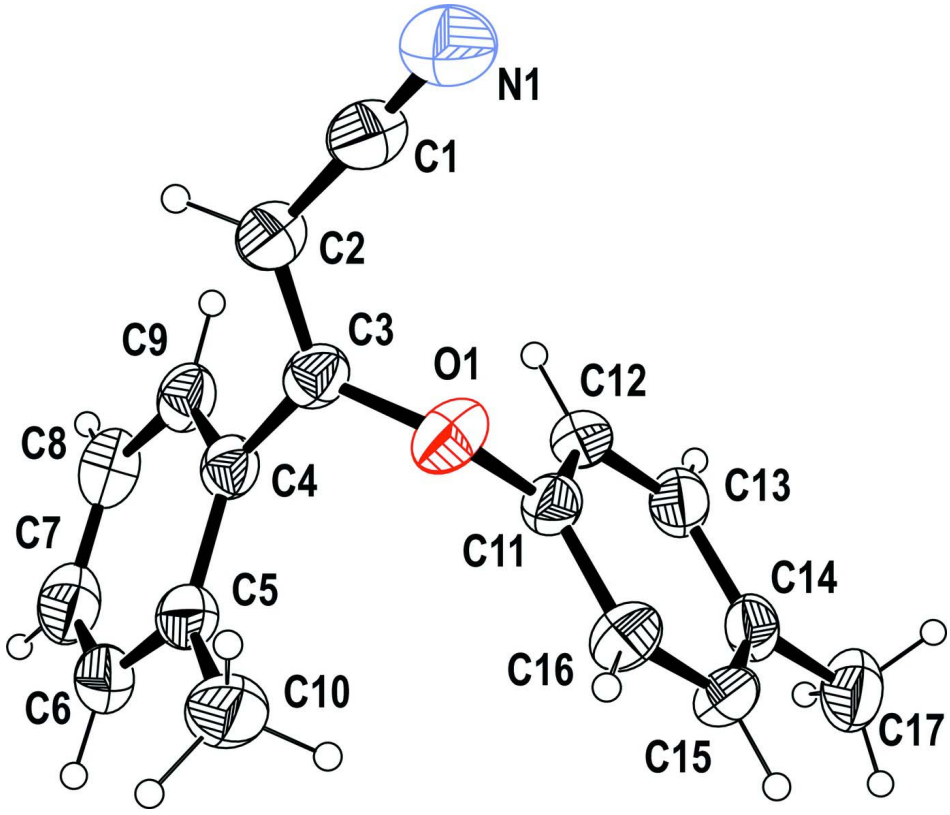

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

(*Z*)-3-*o*-Tolyl-3-(*p*-tolyloxy)acrylonitrile

Crystal data

$C_{17}H_{15}NO$
$M_r = 249.30$
Tetragonal, $P4_1$
Hall symbol: P 4w
$a = 9.8731$ (6) Å
$c = 14.2455$ (17) Å
$V = 1388.6$ (2) Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.192$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2539 reflections
$\theta = 2.9$–$25.0°$
$\mu = 0.07$ mm^{-1}
$T = 296$ K
Block, colourless
0.40 × 0.37 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.971$, $T_{max} = 0.975$
2539 measured reflections
1277 independent reflections
1028 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
$h = -8 \rightarrow 10$
$k = -1 \rightarrow 11$
$l = -16 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.03$
1277 reflections
172 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.0136P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > \sigma(F^2)$ 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}
N1	0.6863 (4)	0.6337 (4)	−0.0783 (3)	0.1013 (11)
O1	0.8869 (2)	0.4406 (2)	0.07086 (17)	0.0694 (6)
C1	0.6991 (4)	0.6132 (4)	0.0003 (3)	0.0744 (10)
C2	0.7108 (3)	0.5867 (3)	0.0981 (2)	0.0684 (9)
H2	0.6554	0.6339	0.1395	0.082*
C3	0.7979 (3)	0.4971 (3)	0.1321 (2)	0.0566 (8)
C4	0.8057 (3)	0.4605 (3)	0.2332 (2)	0.0548 (7)
C5	0.9274 (3)	0.4663 (3)	0.2842 (2)	0.0631 (9)
C6	0.9215 (4)	0.4387 (4)	0.3795 (3)	0.0772 (10)
H6	1.0008	0.4433	0.4146	0.093*
C7	0.8028 (5)	0.4049 (4)	0.4239 (3)	0.0850 (11)
H7	0.8028	0.3863	0.4879	0.102*
C8	0.6850 (4)	0.3986 (4)	0.3743 (3)	0.0751 (10)
H8	0.6046	0.3749	0.4041	0.090*
C9	0.6856 (3)	0.4278 (3)	0.2792 (2)	0.0624 (8)
H9	0.6048	0.4256	0.2457	0.075*
C10	1.0598 (4)	0.5058 (4)	0.2403 (3)	0.0883 (12)
H10A	1.1021	0.4271	0.2136	0.132*
H10B	1.1180	0.5441	0.2872	0.132*
H10C	1.0439	0.5714	0.1918	0.132*
C11	0.9107 (3)	0.3006 (3)	0.0749 (2)	0.0553 (7)
C12	0.8072 (3)	0.2094 (3)	0.0842 (2)	0.0616 (8)
H12	0.7185	0.2389	0.0922	0.074*
C13	0.8366 (3)	0.0734 (3)	0.0815 (2)	0.0684 (9)
H13	0.7662	0.0115	0.0878	0.082*
C14	0.9668 (3)	0.0254 (3)	0.0699 (2)	0.0619 (8)

C15	1.0682 (3)	0.1212 (4)	0.0605 (2)	0.0664 (9)
H15	1.1571	0.0923	0.0527	0.080*
C16	1.0413 (3)	0.2578 (3)	0.0624 (2)	0.0665 (8)
H16	1.1110	0.3203	0.0554	0.080*
C17	0.9986 (5)	−0.1231 (4)	0.0674 (3)	0.0916 (12)
H17A	0.9627	−0.1619	0.0108	0.137*
H17B	0.9583	−0.1667	0.1207	0.137*
H17C	1.0950	−0.1357	0.0689	0.137*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.103 (3)	0.108 (3)	0.094 (3)	0.0227 (19)	−0.015 (2)	0.010 (2)
O1	0.0669 (13)	0.0668 (13)	0.0746 (14)	0.0157 (10)	0.0185 (11)	0.0127 (12)
C1	0.067 (2)	0.072 (2)	0.084 (3)	0.0144 (17)	−0.008 (2)	0.001 (2)
C2	0.063 (2)	0.064 (2)	0.078 (2)	0.0093 (15)	−0.0049 (17)	−0.0066 (17)
C3	0.0467 (16)	0.0494 (17)	0.074 (2)	−0.0008 (12)	0.0016 (15)	−0.0041 (15)
C4	0.0553 (18)	0.0434 (15)	0.0658 (18)	−0.0004 (12)	−0.0002 (15)	−0.0072 (14)
C5	0.061 (2)	0.0514 (17)	0.077 (2)	0.0031 (13)	−0.0074 (16)	−0.0109 (16)
C6	0.088 (3)	0.067 (2)	0.077 (2)	0.0161 (17)	−0.017 (2)	−0.0199 (19)
C7	0.121 (4)	0.067 (2)	0.068 (2)	0.018 (2)	0.005 (2)	−0.0021 (19)
C8	0.089 (3)	0.059 (2)	0.078 (2)	−0.0003 (17)	0.023 (2)	−0.0041 (18)
C9	0.0614 (19)	0.0491 (17)	0.077 (2)	−0.0019 (13)	0.0068 (17)	−0.0099 (15)
C10	0.057 (2)	0.091 (3)	0.117 (3)	−0.0069 (18)	−0.005 (2)	−0.017 (2)
C11	0.0558 (17)	0.0632 (18)	0.0469 (15)	0.0122 (13)	0.0033 (14)	−0.0001 (15)
C12	0.0468 (17)	0.076 (2)	0.0620 (19)	0.0082 (14)	−0.0024 (15)	−0.0101 (17)
C13	0.065 (2)	0.073 (2)	0.067 (2)	−0.0043 (15)	0.0040 (17)	−0.0162 (17)
C14	0.074 (2)	0.0666 (19)	0.0447 (14)	0.0082 (15)	0.0018 (16)	−0.0084 (15)
C15	0.0545 (18)	0.077 (2)	0.068 (2)	0.0224 (15)	0.0023 (16)	−0.0042 (18)
C16	0.0511 (17)	0.073 (2)	0.076 (2)	0.0045 (15)	0.0126 (16)	0.0005 (18)
C17	0.120 (3)	0.076 (2)	0.078 (2)	0.021 (2)	0.006 (2)	−0.013 (2)

Geometric parameters (Å, º)

N1—C1	1.145 (5)	C10—H10A	0.9600
O1—C3	1.358 (4)	C10—H10B	0.9600
O1—C11	1.403 (4)	C10—H10C	0.9600
C1—C2	1.421 (5)	C11—C12	1.369 (5)
C2—C3	1.326 (4)	C11—C16	1.368 (4)
C2—H2	0.9300	C12—C13	1.374 (5)
C3—C4	1.487 (4)	C12—H12	0.9300
C4—C9	1.393 (4)	C13—C14	1.380 (5)
C4—C5	1.406 (4)	C13—H13	0.9300
C5—C6	1.386 (5)	C14—C15	1.383 (5)
C5—C10	1.501 (5)	C14—C17	1.500 (5)
C6—C7	1.373 (6)	C15—C16	1.375 (5)
C6—H6	0.9300	C15—H15	0.9300
C7—C8	1.362 (6)	C16—H16	0.9300
C7—H7	0.9300	C17—H17A	0.9600
C8—C9	1.384 (5)	C17—H17B	0.9600

C8—H8	0.9300	C17—H17C	0.9600
C9—H9	0.9300		
C3—O1—C11	119.2 (2)	H10A—C10—H10B	109.5
N1—C1—C2	178.3 (4)	C5—C10—H10C	109.5
C3—C2—C1	122.2 (3)	H10A—C10—H10C	109.5
C3—C2—H2	118.9	H10B—C10—H10C	109.5
C1—C2—H2	118.9	C12—C11—C16	120.8 (3)
C2—C3—O1	117.3 (3)	C12—C11—O1	121.8 (2)
C2—C3—C4	123.4 (3)	C16—C11—O1	117.2 (3)
O1—C3—C4	119.3 (3)	C11—C12—C13	118.9 (3)
C9—C4—C5	119.6 (3)	C11—C12—H12	120.6
C9—C4—C3	117.9 (3)	C13—C12—H12	120.6
C5—C4—C3	122.3 (3)	C12—C13—C14	122.4 (3)
C6—C5—C4	117.5 (3)	C12—C13—H13	118.8
C6—C5—C10	119.8 (3)	C14—C13—H13	118.8
C4—C5—C10	122.6 (3)	C13—C14—C15	116.8 (3)
C7—C6—C5	122.4 (4)	C13—C14—C17	122.2 (3)
C7—C6—H6	118.8	C15—C14—C17	121.0 (3)
C5—C6—H6	118.8	C16—C15—C14	122.0 (3)
C8—C7—C6	120.0 (4)	C16—C15—H15	119.0
C8—C7—H7	120.0	C14—C15—H15	119.0
C6—C7—H7	120.0	C11—C16—C15	119.2 (3)
C7—C8—C9	119.6 (4)	C11—C16—H16	120.4
C7—C8—H8	120.2	C15—C16—H16	120.4
C9—C8—H8	120.2	C14—C17—H17A	109.5
C8—C9—C4	120.8 (3)	C14—C17—H17B	109.5
C8—C9—H9	119.6	H17A—C17—H17B	109.5
C4—C9—H9	119.6	C14—C17—H17C	109.5
C5—C10—H10A	109.5	H17A—C17—H17C	109.5
C5—C10—H10B	109.5	H17B—C17—H17C	109.5
C1—C2—C3—O1	6.7 (5)	C7—C8—C9—C4	1.5 (5)
C1—C2—C3—C4	−175.6 (3)	C5—C4—C9—C8	−1.2 (4)
C11—O1—C3—C2	−135.9 (3)	C3—C4—C9—C8	−177.1 (3)
C11—O1—C3—C4	46.3 (4)	C3—O1—C11—C12	44.3 (4)
C2—C3—C4—C9	49.1 (4)	C3—O1—C11—C16	−140.2 (3)
O1—C3—C4—C9	−133.3 (3)	C16—C11—C12—C13	0.5 (5)
C2—C3—C4—C5	−126.8 (3)	O1—C11—C12—C13	175.8 (3)
O1—C3—C4—C5	50.8 (4)	C11—C12—C13—C14	0.1 (5)
C9—C4—C5—C6	0.0 (4)	C12—C13—C14—C15	−0.2 (5)
C3—C4—C5—C6	175.7 (3)	C12—C13—C14—C17	179.8 (3)
C9—C4—C5—C10	−177.6 (3)	C13—C14—C15—C16	−0.2 (5)
C3—C4—C5—C10	−1.9 (4)	C17—C14—C15—C16	179.9 (3)
C4—C5—C6—C7	0.9 (5)	C12—C11—C16—C15	−0.8 (5)
C10—C5—C6—C7	178.6 (3)	O1—C11—C16—C15	−176.4 (3)
C5—C6—C7—C8	−0.6 (5)	C14—C15—C16—C11	0.7 (5)
C6—C7—C8—C9	−0.7 (5)		