Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

p-Anisolecarbonitrile

M. J. Gerald Lesley,[a] Mark R. Pineau,[a] Allen D. Hunter[b]* and Matthias Zeller[b]

[a]Department of Chemistry, Southern Connecticut State University, 501 Crescent St, Jennings Hall Room 308 (JE308), New Haven, CT 06515-1355, USA, and [b]Department of Chemistry, Youngstown State University, One University Plaza, Youngstown, OH 44555, USA

Correspondence e-mail: adhunter@ysu.edu

Received 1 September 2004
Accepted 14 September 2004
Online 9 October 2004

Key indicators

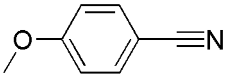
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of *p*-anisolecarbonitrile, C_8H_7NO, was determined by single-crystal X-ray diffraction at 100 K. It crystallizes in the monoclinic space group $P2_1/c$ with two crystallographically independent molecules in the asymmetric unit.

Comment

In the course of our work on the synthesis of boronimines, we were able to isolate single crystals of one of the starting materials, *viz.* *p*-anisolecarbonitrile, (I). It was found to crystallize in the monoclinic space group $P2_1/c$ with two crystallographically independent molecules in the asymmetric unit (Fig. 1). All bond lengths and angles are in the expected ranges and the geometries of both molecules are basically identical with a weighted r.m.s. deviation of only 0.0293 Å. The molecules are planar with the methoxy groups lying in the plane of the aromatic rings.



(I)

The structure consists of sheets of molecules parallel to the (100) plane, with the molecules themselves slightly tilted out these planes. Parallel sheets stack, forming an *AABBAABB*-type layered structure where all the *A* layers contain one of the two independent molecules in the asymmetric unit and the *B* layers are made up of the second crystallograpically unique molecule (Fig. 2). Centers of symmetry are found within each *AA* and *BB* layer, and the distances between the *AA*, the *AB* and the *BB* planes (by way of the benzene ring centers) are 1.8246 (14), 1.8019 (12) and 1.8156 (14) Å, respectively. In each layer the molecules are offset with respect to the layer above and below, thus allowing for close packing. For one of the symmetry-independent molecules, the molecular axis is roughly aligned with the *c* axis, while the second molecule is tilted by approximately 30°.

Experimental

Solid anisolecarbonitrile (1.000 g, 7.51 mmol) was dissolved in tetrahydrofuran (THF, 60 ml) and a solution of hexylborane (0.810 g, 8.26 mmol) in THF (10 ml) was added dropwise via syringe under a nitrogen atmosphere. The reaction mixture was stirred at ambient temperature for 24 h and washed with water (2 × 20 l). The organic layer was dried over $MgSO_4$, filtered, and the filtrate was reduced *in vacuo* yielding a pale-yellow solid of the crude yellow aldiminoborane dimer (1.285 g, 74.0%). A sample (0.500 g, 1.08 mmol) was reacted with *p*-tolylacetylene (0.264 g, 2.27 mmol) in toluene at 363 K for 24 h. Careful layering with hexanes yielded two types of single crystals of X-ray quality, which were found to be *p*-anisolenitrile and tris(*p*-methoxybenzyl)amine.

Crystal data

C_8H_7NO
$M_r = 133.15$
Monoclinic, $P2_1/c$
$a = 7.5924$ (7) Å
$b = 8.6639$ (8) Å
$c = 21.7191$ (19) Å
$\beta = 107.396$ (2)°
$V = 1363.3$ (2) Å^3
$Z = 8$

$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5279 reflections
$\theta = 2.5$–28.3°
$\mu = 0.09$ mm^{-1}
$T = 100$ (2) K
Block, colorless
$0.50 \times 0.46 \times 0.30$ mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS* in *SAINT-Plus*; Bruker, 2003)
$T_{\min} = 0.725$, $T_{\max} = 0.97$
12523 measured reflections

3084 independent reflections
2818 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 28.3°$
$h = -10 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.115$
$S = 1.09$
3084 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.3082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.1516 (16)	C11—N2	1.1508 (15)
C1—C2	1.4326 (15)	C11—C12	1.4361 (15)
C2—C3	1.3948 (15)	C12—C13	1.3972 (15)
C2—C7	1.4015 (15)	C12—C17	1.3990 (15)
C3—C4	1.3827 (16)	C13—C14	1.3868 (15)
C4—C5	1.3943 (15)	C14—C15	1.3922 (15)
C5—O1	1.3575 (13)	C15—O2	1.3584 (12)
C6—C7	1.3734 (16)	C15—C16	1.3990 (15)
C8—O1	1.4274 (14)	C16—C17	1.3730 (16)
N1—C1—C2	178.94 (12)	C13—C12—C17	119.65 (10)
C3—C2—C7	119.78 (10)	C13—C12—C11	120.70 (10)
C3—C2—C1	120.59 (10)	C17—C12—C11	119.65 (10)
C7—C2—C1	119.63 (10)	C14—C13—C12	120.46 (10)
C4—C3—C2	120.32 (10)	C13—C14—C15	119.43 (10)
C3—C4—C5	119.51 (10)	O2—C15—C14	124.34 (10)
O1—C5—C4	124.21 (10)	O2—C15—C16	115.55 (9)
O1—C5—C6	115.44 (9)	C14—C15—C16	120.11 (10)
C4—C5—C6	120.35 (10)	C17—C16—C15	120.40 (10)
C7—C6—C5	120.03 (10)	C16—C17—C12	119.94 (10)
C6—C7—C2	120.01 (10)	C5—O1—C8	117.77 (9)
N2—C11—C12	179.32 (13)	C15—O2—C18	117.58 (8)

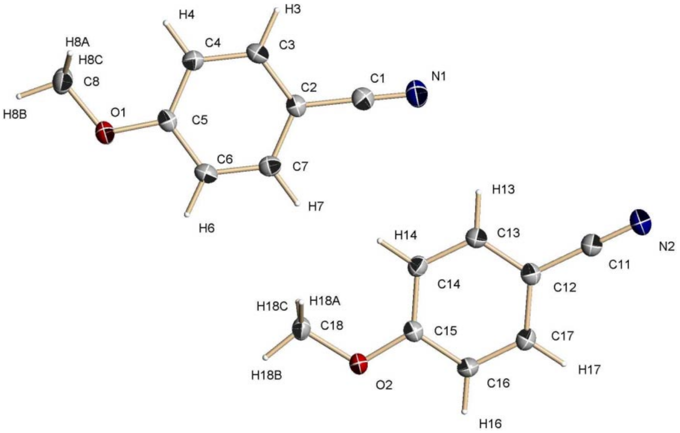


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids.

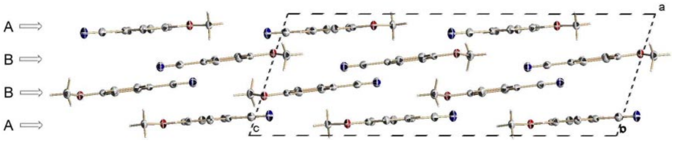


Figure 2
Packing representation showing the layered *AABBAA* pattern.

Methyl H atoms were positioned geometrically with a C—H distance of 0.98 Å and were refined as riding, with an isotropic displacement parameter 1.5 times that of the $U_{\rm eq}$ value of the parent C atom. All other H atoms were located in a difference density Fourier map and were isotropically refined, giving C—H = 0.944 (15)–1.004 (15) Å. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000).

Data collection: *SMART* (Bruker, 1997–2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

MZ was supported by NSF grant 0111511, CLP by ACS PRF grant 37228-B3 and the diffractometer was funded by NSF grant 0087210, by the Ohio Board of Regents grant CAP-491, and by YSU.

References

Bruker (1997–2002). *SMART for WNT*/2000. Version 5.630. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT-Plus*. Version 6.45. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Herbstein, F. H. (2000). *Acta Cryst.* B**56**, 547–557.

o1938 M. J. Gerald Lesley *et al.* • C_8H_7NO *Acta Cryst.* (2004). E**60**, o1937–o1938