Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
O1	0.2393 (2)	0.4422 (2)	0.1670 (2)	0.0663 (4)
O2	0.0070 (2)	0.2891 (2)	0.1023 (2)	0.0860 (5)
C1	0.3402 (2)	0.1541 (2)	0.3451 (2)	0.0370 (4)
C2	0.1858 (3)	0.3089 (2)	0.1932 (2)	0.0404 (5)
B1	0.6253 (3)	0.0983 (3)	0.3941 (3)	0.0435 (5)
B2	0.4480 (3)	0.2554 (3)	0.5596 (3)	0.0419 (5)
B3	0.2349 (3)	0.1632 (3)	0.5394 (3)	0.0429 (5)
B4	0.2813 (3)	−0.0511 (3)	0.3608 (3)	0.0434 (5)
B5	0.5225 (3)	−0.0924 (3)	0.2703 (3)	0.0433 (5)

Table 2. *Selected geometric parameters* (Å, °)

O1—C2	1.221 (1)	B1—B5	1.795 (2)
O2—C2	1.262 (1)	B1—B3′	1.759 (2)
C2—C1	1.515 (1)	B1—B4′	1.753 (2)
C1—B1	1.712 (2)	B2—B3	1.794 (2)
C1—B2	1.708 (2)	B2—B4′	1.756 (2)
C1—B3	1.709 (2)	B2—B5′	1.760 (2)
C1—B4	1.716 (2)	B3—B4	1.777 (2)
C1—B5	1.708 (2)	B3—B5′	1.761 (2)
B1—B2	1.771 (2)	B4—B5	1.784 (2)
O1—C2—O2	124.7 (1)	C1—B2—B5′	103.99 (8)
O1—C2—C1	119.34 (9)	B1—B2—B3	108.10 (8)
O2—C2—C1	115.92 (9)	B1—B2—B4′	59.61 (7)
C2—C1—B1	116.22 (8)	B3—B2—B5′	59.40 (7)
C2—C1—B2	116.43 (8)	B4′—B2—B5′	60.98 (7)
C2—C1—B3	118.09 (8)	C1—B3—B1′	104.33 (8)
C2—C1—B4	118.77 (8)	C1—B3—B2	58.30 (6)
C2—C1—B5	117.83 (8)	C1—B3—B4	58.96 (6)
B1—C1—B2	62.37 (7)	C1—B3—B5′	103.92 (8)
B1—C1—B3	115.09 (8)	B1′—B3—B4	59.45 (7)
B1—C1—B4	115.43 (8)	B1′—B3—B5′	61.31 (7)
B1—C1—B5	63.31 (7)	B2—B3—B4	108.15 (8)
B2—C1—B3	63.36 (7)	B2—B3—B5′	59.33 (7)
B2—C1—B4	115.24 (8)	C1—B4—B1′	104.25 (8)
B2—C1—C5	115.00 (8)	C1—B4—B2′	104.01 (8)
B3—C1—B4	62.50 (7)	C1—B4—B3	58.54 (6)
B3—C1—B5	114.71 (7)	C1—B4—B5	58.38 (6)
B4—C1—B5	62.80 (7)	B1′—B4—B2′	60.62 (7)
C1—B1—B2	58.70 (7)	B1′—B4—B3	59.77 (7)
C1—B1—B3′	103.85 (8)	B2′—B4—B5	59.62 (7)
C1—B1—B4′	104.31 (8)	B3—B4—B5	107.80 (8)
C1—B1—B5	58.24 (6)	C1—B5—B1	58.45 (7)
B2—B1—B4′	59.76 (7)	C1—B5—B2′	104.18 (8)
B2—B1—B5	107.79 (8)	C1—B5—B3′	103.92 (8)
B3′—B1—B5	59.40 (7)	C1—B5—B4	58.83 (6)
B4′—B1—B3′	60.78 (7)	B1—B5—B3′	59.28 (7)
C1—B2—B1	58.92 (7)	B1—B5—B4	108.15 (9)
C1—B2—B3	58.34 (6)	B2′—B5—B3′	61.27 (7)
C1—B2—B4′	104.36 (8)	B2′—B5—B4	59.40 (7)

For the H atom of the carboxy group, two sites were found by difference Fourier synthesis, bonded to O2 and O1 (a disorder in the orientation of the carboxy group is present). The sites were given occupancies of 0.7 and 0.3, respectively, and refined using a riding model with $U_{iso}(H) = U_{eq}(O)$. Refinement was by full-matrix least squares. Program(s) used to solve structure: *MULTAN*11/82 (Main *et al.*, 1982). Program(s) used to refine structure: *SDP/PDP* (Enraf-Nonius, 1985). All calculations were run on a MicroVAXII computer.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, bond distances and angles involving H atoms, and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71774 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: NA1058]

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N-[2-(7-Methoxy-1-naphthyl)ethyl]-acetamide, a Potent Melatonin Analog

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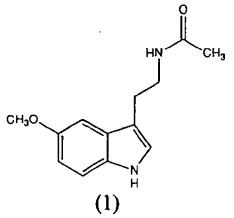
Abstract

The four crystallographically independent molecules present in the unit cell of *N*-[2-(7-methoxy-1-naphthyl)-ethyl]acetamide, $C_{15}H_{17}NO_2$, are very similar; the naphthalene ring is planar, the methoxy substituent is staggered

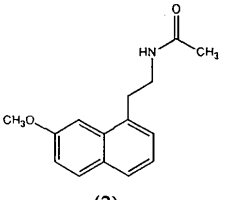
and the side chain is oriented so that the amide and aromatic groups are approximately parallel. This conformation of the longer side chain is different from the fully extended conformation observed in the neurohormone melatonin.

Comment

The neurohormone melatonin [*N*-acetyl-5-methoxytryptamine, (1)] is mainly secreted by the pineal gland. This secretion is influenced by the daily and seasonal changes in the light-darkness cycle, the highest levels being observed during the dark period. Melatonin has been shown to be involved in the regulation of various physiological processes including biological rhythms and neuroendocrine functions. It offers, therefore, considerable interest for future therapeutic prospects such as the treatment of disturbed circadian rhythms.



(1)



(2)

This interest prompted us to develop new melatonin receptor ligands and led to the synthesis of a naphthalenic bioisostere, *N*-[2-(7-methoxy-1-naphthyl)-ethyl]acetamide (2) (Yous, Andrieux & Howell, 1992). This compound shows higher affinity and potency than melatonin (Dubucovich, North, Oakley & Hagan, 1993) and therapeutic potential as a chronobiotic drug for the treatment of circadian rhythm disorders (Bonnefond, Martinet, Lesieur, Adam & Guardiola, 1993; Redman & Guardiola, 1993).

There are four molecules in the asymmetric part of the unit cell. All four molecules are very similar; one of them is shown in Fig. 1. An approximate non-crystallographic center of symmetry located at 0.625, 0.4, 0.375 is observed between the two pairs of molecules *A*,*B* and *C*,*D*.

In each of the four independent molecules the naphthalene ring is planar within experimental error. The maximum deviations from the mean plane through the ten atoms are: C3′ 0.023 (6) Å in molecule *A*, C3′ 0.019 (5) Å in molecule *B*, C1′ 0.035 (5) Å in molecule *C* and C2′ 0.026 (7) Å in molecule *D*. The methoxy group is close to the plane of the ring and the conformation about the C7′—O9 bond is staggered (*sp*) with torsion angles C8′—C7′—O9—C10 of −2.8 (9), −6.3 (10), −4.2 (8) and −3.5 (9)° for molecules *A*, *B*, *C* and *D*, respectively. The longer side chain also has a similar conformation in the four independent molecules. The amide and the naphthalene planes are approximately parallel, the dihedral angles between the mean planes being 12, 16, 8 and 13° in molecules *A*, *B*, *C* and *D*, respectively. This conformation has been observed for one of the two independent molecules of *N*-cyclopropylcarbonyl-2-(7-methoxy-1-naphthyl)ethylamine, another melatoninergic agonist (Tinant, Declercq, Poupaert & Lesieur, 1993). However, this conformation is different from that of the neurohormone. In melatonin, the side chain adopts a fully extended conformation with all the non-H atoms in the same plane as the indole ring (Mostad & Romming, 1974; Quarles, Templeton & Zalkin, 1974; Wakahara, Fujiwara & Tomita, 1972). The average distance between the methoxy O atom O9 and the amide H atom H2, *i.e.* the two presumed polar anchoring points on the receptor (Lesieur, 1992), is 7.01 Å. By comparison this distance is 7.34 Å in melatonin (Mostad & Romming, 1974) and 6.98 Å in molecule *A* of *N*-cyclopropylcarbonyl-2-(7-methoxy-1-naphthyl)ethylamine (Tinant *et al.*, 1993).

The molecules are arranged in dimers by hydrogen bonding between the carbonyl O atoms and the amide H atoms. The geometry of the four hydrogen bonds observed in the structure is given in Table 3.

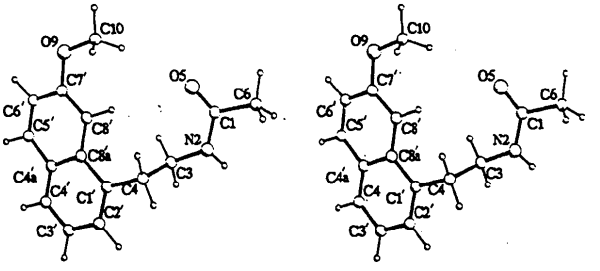


Fig. 1. Stereoview of one of the four independent molecules, showing the atom-numbering scheme. For each independent molecule the atom labels are appended by *A*, *B*, *C* or *D* for molecules *A*, *B*, *C* and *D*, respectively.

Experimental

Crystal data

$C_{15}H_{17}NO_2$
M_r = 243.30
Orthorhombic
$Pca2_1$
a = 31.501 (4) Å
b = 9.5280 (10) Å
c = 17.906 (2) Å
V = 5374.3 (11) Å^3
Z = 16
D_x = 1.203 Mg m^{-3}
Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 29 reflections
θ = 12–30°
μ = 0.603 mm^{-1}
T = 293 (2) K
Parallelepiped
0.15 × 0.10 × 0.08 mm
Colorless

Data collection

Huber four-circle diffractometer
$\theta/2\theta$ scans
Absorption correction: none
4913 measured reflections
4913 independent reflections
2496 observed reflections [$I > 2\sigma(I)$]
θ_{max} = 67.50°
h = 0 → 37
k = 0 → 10
l = 0 → 21
1 standard reflection monitored every 50 reflections
intensity variation: none

Refinement

Refinement on F^2
$R(F) = 0.057$
$wR(F^2) = 0.125$
$S = 1.165$
4913 reflections
661 parameters
Only H-atom U's refined (one common value for all H atoms)
Calculated weights $w = 1/[\sigma^2(F_o^2) + (0.0796P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.046$
$\Delta\rho_{max} = 0.143$ e Å^{-3}
$\Delta\rho_{min} = -0.161$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C1′*A*	0.8788 (2)	0.9266 (6)	0.4821†	0.066 (2)
C2′*A*	0.9027 (2)	0.8070 (7)	0.4909 (5)	0.083 (2)
C3′*A*	0.9460 (2)	0.8166 (9)	0.5041 (5)	0.094 (2)
C4′*A*	0.9649 (2)	0.9414 (9)	0.5116 (5)	0.092 (2)
C4′a*A*	0.9422 (2)	1.0667 (8)	0.5044 (4)	0.073 (2)
C5′*A*	0.9604 (2)	1.2015 (8)	0.5112 (5)	0.086 (2)
C6′*A*	0.9381 (2)	1.3198 (8)	0.5019 (5)	0.088 (2)
C7′*A*	0.8945 (2)	1.3131 (7)	0.4861 (4)	0.0653 (14)
C8′*A*	0.8753 (2)	1.1869 (6)	0.4800 (4)	0.0643 (15)
C8′a*A*	0.8982 (2)	1.0605 (6)	0.4889 (4)	0.0589 (13)
O9*A*	0.87520 (13)	1.4412 (4)	0.4789 (4)	0.0807 (12)
C10*A*	0.8311 (2)	1.4390 (6)	0.4601 (5)	0.093 (2)
C1*A*	0.7402 (2)	1.0474 (7)	0.5443 (5)	0.076 (2)
N2*A*	0.76229 (13)	0.9309 (5)	0.5428 (4)	0.0712 (14)
C3*A*	0.8082 (2)	0.9325 (6)	0.5478 (5)	0.073 (2)
C4*A*	0.8306 (2)	0.9139 (6)	0.4723 (5)	0.072 (2)
O5*A*	0.75583 (15)	1.1639 (4)	0.5478 (5)	0.1022 (15)
C6*A*	0.6929 (2)	1.0266 (7)	0.5454 (6)	0.103 (2)
C1′*B*	0.6974 (2)	0.3849 (6)	0.3080 (5)	0.0612 (14)
C2′*B*	0.6944 (2)	0.2531 (7)	0.2790 (5)	0.081 (2)
C3′*B*	0.6710 (2)	0.2234 (8)	0.2147 (6)	0.100 (2)
C4′*B*	0.6516 (2)	0.3292 (9)	0.1795 (5)	0.087 (2)
C4′a*B*	0.6529 (2)	0.4676 (7)	0.2067 (5)	0.070 (2)
C5′*B*	0.6329 (2)	0.5788 (10)	0.1707 (5)	0.091 (2)
C6′*B*	0.6339 (2)	0.7103 (10)	0.1967 (5)	0.096 (2)
C7′*B*	0.6564 (2)	0.7396 (7)	0.2629 (5)	0.085 (2)
C8′*B*	0.6775 (2)	0.6357 (6)	0.3002 (5)	0.068 (2)
C8′a*B*	0.67659 (15)	0.4975 (6)	0.2723 (4)	0.0558 (14)
O9*B*	0.6540 (2)	0.8732 (5)	0.2862 (5)	0.125 (2)
C10*B*	0.6706 (3)	0.9070 (7)	0.3570 (6)	0.132 (3)
C1*B*	0.7296 (2)	0.5539 (7)	0.5418 (5)	0.065 (2)
N2*B*	0.71674 (15)	0.4319 (5)	0.5161 (4)	0.0630 (13)
C3*B*	0.6931 (2)	0.4191 (6)	0.4467 (4)	0.0649 (15)
C4*B*	0.7219 (2)	0.4076 (6)	0.3792 (4)	0.067 (2)
O5*B*	0.72237 (12)	0.6646 (5)	0.5090 (4)	0.0885 (14)
C6*B*	0.7536 (2)	0.5486 (7)	0.6138 (5)	0.098 (2)
C1′*C*	0.5649 (2)	0.4155 (6)	0.4611 (5)	0.072 (2)
C2′*C*	0.5770 (2)	0.2924 (7)	0.4956 (5)	0.094 (2)
C3′*C*	0.6016 (2)	0.2962 (9)	0.5610 (6)	0.093 (2)
C4′*C*	0.6125 (2)	0.4173 (11)	0.5914 (5)	0.096 (2)
C4′a*C*	0.6019 (2)	0.5461 (9)	0.5581 (5)	0.074 (2)
C5′*C*	0.6120 (2)	0.6787 (10)	0.5897 (5)	0.088 (2)
C6′*C*	0.6011 (2)	0.7988 (8)	0.5576 (5)	0.087 (2)
C7′*C*	0.5784 (2)	0.7976 (8)	0.4901 (5)	0.077 (2)
C8′*C*	0.5672 (2)	0.6745 (6)	0.4571 (5)	0.0653 (15)
C8′a*C*	0.5779 (2)	0.5471 (7)	0.4908 (5)	0.0639 (14)
O9*C*	0.56913 (15)	0.9285 (4)	0.4620 (4)	0.0962 (13)
C10*C*	0.5486 (3)	0.9323 (7)	0.3904 (5)	0.113 (3)
C1*C*	0.5227 (2)	0.5643 (6)	0.2276 (4)	0.0596 (15)
N2*C*	0.5377 (2)	0.4439 (5)	0.2528 (4)	0.0724 (13)
C3*C*	0.5647 (2)	0.4355 (6)	0.3220 (5)	0.073 (2)
C4*C*	0.5372 (2)	0.4114 (6)	0.3900 (4)	0.077 (2)
O5*C*	0.52864 (12)	0.6772 (4)	0.2586 (4)	0.0829 (12)
C6*C*	0.4990 (2)	0.5529 (7)	0.1554 (5)	0.088 (2)
C1′*D*	0.3792 (2)	−0.0534 (7)	0.2801 (4)	0.074 (2)
C2′*D*	0.3556 (2)	−0.1724 (7)	0.2706 (5)	0.097 (2)
C3′*D*	0.3107 (2)	−0.1628 (9)	0.2572 (6)	0.112 (3)
C4′*D*	0.2918 (2)	−0.0383 (9)	0.2569 (5)	0.099 (2)
C4′a*D*	0.3145 (2)	0.0858 (8)	0.2671 (5)	0.078 (2)
C5′*D*	0.2950 (2)	0.2205 (9)	0.2683 (5)	0.090 (2)
C6′*D*	0.3167 (2)	0.3375 (8)	0.2796 (5)	0.089 (2)
C7′*D*	0.3608 (2)	0.3323 (7)	0.2895 (4)	0.070 (2)
C8′*D*	0.3816 (2)	0.2067 (6)	0.2898 (4)	0.070 (2)
C8′a*D*	0.3594 (2)	0.0785 (7)	0.2791 (4)	0.068 (2)
O9*D*	0.38048 (14)	0.4589 (4)	0.2990 (4)	0.0915 (13)
C10*D*	0.4249 (2)	0.4576 (7)	0.3140 (6)	0.105 (2)
C1*D*	0.5163 (2)	0.0671 (6)	0.2128 (4)	0.0641 (15)
N2*D*	0.49416 (15)	−0.0482 (5)	0.2174 (4)	0.0683 (13)
C3*D*	0.4481 (2)	−0.0484 (6)	0.2152 (5)	0.071 (2)
C4*D*	0.4263 (2)	−0.0680 (6)	0.2905 (4)	0.075 (2)
O5*D*	0.49997 (13)	0.1838 (4)	0.2106 (4)	0.0933 (14)
C6*D*	0.5641 (2)	0.0524 (7)	0.2085 (5)	0.086 (2)

† Coordinate fixed to define origin.

Table 2. *Selected geometric parameters* (Å, °)

C1′*A*—C2′*A*	1.376 (7)	C1′*B*—C2′*B*	1.362 (8)
C1′*A*—C8′a*A*	1.420 (7)	C1′*B*—C8′a*B*	1.410 (7)
C1′*A*—C4*A*	1.532 (7)	C1′*B*—C4*B*	1.505 (8)
C2′*A*—C3′*A*	1.386 (9)	C2′*B*—C3′*B*	1.397 (9)
C3′*A*—C4′*A*	1.336 (9)	C3′*B*—C4′*B*	1.337 (9)
C4′*A*—C4′a*A*	1.398 (8)	C4′*B*—C4′a*B*	1.407 (8)
C4′a*A*—C5′*A*	1.412 (8)	C4′a*B*—C5′*B*	1.390 (9)
C4′a*A*—C8′a*A*	1.415 (7)	C4′a*B*—C8′a*B*	1.420 (8)
C5′*A*—C6′*A*	1.338 (8)	C5′*B*—C6′*B*	1.336 (10)
C6′*A*—C7′*A*	1.404 (8)	C6′*B*—C7′*B*	1.411 (10)
C7′*A*—C8′*A*	1.350 (7)	C7′*B*—O9*B*	1.341 (7)
C7′*A*—O9*A*	1.370 (6)	C7′*B*—C8′*B*	1.366 (8)
C8′*A*—C8′a*A*	1.412 (7)	C8′*B*—C8′a*B*	1.409 (8)
O9*A*—C10*A*	1.431 (7)	O9*B*—C10*B*	1.409 (10)
C1*A*—O5*A*	1.216 (6)	C1*B*—O5*B*	1.228 (7)
C1*A*—N2*A*	1.310 (6)	C1*B*—N2*B*	1.314 (7)
C1*A*—C6*A*	1.504 (8)	C1*B*—C6*B*	1.496 (9)
N2*A*—C3*A*	1.448 (6)	N2*B*—C3*B*	1.453 (7)
C3*A*—C4*A*	1.536 (8)	C3*B*—C4*B*	1.516 (7)
C1′*C*—C2′*C*	1.380 (8)	C1′*D*—C2′*D*	1.366 (8)
C1′*C*—C8′a*C*	1.422 (8)	C1′*D*—C8′a*D*	1.403 (7)
C1′*C*—C4*C*	1.543 (8)	C1′*D*—C4*D*	1.500 (7)
C2′*C*—C3′*C*	1.405 (10)	C2′*D*—C3′*D*	1.438 (9)
C3′*C*—C4′*C*	1.321 (9)	C3′*D*—C4′*D*	1.327 (10)
C4′*C*—C4′a*C*	1.404 (10)	C4′*D*—C4′a*D*	1.394 (9)
C4′a*C*—C5′*C*	1.420 (9)	C4′a*D*—C5′*D*	1.422 (9)
C4′a*C*—C8′a*C*	1.423 (8)	C4′a*D*—C8′a*D*	1.433 (7)
C5′*C*—C6′*C*	1.325 (9)	C5′*D*—C6′*D*	1.324 (9)
C6′*C*—C7′*C*	1.406 (9)	C6′*D*—C7′*D*	1.399 (8)
C7′*C*—C8′*C*	1.360 (8)	C7′*D*—C8′*D*	1.366 (7)
C7′*C*—O9*C*	1.377 (7)	C7′*D*—O9*D*	1.367 (7)
C8′*C*—C8′a*C*	1.397 (8)	C8′*D*—C8′a*D*	1.420 (7)
O9*C*—C10*C*	1.436 (8)	O9*D*—C10*D*	1.426 (7)
C1*C*—O5*C*	1.226 (6)	C1*D*—O5*D*	1.226 (6)
C1*C*—N2*C*	1.321 (6)	C1*D*—N2*D*	1.305 (6)
C1*C*—C6*C*	1.496 (8)	C1*D*—C6*D*	1.514 (8)
N2*C*—C3*C*	1.504 (7)	N2*D*—C3*D*	1.452 (7)
C3*C*—C4*C*	1.512 (8)	C3*D*—C4*D*	1.524 (8)
C2′*A*—C1′*A*—C8′a*A*	119.9 (5)	C2′*B*—C1′*B*—C8′a*B*	119.8 (6)
C2′*A*—C1′*A*—C4*A*	119.4 (6)	C2′*B*—C1′*B*—C4*B*	119.3 (5)
C8′a*A*—C1′*A*—C4*A*	120.5 (5)	C8′a*B*—C1′*B*—C4*B*	120.9 (5)
C1′*A*—C2′*A*—C3′*A*	120.3 (6)	C1′*B*—C2′*B*—C3′*B*	122.5 (7)
C4′*A*—C3′*A*—C2′*A*	120.9 (7)	C4′*B*—C3′*B*—C2′*B*	118.5 (7)
C3′*A*—C4′*A*—C4′a*A*	121.5 (6)	C3′*B*—C4′*B*—C4′a*B*	122.0 (7)
C4′*A*—C4′a*A*—C5′*A*	124.1 (6)	C5′*B*—C4′a*B*—C4′*B*	122.8 (7)
C4′*A*—C4′a*A*—C8′a*A*	118.9 (6)	C5′*B*—C4′a*B*—C8′a*B*	117.9 (6)
C5′*A*—C4′a*A*—C8′a*A*	117.0 (6)	C4′*B*—C4′a*B*—C8′a*B*	119.3 (6)
C6′*A*—C5′*A*—C4′a*A*	122.8 (6)	C6′*B*—C5′*B*—C4′a*B*	122.9 (7)
C5′*A*—C6′*A*—C7′*A*	120.0 (6)	C5′*B*—C6′*B*—C7′*B*	119.3 (7)
C8′*A*—C7′*A*—O9*A*	125.9 (5)	O9*B*—C7′*B*—C8′*B*	124.3 (7)
C8′*A*—C7′*A*—C6′*A*	119.7 (6)	O9*B*—C7′*B*—C6′*B*	114.9 (7)

O9A—C7′A—C6′A	114.4 (6)	C8′B—C7′B—C6′B	120.8 (7)
C7′A—C8′A—C8′aA	121.5 (5)	C7′B—C8′B—C8′aB	119.6 (6)
C8′A—C8′aA—C4′aA	119.1 (5)	C8′B—C8′aB—C1′B	122.7 (6)
C8′A—C8′aA—C1′A	122.5 (5)	C8′B—C8′aB—C4′aB	119.4 (6)
C4′aA—C8′aA—C1′A	118.4 (5)	C1′B—C8′aB—C4′aB	117.8 (6)
C7′A—O9A—C10A	116.2 (4)	C7′B—O9B—C10B	118.4 (6)
O5A—C1A—N2A	124.1 (6)	O5B—C1B—N2B	122.4 (6)
O5A—C1A—C6A	121.3 (6)	O5B—C1B—C6B	122.3 (6)
N2A—C1A—C6A	114.5 (5)	N2B—C1B—C6B	115.3 (6)
C1A—N2A—C3A	121.3 (5)	C1B—N2B—C3B	122.1 (5)
N2A—C3A—C4A	113.8 (5)	N2B—C3B—C4B	112.4 (4)
C1′A—C4A—C3A	110.3 (5)	C1′B—C4B—C3B	112.3 (4)
C2′C—C1′C—C8′aC	120.2 (6)	C2′D—C1′D—C8′aD	120.0 (6)
C2′C—C1′C—C4C	120.2 (6)	C2′D—C1′D—C4D	118.4 (6)
C8′aC—C1′C—C4C	119.6 (5)	C8′aD—C1′D—C4D	121.6 (5)
C1′C—C2′C—C3′C	120.2 (7)	C1′D—C2′D—C3′D	120.2 (7)
C4′C—C3′C—C2′C	120.6 (7)	C4′D—C3′D—C2′D	119.9 (7)
C3′C—C4′C—C4′aC	121.8 (7)	C3′D—C4′D—C4′aD	121.9 (7)
C4′C—C4′aC—C5′C	123.8 (7)	C4′D—C4′aD—C5′D	123.1 (6)
C4′C—C4′aC—C8′aC	119.4 (7)	C4′D—C4′aD—C8′aD	119.0 (6)
C5′C—C4′aC—C8′aC	116.8 (7)	C5′D—C4′aD—C8′aD	117.9 (6)
C6′C—C5′C—C4′aC	122.5 (6)	C6′D—C5′D—C4′aD	122.6 (6)
C5′C—C6′C—C7′C	119.8 (7)	C5′D—C6′D—C7′D	120.2 (6)
C8′C—C7′C—O9C	124.6 (6)	C8′D—C7′D—O9D	123.6 (5)
C8′C—C7′C—C6′C	120.9 (7)	C8′D—C7′D—C6′D	120.6 (6)
O9C—C7′C—C6′C	114.5 (7)	O9D—C7′D—C6′D	115.8 (6)
C7′C—C8′C—C8′aC	119.9 (6)	C7′D—C8′D—C8′aD	121.0 (5)
C8′C—C8′aC—C1′C	122.3 (6)	C1′D—C8′aD—C8′D	123.3 (5)
C8′C—C8′aC—C4′aC	120.0 (6)	C1′D—C8′aD—C4′aD	119.0 (6)
C1′C—C8′aC—C4′aC	117.7 (6)	C8′D—C8′aD—C4′aD	117.7 (6)
C7′C—O9C—C10C	116.4 (5)	C7′D—O9D—C10D	117.5 (5)
O5C—C1C—N2C	123.5 (5)	O5D—C1D—N2D	122.7 (5)
O5C—C1C—C6C	122.1 (6)	O5D—C1D—C6D	120.1 (5)
N2C—C1C—C6C	114.3 (6)	N2D—C1D—C6D	117.2 (5)
C1C—N2C—C3C	122.1 (5)	C1D—N2D—C3D	122.3 (5)
N2C—C3C—C4C	110.3 (4)	N2D—C3D—C4D	115.2 (5)
C3C—C4C—C1′C	109.7 (4)	C1′D—C4D—C3D	108.9 (5)

O5A—C1A—N2A—C3A	2.2 (10)
C1A—N2A—C3A—C4A	−101.1 (7)
C2′A—C1′A—C4A—C3A	95.4 (6)
N2A—C3A—C4A—C1′A	176.3 (5)
O5B—C1B—N2B—C3B	0.2 (8)
C1B—N2B—C3B—C4B	86.8 (6)
C2′B—C1′B—C4B—C3B	−100.4 (6)
N2B—C3B—C4B—C1′B	176.2 (5)
O5C—C1C—N2C—C3C	−1.5 (9)
C1C—N2C—C3C—C4C	91.3 (6)
N2C—C3C—C4C—C1′C	−175.2 (5)
C2′C—C1′C—C4C—C3C	−101.5 (6)
O5D—C1D—N2D—C3D	4.3 (9)
C1D—N2D—C3D—C4D	−103.0 (7)
C2′D—C1′D—C4D—C3D	95.7 (7)
N2D—C3D—C4D—C1′D	175.2 (5)

Table 3. *Hydrogen-bonding geometry* (Å, °)

	N···O	H···O	N—H···O
N2A—H···O5B	2.896 (8)	2.02 (5)	176 (1)
N2B—H···O5A^{i}	2.891 (7)	2.05 (5)	164 (1)
N2C—H···O5D	2.852 (8)	1.82 (5)	166 (1)
N2D—H···O5C^{i}	2.927 (8)	2.03 (5)	162 (1)

Symmetry code: (i) $x, y-1, z$.

Data collection, cell refinement and data reduction: local program. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program used to refine structure: *SHELXL* (Sheldrick, 1994). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978). Software used to prepare material for publication: *SHELXL*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71834 (41 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA1082]

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2-Methyl-4-(4-pyridyl)-3-butyn-2-ol: a Two-Dimensional Hydrogen-Bond Network

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Abstract

The asymmetric unit of $C_{10}H_{11}NO$ consists of two chemically similar but crystallographically distinct molecules of 2-methyl-4-(4-pyridyl)-3-butyn-2-ol which are linked *via* a head-to-tail hydrogen bond