Asian Journal of Chemistry; Vol. 25, No. 9 (2013), 5115-5116

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2013.14314

NOTE

Synthesis and Supramolecular Structure of 2-Acetyl-1-naphthol

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(*Received*: 16 July 2012; *Accepted*: 25 March 2013) AJC-13154

2-Acetyl-1-naphthol with the molecular formula $C_{12}H_{10}O_2$, is stabilized by intramolecular O2-H2···O1 hydrogen bond forming a six-membered ring, nearly planar with the naphthone ring and the distances from C1 atom of acetyl group to mean plane of the three six-membered ring is 0.112(3) Å. Moreover, the structure is stabilized by intermolecular C-H···π and π-π stacking interactions.

Key Words: Naphthol, Synthesis, Supramolecular structure.

Naphthaldehyde, hydroxy-naphthaldehyde and their derivatives are an important class of intermediates[1-3] which condenses with primary amines to afford Schiff bases[4,5] that are one of most versatile mixed-donor ligands in the field of coordination chemistry[6-8]. In this paper, we report on the synthesis and the X-ray single-crystal structure of the 2-acetyl-1-naphthol.

A sample of 2-methoxy naphthalene was obtained from Alfa Aesar and used without further purification. The other reagents and solvents were analytical grade reagents from Tianjin Chemical Reagent Factory. C, H and O analyses were carried out with a GmbH VariuoEL V3.00 automatic elemental analyzer. X-Ray single crystal structure was determined on a Bruker Smart 1000 CCD area detector. Melting points were measured by the use of a microscopic melting point apparatus made in Beijing Taike Instrument Limited Company and the thermometer was uncorrected.

Synthesis: A solution of 2-methoxy naphthalene (0.1 mmol), acetyl chloride (0.1 mmol) in 30 mL ethanol in the presence of $AlCl_3$ was refluxed for 5 h and then cooled to room temperature and filtered. Pale-yellow needle-like single crystals suitable for X-ray diffraction studies were obtained after several weeks by slow evaporation from a methanol-ethyl ether (1:3) mixed solution of the title compound.

X-Ray structure determination: The single crystal of the 2-acetyl-1-naphthol, with approximate dimensions of 0.55 mm × 0.50 mm × 0.38 mm was placed on a Bruker Smart 1000 diffractmeter equipped with Apex CCD area detector. The diffraction data were collected using a graphite monochromated MoK_α radition (λ = 0.71073 Å) at 298(2) K. The structure was solved by using the program SHELXS-97 and Fourier difference techniques and refined by full-matrix least-squares method on F^2 using SHELXL-97. Details of the data collection and refinements of the title compound are given in Table-1. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were added theoretically. CCDC: 712170.

TABLE-1
CRYSTAL DATA AND STRUCTURE REFINEMENT FOR THE 2-ACETYL-1-NAPHTHOL

Empirical formula	$C_{12}H_{10}O_2$
Formula weight	186.20
Temperature (K)	298(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 2_1/n
Cell dimensions, (Å, deg)	a = 7.6246(9), b = 7.0312(7), c = 17.4709(16), β = 92.432(1)
Volume (Å^3)	935.77(17)
Z	4
Density (calculated) (mg/m^3)	1.322
Absorption coefficient (mm^{-1})	0.089
$F_{(000)}$	392.0
Index ranges	-9 ≤ h ≤ 8, -8 ≤ k ≤ 7, -20 ≤ l ≤ 19
Reflections collected	4497/1643 [$R_{(int)}$ = 0.0454]
Independent reflections	1494
Data/restraints/parameters	1643/0/129
Goodness of fit indicator	1.071
R [I > 2σ(I)]	R_1 = 0.0421, wR_2 = 0.1332
Largest diff. peak and hole (e Å^{-3})	0.152 and -0.154

TABLE-2
SELECTED BOND DISTANCES (Å) AND ANGLES (°) FOR THE TITLE COMPOUND

Bond	Lengths	Bond	Lengths	Bond	Lengths
O1-C2	1.240(3)	C3-C8	1.429(3)	C7-C12	1.413(3)
O2-C3	1.341(2)	C4-C5	1.413(3)	C8-C9	1.413(3)
C1-C2	1.489(3)	C5-C6	1.352(3)	C9-C10	1.367(3)
C2-C4	1.467(3)	C6-C7	1.412(3)	C10-C11	1.379(3)
C3-C4	1.385(3)	C7-C8	1.408(3)	C11-C12	1.358(3)
Bond	Angles	Bond	Angles	Bond	Angles
O1-C2-C4	119.9(2)	C3-C4-C2	120.0(2)	C7-C8-C9	119.29(19)
O1-C2-C1	119.4(2)	C5-C4-C2	121.6(2)	C7-C8-C3	118.51(18)
C4-C2-C1	120.7(2)	C6-C5-C4	121.8(2)	C9-C8-C3	122.19(19)
O2-C3-C4	122.49(18)	C5-C6-C7	120.67(19)	C10-C9-C8	120.4(2)
O2-C3-C8	116.45(19)	C8-C7-C6	119.51(18)	C9-C10-C11	120.5(2)
C4-C3-C8	121.06(17)	C8-C7-C12	117.91(19)	C12-C11-C10	120.5(2)
C3-C4-C5	118.45(17)	C6-C7-C12	122.58(19)	C11-C12-C7	121.4(2)

X-Ray crystallographic analysis revealed the crystal structure of the title compound. And the structure is shown in Fig. 1. Selected bond distances and angles are listed in Table-2. The single crystal structure of the title compound is built up by only the $C_{12}H_{10}O_2$ molecule. An intramolecular O2-H2···O1 hydrogen bond between the hydroxyl group and the O atom of carbonyl group forms a six-membered ring in each molecule (Table-3), which is nearly coplanar with the naphthone ring and the distances from C1 atom of acetyl group to mean plane of the three six-membered ring is 0.112(3) Å. There are weak intermolecular π-π stacking interactions between neighbouring aromatic rings (C3-C8) with centroid-to-centroid distances of 3.844(2) Å (Fig. 2). Moreover, the structure is stabilized by intermolecular C-H···π stacking interactions.

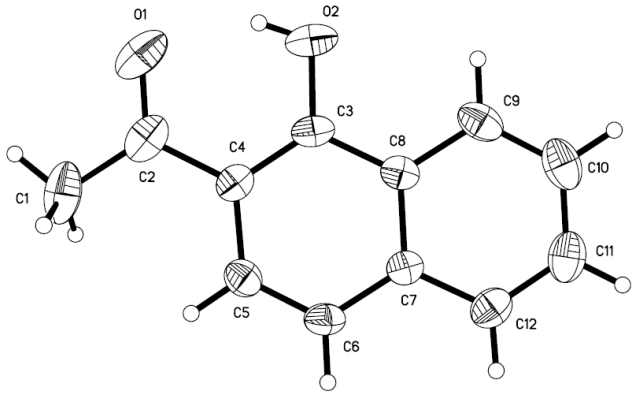

Fig. 1. Molecule structure of the title compound with atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30 % probability level

TABLE-3
HYDROGEN BOND [Å, °] FOR THE TITLE COMPOUND

D-H···A	d(D-H)	d(H···A)	∠DHA	d(D···A)
O2-H2···O1	0.82	1.80	146	2.526(3)

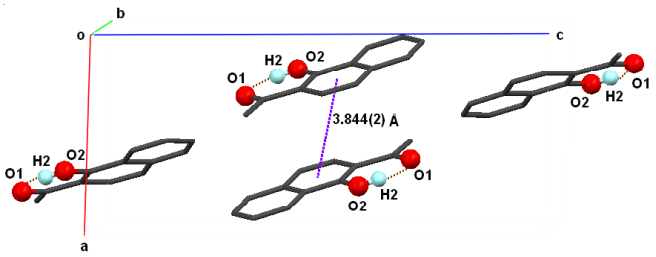

Fig. 2. A perspective view of the intramolecular hydrogen-bond and π-π stacking interactions together with the centroid-centroid contacts

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