Crystal structure of 1,3-di(1-naphthyl)propan-2-one, C₂₃H₁₈O

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Abstract

C₂₃H₁₈O, monoclinic, *P*12₁/*c*1 (no. 14), *a* = 12.614(1) Å, *b* = 10.142(1) Å, *c* = 12.967(1) Å, β = 98.00(1)°, *V* = 1642.7 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.059, *wR*_{ref}(*F*²) = 0.173, *T* = 193 K.

Source of material

1-Naphthylacetic acid anhydride (42 mmol) and 50 ml of pyridine were refluxed for 2.5 h. After evaporation of the solvent, the residue was dissolved in 100 ml aqueous sodium hydroxide solution and extracted with toluene. To the combined organic phases 5 g of active carbon and 5 g of sodium sulfate were added. The mixture was stirred for 1 h, filtered over celite and evaporated. Distillation followed by crystallization from acetone yielded the pure product (m.p. 108 °C, [1]).

Discussion

Although the 1,3-diaryl substituted propan-2-ones are useful starting materials in the carbocyclic ring formation [2] and despite their potential property of supramolecular interactions (C–H...O, C–H... π , π ... π) derived from the functional sites [3], reports on crystal structures of respective compounds are very rare. Actually, there is only one structure description which com-

prises a manganese carbonyl complex of 1,3-diphenylpropan-2-one [4]. This prompted us to determine the crystal structure of the title compound.

A twisted conformation with reference to the planes defined by the naphthyl units (C3–C12/C14–C23, 61.58(5)°) and the carbonyl group (C1–O1/C3–C12, 54.60°; C1–O1/C14–C23, 1.32°) gives rise to an intramolecular C–H... π contact (*d*(C2–H2A...cg₃) = 2.37 Å; cg₃ means the centroid of the ring with atoms C14–C18 and C23). In the packing, each of the molecules is connected via a bifurcated C–H...O...H–C type interaction (three center bond [5,6]) to form supramolecular zigzag strands in the *a,c* plane (figure, bottom). These strands are assembled by means of weaker C–H... π contacts and face-to-face π ... π -stacking interactions (*d*(cg₄...cg₄) = 3.79 Å, cg₄ defined as centroid of the aromatic ring C18 – C23) that stabilize the crystal packing. Thus, a variety of supramolecular interactions corresponding to the functional sites of the title molecule are effected in the crystal structure.

Table 1. Data collection and handling.

Crystal:	colorless plate, size 0.15 × 0.25 × 0.45 mm
Wavelength:	Cu K α radiation (1.54178 Å)
μ :	5.80 cm ^{−1}
Diffractionmeter, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{\max}$:	120.06°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	2561, 2435
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1838
<i>N</i> (<i>param</i>) _{refined} :	218
Programs:	SHELXS-97 [7], SHELXL-97 [8], ORTEP-3 [9]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2A)	4e	0.1866	0.0712	0.5373	0.058
H(2B)	4e	0.0862	0.1307	0.5841	0.058
H(4)	4e	0.1586	−0.0170	0.3716	0.062
H(5)	4e	0.0511	−0.0629	0.2116	0.065
H(6)	4e	−0.1112	0.0423	0.1696	0.057
H(8)	4e	−0.2463	0.2003	0.2154	0.060
H(9)	4e	−0.3066	0.3462	0.3293	0.067
H(10)	4e	−0.2050	0.3861	0.4904	0.063
H(11)	4e	−0.0417	0.2887	0.5359	0.056
H(13A)	4e	0.2004	0.3234	0.6906	0.057
H(13B)	4e	0.2871	0.3936	0.6303	0.057
H(15)	4e	0.2568	0.1489	0.7993	0.063
H(16)	4e	0.3796	−0.0173	0.8610	0.069
H(17)	4e	0.5263	−0.0584	0.7798	0.066
H(19)	4e	0.6367	−0.0060	0.6412	0.066
H(20)	4e	0.6662	0.1158	0.4987	0.070
H(21)	4e	0.5441	0.2815	0.4336	0.066
H(22)	4e	0.3943	0.3224	0.5113	0.054

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	4e	0.1760(2)	0.3509(2)	0.4622(2)	0.049(1)	0.045(1)	0.058(1)	−0.0025(9)	−0.0014(9)	0.008(1)
C(1)	4e	0.1836(2)	0.2748(3)	0.5352(2)	0.029(2)	0.047(2)	0.055(2)	0.002(1)	−0.002(1)	−0.000(1)
C(2)	4e	0.1302(2)	0.1396(3)	0.5269(2)	0.036(2)	0.045(2)	0.061(2)	−0.000(1)	−0.008(1)	0.004(1)
C(3)	4e	0.0600(2)	0.1130(3)	0.4250(2)	0.038(2)	0.038(2)	0.051(2)	−0.004(1)	0.000(1)	0.002(1)
C(4)	4e	0.0916(2)	0.0263(3)	0.3553(2)	0.033(2)	0.046(2)	0.073(2)	0.004(1)	0.003(1)	0.009(2)
C(5)	4e	0.0272(2)	−0.0015(3)	0.2586(3)	0.056(2)	0.044(2)	0.064(2)	−0.000(1)	0.014(2)	−0.004(2)
C(6)	4e	−0.0682(2)	0.0601(3)	0.2342(2)	0.053(2)	0.042(2)	0.045(2)	−0.007(1)	−0.002(1)	−0.003(1)
C(7)	4e	−0.1039(2)	0.1510(2)	0.3046(2)	0.036(2)	0.035(1)	0.046(2)	−0.006(1)	−0.003(1)	0.002(1)
C(8)	4e	−0.2037(2)	0.2170(3)	0.2804(2)	0.043(2)	0.044(2)	0.061(2)	−0.006(1)	−0.005(1)	0.002(1)
C(9)	4e	−0.2398(2)	0.3029(3)	0.3475(3)	0.037(2)	0.053(2)	0.076(2)	0.002(1)	−0.002(2)	0.010(2)
C(10)	4e	−0.1786(2)	0.3272(3)	0.4430(3)	0.039(2)	0.048(2)	0.071(2)	0.005(1)	0.007(2)	0.002(2)
C(11)	4e	−0.0822(2)	0.2689(3)	0.4704(2)	0.047(2)	0.045(2)	0.045(2)	−0.006(1)	−0.001(1)	−0.002(1)
C(12)	4e	−0.0404(2)	0.1770(2)	0.4009(2)	0.039(2)	0.034(1)	0.047(2)	−0.007(1)	−0.000(1)	0.002(1)
C(13)	4e	0.2494(2)	0.3093(3)	0.6382(2)	0.033(2)	0.050(2)	0.058(2)	0.004(1)	0.000(1)	−0.007(1)
C(14)	4e	0.3312(2)	0.2061(3)	0.6791(2)	0.032(2)	0.043(2)	0.046(2)	−0.008(1)	−0.007(1)	−0.005(1)
C(15)	4e	0.3171(2)	0.1328(3)	0.7645(2)	0.044(2)	0.063(2)	0.047(2)	−0.013(1)	−0.002(1)	−0.003(2)
C(16)	4e	0.3909(3)	0.0332(3)	0.8018(2)	0.060(2)	0.056(2)	0.052(2)	−0.017(2)	−0.013(2)	0.010(2)
C(17)	4e	0.4776(2)	0.0092(3)	0.7540(2)	0.050(2)	0.046(2)	0.061(2)	−0.006(1)	−0.020(2)	0.007(2)
C(18)	4e	0.4965(2)	0.0832(3)	0.6663(2)	0.037(2)	0.040(2)	0.054(2)	−0.004(1)	−0.014(1)	−0.001(1)
C(19)	4e	0.5871(2)	0.0607(3)	0.6157(3)	0.036(2)	0.048(2)	0.075(2)	0.005(1)	−0.013(2)	−0.001(2)
C(20)	4e	0.6047(2)	0.1323(3)	0.5314(3)	0.038(2)	0.061(2)	0.075(2)	0.002(1)	0.003(2)	−0.006(2)
C(21)	4e	0.5316(2)	0.2313(3)	0.4926(2)	0.045(2)	0.058(2)	0.060(2)	0.000(1)	0.004(1)	0.003(2)
C(22)	4e	0.4431(2)	0.2557(3)	0.5389(2)	0.034(2)	0.044(2)	0.056(2)	0.001(1)	−0.002(1)	0.002(1)
C(23)	4e	0.4223(2)	0.1836(3)	0.6275(2)	0.033(1)	0.037(1)	0.048(2)	−0.006(1)	−0.009(1)	−0.002(1)

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