Crystal structure of 1′-(1,2′-binaphthyl) 1-naphthyl ketone, $C_{31}H_{20}O$

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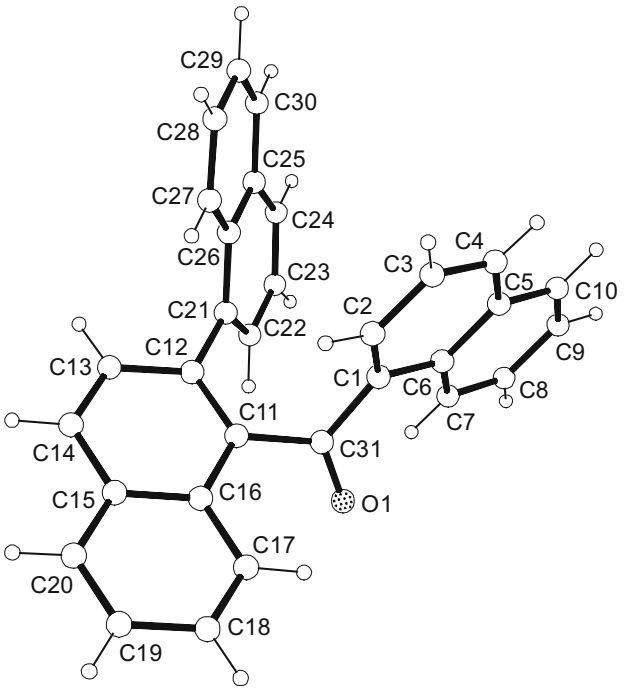

Abstract

$C_{31}H_{20}O$, monoclinic, $P12_1/n1$ (No. 14), a = 11.588(2) Å, b = 12.306(2) Å, c = 15.794(3) Å, β = 105.65(3)°, V = 2168.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.071, $wR_{ref}(F^2)$ = 0.203, T = 298 K.

Source of material

The title compound is formed as by-product in the synthesis of tri(1-naphthyl)methanol via Grignard reaction from 1-naphthoyl chloride and 1-bromonaphthalene in dry diethyl ether and quenching with sat. aqueous ammonium solution. The single crystal for X-ray analysis has been obtained by slow crystallization of the title compound from isopropyl amine at 298 K.

Experimental details

Data collection of three different crystals of the same size of the compound yielded similar $R_{gt}(F)$ values (0.07) with constant min/max residual electron density (~ 0.3/–0.3 e·Å^{-3}). Thus, there is no obvious reason for the relative high R-values.

Discussion

The two naphthyl units connected with the keto group exhibit an dihedral angle of 83.85°, whereas the aromatic groups within the binaphthyl fragment are oriented in an angle of 65.63° to one another. The closest intramolecular distance between the aromatic subunits (C1–C10 and C21–C30) is 3.05Å thus indicating π-π interactions.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.40 × 0.50 × 0.50 mm
Wavelength:	Cu K_α radiation (1.54180 Å)
μ:	5.72 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω/2θ
$2\theta_{max}$:	149.74°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4631, 4411
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2452
$N(param)_{refined}$:	289
Programs:	SHELXS-97 [2], SHELXL-97 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.7652	0.2480	0.2197	0.070
H(3)	4*e*	0.7978	0.2234	0.3698	0.085
H(4)	4*e*	0.7242	0.3451	0.4495	0.090
H(7)	4*e*	0.5354	0.5636	0.1582	0.084
H(8)	4*e*	0.4546	0.6785	0.2407	0.107
H(9)	4*e*	0.4880	0.6494	0.3911	0.119
H(10)	4*e*	0.5998	0.5066	0.4569	0.105
H(13)	4*e*	0.5133	0.0933	–0.0199	0.085
H(14)	4*e*	0.6556	0.0738	–0.0935	0.091
H(17)	4*e*	0.8644	0.4286	0.0611	0.083
H(18)	4*e*	1.0103	0.3978	–0.0086	0.100
H(19)	4*e*	0.9971	0.2526	–0.1038	0.105
H(20)	4*e*	0.8412	0.1336	–0.1255	0.096
H(22)	4*e*	0.4157	0.3827	0.0315	0.080
H(23)	4*e*	0.2549	0.4000	0.0911	0.094
H(24)	4*e*	0.2168	0.2698	0.1818	0.092
H(27)	4*e*	0.6081	0.0684	0.1594	0.073
H(28)	4*e*	0.5735	–0.0549	0.2576	0.084
H(29)	4*e*	0.4047	–0.0423	0.3086	0.089
H(30)	4*e*	0.2724	0.0959	0.2634	0.085

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.6742(2)	0.4956(2)	0.0865(1)	0.118(2)	0.052(1)	0.074(1)	0.002(1)	0.035(1)	0.010(1)
C(1)	4*e*	0.6722(2)	0.3861(2)	0.2090(2)	0.055(2)	0.050(2)	0.051(2)	–0.009(1)	0.015(1)	–0.001(1)
C(2)	4*e*	0.7348(3)	0.2985(2)	0.2517(2)	0.062(2)	0.057(2)	0.056(2)	–0.002(1)	0.016(1)	0.003(1)
C(3)	4*e*	0.7542(3)	0.2830(3)	0.3422(2)	0.075(2)	0.076(2)	0.060(2)	0.002(2)	0.014(2)	0.011(2)
C(4)	4*e*	0.7092(3)	0.3549(3)	0.3891(2)	0.077(2)	0.094(3)	0.053(2)	–0.008(2)	0.016(2)	0.002(2)
C(5)	4*e*	0.6396(3)	0.4450(3)	0.3489(2)	0.068(2)	0.075(2)	0.060(2)	–0.015(2)	0.022(2)	–0.013(2)
C(6)	4*e*	0.6207(2)	0.4629(2)	0.2570(2)	0.053(2)	0.052(2)	0.066(2)	–0.012(1)	0.018(1)	–0.008(1)
C(7)	4*e*	0.5496(3)	0.5514(2)	0.2182(2)	0.074(2)	0.055(2)	0.082(2)	–0.002(2)	0.025(2)	–0.005(2)
C(8)	4*e*	0.5011(3)	0.6199(3)	0.2674(3)	0.086(3)	0.068(2)	0.120(3)	0.002(2)	0.037(2)	–0.016(2)
C(9)	4*e*	0.5210(4)	0.6023(3)	0.3579(3)	0.107(3)	0.087(3)	0.118(4)	–0.004(2)	0.056(3)	–0.040(3)
C(10)	4*e*	0.5877(3)	0.5175(3)	0.3969(3)	0.092(3)	0.095(3)	0.083(2)	–0.009(2)	0.036(2)	–0.027(2)
C(11)	4*e*	0.6694(3)	0.3079(2)	0.0575(2)	0.063(2)	0.051(2)	0.048(2)	–0.003(1)	0.012(1)	0.001(1)
C(12)	4*e*	0.5782(3)	0.2321(2)	0.0465(2)	0.066(2)	0.055(2)	0.051(2)	0.001(1)	0.013(1)	–0.000(1)
C(13)	4*e*	0.5749(3)	0.1440(3)	–0.0116(2)	0.074(2)	0.068(2)	0.069(2)	–0.012(2)	0.015(2)	–0.013(2)
C(14)	4*e*	0.6602(3)	0.1323(3)	–0.0555(2)	0.091(2)	0.073(2)	0.065(2)	–0.004(2)	0.022(2)	–0.018(2)
C(15)	4*e*	0.7551(3)	0.2067(3)	–0.0449(2)	0.075(2)	0.069(2)	0.051(2)	0.004(2)	0.018(2)	0.003(2)
C(16)	4*e*	0.7601(3)	0.2968(2)	0.0122(2)	0.068(2)	0.058(2)	0.047(2)	–0.001(2)	0.017(1)	0.005(1)
C(17)	4*e*	0.8587(3)	0.3688(3)	0.0243(2)	0.077(2)	0.066(2)	0.067(2)	–0.005(2)	0.026(2)	0.007(2)
C(18)	4*e*	0.9454(3)	0.3507(3)	–0.0179(2)	0.082(2)	0.084(3)	0.093(3)	0.001(2)	0.038(2)	0.020(2)
C(19)	4*e*	0.9381(4)	0.2628(3)	–0.0747(2)	0.098(3)	0.092(3)	0.087(3)	0.018(2)	0.051(2)	0.021(2)
C(20)	4*e*	0.8452(3)	0.1922(3)	–0.0877(2)	0.097(3)	0.084(2)	0.066(2)	0.010(2)	0.035(2)	0.002(2)
C(21)	4*e*	0.4790(3)	0.2430(2)	0.0898(2)	0.057(2)	0.058(2)	0.054(2)	–0.005(2)	0.009(1)	–0.004(1)
C(22)	4*e*	0.4025(3)	0.3296(3)	0.0697(2)	0.064(2)	0.063(2)	0.069(2)	–0.001(2)	0.008(2)	0.003(2)
C(23)	4*e*	0.3050(3)	0.3398(3)	0.1052(2)	0.064(2)	0.068(2)	0.097(3)	0.014(2)	0.013(2)	0.004(2)
C(24)	4*e*	0.2832(3)	0.2629(3)	0.1598(2)	0.063(2)	0.075(2)	0.096(3)	0.008(2)	0.028(2)	–0.002(2)
C(25)	4*e*	0.3594(3)	0.1720(2)	0.1841(2)	0.058(2)	0.062(2)	0.062(2)	–0.001(2)	0.014(1)	–0.007(2)
C(26)	4*e*	0.4602(2)	0.1624(2)	0.1499(2)	0.050(2)	0.054(2)	0.051(2)	–0.004(1)	0.007(1)	–0.005(1)
C(27)	4*e*	0.5403(3)	0.0754(2)	0.1798(2)	0.056(2)	0.060(2)	0.066(2)	0.001(1)	0.013(1)	–0.002(2)
C(28)	4*e*	0.5194(3)	0.0015(3)	0.2383(2)	0.077(2)	0.061(2)	0.067(2)	0.005(2)	0.011(2)	0.006(2)
C(29)	4*e*	0.4184(3)	0.0093(3)	0.2694(2)	0.088(2)	0.071(2)	0.065(2)	–0.005(2)	0.023(2)	0.008(2)
C(30)	4*e*	0.3402(3)	0.0918(3)	0.2427(2)	0.074(2)	0.075(2)	0.071(2)	–0.006(2)	0.031(2)	–0.007(2)
C(31)	4*e*	0.6698(3)	0.4041(2)	0.1156(2)	0.064(2)	0.049(2)	0.058(2)	–0.000(1)	0.017(1)	0.005(1)

References

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