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Crystal Structure of *N*-(4-methylphenyl)benzamide

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The title compound N-*(4-methylphenyl)benzamide was determined by single-crystal X-ray diffraction analysis. The crystals are orthorhombic, space group Pbca with* a = *9.1082(18),* b = *9.822(2),* c = *26.125(5) Å,* $\alpha = 90$, $\beta = 90$, $\gamma = 90^\circ$, V = *2337.1(8) Å^3,* Z = *8,* F(000) = *896,* D_c = *1.201 g/cm^3,* μ = *0.076 mm^{-1}, the final* R = *0.0683, and* wR = *0.1718. A total of 17,393 reflections were collected, of which 2049 were independent* (R_{int} = *0.0730). In the crystal packing diagram, intermolecular N—H···O hydrogen bonds stabilize the solid state of the title compound.*

Keywords Benzamide; crystal Structure; phenyl

Introduction

In a continuation of our previous research work on organic compounds [1–4], we obtained the single crystals of the title compound *N*-(4-methylphenyl)benzamide. Fortunately, the single crystal of the title compound was analyzed by X-ray diffraction analysis. In this paper, we present the crystal structural analysis of *N*-(4-methylphenyl)benzamide.

Experimental

Crystal Structure Determination

The crystal of the title compound with dimensions of 0.20 mm × 0.18 mm × 0.10 mm was mounted on a Rigaku Saturn CCD area detector diffractometer with a graphite-monochromated MoKα radiation (λ = 0.71073Å) by using a phi and scan modes at 293(2) K in the range of $2.73^\circ \leq \theta \leq 25.02^\circ$. The crystal belongs to orthorhombic system with space group Pbca and crystal parameters of $a = 9.1082(18)$ Å, $b = 9.822(2)$ Å, $c = 26.125(5)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, V = 2337.1(8) A^3, $D_c = 1.201$ g/cm^3, The absorption coefficient $\mu = 0.076$ mm^{-1}, and $Z = 8$. A summary of crystal data is presented in Table 1.

The structure was solved by direct methods with SHELXS-97 [5] and refined by the full-matrix least squares method on F^2 data using SHELXL-97 [6]. The empirical absorption corrections were applied to all intensity data. H atom of N—H was initially located in a

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Table 1. Crystal data and structure refinement

Empirical formula	$C_{14}H_{13}NO$
Formula weight	211.25
Crystal system	Orthorhombic
Unit cell dimensions	
a (Å)	9.1082(18)
b (Å)	9.822(2)
c (Å)	26.125(5)
Unit cell angles (°)	
α	90
β	90
γ	90
Volume (Å^3)	2337.1(8)
Z	8
Temperature (K)	293(2)
space group	Pbca
Wavelength (Å)	0.71073
Calculated density (g/cm^3)	1.201
Absorption coefficient (mm^{-1})	0.076
F(000)	896
Crystal size (mm)	0.20 × 0.18 × 0.10
Theta range for data collection (°)	2.73–25.02
Reflections collected	17393
Independent reflections	2049 [$R_{(int)} = 0.0730$]
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0683$, w$R_2 = 0.1718$

difference Fourier map and were refined with the restraint Uiso(H) = 1.2Ueq(N). Other H atoms were positioned geometrically and refined using a riding model, with d(C—H) = 0.93–0.97 Å and Uiso(H) = 1.2Ueq(C) or 1.5Ueq(Cmethyl). The final full-matrix least squares refinement gave $R = 0.0683$ and $wR = 0.1718$.

Results and Discussion

The title compound *N*-(4-methylphenyl)benzamide was determined by single-crystal X-ray diffraction analysis. The selected bond lengths and bond angles are listed in Table 2. The structure was solved by direct methods. Anisotropic displacement parameters were applied to all nonhydrogen atoms in full-matrix least-square refinements based on F^2. The hydrogen atoms were set in calculated positions with a common fixed isotropic thermal parameter.

The molecular structure and the packing view of the title compound are shown in Figs. 1 and 2, respectively. The title compound crystallizes in orthorhombic space group Pbca with eight molecules in the unit cell and one molecule in the asymmetric unit. As shown in Fig. 1, the molecular structure contains two phenyl groups joining together through amide group. The H atom of the hydroxy group is transferred to the *N* atom to form amide group. The six-membered rings C1C2C3C4C5C6 and C8C9C10C11C12C13 are almost coplanar with the mean deviations of 0.0042 and 0.0026 Å, respectively. The dihedral angle between

Table 2. Selected bond lengths (Å) and bond angles (°)

Bond lengths			
O(1)-C(7)	1.229(3)	C(3)-C(4)	1.372(4)
N(1)-C(7)	1.347(3)	C(4)-C(5)	1.378(3)
N(1)-C(8)	1.428(3)	C(5)-C(6)	1.392(3)
C(1)-C(6)	1.374(3)	C(6)-C(7)	1.486(3)
C(1)-C(2)	1.377(3)	C(8)-C(13)	1.371(3)
C(2)-C(3)	1.367(4)	C(8)-C(9)	1.380(3)
C(9)-C(10)	1.375(3)	C(11)-C(12)	1.378(4)
C(10)-C(11)	1.370(4)	C(11)-C(14)	1.516(4)
Bond angles			
C(7)-N(1)-C(8)	125.4(2)	C(1)-C(6)-C(7)	118.2(2)
C(6)-C(1)-C(2)	120.8(2)	C(5)-C(6)-C(7)	123.2(2)
C(3)-C(2)-C(1)	120.2(3)	O(1)-C(7)-N(1)	122.0(2)
C(2)-C(3)-C(4)	120.0(3)	O(1)-C(7)-C(6)	120.7(2)
C(3)-C(4)-C(5)	120.1(3)	N(1)-C(7)-C(6)	117.2(2)
C(4)-C(5)-C(6)	120.3(2)	C(13)-C(8)-C(9)	119.1(2)
C(13)-C(8)-N(1)	118.6(2)	C(9)-C(8)-N(1)	122.3(2)
C(10)-C(9)-C(8)	119.7(2)	C(11)-C(10)-C(9)	122.2(3)
C(10)-C(11)-C(12)	117.3(2)	C(10)-C(11)-C(14)	122.1(3)

the two phenyl planes is 63.9°. The bond distances [O(1)-C(7) = 1.229(3) Å, N(1)-C(7) = 1.347(3) Å, N(1)-C(8) = 1.428(3) Å, C(1)-C(6) = 1.374(3) Å, C(1)-C(2) = 1.377(3) Å, C(2)-C(3) = 1.367(4) Å, and C(3)-C(4) = 1.372(4) Å] and bond angles [C(7)-N(1)-C(8) = 125.4(2)°, C(6)-C(1)-C(2) = 120.8(2)°, C(1)-C(6)-C(7) = 118.2(2)°, C(5)-C(6)-C(7) = 123.2(2)°, O(1)-C(7)-N(1) = 122.0(2)°, O(1)-C(7)-C(6) = 120.7(2)°, N(1)-C(7)-C(6) = 117.2(2)°, and C(13)-C(8)-N(1) = 118.6(2)°] are comparable to the analogous compounds [7–19].

As shown in Fig. 2, the crystal packing diagram of the title compound shows that intermolecular N—H···O hydrogen bonds between amide groups stabilize the solid state.

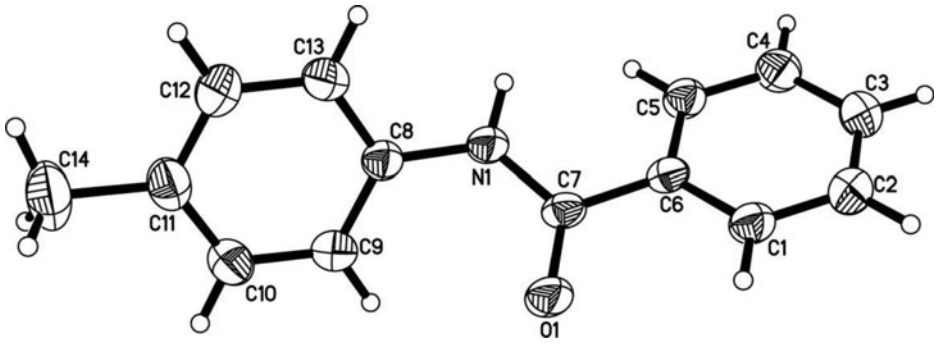

Figure 1. Molecular structure of the title compound.

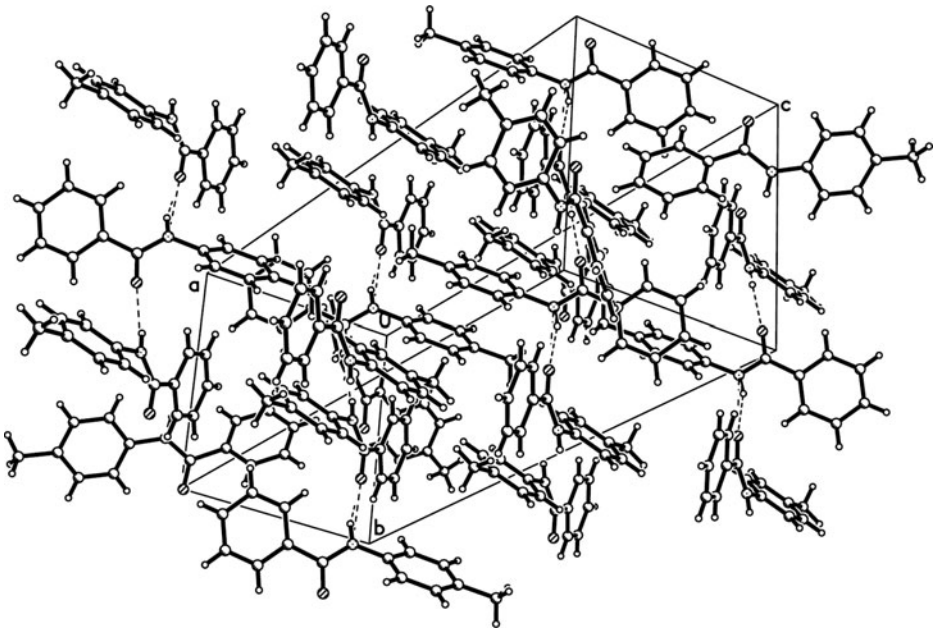

Figure 2. The crystal packing view of the title compound.

Conclusions

In summary, the title compound *N*-(4-methylphenyl)benzamide has been characterized by X-ray diffraction analysis.

Acknowledgments

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Supplemental Materials

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1026963 for the title compound. Copies of the data can be obtained free of charge at http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk.

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