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The crystal structure of 4-chloro-*N*-(2-phenoxyphenyl)benzamide, $C_{19}H_{14}ClNO_2$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.55 × 0.35 × 0.19 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.25 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	13015, 3770, 0.035
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2858
$N(\text{param})_{\text{refined}}$:	212
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

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Abstract

$C_{19}H_{14}ClNO_2$, monoclinic, $P2_1/c$ (no. 14), $a = 19.328(4)$ Å, $b = 7.1086(12)$ Å, $c = 11.627(2)$ Å, $\beta = 99.417(9)^\circ$, $V = 1576.0(5)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0582$, $wR_{\text{ref}}(F^2) = 0.1615$, $T = 200$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was obtained upon reacting *ortho*-phenoxyaniline with *para*-chlorobenzoylchloride. Crystals

suitable for the diffraction study were obtained upon free evaporation of a solution of the compound in chloroform.

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2U_{\text{eq}}(C)$.

The nitrogen-bound H atom was located on a difference Fourier map and refined freely.

Comment

In continuation of our interest in the structural aspects of amides [7–11] we initiated a larger study aimed at elucidating the influence of sterical overcrowding on the conformation as well as bond lengths of differently substituted amides featuring aniline-derivatives as bonding partners. The title compound appeared as an interesting target molecule in this context and, therefore, we sought to determine its molecular and crystal structure. The crystal structure of unsubstituted benzoyl anilide has been reported in the literature [12, 13].

In the molecule, resonance involving the π -electrons of the aromatic systems adjacent to the amide functionality forces the ring systems a common plane. The least-squares planes defined by their respective carbon atoms intersect at an angle of only $9.99(11)^\circ$. The phenoxy substituent, on the

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cl1	0.46244 (4)	1.46598 (13)	0.17349 (7)	0.0816 (3)
O1	0.32530 (12)	0.6944 (3)	−0.09961 (15)	0.0801 (7)
O2	0.19251 (7)	0.5693 (2)	0.20847 (11)	0.0412 (3)
N1	0.28227 (10)	0.6558 (3)	0.06720 (16)	0.0440 (4)
H71	0.2814 (15)	0.703 (4)	0.132 (3)	0.065 (8)*
C1	0.32097 (12)	0.7488 (3)	−0.00174 (18)	0.0459 (5)
C11	0.35632 (10)	0.9240 (3)	0.04752 (17)	0.0409 (5)
C12	0.39947 (12)	1.0151 (4)	−0.0184 (2)	0.0498 (6)
H12	0.406531	0.962345	−0.090642	0.060*
C13	0.43245 (12)	1.1815 (4)	0.0193 (2)	0.0544 (6)
H13	0.462208	1.242865	−0.026397	0.065*
C14	0.42163 (12)	1.2575 (4)	0.1240 (2)	0.0504 (5)
C15	0.37939 (13)	1.1685 (4)	0.19100 (18)	0.0539 (6)
H15	0.372326	1.221815	0.263098	0.065*
C16	0.34737 (13)	1.0020 (4)	0.15346 (17)	0.0500 (6)
H16	0.318746	0.939589	0.200580	0.060*
C21	0.24551 (11)	0.4866 (3)	0.04544 (16)	0.0388 (4)
C22	0.19852 (11)	0.4426 (3)	0.12019 (17)	0.0397 (4)
C23	0.16224 (13)	0.2760 (3)	0.1115 (2)	0.0541 (6)
H23	0.131500	0.247119	0.164947	0.065*
C24	0.17083 (14)	0.1508 (4)	0.0243 (2)	0.0610 (7)
H24	0.145826	0.035167	0.017048	0.073*
C25	0.21555 (14)	0.1939 (4)	−0.0517 (2)	0.0590 (7)
H25	0.220746	0.107722	−0.112195	0.071*
C26	0.25325 (13)	0.3593 (3)	−0.04265 (19)	0.0504 (5)
H26	0.284250	0.386321	−0.096016	0.060*
C31	0.13385 (10)	0.6838 (3)	0.19547 (15)	0.0359 (4)
C32	0.13213 (13)	0.8108 (3)	0.28485 (17)	0.0478 (5)
H32	0.169210	0.814671	0.349461	0.057*
C33	0.07635 (16)	0.9309 (4)	0.2792 (2)	0.0584 (6)
H33	0.075132	1.019235	0.340148	0.070*
C34	0.02188 (15)	0.9258 (4)	0.1864 (2)	0.0583 (6)
H34	−0.016877	1.008849	0.183681	0.070*
C35	0.02442 (13)	0.7985 (4)	0.0975 (2)	0.0521 (6)
H35	−0.012803	0.794624	0.033083	0.063*
C36	0.08020 (11)	0.6771 (3)	0.10094 (17)	0.0417 (5)
H36	0.081816	0.590120	0.039401	0.050*

other hand, adopts a conformation positioning it nearly perpendicular to its aromatic parent moiety with the respective least-squares planes enclosing an angle of 76.99(11)°. The length of the C–O bond as well as the C–N bond in the amide functionality are in good agreement with the values found for other aromatic amides featuring aniline and benzoic acid derivatives whose crystal structural data was deposited with the Cambridge Structural Database [14].

In the crystal structure, C–H···O contacts whose range falls by more than 0.2 Å below the sum of van-der-Waals radii of the atoms participating are observed. While one of the H atoms of the *para*-chlorobenzoic acid moiety has the O atom of the amide functionality as acceptor, the H atom in

para-position to the phenoxy-substituent employs the etheral O atom as acceptor. In terms of graph-set analysis [15, 16], the descriptor for the hydrogen bonding system is C₁¹(5)C₁¹(6) at the unitary level. In total, the molecules are connected to planes perpendicular to the crystallographic *a* axis. While no hydrogen bonds involving the nitrogen-bonded hydrogen atom are present, one can debate the presence of a C–H···π interaction supported by hydrogen atom in *para*-position on the phenoxy substituent as donor and the aromatic system of this very moiety in a symmetry-generated equivalent as acceptor. Furthermore, the presence of a C–Cl···π contact could be debated that sees the aromatic system of the benzoate moiety in a neighbouring molecule as acceptor. The closest inter-centroid distance was measured at 3.8228(16) Å between the two phenyl moieties directly adjacent to the amide functionality.

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