Crystal structure of 5,6-dimethyl-1*H*-benzo[*d*]imidazol-3-ium 2-(4-chlorophenoxy)acetate, $C_{17}H_{17}ClN_2O_3$

Hui-Lian Liu*

Microscale Science Institute, Biology Department, Weifang University, Weifang 261061, Shandong Province, P. R. China

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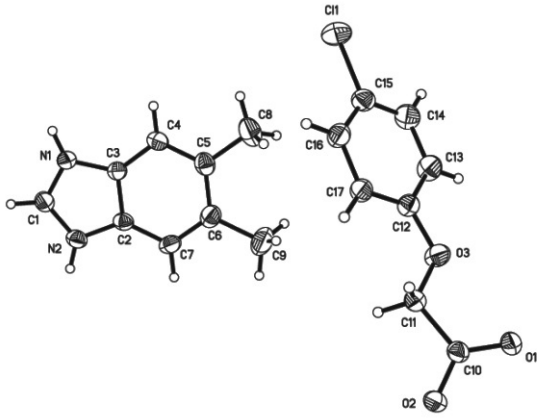

Abstract

$C_{17}H_{17}ClN_2O_3$, monoclinic, $P2_1/c$ (no. 14), a = 10.849(1) Å, b = 15.193(2) Å, c = 10.313(1) Å, β = 98.436(1)°, V = 1681.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.0443, $wR_{ref}(F^2)$ = 0.1236, T = 293 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.43×0.44×0.46 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.43 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ and ω
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12395, 2961
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2584
$N(param)_{refined}$:	210
Programs:	SHELXS-97 [5]

Source of material

The title compound was synthesized by the following procedure. A mixture of 2-(4-chlorophenoxy)acetic acid 1.86g(0.01 mol) and 5,6-dimethyl-1H-benzo[d]imidazole 1.46g(0.02 mol) was stirred with ethanol (50mL) at 367K for 4h. Single crystals suitable for *X*-ray measurements were obtained by recrystallization from ethanol at room temperature.

Discussion

The designs and syntheses of the compounds containing phenoxyacetic acid have received considerable attention over the past two decades. Phenoxyacetic acid and its derivatives are biologically active compounds which are widely used as herbicides and plant-growth substances [1]. Due to their versatile bonding modes with metal ions, they have also been used in the synthesis of mononuclear monomeric and polymeric complexes [2,3]. As part of this ongoing search for new phenoxyacetic acid compounds, the title compound has been synthesized and its structure is reported here. In the title compound, bond lengths and angles fall in the usual ranges. In the crystal structure, the molecules interact through two weak intermolecular N–H···O hydrogen bond.

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	1.0006	0.4261	0.8256	0.058
H(2)	4*e*	0.8852	0.6301	0.6329	0.061
H(1A)	4*e*	0.9892	0.5805	0.8364	0.062
H(4)	4*e*	0.9172	0.2967	0.6374	0.058
H(7)	4*e*	0.7785	0.5473	0.3946	0.064
H(8A)	4*e*	0.8300	0.2040	0.4705	0.123
H(8B)	4*e*	0.8187	0.2416	0.3277	0.123
H(8C)	4*e*	0.7013	0.2385	0.3999	0.123
H(9A)	4*e*	0.6309	0.3742	0.2592	0.144
H(9B)	4*e*	0.7563	0.3734	0.2006	0.144
H(9C)	4*e*	0.6885	0.4628	0.2183	0.144
H(11A)	4*e*	0.2645	0.3249	0.1125	0.060
H(11B)	4*e*	0.1788	0.2446	0.1356	0.060
H(13)	4*e*	0.4846	0.1217	–0.0176	0.073
H(14)	4*e*	0.6269	0.0416	0.1235	0.075
H(16)	4*e*	0.4801	0.1347	0.4289	0.066
H(17)	4*e*	0.3385	0.2179	0.2881	0.060

* Correspondence author (e-mail: huilian.liu@163.com)

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}
Cl(1)	4*e*	0.67061(5)	0.01661(4)	0.39379(6)	0.0736(4)	0.0756(4)	0.0894(4)	0.0249(3)	–0.0066(3)	0.0097(3)
N(1)	4*e*	0.9658(1)	0.45887(9)	0.7627(1)	0.0588(8)	0.0437(7)	0.0417(7)	0.0073(6)	0.0069(6)	0.0042(6)
N(2)	4*e*	0.9000(1)	0.57570(9)	0.6522(1)	0.0618(9)	0.0384(7)	0.0535(8)	0.0060(6)	0.0157(7)	0.0050(6)
O(1)	4*e*	0.1070(1)	0.25422(7)	–0.1435(1)	0.0661(8)	0.0434(6)	0.0428(6)	0.0035(5)	0.0017(5)	–0.0057(5)
O(2)	4*e*	0.0766(1)	0.37442(8)	–0.0303(1)	0.100(1)	0.0493(7)	0.0480(7)	0.0284(7)	–0.0087(6)	–0.0076(6)
O(3)	4*e*	0.3091(1)	0.21520(9)	0.0277(1)	0.0604(7)	0.0709(8)	0.0426(6)	0.0206(6)	0.0105(5)	0.0030(6)
C(1)	4*e*	0.9581(2)	0.5455(1)	0.7651(2)	0.062(1)	0.0460(9)	0.0484(9)	0.0022(8)	0.0110(8)	–0.0023(8)
C(2)	4*e*	0.8671(2)	0.5046(1)	0.5705(2)	0.0445(8)	0.0417(8)	0.0463(9)	0.0065(6)	0.0145(7)	0.0053(7)
C(3)	4*e*	0.9084(1)	0.4299(1)	0.6417(2)	0.0432(8)	0.0434(8)	0.0413(8)	0.0047(6)	0.0112(6)	0.0038(7)
C(4)	4*e*	0.8872(2)	0.3462(1)	0.5897(2)	0.0533(9)	0.0406(8)	0.053(1)	0.0054(7)	0.0147(7)	0.0032(7)
C(5)	4*e*	0.8205(2)	0.3380(1)	0.4656(2)	0.0488(9)	0.059(1)	0.056(1)	0.0019(8)	0.0136(8)	–0.0105(8)
C(6)	4*e*	0.7793(2)	0.4144(1)	0.3916(2)	0.051(1)	0.077(1)	0.047(1)	0.0114(9)	0.0069(8)	–0.0058(9)
C(7)	4*e*	0.8038(2)	0.4973(1)	0.4434(2)	0.054(1)	0.063(1)	0.0440(9)	0.0177(8)	0.0104(7)	0.0108(8)
C(8)	4*e*	0.7899(2)	0.2473(2)	0.4110(3)	0.084(2)	0.072(1)	0.090(2)	–0.006(1)	0.011(1)	–0.029(1)
C(9)	4*e*	0.7071(3)	0.4054(2)	0.2549(2)	0.095(2)	0.128(2)	0.058(1)	0.023(2)	–0.012(1)	–0.017(1)
C(10)	4*e*	0.1285(2)	0.3021(1)	–0.0453(2)	0.0567(9)	0.0378(8)	0.0401(8)	0.0035(7)	0.0066(7)	0.0010(7)
C(11)	4*e*	0.2216(2)	0.2738(1)	0.0714(2)	0.058(1)	0.0453(9)	0.0441(9)	0.0095(7)	0.0036(7)	–0.0043(7)
C(12)	4*e*	0.3949(1)	0.1759(1)	0.1207(2)	0.0417(8)	0.0502(9)	0.0458(9)	0.0014(7)	0.0074(7)	–0.0001(7)
C(13)	4*e*	0.4829(2)	0.1241(1)	0.0722(2)	0.056(1)	0.078(1)	0.051(1)	0.0114(9)	0.0161(8)	–0.0049(9)
C(14)	4*e*	0.5678(2)	0.0762(1)	0.1562(2)	0.049(1)	0.071(1)	0.070(1)	0.0143(9)	0.0130(9)	–0.010(1)
C(15)	4*e*	0.5645(2)	0.0797(1)	0.2887(2)	0.0447(9)	0.0508(9)	0.064(1)	0.0036(7)	0.0009(8)	–0.0004(8)
C(16)	4*e*	0.4803(2)	0.1321(1)	0.3388(2)	0.055(1)	0.062(1)	0.0466(9)	0.0058(8)	0.0035(7)	–0.0014(8)
C(17)	4*e*	0.3950(2)	0.1814(1)	0.2546(2)	0.0476(9)	0.0554(9)	0.0465(9)	0.0082(7)	0.0077(7)	–0.0050(8)

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