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Benzimidazolium 2-(2,4-dichlorophenoxy)acetate monohydrate

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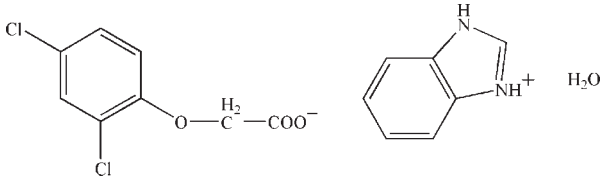
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.102; data-to-parameter ratio = 17.3.

In the crystal of the title hydrated molecular salt, $C_7H_7N_2^+\cdot C_8H_5Cl_2O_3\cdot H_2O$, the components interact by way of N—H···O and O—H···O hydrogen bonds, leading to chains propagating in [100].

Related literature

For background to 2,4-dichlorophenoxyacetic acid, see: Lv (1998).



Experimental

Crystal data

$C_7H_7N_2^+\cdot C_8H_5Cl_2O_3^-\cdot H_2O$
M_r = 357.18
Orthorhombic, $Pna2_1$
a = 4.9322 (10) Å
b = 23.808 (5) Å
c = 13.931 (3) Å
V = 1635.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 293 K
0.20 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
13995 measured reflections
3746 independent reflections
3083 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.102
S = 0.98
3746 reflections
216 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1784 Friedel pairs
Flack parameter: 0.04 (5)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	1.78	2.636 (3)	179
N2—H2A···O3	0.86	1.81	2.667 (3)	172
O1W—H1WA···O3	0.74 (5)	2.11 (5)	2.822 (4)	160 (5)
O1W—H1WB···O1W^{ii}	0.81 (4)	1.95 (4)	2.751 (4)	173 (4)

Symmetry codes: (i) $-x+1, -y+1, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5201).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Lv, F. T. (1998). *Chem. Agent.* **20**, 179.
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supplementary materials

Acta Cryst. (2009). E**65**, o3043 [**doi:10.1107/S1600536809045899**]

Benzimidazolium 2-(2,4-dichlorophenoxy)acetate monohydrate

H.-L. Liu, Q.-Z. Wang and F.-F. Jian

Experimental

A mixture of 2,4-Dichlorophenoxyacetic acid 4.42 g (0.02 mol) and benzimidazole 2.4 g (0.02 mol) was stirred with ethanol (50 ml) at 367 K for 3 h. Colourless bars of (I) were obtained by recrystallization from acetone and ethanol (1:1) at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H and N—H distances of 0.93–0.96 and 0.86 Å, and with U_{iso}=1.2–1.5U_{eq}.

Figures

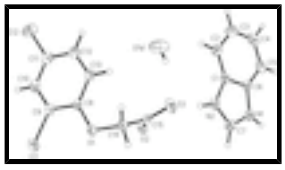


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids.

Benzimidazolium 2-(2,4-dichlorophenoxy)acetate monohydrate

Crystal data

$C_7H_7N_2^+ \cdot C_8H_5Cl_2O_3^- \cdot H_2O$	F_{000} = 736
M_r = 357.18	D_x = 1.450 Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 2216 reflections
a = 4.9322 (10) Å	θ = 3.4–27.5º
b = 23.808 (5) Å	μ = 0.42 mm^{-1}
c = 13.931 (3) Å	*T* = 293 K
V = 1635.9 (6) Å^3	Bar, colorless
Z = 4	0.20 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer	3083 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.069
Monochromator: graphite	θ_{max} = 27.5º

T = 293 K	θ_{min} = 3.4°
ω scans	h = −6→6
Absorption correction: none	k = −30→30
13995 measured reflections	l = −18→18
3746 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.102	$(\Delta/\sigma)_{max} < 0.001$
S = 0.98	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
3746 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
216 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1784 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (5)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.90454 (14)	0.52904 (3)	0.19850 (5)	0.05295 (18)
Cl2	0.18254 (15)	0.69703 (3)	0.23025 (7)	0.0655 (2)
O1	0.9973 (3)	0.57283 (7)	0.00727 (12)	0.0399 (4)
N2	0.5521 (4)	0.57806 (9)	−0.38610 (16)	0.0433 (5)
H2A	0.6477	0.5848	−0.3358	0.052*
O3	0.8577 (4)	0.60800 (8)	−0.23670 (12)	0.0495 (5)
N1	0.3939 (4)	0.53553 (8)	−0.51242 (16)	0.0424 (5)
H1A	0.3716	0.5105	−0.5563	0.051*
O2	0.6808 (3)	0.53999 (7)	−0.14827 (13)	0.0419 (4)
C10	0.5471 (5)	0.61429 (10)	0.2019 (2)	0.0429 (5)

H10A	0.5020	0.6018	0.2631	0.051*
C15	0.8470 (4)	0.57845 (8)	−0.16206 (16)	0.0316 (4)
C13	0.6758 (5)	0.65057 (10)	0.01831 (19)	0.0392 (5)
H13A	0.7166	0.6629	−0.0433	0.047*
C1	0.3528 (5)	0.61244 (10)	−0.42408 (17)	0.0378 (5)
C8	0.8059 (4)	0.60339 (9)	0.05484 (16)	0.0345 (5)
C14	1.0646 (5)	0.59077 (11)	−0.08771 (18)	0.0387 (5)
H14A	1.2313	0.5724	−0.1072	0.046*
H14B	1.0983	0.6309	−0.0867	0.046*
C7	0.5692 (5)	0.53288 (10)	−0.4412 (2)	0.0446 (6)
H7A	0.6888	0.5033	−0.4310	0.054*
C11	0.4222 (5)	0.66116 (11)	0.1635 (2)	0.0437 (6)
C12	0.4859 (5)	0.67944 (11)	0.0727 (2)	0.0450 (6)
H12A	0.4016	0.7112	0.0477	0.054*
C6	0.2510 (5)	0.58563 (10)	−0.50448 (18)	0.0360 (5)
C9	0.7402 (5)	0.58614 (10)	0.14810 (17)	0.0366 (5)
C2	0.2556 (6)	0.66476 (10)	−0.3953 (2)	0.0517 (7)
H2B	0.3238	0.6831	−0.3415	0.062*
C4	−0.0475 (6)	0.66061 (14)	−0.5315 (3)	0.0641 (8)
H4A	−0.1831	0.6780	−0.5671	0.077*
C5	0.0468 (6)	0.60888 (13)	−0.5602 (2)	0.0511 (7)
H5A	−0.0224	0.5906	−0.6139	0.061*
C3	0.0547 (7)	0.68769 (13)	−0.4503 (3)	0.0673 (9)
H3A	−0.0161	0.7225	−0.4331	0.081*
O1W	0.8508 (6)	0.72439 (12)	−0.1984 (3)	0.0798 (9)
H1WA	0.831 (9)	0.696 (2)	−0.219 (4)	0.111 (19)*
H1WB	0.995 (8)	0.7405 (17)	−0.194 (3)	0.088 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0616 (4)	0.0589 (4)	0.0383 (3)	0.0105 (3)	−0.0035 (3)	0.0137 (3)
Cl2	0.0578 (4)	0.0584 (4)	0.0802 (6)	0.0021 (3)	0.0287 (4)	−0.0082 (4)
O1	0.0435 (9)	0.0492 (9)	0.0271 (8)	0.0090 (7)	−0.0022 (7)	0.0020 (7)
N2	0.0522 (12)	0.0432 (11)	0.0344 (11)	−0.0106 (10)	−0.0063 (9)	0.0002 (9)
O3	0.0647 (12)	0.0488 (10)	0.0350 (9)	−0.0190 (8)	−0.0114 (8)	0.0130 (7)
N1	0.0489 (11)	0.0373 (10)	0.0410 (12)	−0.0052 (9)	−0.0017 (10)	−0.0081 (9)
O2	0.0464 (10)	0.0415 (9)	0.0378 (9)	−0.0093 (7)	−0.0024 (8)	0.0054 (7)
C10	0.0419 (12)	0.0494 (13)	0.0373 (12)	−0.0089 (10)	0.0023 (12)	−0.0011 (11)
C15	0.0352 (10)	0.0321 (10)	0.0274 (11)	0.0031 (8)	0.0026 (9)	−0.0011 (8)
C13	0.0471 (12)	0.0393 (11)	0.0313 (12)	−0.0005 (10)	−0.0020 (10)	0.0019 (10)
C1	0.0457 (12)	0.0354 (11)	0.0321 (12)	−0.0084 (10)	0.0051 (10)	0.0021 (9)
C8	0.0356 (11)	0.0380 (11)	0.0300 (11)	−0.0005 (9)	−0.0054 (10)	−0.0027 (9)
C14	0.0354 (12)	0.0497 (13)	0.0310 (11)	0.0018 (10)	−0.0023 (10)	0.0029 (10)
C7	0.0502 (14)	0.0363 (12)	0.0474 (15)	−0.0031 (10)	−0.0030 (12)	−0.0002 (11)
C11	0.0376 (12)	0.0434 (13)	0.0501 (15)	−0.0058 (10)	0.0041 (11)	−0.0061 (11)
C12	0.0462 (13)	0.0397 (12)	0.0491 (16)	0.0029 (10)	−0.0018 (12)	0.0007 (11)
C6	0.0377 (12)	0.0382 (11)	0.0322 (12)	−0.0057 (9)	0.0012 (9)	0.0008 (9)

C9	0.0391 (11)	0.0419 (12)	0.0288 (12)	−0.0036 (10)	−0.0022 (10)	0.0019 (9)
C2	0.0674 (17)	0.0394 (14)	0.0482 (16)	−0.0074 (13)	0.0174 (14)	−0.0081 (12)
C4	0.0554 (16)	0.0667 (19)	0.070 (2)	0.0127 (14)	0.0073 (16)	0.0225 (17)
C5	0.0493 (14)	0.0633 (18)	0.0409 (15)	−0.0074 (13)	−0.0075 (13)	0.0076 (13)
C3	0.078 (2)	0.0415 (15)	0.083 (3)	0.0100 (14)	0.023 (2)	0.0027 (16)
O1W	0.0654 (16)	0.0463 (13)	0.128 (3)	0.0020 (12)	0.0147 (17)	0.0039 (14)

Geometric parameters (Å, °)

Cl1—C9	1.731 (2)	C1—C6	1.384 (3)
Cl2—C11	1.729 (3)	C1—C2	1.394 (3)
O1—C8	1.364 (3)	C8—C9	1.401 (3)
O1—C14	1.429 (3)	C14—H14A	0.9700
N2—C7	1.324 (3)	C14—H14B	0.9700
N2—C1	1.384 (3)	C7—H7A	0.9300
N2—H2A	0.8600	C11—C12	1.375 (4)
O3—C15	1.257 (3)	C12—H12A	0.9300
N1—C7	1.318 (3)	C6—C5	1.387 (4)
N1—C6	1.390 (3)	C2—C3	1.366 (4)
N1—H1A	0.8600	C2—H2B	0.9300
O2—C15	1.244 (3)	C4—C5	1.376 (4)
C10—C11	1.383 (4)	C4—C3	1.396 (5)
C10—C9	1.385 (3)	C4—H4A	0.9300
C10—H10A	0.9300	C5—H5A	0.9300
C15—C14	1.520 (3)	C3—H3A	0.9300
C13—C12	1.387 (3)	O1W—H1WA	0.73 (5)
C13—C8	1.390 (3)	O1W—H1WB	0.81 (4)
C13—H13A	0.9300		
C8—O1—C14	116.82 (18)	N1—C7—N2	110.9 (2)
C7—N2—C1	107.7 (2)	N1—C7—H7A	124.6
C7—N2—H2A	126.2	N2—C7—H7A	124.6
C1—N2—H2A	126.2	C12—C11—C10	120.7 (3)
C7—N1—C6	108.3 (2)	C12—C11—Cl2	119.7 (2)
C7—N1—H1A	125.9	C10—C11—Cl2	119.7 (2)
C6—N1—H1A	125.9	C11—C12—C13	120.0 (2)
C11—C10—C9	119.2 (3)	C11—C12—H12A	120.0
C11—C10—H10A	120.4	C13—C12—H12A	120.0
C9—C10—H10A	120.4	C1—C6—C5	122.2 (2)
O2—C15—O3	124.6 (2)	C1—C6—N1	106.0 (2)
O2—C15—C14	120.1 (2)	C5—C6—N1	131.8 (2)
O3—C15—C14	115.25 (19)	C10—C9—C8	121.3 (2)
C12—C13—C8	120.8 (2)	C10—C9—Cl1	118.83 (19)
C12—C13—H13A	119.6	C8—C9—Cl1	119.89 (18)
C8—C13—H13A	119.6	C3—C2—C1	116.4 (3)
N2—C1—C6	107.1 (2)	C3—C2—H2B	121.8
N2—C1—C2	131.5 (2)	C1—C2—H2B	121.8
C6—C1—C2	121.4 (2)	C5—C4—C3	121.8 (3)
O1—C8—C13	124.9 (2)	C5—C4—H4A	119.1
O1—C8—C9	117.0 (2)	C3—C4—H4A	119.1

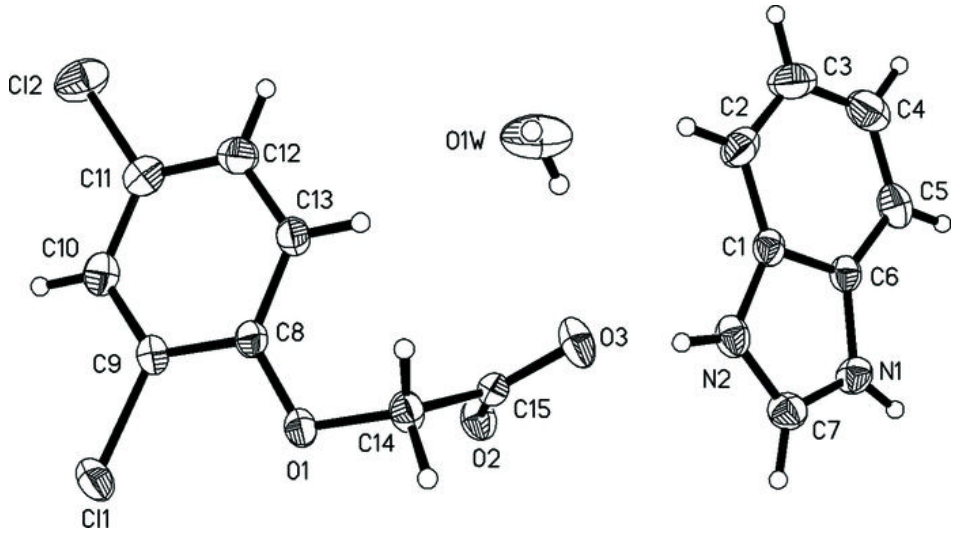
C13—C8—C9	118.0 (2)	C4—C5—C6	116.1 (3)
O1—C14—C15	114.17 (19)	C4—C5—H5A	122.0
O1—C14—H14A	108.7	C6—C5—H5A	122.0
C15—C14—H14A	108.7	C2—C3—C4	122.1 (3)
O1—C14—H14B	108.7	C2—C3—H3A	118.9
C15—C14—H14B	108.7	C4—C3—H3A	118.9
H14A—C14—H14B	107.6	H1WA—O1W—H1WB	126 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.86	1.78	2.636 (3)	179
N2—H2A···O3	0.86	1.81	2.667 (3)	172
O1W—H1WA···O3	0.74 (5)	2.11 (5)	2.822 (4)	160 (5)
O1W—H1WB···O1W^{ii}	0.81 (4)	1.95 (4)	2.751 (4)	173 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, *z*−1/2; (ii) *x*+1/2, −*y*+3/2, *z*.

Fig. 1


Cl2
C12
C11
C13
C10
C8
C9
Cl1
O1
C14
O2
C15
O3
O1W
C3
C2
C4
C5
C1
C6
N2
N1
C7