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2-(4-Chlorobenzoyl)benzoic acid

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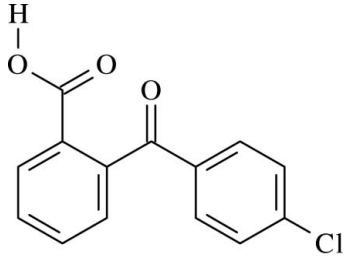
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.110; data-to-parameter ratio = 14.6.

Crystals of the title compound, $C_{14}H_9ClO_3$, are stabilized by O—H···O and C—H···O hydrogen bonds and C—H···π interactions. O—H···O hydrogen bonds generate centrosymmetric dimers. O—H···O and two C—H···O hydrogen bonds generate spirocyclic $R_2^2(8)R_2^1(5)$ ring motifs. The $R_2^2(8)$ and $R_2^1(5)$ ring motifs are connected to each other by C(6) chains and C—H···π interactions. The dihedral angle between the aromatic rings is 88.07 (11)°.

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For related structures, see: Odabaşoğlu *et al.* (2005); Büyükgüngör & Odabaşoğlu (2006); Odabaşoğlu & Büyükgüngör (2006); Odabaşoğlu *et al.* (2006); Ersanlı *et al.* (2005); Etter (1990); Loudon (2002).



Experimental

Crystal data

$C_{14}H_9ClO_3$
M_r = 260.66
Monoclinic, $P2_1/c$
a = 15.3209 (17) Å
b = 7.3171 (6) Å
c = 11.1988 (14) Å
β = 98.467 (10)°
V = 1241.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 296 K
0.72 × 0.44 × 0.27 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.839, T_{max} = 0.919
6666 measured reflections
2381 independent reflections
1611 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.04
2381 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.82	2.6389 (17)	172
C3—H3···O1^{ii}	0.93	2.85	3.413 (2)	120
C4—H4···O1^{ii}	0.93	2.65	3.317 (2)	129
C5—H5···O3^{iii}	0.93	2.83	3.489 (2)	129
C14—H14···Cg^{iv}	0.93	2.77	3.592 (2)	149

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2314).

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supplementary materials

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2-(4-Chlorobenzoyl)benzoic acid

M. Odabasoglu and O. Büyükgüngör

Comment

The present work is part of a structural study of carbonyl compounds (Odabaşoğlu & Büyükgüngör, 2006) and we report here the structure of 3-(4-ethoxyanilino)isobenzofuran-1(3*H*)-one, (I), Fig. 1, Table 1. The dihedral angle between aromatic rings is 88.07 (11)°. The bond lengths and angles are in normal ranges, and comparable with in our previous work on carbonyl compounds (Büyükgüngör & Odabaşoğlu, 2006; Odabaşoğlu & Büyükgüngör, 2006; Odabaşoğlu *et al.*, 2006; Odabaşoğlu *et al.*, 2005; Ersanlı *et al.*, 2005; Allen *et al.*, 1987). The C2—O1 bond distance in (I) is also consistent with the value of the C=O double bond in carbonyl compounds (Loudon, 2002).

The title compound, I, are stabilized by one O—H···O, three C—H···O intermolecular hydrogen bonds and one C—H···π interactions. O—H···O hydrogen bonds generate centrocymmetric dimers. O—H···O and two C—H···O hydrogenbonds generate spirocyclic $R_2^2(8)R_2^1(5)$ ring motifs (Etter, 1990) these motifs are connected by C(6) chains and C—H···π interactions (Fig. 2 and 3).

Experimental

A pure sample of the compound was obtained from Alfa Aeser GmbH & Co KG, Germany, and crystallized by slow evaporation of a solution in ethyl DMF-H_2O (1:1 *v*/*v*) solution at room temperature, m.p. 425–425 K.

Refinement

H atoms were placed in idealized positions with d(C—H) = 0.93 for aromatic, d(C—H) = 0.98Å for methine and d(C—O)=0.82Å for hydroxy and thereafter treated as riding. U_{iso} for H was assigned as 1.2 times U_{eq} of the attached C atoms (1.5 for O)

Figures

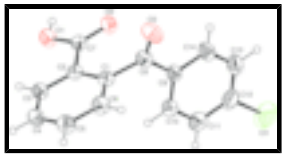

Fig. 1. A view of (I) showing the atomic numbering scheme with displacement ellipsoids drawn at the 50% probability level.

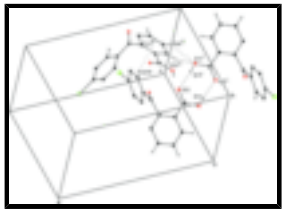

Fig. 2. The $R_2^2(8)R_2^1(5)$ ring motifs and π···π interactions of (I), with C For the sake of clarity, H atoms not involved in the hydrogen bonding motifs shown have been omitted; hydrogen bonds are drawn as dashed lines. [Symmetry codes: (i) −*x*, 1 − *y*, 1 − *z*; (ii) *x* − 1/2, *y*, *z* + 1/2].

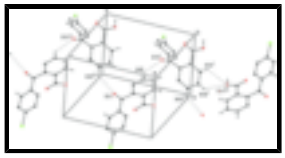

Fig. 3. The C(6) chain and $R_2^1(5)$ ring of (I),, with C For the sake of clarity, H atoms not involved in the hydrogen bonding motifs shown have been omitted; hydrogen bonds are drawn as dashed lines. [Symmetry codes: (i) *x*, 1/2 − *y*, *z* − 1/2; (ii) *x*, 1/2 − *y*, *z* + 1/2; (iii) −*x*, 1 − *y*, 1 − *z*].

2-(4-Chlorobenzoyl)benzoic acid

Crystal data

$C_{14}H_9ClO_3$	F_{000} = 536
M_r = 260.66	D_x = 1.394 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yc	Cell parameters from 6666 reflections
a = 15.3209 (17) Å	θ = 2.1–27.9º
b = 7.3171 (6) Å	μ = 0.30 mm^{-1}
c = 11.1988 (14) Å	*T* = 296 K
β = 98.467 (10)º	Prism, colorless
V = 1241.8 (2) Å^3	0.72 × 0.44 × 0.27 mm
Z = 4	

Data collection

Stoe IPDSII diffractometer	2381 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	1611 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.030
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0º
T = 296 K	θ_{min} = 3.1º
ω scans	*h* = −18→15
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	*k* = −9→9
T_{min} = 0.839, T_{max} = 0.919	*l* = −13→13
6666 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H-atom parameters constrained
$wR(F^2)$ = 0.110	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.074P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
2381 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
C1	0.17454 (12)	0.0458 (2)	0.56843 (15)	0.0466 (4)
C2	0.10791 (12)	0.0997 (2)	0.47700 (15)	0.0438 (4)
C3	0.08082 (13)	−0.0174 (2)	0.38059 (16)	0.0520 (5)
H3	0.0357	0.0182	0.3202	0.062*
C4	0.12036 (14)	−0.1853 (3)	0.37402 (19)	0.0585 (5)
H4	0.1027	−0.2619	0.3086	0.070*
C5	0.18558 (16)	−0.2393 (2)	0.46361 (19)	0.0627 (6)
H5	0.2119	−0.3532	0.4595	0.075*
C6	0.21235 (14)	−0.1254 (2)	0.55999 (18)	0.0593 (5)
H6	0.2566	−0.1639	0.6206	0.071*
C7	0.06322 (12)	0.2779 (2)	0.48544 (15)	0.0449 (4)
C8	0.20686 (13)	0.1576 (2)	0.67855 (16)	0.0518 (5)
C9	0.27299 (12)	0.3042 (2)	0.67000 (16)	0.0509 (5)
C10	0.31668 (15)	0.3224 (3)	0.5719 (2)	0.0702 (6)
H10	0.3037	0.2425	0.5071	0.084*
C11	0.37936 (17)	0.4568 (4)	0.5675 (3)	0.0861 (8)
H11	0.4089	0.4672	0.5009	0.103*
C12	0.39722 (16)	0.5748 (3)	0.6631 (3)	0.0802 (7)
C13	0.35424 (16)	0.5614 (3)	0.7606 (2)	0.0742 (7)
H13	0.3668	0.6430	0.8245	0.089*
C14	0.29228 (15)	0.4270 (3)	0.76445 (18)	0.0624 (6)
H14	0.2629	0.4182	0.8312	0.075*
O1	0.00022 (9)	0.31239 (18)	0.39744 (11)	0.0607 (4)
H1	−0.0213	0.4126	0.4081	0.091*
O2	0.08373 (9)	0.38031 (16)	0.57144 (11)	0.0551 (4)
O3	0.18427 (12)	0.1185 (2)	0.77436 (12)	0.0769 (5)
Cl1	0.47438 (7)	0.74585 (13)	0.65780 (11)	0.1428 (4)

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.0519 (11)	0.0417 (9)	0.0464 (9)	0.0039 (8)	0.0078 (8)	0.0043 (7)
C2	0.0461 (10)	0.0415 (8)	0.0445 (9)	0.0030 (7)	0.0087 (8)	0.0046 (7)
C3	0.0540 (12)	0.0511 (10)	0.0504 (10)	0.0019 (8)	0.0059 (8)	0.0005 (8)
C4	0.0668 (14)	0.0475 (10)	0.0611 (12)	−0.0015 (9)	0.0089 (10)	−0.0075 (9)
C5	0.0741 (15)	0.0390 (9)	0.0757 (14)	0.0078 (9)	0.0126 (11)	−0.0009 (9)
C6	0.0658 (14)	0.0473 (10)	0.0624 (12)	0.0133 (9)	0.0008 (10)	0.0096 (9)
C7	0.0468 (11)	0.0457 (9)	0.0424 (9)	0.0042 (7)	0.0074 (7)	0.0054 (8)
C8	0.0603 (13)	0.0490 (10)	0.0446 (10)	0.0136 (8)	0.0027 (9)	0.0060 (8)
C9	0.0491 (11)	0.0557 (10)	0.0443 (10)	0.0116 (8)	−0.0055 (8)	−0.0032 (8)
C10	0.0603 (14)	0.0828 (15)	0.0676 (13)	−0.0109 (12)	0.0097 (10)	−0.0228 (11)
C11	0.0650 (16)	0.0989 (18)	0.0979 (18)	−0.0186 (14)	0.0237 (13)	−0.0207 (15)
C12	0.0492 (14)	0.0755 (15)	0.112 (2)	−0.0041 (11)	−0.0013 (13)	−0.0195 (14)
C13	0.0692 (16)	0.0642 (13)	0.0816 (15)	0.0087 (11)	−0.0145 (12)	−0.0217 (11)
C14	0.0726 (15)	0.0596 (12)	0.0510 (11)	0.0146 (10)	−0.0039 (10)	−0.0042 (9)
O1	0.0658 (10)	0.0594 (7)	0.0523 (8)	0.0217 (7)	−0.0062 (6)	−0.0014 (6)
O2	0.0574 (9)	0.0466 (7)	0.0574 (8)	0.0108 (6)	−0.0048 (6)	−0.0061 (6)
O3	0.1141 (14)	0.0690 (9)	0.0496 (8)	0.0006 (8)	0.0187 (8)	0.0079 (7)
Cl1	0.0970 (7)	0.1214 (7)	0.2131 (11)	−0.0513 (5)	0.0328 (7)	−0.0505 (7)

Geometric parameters (Å, °)

C1—C6	1.389 (3)	C8—O3	1.209 (2)
C1—C2	1.392 (2)	C8—C9	1.488 (3)
C1—C8	1.502 (2)	C9—C10	1.375 (3)
C2—C3	1.393 (2)	C9—C14	1.386 (3)
C2—C7	1.483 (2)	C10—C11	1.381 (3)
C3—C4	1.377 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.371 (3)
C4—C5	1.366 (3)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.359 (4)
C5—C6	1.378 (3)	C12—Cl1	1.729 (3)
C5—H5	0.9300	C13—C14	1.372 (3)
C6—H6	0.9300	C13—H13	0.9300
C7—O2	1.224 (2)	C14—H14	0.9300
C7—O1	1.299 (2)	O1—H1	0.8200
C6—C1—C2	118.24 (16)	O3—C8—C1	119.80 (18)
C6—C1—C8	117.17 (16)	C9—C8—C1	119.02 (16)
C2—C1—C8	124.56 (15)	C10—C9—C14	118.2 (2)
C1—C2—C3	119.93 (16)	C10—C9—C8	122.50 (17)
C1—C2—C7	119.84 (15)	C14—C9—C8	119.27 (18)
C3—C2—C7	120.17 (16)	C9—C10—C11	121.4 (2)
C4—C3—C2	120.46 (18)	C9—C10—H10	119.3
C4—C3—H3	119.8	C11—C10—H10	119.3
C2—C3—H3	119.8	C12—C11—C10	118.7 (2)
C5—C4—C3	119.95 (18)	C12—C11—H11	120.6
C5—C4—H4	120.0	C10—C11—H11	120.6
C3—C4—H4	120.0	C13—C12—C11	121.2 (2)
C4—C5—C6	120.09 (17)	C13—C12—Cl1	119.6 (2)
C4—C5—H5	120.0	C11—C12—Cl1	119.2 (2)

C6—C5—H5	120.0	C12—C13—C14	119.8 (2)
C5—C6—C1	121.33 (18)	C12—C13—H13	120.1
C5—C6—H6	119.3	C14—C13—H13	120.1
C1—C6—H6	119.3	C13—C14—C9	120.8 (2)
O2—C7—O1	123.66 (15)	C13—C14—H14	119.6
O2—C7—C2	121.41 (15)	C9—C14—H14	119.6
O1—C7—C2	114.90 (15)	C7—O1—H1	109.5
O3—C8—C9	120.93 (17)		
C6—C1—C2—C3	0.1 (3)	C6—C1—C8—C9	99.6 (2)
C8—C1—C2—C3	−177.79 (17)	C2—C1—C8—C9	−82.5 (2)
C6—C1—C2—C7	177.32 (17)	O3—C8—C9—C10	163.2 (2)
C8—C1—C2—C7	−0.6 (3)	C1—C8—C9—C10	−11.0 (3)
C1—C2—C3—C4	−0.9 (3)	O3—C8—C9—C14	−16.3 (3)
C7—C2—C3—C4	−178.14 (17)	C1—C8—C9—C14	169.48 (16)
C2—C3—C4—C5	1.2 (3)	C14—C9—C10—C11	1.1 (3)
C3—C4—C5—C6	−0.6 (3)	C8—C9—C10—C11	−178.4 (2)
C4—C5—C6—C1	−0.3 (3)	C9—C10—C11—C12	−0.6 (4)
C2—C1—C6—C5	0.5 (3)	C10—C11—C12—C13	−0.2 (4)
C8—C1—C6—C5	178.56 (19)	C10—C11—C12—Cl1	−179.1 (2)
C1—C2—C7—O2	0.2 (3)	C11—C12—C13—C14	0.5 (4)
C3—C2—C7—O2	177.39 (18)	Cl1—C12—C13—C14	179.28 (17)
C1—C2—C7—O1	−177.92 (16)	C12—C13—C14—C9	0.1 (3)
C3—C2—C7—O1	−0.7 (2)	C10—C9—C14—C13	−0.9 (3)
C6—C1—C8—O3	−74.7 (2)	C8—C9—C14—C13	178.60 (18)
C2—C1—C8—O3	103.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.82	2.6389 (17)	172
C3—H3···O1^{ii}	0.93	2.85	3.413 (2)	120
C4—H4···O1^{ii}	0.93	2.65	3.317 (2)	129
C5—H5···O3^{iii}	0.93	2.83	3.489 (2)	129
C14—H14···Cg^{iv}	0.93	2.77	3.592 (2)	149

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

Fig. 1

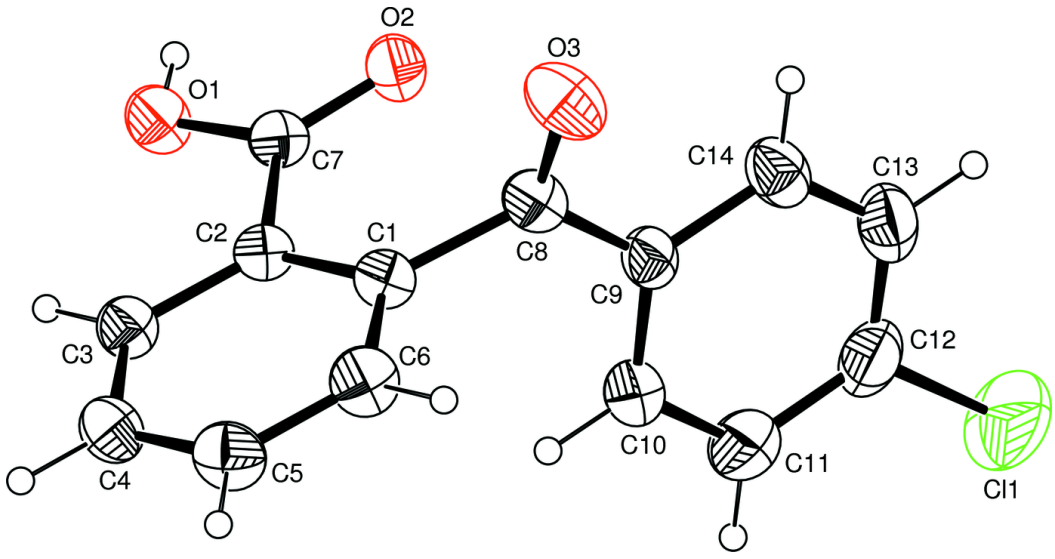

Fig. 2

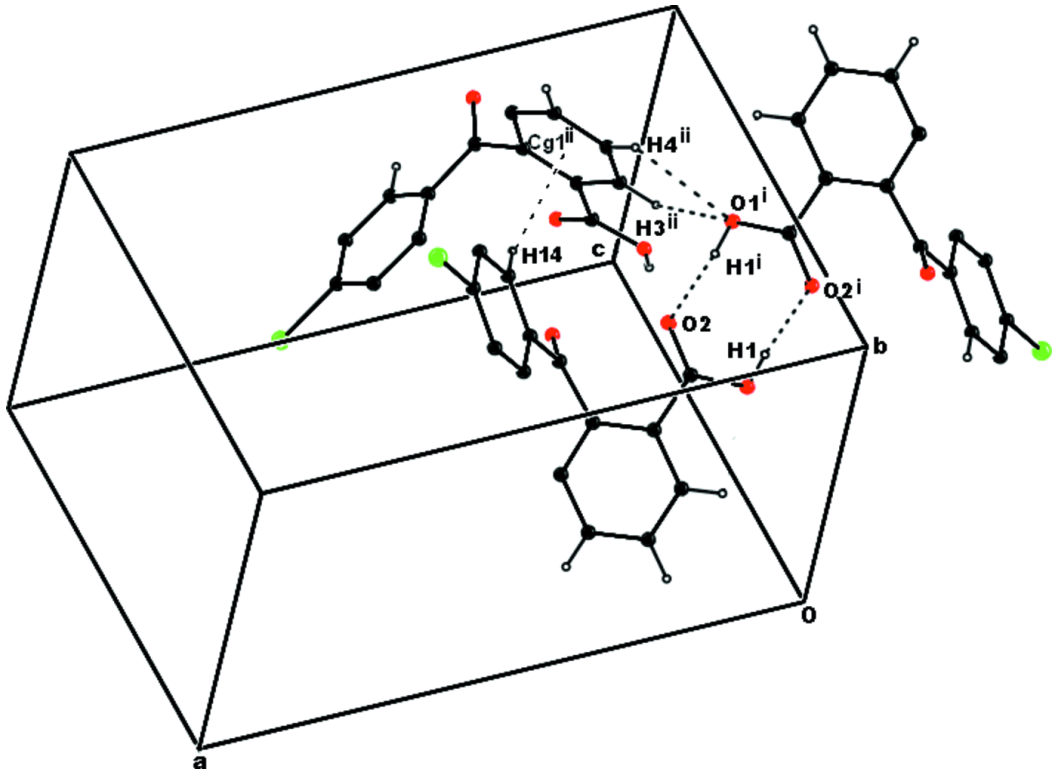

Fig. 3