

4-Amino-3-bromobenzoic acid

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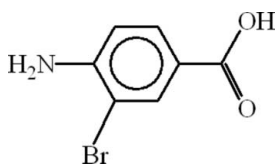
Received 1 February 2009; accepted 24 February 2009

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.030; wR factor = 0.059; data-to-parameter ratio = 18.3.

The asymmetric unit of the title compound, $\text{C}_7\text{H}_6\text{BrNO}_2$, consists of two molecules having a small variation of bond lengths and angles. The title compound forms dimers through pairs of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds involving the carboxylate groups. The dimers are linked into polymeric forms through intermolecular hydrogen bonds, forming $R_2^1(6)$, $R_3^2(8)$ and $R_3^3(15)$ ring motifs.

Related literature

The title compound has been prepared as an intermediate for the synthesis of sulfonamides (Arshad *et al.*, 2009) and benzothiazines (Arshad *et al.*, 2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Pant (1965); Tanaka *et al.* (1967). For the synthesis, see: Krishna Mohan *et al.* (2004).



Experimental

Crystal data

$\text{C}_7\text{H}_6\text{BrNO}_2$	$V = 1511.53$ (11) Å ³
$M_r = 216.04$	$Z = 8$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 24.3968$ (11) Å	$\mu = 5.38$ mm ⁻¹
$b = 4.8388$ (2) Å	$T = 296$ K
$c = 12.8040$ (5) Å	$0.22 \times 0.16 \times 0.14$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	9922 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	3908 independent reflections
$T_{\min} = 0.375$, $T_{\max} = 0.469$	3169 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.059$
 $S = 1.00$
 3908 reflections
 214 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³
 Absolute structure: Flack (1983), 1857 Friedel pairs
 Flack parameter: 0.012 (9)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O4}^{\text{i}}$	0.82	1.76	2.564 (3)	165
$\text{N1}-\text{H1A}\cdots\text{Br1}^{\text{i}}$	0.92 (4)	2.63 (4)	3.081 (4)	111 (3)
$\text{N1}-\text{H1B}\cdots\text{O2}^{\text{ii}}$	0.83 (5)	2.57 (5)	3.313 (4)	149 (4)
$\text{N2}-\text{H2A}\cdots\text{Br2}^{\text{i}}$	0.99 (4)	2.68 (4)	3.099 (4)	106 (2)
$\text{N2}-\text{H2A}\cdots\text{Br1}^{\text{ii}}$	0.99 (4)	2.69 (4)	3.630 (4)	158 (3)
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{iii}}$	0.79 (5)	2.43 (5)	3.216 (4)	179 (6)
$\text{O3}-\text{H3}\cdots\text{O2}^{\text{iv}}$	0.82	1.90	2.723 (3)	178
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{ii}}$	0.93	2.59	3.407 (4)	147
$\text{C12}-\text{H12}\cdots\text{O4}^{\text{v}}$	0.93	2.54	3.470 (4)	174

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

MNA gratefully acknowledges the Higher Education Commission, Islamabad, Pakistan, for providing him with a Scholarship under the Indigenous PhD Program (PIN 042-120607-PS2-183).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2123).

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supplementary materials

Acta Cryst. (2009). E65, o640 [doi:10.1107/S1600536809006825]

4-Amino-3-bromobenzoic acid

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Comment

Different types of aromatic anilines have been used for the synthesis of carboxamides and sulfonamides. The title compound (I), (Fig 1), has been prepared as an intermediate for the synthesis of sulfonamides (Arshad *et al.*, 2009), benzothiazines (Arshad *et al.*, 2008) and different metal complexes.

The crystal structure of *m*-Bromobenzoic acid (Tanaka *et al.*, 1967) and 3,5-Dibromo-*p*-aminobenzoic acid (Pant, 1965) has been published. The title compound consists of an asymmetric unit having two chemical isomers. There is a small variation of bond lengths and bond angles among the two isomers and both isomers form five membered ring (Br/C/C/N/H) through intramolecular H-bond of type N—H...Br. The molecules are dimerized forming $R_2^2(8)$ ring motifs (Bernstein *et al.*, 1995). These dimers are linked to each other through $R_2^1(6)$, $R_3^2(8)$ and $R_3^3(15)$ ring motifs (Table 1), (Fig 2).

Experimental

The title compound was prepared following the same method (Krishna Mohan *et al.*, 2004) available in literature. 4-Amino Benzoic acid (2 g, 0.0146 mol) and ammonium bromide (1.5 g, 0.16 mol) was charged to a flask (25 ml) containing acetic acid (15 ml). Hydrogen peroxide (0.545 g, 0.016 mol) was added drop wise to the above mixture and allowed to stir at room temperature for 3 h. Stirring was stopped and allowed it to settle down. Precipitate obtained was filtered and washed with water and recrystallized in dichloromethane and methanol for X-ray studies.

Refinement

The coordinates of H-atoms of amino groups were refined. H-atoms were positioned geometrically, with O-H = 0.82 Å for OH, C-H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N}, \text{O})$, where $x = 1.2$ for all other H atoms.

Figures

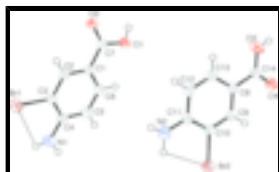


Fig. 1. ORTEP drawing of the title compound, with the atom numbering scheme. The thermal ellipsoids are drawn at the 30% probability level. The dotted lines show the intramolecular H-bonds.

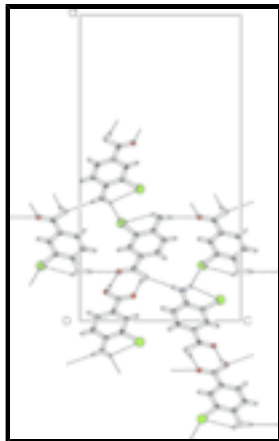


Fig. 2. The projectional view (*PLATON*: Spek, 2009) which shows that molecules are dimerized and form ring motifs.

4-Amino-3-bromobenzoic acid

Crystal data

$C_7H_6BrNO_2$

$M_r = 216.04$

Orthorhombic, $Pna2_1$

Hall symbol: P 2c -2n

$a = 24.3968$ (11) Å

$b = 4.8388$ (2) Å

$c = 12.8040$ (5) Å

$V = 1511.53$ (11) Å³

$Z = 8$

$F_{000} = 848$

$D_x = 1.899$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3169 reflections

$\theta = 1.7$ – 28.7°

$\mu = 5.38$ mm⁻¹

$T = 296$ K

Prismatic, colorless

$0.22 \times 0.16 \times 0.14$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 7.40 pixels mm⁻¹

$T = 296$ K

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2005)

$T_{\min} = 0.375$, $T_{\max} = 0.469$

9922 measured reflections

3908 independent reflections

3169 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 28.7^\circ$

$\theta_{\min} = 1.7^\circ$

$h = -32 \rightarrow 33$

$k = -6 \rightarrow 5$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0107P)^2]$
$wR(F^2) = 0.059$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} < 0.001$
3908 reflections	$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$
214 parameters	$\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1857 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.012 (9)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.320114 (15)	-0.05594 (7)	0.25848 (2)	0.03957 (10)
O1	0.14368 (11)	0.8516 (5)	0.40595 (16)	0.0440 (6)
H1	0.1288	0.9846	0.3781	0.053*
O2	0.16062 (9)	0.7357 (4)	0.24087 (17)	0.0350 (5)
N1	0.33671 (15)	0.0202 (8)	0.4953 (3)	0.0510 (10)
H1A	0.3479 (16)	-0.127 (8)	0.455 (3)	0.061*
H1B	0.3387 (19)	0.004 (8)	0.560 (4)	0.061*
C1	0.21062 (12)	0.5149 (6)	0.3765 (3)	0.0302 (6)
C2	0.23965 (12)	0.3438 (6)	0.3108 (2)	0.0288 (7)
H2	0.2318	0.3416	0.2397	0.035*
C3	0.28043 (13)	0.1752 (6)	0.3501 (2)	0.0275 (7)
C4	0.29402 (14)	0.1757 (7)	0.4569 (3)	0.0339 (8)
C5	0.26337 (14)	0.3430 (8)	0.5214 (3)	0.0428 (9)
H5	0.2702	0.3409	0.5928	0.051*
C6	0.22328 (15)	0.5119 (7)	0.4833 (3)	0.0416 (9)
H6	0.2041	0.6265	0.5287	0.050*
C7	0.16965 (14)	0.7060 (7)	0.3350 (3)	0.0312 (8)
Br2	0.068709 (14)	-0.02802 (6)	0.87184 (3)	0.03738 (9)
O3	-0.09440 (11)	0.8621 (5)	0.66215 (19)	0.0441 (6)
H3	-0.1136	0.9859	0.6862	0.053*
O4	-0.08170 (10)	0.7685 (5)	0.83152 (18)	0.0400 (6)
N2	0.09823 (15)	-0.0184 (7)	0.6365 (3)	0.0468 (9)

supplementary materials

H2A	0.1139 (15)	-0.152 (7)	0.687 (3)	0.056*
H2B	0.1093 (17)	-0.052 (8)	0.580 (4)	0.056*
C8	-0.02918 (14)	0.5234 (6)	0.7088 (3)	0.0284 (7)
C9	-0.00474 (13)	0.3632 (6)	0.7867 (2)	0.0281 (7)
H9	-0.0167	0.3786	0.8554	0.034*
C10	0.03682 (12)	0.1830 (6)	0.7625 (3)	0.0286 (6)
C11	0.05602 (13)	0.1496 (7)	0.6603 (3)	0.0305 (7)
C12	0.03023 (14)	0.3106 (8)	0.5824 (2)	0.0400 (8)
H12	0.0416	0.2949	0.5134	0.048*
C13	-0.01099 (15)	0.4883 (6)	0.6068 (3)	0.0371 (8)
H13	-0.0275	0.5894	0.5537	0.045*
C14	-0.07084 (13)	0.7263 (6)	0.7391 (3)	0.0315 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03529 (19)	0.04090 (18)	0.0425 (2)	0.00405 (15)	0.00077 (17)	-0.0027 (2)
O1	0.0561 (17)	0.0506 (15)	0.0252 (12)	0.0258 (13)	0.0033 (11)	0.0052 (11)
O2	0.0373 (13)	0.0412 (13)	0.0265 (13)	0.0111 (9)	0.0002 (10)	0.0058 (10)
N1	0.049 (2)	0.069 (2)	0.0351 (19)	0.0173 (16)	-0.0101 (17)	0.0089 (16)
C1	0.0271 (15)	0.0389 (15)	0.0246 (15)	0.0026 (13)	-0.0001 (16)	0.0062 (15)
C2	0.0250 (18)	0.0351 (18)	0.0264 (17)	-0.0012 (14)	-0.0023 (13)	0.0040 (14)
C3	0.0254 (17)	0.0300 (16)	0.027 (2)	0.0002 (13)	0.0000 (13)	0.0040 (13)
C4	0.0293 (19)	0.0360 (19)	0.036 (2)	0.0029 (15)	-0.0073 (14)	0.0071 (16)
C5	0.044 (2)	0.060 (2)	0.0246 (17)	0.0105 (19)	-0.0050 (16)	-0.0015 (17)
C6	0.039 (2)	0.051 (2)	0.034 (2)	0.0133 (16)	0.0008 (16)	0.0011 (16)
C7	0.032 (2)	0.0305 (17)	0.0310 (19)	-0.0003 (14)	0.0025 (15)	0.0055 (15)
Br2	0.03815 (19)	0.03913 (17)	0.03487 (17)	0.00381 (15)	-0.00324 (17)	0.0049 (2)
O3	0.0484 (16)	0.0458 (15)	0.0381 (14)	0.0211 (12)	-0.0097 (12)	-0.0080 (12)
O4	0.0403 (16)	0.0471 (15)	0.0326 (13)	0.0124 (12)	-0.0019 (11)	-0.0078 (11)
N2	0.053 (2)	0.054 (2)	0.0327 (18)	0.0179 (16)	0.0056 (16)	-0.0052 (16)
C8	0.0292 (17)	0.0257 (15)	0.0303 (17)	0.0030 (13)	-0.0028 (14)	-0.0054 (13)
C9	0.0309 (18)	0.0323 (16)	0.0212 (16)	-0.0029 (14)	0.0027 (12)	-0.0047 (12)
C10	0.0310 (16)	0.0269 (14)	0.0278 (16)	-0.0003 (12)	-0.0057 (15)	0.0013 (16)
C11	0.0285 (17)	0.0335 (17)	0.0296 (17)	0.0008 (14)	-0.0003 (14)	-0.0041 (15)
C12	0.044 (2)	0.055 (2)	0.0206 (17)	0.0048 (17)	0.0046 (15)	-0.0024 (15)
C13	0.046 (2)	0.0403 (17)	0.0254 (19)	0.0058 (16)	-0.0058 (15)	0.0011 (14)
C14	0.0302 (17)	0.0287 (16)	0.035 (2)	0.0012 (12)	-0.0015 (16)	-0.0019 (14)

Geometric parameters (\AA , $^\circ$)

Br1—C3	1.888 (3)	Br2—C10	1.899 (3)
O1—C7	1.312 (4)	O3—C14	1.316 (4)
O1—H1	0.8200	O3—H3	0.8200
O2—C7	1.234 (3)	O4—C14	1.230 (3)
N1—C4	1.376 (4)	N2—C11	1.347 (5)
N1—H1A	0.92 (4)	N2—H2A	0.99 (4)
N1—H1B	0.83 (4)	N2—H2B	0.79 (4)
C1—C2	1.376 (5)	C8—C13	1.390 (5)

C1—C6	1.402 (5)	C8—C9	1.397 (4)
C1—C7	1.462 (5)	C8—C14	1.465 (4)
C2—C3	1.382 (4)	C9—C10	1.373 (4)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.407 (4)	C10—C11	1.400 (5)
C4—C5	1.377 (5)	C11—C12	1.413 (5)
C5—C6	1.365 (5)	C12—C13	1.360 (5)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—O1—H1	109.5	C14—O3—H3	109.5
C4—N1—H1A	116 (2)	C11—N2—H2A	123 (2)
C4—N1—H1B	117 (3)	C11—N2—H2B	126 (3)
H1A—N1—H1B	118 (4)	H2A—N2—H2B	109 (4)
C2—C1—C6	118.5 (3)	C13—C8—C9	117.8 (3)
C2—C1—C7	120.7 (3)	C13—C8—C14	123.5 (3)
C6—C1—C7	120.7 (3)	C9—C8—C14	118.7 (3)
C1—C2—C3	120.2 (3)	C10—C9—C8	120.5 (3)
C1—C2—H2	119.9	C10—C9—H9	119.7
C3—C2—H2	119.9	C8—C9—H9	119.7
C2—C3—C4	121.5 (3)	C9—C10—C11	122.1 (3)
C2—C3—Br1	119.5 (2)	C9—C10—Br2	118.6 (2)
C4—C3—Br1	119.0 (2)	C11—C10—Br2	119.4 (2)
N1—C4—C5	121.3 (3)	N2—C11—C10	122.5 (3)
N1—C4—C3	121.6 (3)	N2—C11—C12	120.9 (3)
C5—C4—C3	117.1 (3)	C10—C11—C12	116.6 (3)
C6—C5—C4	121.8 (3)	C13—C12—C11	121.0 (3)
C6—C5—H5	119.1	C13—C12—H12	119.5
C4—C5—H5	119.1	C11—C12—H12	119.5
C5—C6—C1	120.8 (3)	C12—C13—C8	122.0 (3)
C5—C6—H6	119.6	C12—C13—H13	119.0
C1—C6—H6	119.6	C8—C13—H13	119.0
O2—C7—O1	121.8 (3)	O4—C14—O3	122.9 (3)
O2—C7—C1	123.4 (3)	O4—C14—C8	121.0 (3)
O1—C7—C1	114.7 (3)	O3—C14—C8	116.1 (3)
C6—C1—C2—C3	-0.4 (4)	C13—C8—C9—C10	1.7 (5)
C7—C1—C2—C3	176.3 (3)	C14—C8—C9—C10	-176.0 (3)
C1—C2—C3—C4	-0.9 (5)	C8—C9—C10—C11	-0.7 (5)
C1—C2—C3—Br1	-179.5 (2)	C8—C9—C10—Br2	179.7 (2)
C2—C3—C4—N1	-176.1 (3)	C9—C10—C11—N2	177.3 (3)
Br1—C3—C4—N1	2.5 (5)	Br2—C10—C11—N2	-3.1 (4)
C2—C3—C4—C5	2.7 (5)	C9—C10—C11—C12	-0.2 (5)
Br1—C3—C4—C5	-178.7 (3)	Br2—C10—C11—C12	179.4 (2)
N1—C4—C5—C6	175.6 (4)	N2—C11—C12—C13	-177.4 (3)
C3—C4—C5—C6	-3.2 (6)	C10—C11—C12—C13	0.1 (5)
C4—C5—C6—C1	2.0 (6)	C11—C12—C13—C8	1.0 (6)
C2—C1—C6—C5	-0.1 (5)	C9—C8—C13—C12	-1.8 (5)
C7—C1—C6—C5	-176.8 (3)	C14—C8—C13—C12	175.7 (3)
C2—C1—C7—O2	-3.7 (5)	C13—C8—C14—O4	-172.8 (3)

supplementary materials

C6—C1—C7—O2	172.9 (3)	C9—C8—C14—O4	4.7 (5)
C2—C1—C7—O1	178.0 (3)	C13—C8—C14—O3	5.7 (5)
C6—C1—C7—O1	-5.3 (5)	C9—C8—C14—O3	-176.8 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots O4 ⁱ	0.82	1.76	2.564 (3)	165
N1—H1A \cdots Br1	0.92 (4)	2.63 (4)	3.081 (4)	111 (3)
N1—H1B \cdots O2 ⁱⁱ	0.83 (5)	2.57 (5)	3.313 (4)	149 (4)
N2—H2A \cdots Br2	0.99 (4)	2.68 (4)	3.099 (4)	106 (2)
N2—H2A \cdots Br1 ⁱⁱ	0.99 (4)	2.69 (4)	3.630 (4)	158 (3)
N2—H2B \cdots O1 ⁱⁱⁱ	0.79 (5)	2.43 (5)	3.216 (4)	179 (6)
O3—H3 \cdots O2 ^{iv}	0.82	1.90	2.723 (3)	178
C5—H5 \cdots O2 ⁱⁱ	0.93	2.59	3.407 (4)	147
C12—H12 \cdots O4 ^v	0.93	2.54	3.470 (4)	174

Symmetry codes: (i) $-x, -y+2, z-1/2$; (ii) $-x+1/2, y-1/2, z+1/2$; (iii) $x, y-1, z$; (iv) $-x, -y+2, z+1/2$; (v) $-x, -y+1, z-1/2$.

Fig. 1

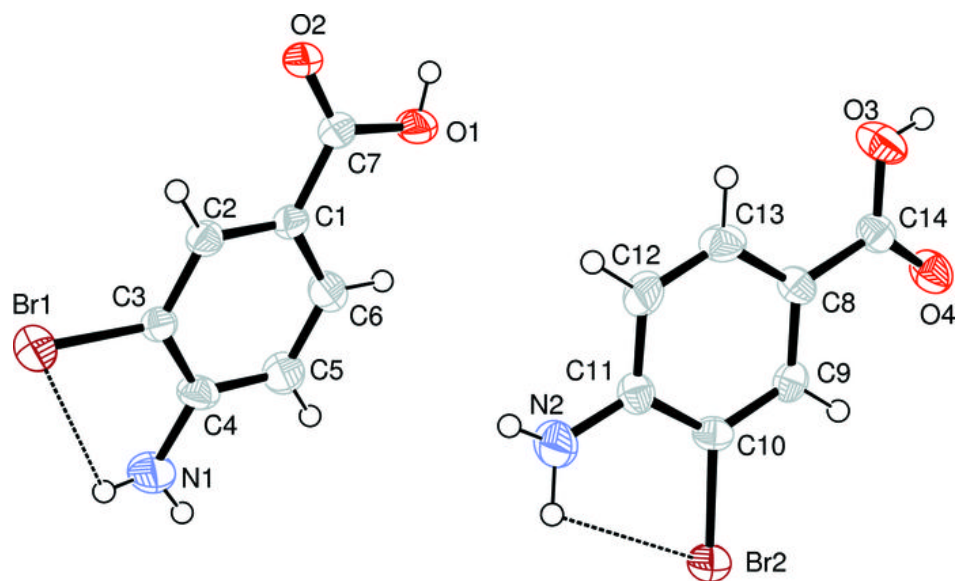


Fig. 2

