

(S)-2-[(2-Hydroxybenzyl)azaniumyl]-4-(methylsulfanyl)butanoate

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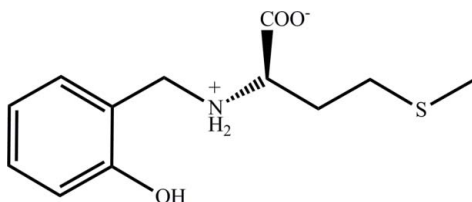
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}–\text{C}) = 0.006$ Å; R factor = 0.059; wR factor = 0.179; data-to-parameter ratio = 14.9.

The zwitterionic title compound, $\text{C}_{12}\text{H}_{17}\text{NO}_3\text{S}$, is a reduced Schiff base derived from (*S*)-*N*-(2-hydroxybenzylidene)-methionine. An intramolecular interaction between the N–H and carboxylate groups forms a roughly planar (r.m.s. deviation = 0.1405 Å) five-membered ring containing the H(N), N, C α , C(carboxylate) and O atoms in a pentagonal conformation. In the crystal, a supramolecular triangle-shaped motif is generated by molecules held together by O–H...O and N–H...O hydrogen bonds.

Related literature

For transition metal complexes containing *N*-(2-hydroxybenzyl)- α -amino acids as ligands, see: Bandyopadhyay *et al.* (2006); Beltrán *et al.* (2002); Ganguly *et al.* (2008); Koh *et al.* (1996); Martell (1989); Maurya (2003); Nefkens & Zwanenburg (1985); Ritsma (1975); Shongwe *et al.* (1999); Sreenivasulu & Vittal (2004); Wilson (1990).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{17}\text{NO}_3\text{S}$
 $M_r = 255.33$
 Triclinic, $P1$
 $a = 5.3221$ (2) Å
 $b = 5.8369$ (2) Å
 $c = 10.5564$ (5) Å

$\alpha = 98.200$ (3)°
 $\beta = 90.780$ (3)°
 $\gamma = 96.849$ (3)°
 $V = 322.10$ (2) Å³
 $Z = 1$
 Mo $K\alpha$ radiation

$\mu = 0.25$ mm⁻¹
 $T = 296$ K

0.53 × 0.44 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.679$, $T_{\max} = 0.746$

7430 measured reflections
 2324 independent reflections
 1966 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.179$
 $S = 1.07$
 2324 reflections
 156 parameters
 3 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.79$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.41$ e Å⁻³
 Absolute structure: Assigned from the known absolute structure of the starting material; the Flack (1983) parameter is consistent with this assignment, 1119 Friedel pairs
 Flack parameter: 0.12 (19)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O1–H1...O2 ⁱ	0.82	1.83	2.641 (3)	168
N1–H1A...O3 ⁱⁱ	0.9	1.83	2.713 (3)	166
N1–H1B...O1 ⁱⁱⁱ	0.9	2.14	2.916 (4)	144
N1–H1B...O2	0.9	2.35	2.687 (3)	102

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SIR2004 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2002).

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supplementary materials

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(S)-2-[(2-Hydroxybenzyl)azaniumyl]-4-(methylsulfanyl)butanoate

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Comment

Considerable attention has been devoted to both Schiff bases and reduced Schiff bases derived from salicylaldehyde and α -amino acids, since their transition metal complexes are closely analogous to the metal-free systems formed as intermediates in many reactions involving the vitamin B6, such as transamination, decarboxylation, α - and β -elimination and racemization (Martell, 1989). In this regard, copper(II) complexes of *N*-(2-hydroxybenzyl)- α -amino acids have been studied as models for the intermediate species that occur in the biological reactions mentioned above (Koh *et al.*, 1996) and such reduced Schiff bases have been used as chelating agents for organoboron (Nefkens *et al.*, 1985; Beltrán *et al.*, 2002) and transition metals such as copper (Koh *et al.*, 1996), zinc (Ritsma, 1975), cobalt (Bandyopadhyay *et al.*, 2006), nickel (Sreenivasulu *et al.*, 2004), manganese (Shongwe *et al.*, 1999), technetium (Wilson, 1990) and vanadium (Maurya, 2003). These ligands are more stable than the Schiff bases from which they originate and are suitable to provide conformationally flexible rings in complexation. This results in different solid state architectures, and the presence of hydrogen bond donors and acceptors enables the design and construction of supramolecular, three-dimensional networks (Ganguly *et al.*, 2008). This paper describes the structural characterization of the reduced Schiff base (*S*)-*N*-(2-hydroxybenzyl)methionine (I).

Figure 1 shows the molecular structure of (I). The crystal structure analysis clearly indicates that the amino acid is a pure enantiomer, since the compound crystallizes in the chiral *P1* space group. In Figure 1 the L-enantiomer is shown with *S* absolute configuration at C8, in agreement with the synthetic precursor, L-(*S*)-methionine. The carboxylic acid has been found in the deprotonated —(COO)^- form, with the C9—O2 and C9—O3 bond distances being very similar. Meanwhile, N1 is protonated in the NH_2^+ form. Therefore compound (I) crystallizes as a zwitterion. The angle N1—C8—C9 is lower in comparison to the angles N1—C8—C10 and C10—C8—C9. This asymmetry in the angles at the C8 is due to the presence of an intramolecular interaction between the N—H and carboxylate groups forming a roughly planar five-membered ring containing H, N, C α , C and O atoms in a pentagonal (C_5) conformation.

A very interesting feature encountered in the crystal lattice of (I) is related to the formation of supramolecular triangle-shaped motifs [$R^2_3(8)$] involving molecules held together by O—H \cdots O and N—H \cdots O hydrogen bonds (Figure 2, Table 1). Other hydrogen bonding interactions govern the molecular arrangement in parallel strings extending along the (001) crystallographic plane (Figure 3).

Experimental

The synthesis of the title compound (I) was performed according to the method previously employed for similar Schiff bases (Koh, *et al.*, 1996), starting from L-(*S*)-methionine. Recrystallization of (I) from a methanol solution produced single crystals suitable for X-ray diffraction.

Refinement

H atoms were located in a difference Fourier map and placed in idealized positions using the riding-model technique, with distances C—H = 0.93–0.97 Å, N—H = 0.90 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The best refinement was obtained using the multi-scan *SADABS* (Sheldrick, 1996) correction. The restraints were generated automatically by *SHELXL97* to fix the origin.

Figures

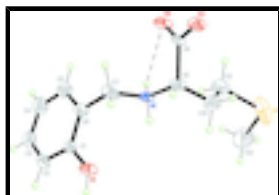


Fig. 1. : *ORTEP* drawing with numbering of the atoms. Non H-atoms are represented as displacement ellipsoids plotted at the 50% probability level, while H-atoms bound to heteroatoms are shown as small spheres of arbitrary radius. The intramolecular H-bond is represented by a dashed line.

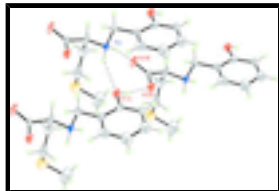


Fig. 2. : Supramolecular arrangement of (I): a perpendicular view of the triangular-shaped ring [$R^2_3(8)$], involving three molecules interconnected through the H-bonding interactions N1—H1A...O3, N1—H1B...O1 and O1—H1...O2. Dotted lines indicate H-bonding interactions.

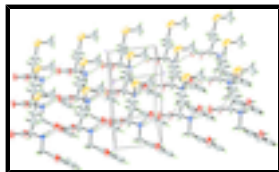


Fig. 3. : Crystal packing of (I): molecular arrangement in parallel strings extending along the (001) crystallographic plane.

(S)-2-[(2-Hydroxybenzyl)azaniumyl]-4-(methylsulfanyl)butanoate

Crystal data

$\text{C}_{12}\text{H}_{17}\text{NO}_3\text{S}$

$M_r = 255.33$

Triclinic, *P*1

Hall symbol: P 1

$a = 5.3221(2) \text{ \AA}$

$b = 5.8369(2) \text{ \AA}$

$c = 10.5564(5) \text{ \AA}$

$\alpha = 98.200(3)^\circ$

$\beta = 90.780(3)^\circ$

$\gamma = 96.849(3)^\circ$

$V = 322.10(2) \text{ \AA}^3$

$Z = 1$

$F(000) = 136$

$D_x = 1.316 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4292 reflections

$\theta = 3.6\text{--}27.0^\circ$

$\mu = 0.25 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Prismatic, yellow

$0.53 \times 0.44 \times 0.16 \text{ mm}$

Data collection

Bruker APEXII CCD

1966 reflections with $I > 2\sigma(I)$

diffractometer
 graphite $R_{\text{int}} = 0.016$
 φ and ω scans $\theta_{\text{max}} = 26^\circ$, $\theta_{\text{min}} = 3.8^\circ$
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996) $h = -6 \rightarrow 6$
 $T_{\text{min}} = 0.679$, $T_{\text{max}} = 0.746$ $k = -7 \rightarrow 7$
 7430 measured reflections $l = -13 \rightarrow 13$
 2324 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.059$ H-atom parameters constrained
 $wR(F^2) = 0.179$ $w = 1/[\sigma^2(F_o^2) + (0.1065P)^2 + 0.1553P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.07$ $(\Delta/\sigma)_{\text{max}} < 0.001$
 2324 reflections $\Delta\rho_{\text{max}} = 0.79 \text{ e } \text{\AA}^{-3}$
 156 parameters $\Delta\rho_{\text{min}} = -0.41 \text{ e } \text{\AA}^{-3}$
 3 restraints Absolute structure: Assigned from the known absolute structure of the starting material; the Flack (1983) parameter is consistent with this assignment, 1119 Friedel-pairs
 Primary atom site location: structure-invariant direct methods Flack parameter: 0.12 (19)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1397 (7)	0.8261 (5)	0.6478 (4)	0.0378 (8)
C2	0.1286 (8)	1.0229 (6)	0.7378 (4)	0.0480 (10)
H2	0.0037	1.1192	0.7301	0.058*
C3	0.3045 (9)	1.0752 (9)	0.8391 (4)	0.0595 (11)
H3	0.2993	1.2085	0.8984	0.071*
C4	0.4846 (11)	0.9326 (10)	0.8521 (5)	0.0719 (14)

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H4	0.6064	0.9719	0.918	0.086*
C5	0.4866 (8)	0.7305 (8)	0.7677 (5)	0.0592 (11)
H5	0.6034	0.6289	0.7807	0.071*
C6	0.3176 (7)	0.6750 (6)	0.6635 (4)	0.0437 (9)
C7	0.3226 (7)	0.4586 (6)	0.5712 (5)	0.0523 (11)
H7A	0.1526	0.4057	0.5364	0.063*
H7B	0.3754	0.3381	0.6164	0.063*
N1	0.4971 (5)	0.4903 (4)	0.4628 (3)	0.0365 (7)
H1A	0.4664	0.6175	0.4288	0.044*
H1B	0.6586	0.5129	0.4927	0.044*
C12	0.982 (2)	0.7692 (13)	0.1065 (9)	0.125 (3)
H12A	0.8321	0.8384	0.0902	0.187*
H12B	1.1162	0.8272	0.0553	0.187*
H12C	1.0313	0.8083	0.1955	0.187*
C8	0.4605 (9)	0.2821 (6)	0.3620 (4)	0.0528 (11)
H8	0.2775	0.234	0.3533	0.063*
C9	0.5770 (7)	0.0784 (5)	0.4082 (4)	0.0396 (8)
O1	-0.0230 (5)	0.7724 (4)	0.5440 (3)	0.0481 (7)
H1	-0.0734	0.8918	0.5264	0.072*
O2	0.7473 (5)	0.1274 (4)	0.4933 (3)	0.0542 (8)
O3	0.4885 (6)	-0.1164 (4)	0.3543 (3)	0.0543 (8)
S1	0.9203 (4)	0.4659 (3)	0.0671 (2)	0.1140 (8)
C10	0.5426 (11)	0.3361 (8)	0.2347 (5)	0.0673 (14)
H10A	0.4849	0.2056	0.1691	0.081*
H10B	0.4698	0.472	0.2149	0.081*
C11	0.8008 (11)	0.3782 (9)	0.2368 (6)	0.0749 (15)
H11A	0.8727	0.24	0.2535	0.09*
H11B	0.8581	0.5041	0.3051	0.09*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0352 (18)	0.0332 (17)	0.047 (2)	0.0050 (13)	0.0058 (17)	0.0120 (14)
C2	0.049 (2)	0.0382 (19)	0.060 (2)	0.0137 (15)	0.015 (2)	0.0095 (17)
C3	0.064 (3)	0.068 (3)	0.045 (2)	0.008 (2)	0.007 (2)	0.0004 (19)
C4	0.070 (3)	0.091 (4)	0.054 (3)	0.013 (3)	0.000 (3)	0.005 (3)
C5	0.047 (2)	0.071 (3)	0.065 (3)	0.013 (2)	0.002 (2)	0.025 (2)
C6	0.0355 (19)	0.0368 (18)	0.063 (2)	0.0053 (14)	0.0139 (19)	0.0199 (16)
C7	0.037 (2)	0.0255 (16)	0.096 (3)	0.0053 (13)	0.014 (2)	0.0138 (19)
N1	0.0462 (16)	0.0128 (11)	0.0509 (17)	0.0053 (10)	-0.0084 (14)	0.0058 (10)
C12	0.183 (9)	0.078 (4)	0.121 (6)	0.010 (5)	0.017 (6)	0.043 (4)
C8	0.079 (3)	0.0190 (15)	0.059 (2)	0.0112 (16)	-0.025 (2)	0.0016 (15)
C9	0.052 (2)	0.0163 (15)	0.0514 (19)	0.0096 (13)	0.0019 (19)	0.0044 (13)
O1	0.0499 (16)	0.0286 (12)	0.0668 (18)	0.0114 (10)	-0.0099 (15)	0.0056 (11)
O2	0.0539 (16)	0.0272 (12)	0.082 (2)	0.0108 (10)	-0.0169 (16)	0.0075 (12)
O3	0.081 (2)	0.0182 (12)	0.0622 (17)	0.0056 (11)	-0.0112 (16)	0.0037 (11)
S1	0.1068 (14)	0.1004 (13)	0.1180 (14)	-0.0026 (10)	0.0483 (12)	-0.0327 (11)
C10	0.092 (4)	0.046 (2)	0.064 (3)	0.011 (2)	-0.016 (3)	0.007 (2)

C11 0.087 (4) 0.057 (3) 0.078 (3) 0.026 (2) -0.033 (3) -0.009 (2)

Geometric parameters (Å, °)

C1—O1	1.365 (5)	N1—H1B	0.9
C1—C2	1.389 (5)	C12—S1	1.749 (8)
C1—C6	1.392 (5)	C12—H12A	0.96
C2—C3	1.387 (7)	C12—H12B	0.96
C2—H2	0.93	C12—H12C	0.96
C3—C4	1.360 (7)	C8—C10	1.483 (7)
C3—H3	0.93	C8—C9	1.539 (4)
C4—C5	1.375 (7)	C8—H8	0.98
C4—H4	0.93	C9—O3	1.232 (4)
C5—C6	1.388 (6)	C9—O2	1.246 (5)
C5—H5	0.93	O1—H1	0.82
C6—C7	1.484 (6)	S1—C11	2.023 (7)
C7—N1	1.502 (5)	C10—C11	1.366 (8)
C7—H7A	0.97	C10—H10A	0.97
C7—H7B	0.97	C10—H10B	0.97
N1—C8	1.489 (4)	C11—H11A	0.97
N1—H1A	0.9	C11—H11B	0.97
O1—C1—C2	121.9 (3)	S1—C12—H12A	109.5
O1—C1—C6	118.1 (3)	S1—C12—H12B	109.5
C2—C1—C6	120.0 (3)	H12A—C12—H12B	109.5
C3—C2—C1	119.7 (4)	S1—C12—H12C	109.5
C3—C2—H2	120.1	H12A—C12—H12C	109.5
C1—C2—H2	120.1	H12B—C12—H12C	109.5
C4—C3—C2	120.3 (4)	C10—C8—N1	112.6 (3)
C4—C3—H3	119.8	C10—C8—C9	115.0 (4)
C2—C3—H3	119.8	N1—C8—C9	109.9 (3)
C3—C4—C5	120.0 (5)	C10—C8—H8	106.2
C3—C4—H4	120	N1—C8—H8	106.2
C5—C4—H4	120	C9—C8—H8	106.2
C4—C5—C6	121.2 (4)	O3—C9—O2	127.9 (3)
C4—C5—H5	119.4	O3—C9—C8	114.6 (3)
C6—C5—H5	119.4	O2—C9—C8	117.5 (3)
C5—C6—C1	118.4 (4)	C1—O1—H1	109.5
C5—C6—C7	121.2 (4)	C12—S1—C11	100.5 (3)
C1—C6—C7	120.4 (4)	C11—C10—C8	108.8 (4)
C6—C7—N1	113.2 (3)	C11—C10—H10A	109.9
C6—C7—H7A	108.9	C8—C10—H10A	109.9
N1—C7—H7A	108.9	C11—C10—H10B	109.9
C6—C7—H7B	108.9	C8—C10—H10B	109.9
N1—C7—H7B	108.9	H10A—C10—H10B	108.3
H7A—C7—H7B	107.8	C10—C11—S1	110.1 (4)
C8—N1—C7	110.7 (3)	C10—C11—H11A	109.6
C8—N1—H1A	109.5	S1—C11—H11A	109.6
C7—N1—H1A	109.5	C10—C11—H11B	109.6
C8—N1—H1B	109.5	S1—C11—H11B	109.6

supplementary materials

C7—N1—H1B	109.5	H11A—C11—H11B	108.1
H1A—N1—H1B	108.1		
O1—C1—C2—C3	-177.5 (4)	C1—C6—C7—N1	91.8 (4)
C6—C1—C2—C3	3.7 (6)	C6—C7—N1—C8	-169.9 (3)
C1—C2—C3—C4	-1.2 (7)	C7—N1—C8—C10	156.6 (4)
C2—C3—C4—C5	-2.7 (8)	C7—N1—C8—C9	-73.8 (4)
C3—C4—C5—C6	4.3 (8)	C10—C8—C9—O3	-74.6 (5)
C4—C5—C6—C1	-1.8 (6)	N1—C8—C9—O3	157.1 (3)
C4—C5—C6—C7	179.0 (5)	C10—C8—C9—O2	105.0 (4)
O1—C1—C6—C5	178.9 (4)	N1—C8—C9—O2	-23.4 (5)
C2—C1—C6—C5	-2.2 (5)	N1—C8—C10—C11	71.0 (5)
O1—C1—C6—C7	-1.8 (5)	C9—C8—C10—C11	-55.9 (5)
C2—C1—C6—C7	177.1 (4)	C8—C10—C11—S1	-177.7 (3)
C5—C6—C7—N1	-89.0 (5)	C12—S1—C11—C10	100.9 (5)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.82	1.83	2.641 (3)	168
N1—H1A \cdots O3 ⁱⁱ	0.9	1.83	2.713 (3)	166
N1—H1B \cdots O1 ⁱⁱⁱ	0.9	2.14	2.916 (4)	144
N1—H1B \cdots O2	0.9	2.35	2.687 (3)	102

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

Fig. 1

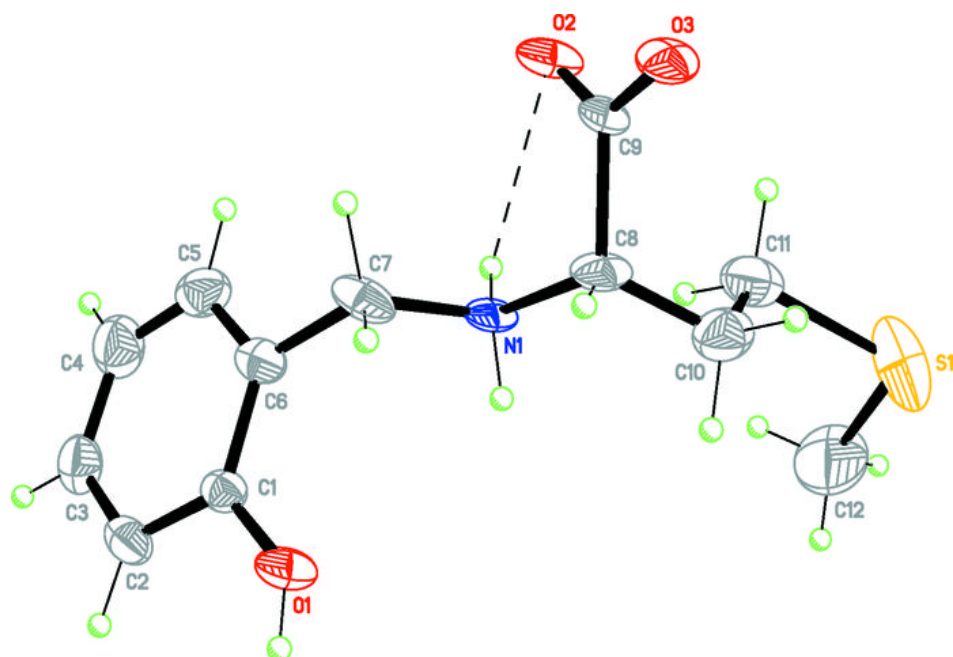


Fig. 2

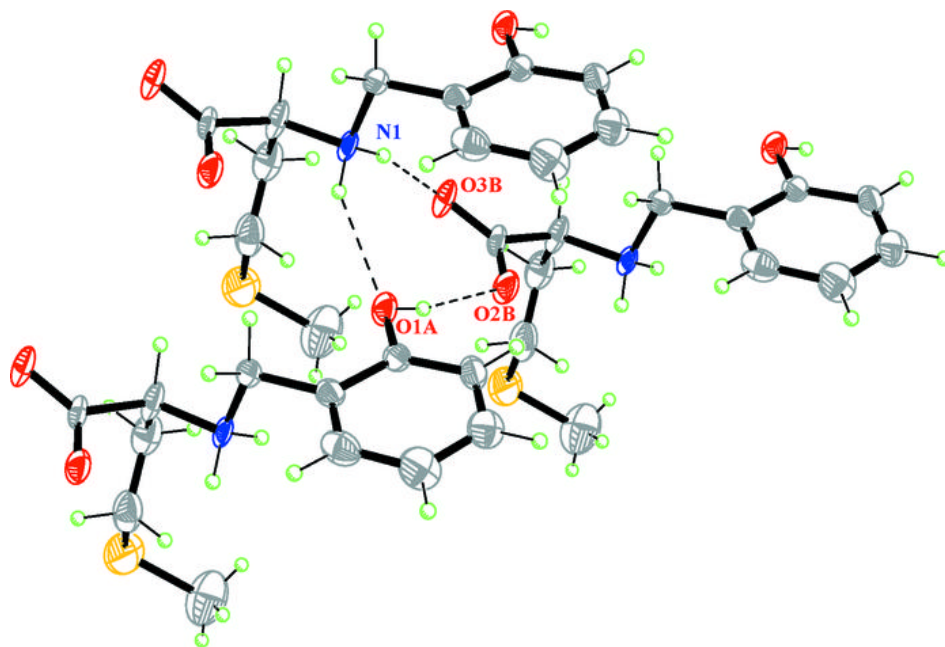


Fig. 3

