# ORIGINAL PAPER

# Synthesis and Crystal Structures of Two Schiff Bases of 2-(Methylthio)aniline with Halogenated Salicylaldehydes

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Abstract The crystal structures of the new compounds 5-bromo-*N*-[2-(methylthio)-phenyl]salicylaldimine (1), and 3,5-dichloro-*N*-[2-(methylthio)phenyl]salicylaldimine (2) were obtained by single crystal X-ray diffraction. Compound 1 crystallizes in the monoclinic space group  $P2_1/c$  with a = 14.1479(14) Å, b = 5.3058(3) Å, c = 19.104(3) Å;  $\beta = 106.218(10)^\circ$ ; and Z = 4. Compound 2 crystallizes in the triclinic space group  $P\overline{1}$  with a = 11.2249(10) Å, b = 13.863(2) Å, c = 13.9055(9) Å; and  $\alpha = 99.378(15)^\circ$ ,  $\beta = 102.866(7)^\circ$ ,  $\gamma = 91.375(11)^\circ$ ; and Z = 6. Details of the synthesis, structures, and spectroscopic properties of the new compounds are discussed.

**Keywords** Schiff base · X-ray structure · Sulfur compounds · Hydrogen bonds

## Introduction

In 1864, German chemist Hugo Schiff developed a new class of organic compound [1]. This group of compounds, imines, are often referred to as Schiff bases in his honor. The preparation of these compounds is simple and elegant. They are prepared by condensing a carbonyl compound with an amine, generally in refluxing alcohol. Schiff bases are often used as ligands in inorganic chemistry. The most common examples of these ligands are prepared from salicylaldehyde derivatives to form a Schiff base ligand. These ligands have been studied extensively due to their

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Department of Chemistry, Illinois State University, Campus Box 4160, Normal, IL 61790, USA e-mail: chamaker@ilstu.edu ease of synthesis and their ability to be readily varied both sterically and electronically.

The chemistry of Schiff bases is very diverse. The ligands can coordinate in anywhere from a monodentate [2] to a nonadentate [3] fashion to a metal ion. Schiff bases and their metal complexes have been studied for use as antibacterial agents [4–6], antifungal agents [7, 8], antitumor drugs [9–11], catalysts [12–14], and in coordination chemistry [15–18].

Although the binding ability of Schiff bases to metals has been extensively studied, their interactions with each other have not been studied as much. In Schiff base compounds, the imine nitrogen can act as an inter- or intramolecular hydrogen-bond acceptor and the hydroxyl oxygen in salicylaldehyde derivatives can act as an intermolecular hydrogen-bond acceptor. Hydrogen bonding interactions are important because of their application in the pharmaceutical industry. The type and strength of the interactions between the molecules in the formulation can affect the uptake of the medication in the body.

Our group is interested in the synthesis, structure, and coordination chemistry of novel, mixed-donor Schiff base ligands [19–25]. As a part of our ongoing studies into the structure and utility of sulfur-containing Schiff base ligands, we report the synthesis, spectral properties, and crystal structures of the Schiff bases prepared from the condensation of 2-(methylthio)aniline with two halogenated salicylaldehyde derivatives.

# Experimental

## General Experimental

All chemicals were purchased from commercial sources and used as received. <sup>1</sup>H and <sup>13</sup>C NMR spectra were

C. G. Hamaker (🖂) · O. S. Maryashina ·

recorded in CD<sub>2</sub>Cl<sub>2</sub> on a Varian Gemini 400 MHz NMR spectrometer and recorded in ppm relative to residual CHDCl<sub>2</sub> in CD<sub>2</sub>Cl<sub>2</sub> at 5.32 ppm for <sup>1</sup>H and CD<sub>2</sub>Cl<sub>2</sub> at 54.0 ppm for <sup>13</sup>C. IR spectra were collected on a Perkin Elmer Spectrum One FTIR equipped with a universal ATR attachment. UV/visible spectra were recorded in CH<sub>2</sub>Cl<sub>2</sub> solution on a Cary 5E spectrometer. Melting points are uncorrected. Elemental analyses were obtained from the School of Chemical Sciences Microanalysis Laboratory at the University of Illinois at Urbana-Champaign.

## Synthesis of Schiff Bases

#### 5-Bromo-N-[2-(methylthio)phenyl]salicylaldimine (1)

A 100 mL roundbottom flask was charged with 60 mL of ethanol, 1.5339 g (11.018 mmol) of 2-(methylthio)aniline, and 2.0646 g (10.809 mmol) of 3,5-dichlorosalicylaldeyde. The resulting mixture changed from yellow to orange in color and was refluxed for 30 min. The mixture was cooled to room temperature and the product allowed to crystallize at -30 °C overnight. The precipitate was filtered off and washed with diethyl ether to yield 3.076 g (91%) of **1** as an orange solid. Single crystals of 1 suitable for X-ray diffraction were grown by solvent diffusion of hexanes (mixture of all five isomers, Fischer Scientific) into a methylene chloride solution of **1**. MP: 107–108 °C. IR: 1611 cm<sup>-1</sup> (C=N). UV/ vis;  $\lambda_{max}(\epsilon)$ : 272 nm (18800 M<sup>-1</sup> cm<sup>-1</sup>), 368 nm (9200 M<sup>-1</sup> cm<sup>-1</sup>). <sup>1</sup>H NMR: δ 13.13 (s, 1H, OH); 8.51 (s, 1H, CH=N); 7.48 (d, 1H,  $H_{Ar}$ , J = 2.8 Hz); 7.43 (dd, 1H,  $H_{Ar}$ , J = 8.8 and 2.4 Hz); 7.25 (m, 2H, H<sub>Ar</sub>); 7.17 (d, 2H, H<sub>Ar</sub>, J = 4.0 Hz); 6.91 (d, 1H, H<sub>Ar</sub>, J = 8.8 Hz); 2.46 ppm (s, 3H, SCH<sub>3</sub>). <sup>13</sup>C NMR:  $\delta$  160.6, 160.5, 144.9, 136.1, 135.8, 134.8, 128.4, 125.7, 125.3, 121.2, 119.7, 117.5, 118.8, 15.0 ppm. Analysis calc. (found) for C14H12BrNOS: C, 52.18 (52.24); H, 3.75 (3.60); N, 4.35 (4.20).

#### 3,5-Dichloro-N-[2-(methylthio)phenyl]salicylaldimine (2)

A 100 mL roundbottom flask was charged with 30 mL of ethanol, 1.4250 g (10.236 mmol) of 2-(methylthio)aniline, and 1.9790 g (9.845 mmol) of 5-bromosalicylaldeyde. The resulting mixture was refluxed for 60 min and cooled to room temperature. The mixture was moved into a freezer at -30 °C and the product was allowed to crystallize overnight. The precipitate was filtered off and washed with diethyl ether to yield 2.957 g (93%) of **2** as an orange solid. Single crystals of **2** suitable for X-ray diffraction were grown by solvent diffusion of hexanes (mixture of all five isomers, Fischer Scientific) into a methylene chloride solution of **2**. MP: 116–117 °C. IR: 1611 cm<sup>-1</sup> (C=N). UV/vis;  $\lambda_{max}(\varepsilon)$ : 273 nm (18000 M<sup>-1</sup> cm<sup>-1</sup>), 370 nm (8470 M<sup>-1</sup> cm<sup>-1</sup>). <sup>1</sup>H NMR:  $\delta$  13.91 (s, 1H, OH); 8.56 (s, 1H, CH=N); 7.43 (d, 1H, H<sub>Ar</sub>,

J = 2.4 Hz); 7.30 (m, 2H, H<sub>Ar</sub>); 7.25 (d, 1H, H<sub>Ar</sub>, J = 7.2 Hz); 7.20 (m, 2H, H<sub>Ar</sub>); 2.48 ppm (s, 3H, SCH<sub>3</sub>). <sup>13</sup>C NMR:  $\delta$  160.0, 156.2, 144.2, 136.2, 133.1, 130.4, 129.0, 125.9, 125.7, 123.8, 123.1, 121.1, 117.6, 15.2 ppm. Analysis calc. (found) for C<sub>14</sub>H<sub>11</sub>Cl<sub>2</sub>NOS: C, 53.86 (53.41); H, 3.55 (3.39); N, 4.49 (4.36).

#### X-ray Crystallography General

Crystal and data collection parameters are given in Table 1. Data for 1 and 2 were collected on a Bruker-Nonius CAD4/ Mach3 diffractometer equipped with an Oxford Cryostreams Cobra cryostat using Mo-K $\alpha$  ( $\lambda = 0.71073$  Å) radiation at 173(2) K. Data collection and cell refinement was performed using CAD4 express [26]. Data reduction was carried out using XCAD4 [27]. Unit cell parameters were obtained from a least-squares refinement of 25 centered reflections. The data were corrected for absorption through the use of empirical psi-scans [28]. Solution and data analysis were performed using the WinGX software package. The structures were solved by direct methods using SIR-92 [29] for compound 1 and SIR-2004 [30] for compound 2. The refinements were completed using the program SHELXL-97 [31]. Hydrogen atoms attached to carbon were assigned positions based on the geometries of their attached carbons. The hydroxyl hydrogens were assigned positions based on the Fourier difference map.

# **Results and Discussion**

The compounds were prepared by refluxing equimolar amounts of substituted salicylaldehyde and 2-(methyl-thio)aniline in absolute ethanol (Fig. 1). Both compounds were isolated as orange solids in better than 90% yield.

# IR and UV/vis Spectroscopy

Both of the compounds have a strong absorbance at  $1611 \text{ cm}^{-1}$  in the infrared, confirming the presence of the imine moiety. Additionally, both **1** and **2** have similar UV/ vis spectra in methylene chloride solution; both compounds have strong absorptions near 270 and 370 nm.

# <sup>1</sup>H NMR Spectroscopy

Both compounds have simple and similar <sup>1</sup>H NMR spectra in  $CD_2Cl_2$  solution. The SCH<sub>3</sub> resonance is at 2.46 and 2.48 ppm in **1** and **2**, respectively. The N=CH resonance for both compounds is also similar (8.51 ppm in **1** and 8.56 ppm in **2**). Both compounds exhibit sharp OH resonances, indicative of strong intramolecular hydrogen bonding, at 13.13 ppm in **1** and 13.91 ppm in **2**.

 Table 1
 Summary of structure

 determination of compounds 1
 and 2

Compound	1	2
CCDC entry no.	703374	703375
Empirical formula	C <sub>14</sub> H <sub>12</sub> BrNOS	C <sub>14</sub> H <sub>11</sub> Cl <sub>2</sub> NOS
Formula weight	322.22	312.20
Color and habit	Yellow needle	Orange block
Crystal size (mm)	$0.42 \times 0.25 \times 0.18$	$0.45 \times 0.45 \times 0.35$
Temperature (K)	173(2)	173(2)
Space group	$P2_{1}/c$	$P\bar{1}$
<i>a</i> (Å)	14.1479(14)	11.2249(10)
<i>b</i> (Å)	5.0358(3)	13.863(2)
<i>c</i> (Å)	19.104(2)	13.9055(9)
a (°)	90	99.378(15)
β (°)	106.218(10)	102.866(7)
γ (°)	90	91.376(11)
V (Å <sup>3</sup> )	1306.9(2)	2077.2(4)
Ζ	4	6
$D_{\text{calc}}$ (Mg/m <sup>3</sup> )	1.638	1.497
Absorption coeff $(mm^{-1})$	3.291	0.609
Absorpton correction	$\psi$ -Scans	$\psi$ -Scans
Max. and min. transmission	0.5522 and 0.4038	0.8071 and 0.7444
<i>F</i> (000)	648	960
<i>R</i> indices $[I > 2\sigma(I)]$	$R_1 = 0.0284, wR_2 = 0.0695$	$R_1 = 0.0325, wR_2 = 0.0851$
R indices (all data)	$R_1 = 0.0489, wR_2 = 0.0761$	$R_1 = 0.0490, wR_2 = 0.0947$
Goodness-of-fit on $F^2$	1.048	1.048
Largest peak/hole (e $Å^{-3}$ )	0.548 and -0.385	0.405  and  -0.441



Fig. 1 Preparation and structure of compounds 1 and 2

Molecular Structures of 1 and 2

The molecular structures for compounds 1 and 2 were determined by single crystal X-ray diffraction and the

asymmetric units for each are shown in Figs. 2 and 3, respectively. Selected bond lengths and angles are given in Tables 2 and 3. Compound 1 crystallizes in the monoclinic space group  $P2_1/c$  with one molecule in the asymmetric unit while compound 2 crystallizes in the triclinic space group  $P\overline{1}$  with three independent molecules in the asymmetric unit.

Compound **1** is non-planar, with a dihedral angle between the two aromatic rings of  $19.03(12)^{\circ}$  (Fig. 2, Table 4). The molecule is stabilized by an intramolecular O1–H1…N9 hydrogen bond (Table 5). There is, at best, a *very weak* intramolecular O1–H1…S16 interaction (the H1…S16 distance is approximately 0.03 Å less than the sum of the van der Waal's radii; the O1…S16 distance is longer than the sum of the van der Waal's radii). This *very weak* interaction explains why the dihedral angle between the aromatic rings smaller than that of some related compounds without O–H…S interactions [23–25], but the molecule is non-planar. The bond lengths and angles (Tables 2, 3) are similar to reported compounds [22–25]. There are no significant intermolecular interactions in **1** and the packing is a result van der Waal's forces.

In compound 2 (Fig. 3), which has a Z' of three, two of the three independent molecules are nearly planar; molecule *a* has a dihedral angle between the aromatic rings of



Fig. 2 The molecular structure of 1 showing the atom numbering scheme. Displacement *ellipsoids* are drawn at the 50% probability level. Hydrogen atoms are drawn as *spheres* of arbitrary size. *Dashed lines* indicate intramolecular hydrogen bonds

1.51(2)° while molecule *b* has a dihedral angle between the aromatic rings of 4.24(2)°. An overlay of molecules *a* and *b*, generated using the program Mercury [32], is shown in Fig. 4 illustrating the similarity between the molecules. Molecule *c* is non-planar with a dihedral angle between the aromatic rings of  $55.37(5)^\circ$ , which can be seen in the overlay of molecules *a* and *c* in Fig. 5. Molecules *a* and *b* have strong O1–H1…N9 and O1–H1…S16 hydrogen bonds while molecule *c* has only a strong O1–H1…N9 hydrogen bond (Table 6). The bond angles and distances in **2** (Tables 2, 3) are in agreement with similar compounds [22–25]. The packing in **2** is held together by a C–H…O

Table 2 Summary of selected bond distances (Å) for compounds 1 and 2

Bond	Length in 1	Length in 2a	Length in 2b	Length in 2c
O1–C2	1.345(3)	1.346(2)	1.343(2)	1.347(2)
C7–C8	1.450(3)	1.456(2)	1.458(2)	1.457(2)
C8-N9	1.283(3)	1.283(2)	1.282(2)	1.283(2)
N9-C10	1.417(3)	1.419(2)	1.421(2)	1.423(2)
C15–S16	1.761(3)	1.7641(17)	1.7638(18)	1.7611(18)
S16–C17	1.801(3)	1.7947(19)	1.799(2)	1.793(2)

Table 3 Summary of selected bond angles (°) for compounds 1 and 2

Bond	Angle in 1	Angle in 2a	Angle in 2b	Angle in 2c
C7-C8-N9	121.7(2)	120.65(15)	121.23(16)	120.73(15)
C8-N9-C10	121.6(2)	124.13(15)	123.11(15)	119.96(14)
C15-S16-C17	103.14(13)	103.55(9)	103.59(9)	103.26(10)

Table 4 Dihedral angle between phenyl rings C2–C7 and C10–C15  $(^\circ)$  for compounds 1 and 2

Angle in 1	Angle in 2a	Angle in 2b	Angle in 2c
14.03(12)	1.51(2)	4.24(2)	55.37(5)

Table 5 Intramolecular hydrogen-bond geometry (Å, °) in compound 1

D–H···A	D-H	Н…А	D····A	D−H…A
O1-H1N9	0.80(4)	1.93(4)	2.652(3)	150(4)

**Fig. 3** The molecular structure of the asymmetric unit of **2** showing the full atom numbering scheme for molecule *c* and partial atom numbering schemes for molecules *a* and *b* (all three molecules have the same numbering scheme). Displacement *ellipsoids* are drawn at the 50% probability level. Hydrogen atoms are drawn as *spheres* of arbitrary size. *Dashed lines* indicate intramolecular hydrogen bonds





Fig. 4 Overlay of molecules *a* and *b* of compound 2 generated using the program Mercury



**Fig. 5** Overlay of molecules *a* and *c* of compound **2** generated using the program Mercury

Table 6 Intramolecular hydrogen-bond geometry (Å, °) in compound  $\mathbf{2}$ 

D–H	$H \cdots A$	$D \cdots A$	D–H···A
0.83(3)	1.80(3)	2.567(2)	154(3)
0.83(3)	2.73(3)	3.3369(15)	131(3)
0.90(3)	1.76(3)	2.597(2)	154(3)
0.90(3)	2.77(3)	3.4135(14)	130(3)
0.83(3)	1.83(3)	2.595(2)	152(3)
	<i>D</i> –H 0.83(3) 0.83(3) 0.90(3) 0.90(3) 0.83(3)	D−H         H…A           0.83(3)         1.80(3)           0.83(3)         2.73(3)           0.90(3)         1.76(3)           0.90(3)         2.77(3)           0.83(3)         1.83(3)	D-H         H···A         D···A           0.83(3)         1.80(3)         2.567(2)           0.83(3)         2.73(3)         3.3369(15)           0.90(3)         1.76(3)         2.597(2)           0.90(3)         2.77(3)         3.4135(14)           0.83(3)         1.83(3)         2.595(2)

hydrogen bond, a Cl···Cl interaction, and a C–H··· $\pi$  interaction (Table 7). Additionally, there are weak  $\pi$ - $\pi$  interactions in **2** leading to the formation of  $\pi$ -stacks of *a* and *b* molecules that run parallel to the *b*-axis (Fig. 6). The distance between the interacting rings is Cg(1)··· Cg(2)<sup>*i*</sup> = 3.69 Å; Cg(1)···Cg(4)<sup>*i*</sup> = 3.73 Å; Cg(2)···Cg(3)<sup>*i*</sup> = 3.61 Å; Cg(3)···Cg(4)<sup>*iv*</sup> = 4.02 Å [Cg(1) is center of gravity of ring C2a–C3a–C4a–C5a–C6a–C7a; Cg(2) is the center of gravity of ring C10a–C11a–C12a–C13a–C14a– C15a; Cg(3) is the center of gravity of ring C2b–C3b–C4b– C5b–C6b–C7b; Cg(4) is the center of gravity of ring C10b–C11b–C12b–C13b–C14b–C15b]; symmetry operations: *i* = -*x* + 1, -*y* + 1, -*z*; *iv* = -*x* + 1, -*y*, -*z*].

There has been significant interest recently in structures with Z' > 1 [33–36]. Of all of the structures published in the Cambridge Structural Database, 8.8% of all structures and 11.5% of all organic structures had Z' > 1 [36]. Steed and co-workers have identified several types of intermolecular interactions which, when combined with each other, can lead to crystal structures with Z' > 1, due to what they term "synthon frustration" [33]. Compound **2** has three of **Table 7** Intermolecular interactions (Å,  $^{\circ}$ ) in compound 2

			-		
D–H…A	D–H	$H \cdots A$	$D \cdots A$	D–H···A	
C8c–H8c…O1a <sup>i</sup>	0.95	2.44	3.339(2)	158	
C6b–H6b…Cg(6) <sup>ii</sup>	0.95	2.90	3.84	170	
D···A	D···A				
Cl5a…Cl5a <sup>iii</sup>	3.3618(10)				

(i) -x + 1, -y + 1, -z; (ii) x, y, z - 1; (iii) -x + 1, -y + 1, -z + 1; Cg(6) is the center of gravity of ring C10c–C11c–C12c–C13c–C14c–C15c



Fig. 6 Packing diagram for compound 2, viewed down the *a* axis. *Dashed lines* indicate intermolecular hydrogen-bonding and Cl…Cl interactions

the identified interactions, a Cl···Cl contact, a C–H··· $\pi$  contact, and  $\pi$ - $\pi$  stacking. The presence of these three interactions probably contributes to the unusual Z' value of 3 in compound **2**. Another potential factor in the unusual Z' is the fact that one of the molecules has a significantly shape than the other two molecules in the asymmetric unit.

In two related molecules [24, 25] without any hydroxyl groups to form intramolecular hydrogen bonds, the molecules deviate significantly from planarity. Also in agreement with the current results, the compound 3-methoxy-N-[2-(methylthio)phenyl]salicylaldimine has both O–H…N and O–H…S intramolecular hydrogen bonds, and it is nearly planar with a dihedral angle of 6.78(7)° between the aromatic rings [22].

### **Supplementary Material**

CCDC-703374 and CCDC-703375 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/ data\_request/cif, or by emailing data\_request@ccdc.cam. ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

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