Synthesis, Characterization, Biological Acvtivity and Crystal Structures of 2(3',4'-Dimethoxy Phenyl imino)–3–o-Fluorophenyl Carboxamido-4,5-Trimethylene Thiophene(I) and 2(3',4',5'- Trimethoxy Phenyl imino)-3-o-Fluorophenyl Carboxamido-4,5-Trimethylene Thiophene (II)

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Abstract —The title compounds (I and II) have been prepared, characterized and crystallized to determine their crystal structures. The compounds I and II crystallize in space groups, $Pna2_1$ and $P2_1/c$, respectively. The former has cell parameters: a = 8.3701(5), b = 19.8697(15), c = 12.3072(9) Å (orthorhombic system) with four asymmetric molecules in the unit cell. The molecule exhibits extensive hydrogen bonding in the crystal lattice with C-H---O, C-H---F, N-H---N and C-H---S interactions with bridge distances vary from 2.839(3) to 3.307(3) Å. The predominant extensive hydrogen bonding is responsible for the arrangement of molecules in the unit cell. The intra and inter molecular hydrogen bonding play a greater role in the stability of the molecules in the lattice. Similarly compound II crystallizes in space group, P21/c with unit cell parameters: a = 12.0085(5), b = 9.1071(4), c = 20.8623(8) Å, β = 103.723° (3) with four asymmetric molecules in the unit cell. The compound II contains one extra –OCH3 group compared to compound I. Compound II also displays an extensive hydrogen bonding network of the type C-H---O, C-H---F, N-H---N and C-H---S with varying hydrogen bond distances from 2.808(2) to 3.441(2) Å. Both the compounds exhibit antimicrobial and antibacterial activities.

Index Terms— Activity, Antibacterial, Characterization, Crystal, Dimethoxy, Fluoro Phenyl, Hydrogen bonding, Structure

1 Introduction

Thiophenes belongs to the family of well-known heterocyclic compounds. Due to their wide range of theraphatic properties substituted thiophenes and their bihetetrocycles have received considerable importance [1]. A number of Schiff bases and thiophenes derivatives have been synthesized, characterized and reported to have significant and diverse biological activities such as antimicrobial [2], analgesic [3], anti-inflammatory [4], antioxidant [5], antitumor [6] and local anesthetic [7] activities. It may be noted that thiophenes can be fused with different heterocyclic nuclei giving rise to newer compounds with enhanced biological activities. Compounds such as thiopyrimidines have occupied pivotal positions among the thiophenes derivatives. Several of these derivatives showed antiallergic [8], antibacterial [9], antidepressant [10], antidiabetic [11], analgesic and anti-inflammatory [12] activities. In view of these compounds there is an ambition to synthesize certain tetrahydrobenzothiophene derivatives and evaluate them for their antimicrobial, antifungal and anti-bacterial activity. Here we report preparation, characterization, crystal structure elucidation and anti-bacterial activity of the two title compounds I and II. It has been found that both the structures show an extensive hydrogen bonding network required for the stability of the molecules in the crystalline lattice.

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2 Preparation and Characterization of Compounds

2.1 Synthesis of 2-amino 3-o-fluoro phenyl -4,5-trimethylene thiophene

A mixture of o-fluoro cyanoacetamide and cyclopentanone taken in the ratio 1:1 with 2ml of glacial acetic acid and 2g of ammonium acetate was taken in 80ml of pure and dry benzene in a round bottom flask and the reaction mixture was refluxed on a water bath involving clean stark apparatus for about ten hours. The reaction mixture was cooled, poured into a separating funnel and the mixture was washed successively with 10% sodium carbonate solution followed by double dis-

tilled water. The organic layer was transferred to a round bottom flask and distilled to remove any traces of benzene which was then collected. The syrupy residue obtained was then transferred to a 100 ml capacity conical flask. To this flask 1.3 g of sulfur was added followed by 30 ml of ethanol and reaction mixture was thoroughly stirred at a temperature between 45-50°C in the presence of diethyl amine until the sulfur goes into the solution. The solvent was removed by evaporation under vacuum.

2.2 Synthesis of Compound I and II

Compound I was synthesized with equimolar mixture (0.05 mole) of 2-amino-3–o-fluoro phenyl-4,5-trimethylene thiophene and 3,4-dimethoxy benzaldehyde was refluxed with a few drops of glacial acetic acid in ethanol for about two hours and then the reaction mixture was cooled to obtain the crystals. The compound was recrystallized from isopropanol. Compound II was synthesized by taking 3,4,5- trimethoxy benzaldehyde with 2-amino-3–o-fluoro phenyl -4,5-trimethylene thiophene by taking equimolar mixture of these two reactants. The reaction mixture was cooled and recrystallized from isopropanol.

2.3 Characterization of compounds I and II

2.3.1 FT-IR spectra

The formation of the title compounds I and II has been further characterized by FT-IR and ^{1}H NMR spectra. In addition to this information substantial proof for the occurance of the title compounds has been provided by differences in their melting points and Rf values by TLC method from that of the parent compound. The IR spectra predicts that the formation of Schiff bases of the two compounds. The presence of specific IR peaks at 1532 cm^{-1} in both the Shciff bases indicate the N=CH- peak. The other important peaks include 3535 (--NH-), 3170 (Arom-CH), 2924 (Ali-CH), 1627(C=O) 1543 (C=N), 1298(C-O); 1267(C-N), 749(C-S).

2.3.2 ^{1}H NMR

The results of the proton NMR of the two compounds I and II are given as: 8.89 (s, 1H, -N=CH-); 8.30 (s,1H, CH ArH phenyl ring); 7.7-7.6 (m,2H,CH,ArH, phenylring), 3.8(s, 6H , -OCH3 for dimethoxy gps) , 3.8 - 3.6 (s, 9H , -OCH3 for trimethoxy gps), 2.55(m,4H, -CH2- of cyclopentane ring); 1.95(m,2H, -CH2- of cyclopentane ring).

2.3.3 Mass Spectra

The mass spectrum of both the compounds I and II showed molecular ion peaks at 408 & 438, respectively which is one more than the actual molecular weight of compounds and is the M+1 peak of the compounds I and II.

3 Crystal Structure Determination of compounds I and II

Nice parallelo piped crystals of the title compounds with moderately yellow color were grown from a solution of the compounds in isopropanol at room temperature (25°C) by slow evaporation technique [20]. A suitable crystal was selected after examining it under an analytical polarizing microscope for its uniform extinction for data collection. Unit cell parameters were obtained from a set of different weighted intensity reciprocal lattice points. These parameters were refined and based on these unit cell parameters a set of weighted reflection intensities were collected from different parts of the reciprocal space after applying corrections for Lorentz and polarization effects [20]. These intensities were normalized and used in the structure determination of the molecule by direct method of phase determination [20]. The structures of the molecules were obtained and refined by the several cycles of the least-squares method by incorporating isothermal and anisothermal parameters for non-hydrogen. All the positions of hydrogen atoms are geometrically fixed and their parameters were not refined. The final R with value of R=0.0358 with weighting factor of 0.0782 for compound I and R=0.0392 with weighting factor of 0.0959 were obtained. The refinement of the structures was consistent because the parameters obtained are within the allowed permissible range. SHELXL97 was used in the structure determination and refinement of the structure. The molecular ORTEP thermal ellipsoid plots are depicted in Figs. 1a and 1b and the crystal packing of the asymmetric molecules are given in Figs. 2a and 2b for the compounds I and II, respectively. The data collection parameters and other associated parameters both compunds for are given in Tables 1A and 1B.

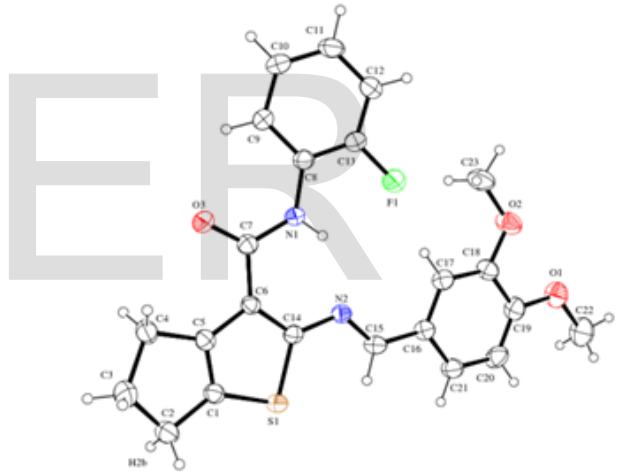

Fig.1a An ORTEP diagram with 50% thermal ellipsoid probability for the compound I. Flourine and oxygen atoms are indicated by green and red colors.

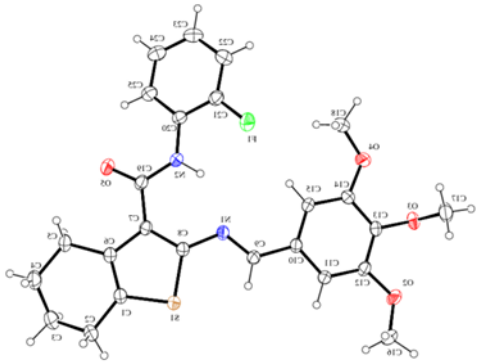

Fig.1b An ORTEP diagram with 50% thermal ellipsoid probability for the compound II.

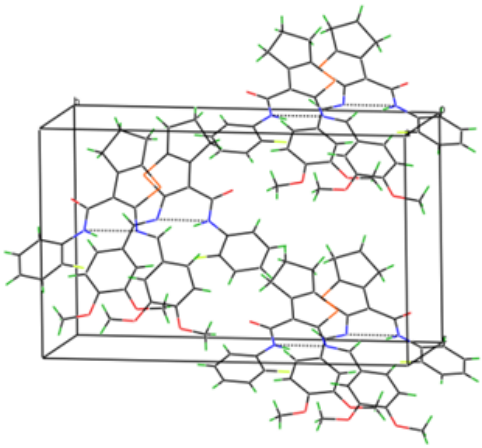

Fig. 2a Crystal packing diagram for the compound I

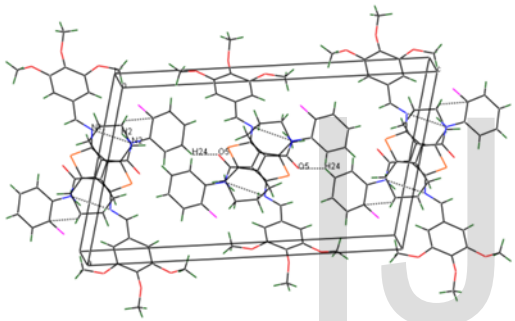

Fig. 2b Crystal packing diagram for the compound II

TABLE 1A
CRYSTAL DATA FOR COMPOUND I

Parameter	Compound I
Empirical formula	C23 H21 F N2 O3 S
Formula weight	424.48
Temperature	293(2) K
Wavelength	0.71073 Å
Space group	Pna21
Unit cell dimensions	a = 8.3701(5) Å b = 19.8697(15) Å c = 12.3072(9) Å
Volume	2046.8(2) Å^3
Z, Calculated density	4, 1.377 Mg/m^3
Absorption coefficient	0.195 mm^{-1}
F(000)	888
Crystal size	(0.30 x 0.20 x 0.20)mm
Theta range for data collection	2.64 to 24.91°
Limiting indices	-9<=h<=9, -23<=k<=23, -14<=l<=14
Reflections collected / unique	16624 / 3525 [R(int) = 0.0393]
Completeness to theta	24.91 99.3 %
Max. and min. transmission	0.952 and 0.911
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3525 / 1 / 273
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0781
R indices (all data)	R1 = 0.0497, wR2 = 0.0844

TABLE 2A
CRYSTAL DATA FOR COMPOUND 2

Parameter	Compound II
Empirical formula	C25 H25 F N2 O4 S
Formula weight	468.53
Temperature	293(2) K
Wavelength	0.71073 Å
Space group	P21/c
Unit cell dimensions	a = 12.0085(5)Å alpha = 90° b = 9.1071(4)Å beta = 103.723(3)° c = 20.8623(8)Å gamma = 90°
Volume	2216.43(16) Å^3
Z, Calculated density	4, 1.404 Mg/m^3
Absorption coefficient	0.191 mm^{-1}
F(000)	984
Crystal size	(0.30 x 0.20 x 0.20) mm
Theta range for data collection	2.33 to 25.00°
Limiting indices	-14<=h<=13, -10<=k<=10, -24<=l<=24
Reflections collected / unique	19566 / 3894 [R(int) = 0.0362]
Completeness to theta	25.00 99.8 %
Max. and min. transmission	0.972 and 0.941
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3894 / 0 / 305
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0959
R indices (all data)	R1 = 0.0536, wR2 = 0.1052

4 RESULTS AND DISCUSSION

The final atomic fractional coordinate (x10^4 Å) and their equivalent isotropic displacement parameters (Å^{2}x10^3) of the non-hydrogen atoms are given in Table 2a and Table 2b respectively. The bond distances and bond angles are given in Table 3 for the molecules I and II. It is seen from the table that the bond distances and angles in both the compounds I and II are within the normal range with 3 times of e.s.ds. The molecules are packed in the unit cells nicely by inter and intra hydrogen bondings (Table 4A and Table 4B). The fluorine F atom in compound I is involved in hydrogen bonding of the type: C(17)–H(17)---F, 3.307 (3) Å and C(23)–H(23)----F with hydrogen bond distance 3.121(4)Å. Also sulfur atom is involved in hydrogen bonding of the type C(15)-H(15)---S with hydrogen bridge distance 2.986(3) Å. In the case of compound II, F atom is involoved in hydrogen bonding of the type: C(15)-H(15)---F with hydrogen bond distance 3.143(2)Å and S atom is also involved in the hydrogen bonding of the type: C(9)-H(9)---S with hydrogen bridge distsnce 2.969 (2) Å. In both compounds I and II, both nitrogen atoms are involved in the hydrogen bonding interactions of the type: N(1)-H(1)---N(2) with bridge distances 2.839(3) and 2.808(2) Å, respectively.There are also hydrogen bonding ineractions in compound I of the type: C(9)-H(9)---O(3) with hydrogen bond distance 2.868(3) Å. Whereas in compound II, the two O atoms are involved in hydrogen bondings of the type: C(11)-H(11)---O(3) and C(25)-H(25)---O(5) with hydrogen bond distances 3.441(2) and 2.853(3) Å, respectively. In compound I, due to extensive hydrogen bonding network, the molecules are arranged in a spiral manner in the unit cell. In compound II, the hydrogen bonding scheme is mainly responsible for the packing of molecules parallel to the longest c-axis. The packing consideration in both the molecules due to extensive hydrogen bonding leads to stability of the molecules in the unit cell.

The two compounds have been screened for their antimicrobial activity. It has been found from the screening results that the two compounds exhibit a potential candidate for their antibacterial activity when tested with E.coli. The presence of electron withdrawing group and methoxy groups in both the compounds have made them good antibacterial agents in comparison to standard drug ampicillin. The values obtained have been found to be 16 and 17 mm using cup-plate method against ampicillin which is 21 mm. In this connection, probably the electron withdrawing groups and methoxy groups play a greater role in the antibacterial property of the compounds I and II. These values are comparable with the observed values by earlier workers [1]. It may be noted here that compound II with its three methoxy groups show a higher antibacterial activity than compound I.

The antibacterial activity may be attributed to the inter and intra hydrogen bonding interactions and also the propensity of the molecules to pack together as dimers involving N-H---N and C-H…O bonding interactions along with C-H---S and C-H---F interactions lead to the possible variation in the nature of packing motifs. These kind of interactions involving O-H---O, C-H---O and C-H---Cl interactions may be responsible for the biological activity of the molecues which is responsible for molecular basis for drug design as observed in the case of crystal structure of atovaquone [22].

TABLE 2A
ATOMIC COORDINATES (X10^4) AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (A^2 X 10^3) FOR COMPOUND I

	x	y	z	U(eq)
C(1)	750(3)	7386(1)	1950(2)	44(1)
C(2)	-123(3)	7440(2)	902(2)	59(1)
C(3)	-243(4)	6714(2)	545(3)	72(1)
C(4)	273(3)	6256(1)	1498(2)	53(1)
C(5)	1003(3)	6751(1)	2277(2)	41(1)
C(6)	1900(3)	6703(1)	3261(2)	37(1)
C(7)	2271(3)	6036(1)	3739(2)	41(1)
C(8)	3940(3)	5474(1)	5129(2)	45(1)
C(9)	3419(4)	4815(1)	5011(3)	67(1)
C(10)	4127(4)	4320(2)	5625(3)	80(1)
C(11)	5303(3)	4448(2)	6357(3)	64(1)
C(12)	5820(3)	5096(1)	6491(3)	59(1)
C(13)	5115(3)	5583(1)	5875(3)	53(1)
C(14)	2332(3)	7331(1)	3645(2)	37(1)
C(15)	3583(3)	8067(1)	4807(2)	45(1)
C(16)	4504(3)	8292(1)	5740(2)	43(1)
C(17)	5222(3)	7852(1)	6474(2)	47(1)
C(18)	6062(3)	8095(1)	7342(2)	50(1)
C(19)	6228(3)	8791(2)	7490(2)	54(1)
C(20)	5515(4)	9224(2)	6771(2)	63(1)
C(21)	4671(3)	8975(1)	5891(2)	54(1)
C(22)	7235(5)	9686(2)	8576(3)	90(1)
C(23)	6574(4)	7013(2)	8068(2)	71(1)
N(1)	3345(2)	6032(1)	4570(2)	46(1)
N(2)	3250(2)	7460(1)	4559(2)	40(1)
O(1)	7103(3)	8981(1)	8366(2)	73(1)
O(2)	6803(3)	7714(1)	8114(2)	72(1)
O(3)	1643(2)	5526(1)	3383(2)	57(1)
F(1)	5649(2)	6228(1)	5964(2)	98(1)
S(1)	1563(1)	7971(1)	2813(1)	47(1)

TABLE 2B
ATOMIC COORDINATES (X10^4) AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (A^2 X 10^3) FOR COMPOUND II

	x	y	z	U(eq)
C(1)	4857(2)	-3211(2)	5675(1)	36(1)
C(2)	4072(2)	-4139(3)	5965(1)	45(1)
C(3)	2878(2)	-4088(3)	5517(1)	58(1)
C(4)	2899(2)	-4351(3)	4820(1)	53(1)
C(5)	3610(2)	-3251(2)	4537(1)	40(1)
C(6)	4677(2)	-2777(2)	5038(1)	32(1)
C(7)	5569(2)	-1825(2)	4926(1)	31(1)
C(8)	6402(2)	-1561(2)	5497(1)	32(1)
C(9)	7949(2)	-350(2)	6148(1)	35(1)
C(10)	8918(2)	653(2)	6308(1)	33(1)
C(11)	9443(2)	817(2)	6976(1)	37(1)
C(12)	10334(2)	1802(2)	7171(1)	36(1)
C(13)	10701(2)	2636(2)	6705(1)	34(1)
C(14)	10193(2)	2445(2)	6037(1)	37(1)
C(15)	9304(2)	1455(2)	5836(1)	36(1)
C(16)	10818(2)	968(3)	8280(1)	59(1)
C(17)	12666(2)	3216(3)	6959(1)	58(1)
C(18)	10387(2)	2959(3)	4953(1)	63(1)
C(19)	5549(2)	-1233(2)	4257(1)	38(1)
C(20)	6621(2)	277(2)	3624(1)	37(1)
C(21)	7705(2)	778(2)	3629(1)	42(1)
C(22)	7987(2)	1480(3)	3111(1)	60(1)
C(23)	7142(2)	1697(3)	2545(1)	70(1)
C(24)	6050(2)	1209(3)	2515(1)	64(1)
C(25)	5783(2)	491(3)	3043(1)	49(1)
N(1)	7349(1)	-629(2)	5567(1)	33(1)
N(2)	6448(2)	-380(2)	4201(1)	39(1)
O(2)	10901(1)	2050(2)	7813(1)	54(1)
O(3)	11525(1)	3698(2)	6903(1)	44(1)
O(4)	10638(1)	3305(2)	5624(1)	59(1)
O(5)	4765(2)	-1517(2)	3786(1)	72(1)
S(1)	6099(1)	-2504(1)	6161(1)	40(1)
F(1)	8527(1)	569(2)	4200(1)	56(1)

TABLE 3
BOND LENGTHS [A] AND ANGLES [DEG] OF COMPOUNDS I AND II

Compound I		Compound II	
C(1)-C(5)	1.341(3)	C(1)-C(6)	1.354(3)
C(1)-C(2)	1.487(4)	C(1)-C(2)	1.497(3)
C(1)-S(1)	1.715(3)	C(1)-S(1)	1.7176(19)
C(2)-C(3)	1.511(4)	C(2)-C(3)	1.515(3)
C(2)-H(2A)	0.9700	C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700	C(2)-H(2B)	0.9700
C(3)-C(4)	1.546(4)	C(3)-C(4)	1.479(3)
C(3)-H(3A)	0.9700	C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700	C(3)-H(3B)	0.9700
C(4)-C(5)	1.503(4)	C(4)-C(5)	1.523(3)
C(4)-H(4A)	0.9700	C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700	C(4)-H(4B)	0.9700
C(5)-C(6)	1.428(3)	C(5)-C(6)	1.512(3)
C(6)-C(14)	1.384(3)	C(5)-H(5A)	0.9700
C(6)-C(7)	1.481(3)	C(5)-H(5B)	0.9700
C(7)-O(3)	1.222(3)	C(6)-C(7)	1.440(3)
C(7)-N(1)	1.362(3)	C(7)-C(8)	1.383(3)
C(8)-C(13)	1.362(4)	C(7)-C(19)	1.490(3)
C(8)-C(9)	1.388(4)	C(8)-N(1)	1.399(2)
C(8)-N(1)	1.397(3)	C(8)-S(1)	1.740(2)
C(9)-C(10)	1.375(4)	C(9)-N(1)	1.279(2)
C(9)-H(9)	0.9300	C(9)-C(10)	1.455(3)
C(10)-C(11)	1.358(4)	C(9)-H(9)	0.9300
C(10)-H(10)	0.9300	C(10)-C(15)	1.391(3)
C(11)-C(12)	1.368(4)	C(10)-C(11)	1.395(3)
C(11)-H(11)	0.9300	C(11)-C(12)	1.382(3)
C(12)-C(13)	1.363(4)	C(11)-H(11)	0.9300
C(12)-H(12)	0.9300	C(12)-O(2)	1.370(2)
C(13)-F(1)	1.362(3)	C(12)-C(13)	1.385(3)
C(14)-N(2)	1.386(3)	C(13)-O(3)	1.376(2)
C(14)-S(1)	1.754(2)	C(13)-C(14)	1.393(3)
C(15)-N(2)	1.274(3)	C(14)-O(4)	1.364(2)
C(15)-C(16)	1.453(4)	C(14)-C(15)	1.384(3)
C(15)-H(15)	0.9300	C(15)-H(15)	0.9300
C(16)-C(21)	1.378(3)	C(16)-O(2)	1.405(3)
C(16)-C(17)	1.393(3)	C(16)-H(16A)	0.9600
C(17)-C(18)	1.367(4)	C(16)-H(16B)	0.9600
C(17)-H(17)	0.9300	C(16)-H(16C)	0.9600
C(18)-O(2)	1.365(3)	C(17)-O(3)	1.417(3)
C(18)-C(19)	1.402(4)	C(17)-H(17A)	0.9600
C(19)-O(1)	1.356(3)	C(17)-H(17B)	0.9600
C(19)-C(20)	1.371(4)	C(17)-H(17C)	0.9600
C(20)-C(21)	1.384(4)	C(18)-O(4)	1.397(3)
C(20)-H(20)	0.9300	C(18)-H(18A)	0.9600
C(21)-H(21)	0.9300	C(18)-H(18B)	0.9600
C(22)-O(1)	1.429(4)	C(18)-H(18C)	0.9600
C(22)-H(22A)	0.9600	C(19)-O(5)	1.217(2)
C(22)-H(22B)	0.9600	C(19)-N(2)	1.358(3)
C(22)-H(22C)	0.9600	C(20)-C(21)	1.377(3)
C(23)-O(2)	1.407(3)	C(20)-C(25)	1.393(3)
C(23)-H(23A)	0.9600	C(20)-N(2)	1.403(3)
C(23)-H(23B)	0.9600	C(21)-C(22)	1.366(3)
C(23)-H(23C)	0.9600	C(21)-F(1)	1.369(2)
N(1)-H(1)	0.8600	C(22)-C(23)	1.375(4)
		C(22)-H(22)	0.9300
C(5)-C(1)-C(2)	114.0(2)	C(23)-C(24)	1.372(4)
C(5)-C(1)-S(1)	112.86(19)	C(23)-H(23)	0.9300
C(2)-C(1)-S(1)	133.1(2)	C(24)-C(25)	1.382(3)
C(1)-C(2)-C(3)	102.4(2)	C(24)-H(24)	0.9300
C(1)-C(2)-H(2A)	111.3	C(25)-H(25)	0.9300
C(3)-C(2)-H(2A)	111.3	N(2)-H(2)	0.90(2)
C(1)-C(2)-H(2B)	111.3		
C(3)-C(2)-H(2B)	111.3	C(6)-C(1)-C(2)	126.38(18)
H(2A)-C(2)-H(2B)	109.2	C(6)-C(1)-S(1)	112.61(15)
C(2)-C(3)-C(4)	108.8(2)	C(2)-C(1)-S(1)	120.94(15)
C(2)-C(3)-H(3A)	109.9	C(1)-C(2)-C(3)	109.08(19)
C(4)-C(3)-H(3A)	109.9	C(1)-C(2)-H(2A)	109.9
C(2)-C(3)-H(3B)	109.9	C(3)-C(2)-H(2A)	109.9
C(4)-C(3)-H(3B)	109.9	C(1)-C(2)-H(2B)	109.9
H(3A)-C(3)-H(3B)	108.3	C(3)-C(2)-H(2B)	109.9
C(5)-C(4)-C(3)	102.3(2)	H(2A)-C(2)-H(2B)	108.3
C(5)-C(4)-H(4A)	111.3	C(4)-C(3)-C(2)	111.6(2)
C(3)-C(4)-H(4A)	111.3	C(4)-C(3)-H(3A)	109.3
C(5)-C(4)-H(4B)	111.3	C(2)-C(3)-H(3A)	109.3
C(3)-C(4)-H(4B)	111.3	C(4)-C(3)-H(3B)	109.3
H(4A)-C(4)-H(4B)	109.2	C(2)-C(3)-H(3B)	109.3
C(1)-C(5)-C(6)	113.6(2)	H(3A)-C(3)-H(3B)	108.0
C(1)-C(5)-C(4)	111.1(2)	C(3)-C(4)-C(5)	114.62(19)
C(6)-C(5)-C(4)	135.3(2)	C(3)-C(4)-H(4A)	108.6
C(14)-C(6)-C(5)	111.5(2)	C(5)-C(4)-H(4A)	108.6
C(14)-C(6)-C(7)	128.1(2)	C(3)-C(4)-H(4B)	108.6
C(5)-C(6)-C(7)	120.5(2)	C(5)-C(4)-H(4B)	108.6
O(3)-C(7)-N(1)	123.1(2)	H(4A)-C(4)-H(4B)	107.6
O(3)-C(7)-C(6)	120.6(2)	C(6)-C(5)-C(4)	112.37(18)
N(1)-C(7)-C(6)	116.3(2)	C(6)-C(5)-H(5A)	109.1
C(13)-C(8)-C(9)	116.6(2)	C(4)-C(5)-H(5A)	109.1
C(13)-C(8)-N(1)	117.6(2)	C(6)-C(5)-H(5B)	109.1
C(9)-C(8)-N(1)	125.8(2)	C(4)-C(5)-H(5B)	109.1
C(10)-C(9)-C(8)	118.9(3)	H(5A)-C(5)-H(5B)	107.9
C(10)-C(9)-H(9)	120.6	C(1)-C(6)-C(7)	112.56(17)
C(8)-C(9)-H(9)	120.6	C(1)-C(6)-C(5)	120.44(18)
C(11)-C(10)-C(9)	122.8(3)	C(7)-C(6)-C(5)	126.96(17)
C(11)-C(10)-H(10)	118.6	C(8)-C(7)-C(6)	112.21(17)
C(9)-C(10)-H(10)	118.6	C(8)-C(7)-C(19)	126.29(17)
C(10)-C(11)-C(12)	119.0(3)	C(6)-C(7)-C(19)	121.50(16)
C(10)-C(11)-H(11)	120.5	C(7)-C(8)-N(1)	126.79(17)
C(12)-C(11)-H(11)	120.5	C(7)-C(8)-S(1)	110.85(14)
C(13)-C(12)-C(11)	117.7(3)	N(1)-C(8)-S(1)	122.32(14)
C(13)-C(12)-H(12)	121.2	N(1)-C(9)-C(10)	125.63(18)
C(11)-C(12)-H(12)	121.2	N(1)-C(9)-H(9)	117.2
C(8)-C(13)-F(1)	116.1(2)	C(10)-C(9)-H(9)	117.2
C(8)-C(13)-C(12)	125.0(3)	C(15)-C(10)-C(11)	120.27(17)
F(1)-C(13)-C(12)	118.8(2)	C(15)-C(10)-C(9)	123.34(18)
C(6)-C(14)-N(2)	126.1(2)	C(11)-C(10)-C(9)	116.36(17)
C(6)-C(14)-S(1)	110.99(18)	C(12)-C(11)-C(10)	119.89(18)
N(2)-C(14)-S(1)	122.94(18)	C(12)-C(11)-H(11)	120.1
N(2)-C(15)-C(16)	126.6(2)	C(10)-C(11)-H(11)	120.1
N(2)-C(15)-H(15)	116.7	O(2)-C(12)-C(11)	124.42(18)
C(16)-C(15)-H(15)	116.7	O(2)-C(12)-C(13)	115.41(17)
C(21)-C(16)-C(17)	119.1(2)	C(11)-C(12)-C(13)	120.16(18)

C(21)-C(16)-C(15)	117.6(2)	O(3)-C(13)-C(12)	120.04(18)
C(17)-C(16)-C(15)	123.3(2)	O(3)-C(13)-C(14)	120.11(18)
C(18)-C(17)-C(16)	120.5(2)	C(12)-C(13)-C(14)	119.78(17)
C(18)-C(17)-H(17)	119.8	O(4)-C(14)-C(15)	124.96(19)
C(16)-C(17)-H(17)	119.8	O(4)-C(14)-C(13)	114.52(17)
O(2)-C(18)-C(17)	125.6(2)	C(15)-C(14)-C(13)	120.52(18)
O(2)-C(18)-C(19)	114.3(2)	C(14)-C(15)-C(10)	119.34(18)
C(17)-C(18)-C(19)	120.1(3)	C(14)-C(15)-H(15)	120.3
O(1)-C(19)-C(20)	125.0(3)	C(10)-C(15)-H(15)	120.3
O(1)-C(19)-C(18)	115.5(3)	O(2)-C(16)-H(16A)	109.5
C(20)-C(19)-C(18)	119.5(3)	O(2)-C(16)-H(16B)	109.5
C(19)-C(20)-C(21)	120.1(3)	H(16A)-C(16)-H(16B)	109.5
C(19)-C(20)-H(20)	119.9	O(2)-C(16)-H(16C)	109.5
C(21)-C(20)-H(20)	119.9	H(16A)-C(16)-H(16C)	109.5
C(16)-C(21)-C(20)	120.7(3)	H(16B)-C(16)-H(16C)	109.5
C(16)-C(21)-H(21)	119.7	O(3)-C(17)-H(17A)	109.5
C(20)-C(21)-H(21)	119.7	O(3)-C(17)-H(17B)	109.5
O(1)-C(22)-H(22A)	109.5	H(17A)-C(17)-H(17B)	109.5
O(1)-C(22)-H(22B)	109.5	O(3)-C(17)-H(17C)	109.5
H(22A)-C(22)-H(22B)	109.5	H(17A)-C(17)-H(17C)	109.5
O(1)-C(22)-H(22C)	109.5	H(17B)-C(17)-H(17C)	109.5
H(22A)-C(22)-H(22C)	109.5	O(4)-C(18)-H(18A)	109.5
H(22B)-C(22)-H(22C)	109.5	O(4)-C(18)-H(18B)	109.5
O(2)-C(23)-H(23A)	109.5	H(18A)-C(18)-H(18B)	109.5
O(2)-C(23)-H(23B)	109.5	O(4)-C(18)-H(18C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(18A)-C(18)-H(18C)	109.5
O(2)-C(23)-H(23C)	109.5	H(18B)-C(18)-H(18C)	109.5
H(23A)-C(23)-H(23C)	109.5	O(5)-C(19)-N(2)	122.04(19)
H(23B)-C(23)-H(23C)	109.5	O(5)-C(19)-C(7)	121.11(19)
C(7)-N(1)-C(8)	127.7(2)	N(2)-C(19)-C(7)	116.85(17)
C(7)-N(1)-H(1)	116.2	C(21)-C(20)-C(25)	116.56(19)
C(8)-N(1)-H(1)	116.2	C(21)-C(20)-N(2)	117.78(18)
C(15)-N(2)-C(14)	119.4(2)	C(25)-C(20)-N(2)	125.66(19)
C(19)-O(1)-C(22)	117.3(3)	C(22)-C(21)-F(1)	119.4(2)
C(18)-O(2)-C(23)	117.3(2)	C(22)-C(21)-C(20)	124.1(2)
C(1)-S(1)-C(14)	90.98(12)	F(1)-C(21)-C(20)	116.50(18)
		C(21)-C(22)-C(23)	118.4(2)
		C(21)-C(22)-H(22)	120.8
		C(23)-C(22)-H(22)	120.8
		C(24)-C(23)-C(22)	119.7(2)
		C(24)-C(23)-H(23)	120.2
		C(22)-C(23)-H(23)	120.2
		C(23)-C(24)-C(25)	121.1(2)
		C(23)-C(24)-H(24)	119.4
		C(25)-C(24)-H(24)	119.4
		C(24)-C(25)-C(20)	120.2(2)
		C(24)-C(25)-H(25)	119.9
		C(20)-C(25)-H(25)	119.9
		C(9)-N(1)-C(8)	118.74(16)
		C(19)-N(2)-C(20)	126.92(17)
		C(19)-N(2)-H(2)	116.2(14)
		C(20)-N(2)-H(2)	116.8(14)
		C(12)-O(2)-C(16)	117.48(17)
		C(13)-O(3)-C(17)	114.85(17)
		C(14)-O(4)-C(18)	118.64(17)
		C(1)-S(1)-C(8)	91.76(9)

TABLE 4A
HYDROGEN BONDS [A AND DEG] OF COMPOUNDS I

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9)...O(3)	0.93	2.29	2.868(3)	119.6
C(15)-H(15)...S(1)	0.93	2.48	2.986(3)	114.4
C(17)-H(17)...F(1)	0.93	2.40	3.307(3)	164.1
C(23)-H(23C)...F(1)	0.96	2.42	3.121(4)	129.7
N(1)-H(1)...N(2)	0.86	2.12	2.839(3)	140.7

TABLE 4B
HYDROGEN BONDS [A AND DEG] OF COMPOUNDS II

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9)...S(1)	0.93	2.47	2.969(2)	114.1
C(11)-H(11)...O(3)#1	0.93	2.51	3.441(2)	177.5
C(15)-H(15)...F(1)	0.93	2.51	3.413(2)	164.6
C(25)-H(25)...O(5)	0.93	2.30	2.853(3)	117.7
N(2)-H(2)...N(1)	0.90(2)	2.05(2)	2.808(2)	141.2(18)

TABLE 5A
ANISOTROPIC DISPLACEMENT PARAMETERS ($A^2 \times 10^3$) OF COMPOUNDS I

	U11	U22	U33	U23	U13	U12
C(1)	40(1)	49(2)	43(2)	8(1)	-1(1)	-1(1)
C(2)	56(2)	67(2)	53(2)	15(2)	-9(1)	-5(1)
C(3)	86(2)	75(2)	55(2)	1(2)	-18(2)	-17(2)
C(4)	50(1)	56(2)	52(2)	-3(2)	-10(1)	2(1)
C(5)	36(1)	49(2)	40(1)	2(1)	2(1)	0(1)
C(6)	34(1)	39(1)	38(1)	3(1)	0(1)	2(1)
C(7)	41(1)	40(2)	42(1)	-2(1)	1(1)	2(1)
C(8)	42(1)	40(2)	52(2)	5(1)	-1(1)	2(1)
C(9)	71(2)	42(2)	87(2)	12(2)	-32(2)	-12(1)
C(10)	83(2)	40(2)	118(3)	21(2)	-32(2)	-8(2)
C(11)	64(2)	53(2)	76(2)	27(2)	-7(2)	5(2)
C(12)	62(2)	53(2)	63(2)	3(2)	-19(2)	4(1)
C(13)	58(2)	37(2)	64(2)	0(1)	-11(2)	1(1)
C(14)	33(1)	39(1)	39(1)	5(1)	5(1)	1(1)
C(15)	56(2)	40(2)	40(2)	4(1)	2(1)	7(1)
C(16)	51(2)	43(2)	36(2)	-4(1)	4(1)	1(1)
C(17)	56(2)	43(1)	42(2)	-5(1)	4(1)	2(1)
C(18)	57(2)	54(2)	40(2)	-2(1)	-1(1)	7(1)
C(19)	61(2)	60(2)	41(2)	-11(1)	1(1)	-7(1)
C(20)	83(2)	44(2)	60(2)	-7(2)	-2(2)	-11(1)
C(21)	70(2)	44(2)	48(2)	1(1)	-6(2)	0(1)
C(22)	108(3)	81(3)	81(3)	-30(2)	-21(2)	-16(2)
C(23)	93(2)	68(2)	52(2)	7(2)	-14(2)	14(2)
N(1)	51(1)	32(1)	55(1)	4(1)	-13(1)	-1(1)
N(2)	42(1)	40(1)	37(1)	2(1)	2(1)	0(1)
O(1)	89(2)	67(2)	64(1)	-20(1)	-17(1)	-6(1)
O(2)	97(2)	64(1)	54(1)	-8(1)	-25(1)	14(1)
O(3)	74(1)	37(1)	61(1)	-4(1)	-18(1)	-3(1)
F(1)	113(2)	45(1)	137(2)	0(1)	-71(2)	-2(1)
S(1)	50(1)	42(1)	50(1)	9(1)	-4(1)	0(1)

TABLE 5B
ANISOTROPIC DISPLACEMENT PARAMETERS ($A^2 \times 10^3$) OF COMPOUNDS II

	U11	U22	U33	U23	U13	U12
C(1)	31(1)	33(1)	40(1)	0(1)	4(1)	-3(1)
C(2)	40(1)	47(1)	49(1)	2(1)	10(1)	-11(1)
C(3)	42(1)	67(2)	66(2)	-3(1)	14(1)	-16(1)
C(4)	38(1)	57(2)	60(2)	-4(1)	1(1)	-12(1)
C(5)	32(1)	36(1)	47(1)	-2(1)	-2(1)	-4(1)
C(6)	29(1)	28(1)	38(1)	-1(1)	3(1)	1(1)
C(7)	32(1)	27(1)	33(1)	-3(1)	3(1)	0(1)
C(8)	31(1)	31(1)	34(1)	-1(1)	6(1)	-1(1)
C(9)	34(1)	36(1)	33(1)	4(1)	3(1)	-4(1)
C(10)	28(1)	32(1)	35(1)	0(1)	2(1)	-2(1)
C(11)	39(1)	39(1)	32(1)	4(1)	3(1)	-8(1)
C(12)	37(1)	36(1)	31(1)	-4(1)	0(1)	-3(1)
C(13)	30(1)	31(1)	40(1)	-6(1)	5(1)	-5(1)
C(14)	37(1)	37(1)	37(1)	2(1)	10(1)	-6(1)
C(15)	35(1)	41(1)	30(1)	-2(1)	2(1)	-5(1)
C(16)	63(2)	75(2)	32(1)	6(1)	-4(1)	-16(1)
C(17)	35(1)	68(2)	67(2)	-4(1)	6(1)	-11(1)
C(18)	65(2)	81(2)	45(2)	4(1)	20(1)	-27(1)
C(19)	41(1)	35(1)	33(1)	-3(1)	2(1)	-4(1)
C(20)	43(1)	37(1)	31(1)	-2(1)	9(1)	0(1)
C(21)	43(1)	47(1)	37(1)	-7(1)	8(1)	-2(1)
C(22)	58(2)	74(2)	54(2)	-4(1)	25(1)	-16(1)
C(23)	81(2)	90(2)	41(2)	10(1)	22(1)	-16(2)
C(24)	71(2)	80(2)	37(1)	11(1)	5(1)	-7(2)
C(25)	47(1)	63(2)	37(1)	5(1)	6(1)	-3(1)
N(1)	31(1)	32(1)	34(1)	-1(1)	3(1)	-4(1)
N(2)	36(1)	48(1)	29(1)	2(1)	1(1)	-7(1)
O(2)	63(1)	58(1)	33(1)	-3(1)	-4(1)	-25(1)
O(3)	37(1)	39(1)	55(1)	-10(1)	8(1)	-11(1)
O(4)	68(1)	67(1)	42(1)	1(1)	13(1)	-35(1)
O(5)	73(1)	93(1)	37(1)	9(1)	-10(1)	-45(1)
S(1)	37(1)	47(1)	34(1)	3(1)	3(1)	-11(1)
F(1)	39(1)	73(1)	52(1)	-3(1)	2(1)	-5(1)

TABLE 6A
HYDROGEN COORDINATES($x10^4$) AND ISOTROPIC DISPLACEMENT PARAMETERS ($A^2 \times 10^3$) OF COMPOUNDS I

	x	y	z	U(eq)
H(2A)	470	7707	379	71
H(2B)	-1173	7637	1003	71
H(3A)	445	6637	-77	86
H(3B)	-1333	6611	335	86
H(4A)	-638	6030	1820	63
H(4B)	1047	5923	1265	63
H(9)	2605	4710	4526	80
H(10)	3785	3878	5535	96
H(11)	5751	4100	6760	77
H(12)	6623	5200	6985	71
H(15)	3197	8399	4344	54
H(17)	5129	7390	6373	56
H(20)	5598	9687	6875	75
H(21)	4213	9272	5398	65
H(22A)	7735	9903	7967	135
H(22B)	7870	9756	9215	135
H(22C)	6190	9873	8686	135
H(23A)	5453	6914	8115	107
H(23B)	7124	6804	8663	107
H(23C)	6988	6843	7394	107
H(1)	3698	6418	4774	55

TABLE 6B
HYDROGEN COORDINATES($x10^4$) AND ISOTROPIC DISPLACEMENT PARAMETERS ($A^2 \times 10^3$) OF COMPOUNDS II

	x	y	z	U(eq)
H(2A)	4054	-3773	6400	54
H(2B)	4347	-5144	6011	54
H(3A)	2403	-4827	5656	70
H(3B)	2539	-3135	5555	70
H(4A)	2118	-4329	4554	64
H(4B)	3201	-5328	4784	64
H(5A)	3829	-3689	4161	48
H(5B)	3145	-2393	4382	48
H(9)	7748	-830	6497	42
H(11)	9194	264	7290	45
H(15)	8967	1328	5390	44
H(16A)	10043	919	8326	89
H(16B)	11319	1213	8697	89
H(16C)	11035	34	8134	89
H(17A)	12827	2404	7260	87
H(17B)	13187	4005	7121	87
H(17C)	12758	2914	6534	87
H(18A)	10563	1944	4899	94
H(18B)	10839	3564	4735	94
H(18C)	9588	3129	4763	94
H(22)	8732	1802	3139	72
H(23)	7311	2172	2185	84
H(24)	5479	1366	2134	77
H(25)	5042	149	3010	59
H(2)	7002(18)	-250(20)	4572(11)	43(6)

TABLE 7
TORSION ANGLES [DEG] OF COMPOUNDS I AND COMPOUND II

Compound I		Compound II	
C(5)-C(1)-C(2)-C(3)	-5.7(3)	C(6)-C(1)-C(2)-C(3)	-19.7(3)
S(1)-C(1)-C(2)-C(3)	171.8(2)	S(1)-C(1)-C(2)-C(3)	157.13(17)
C(1)-C(2)-C(3)-C(4)	10.8(3)	C(1)-C(2)-C(3)-C(4)	48.2(3)
C(2)-C(3)-C(4)-C(5)	-11.8(3)	C(2)-C(3)-C(4)-C(5)	-59.6(3)
C(2)-C(1)-C(5)-C(6)	177.5(2)	C(3)-C(4)-C(5)-C(6)	36.7(3)
S(1)-C(1)-C(5)-C(6)	-0.5(3)	C(2)-C(1)-C(6)-C(7)	176.80(19)
C(2)-C(1)-C(5)-C(4)	-1.9(3)	S(1)-C(1)-C(6)-C(7)	-0.2(2)
S(1)-C(1)-C(5)-C(4)	-179.97(18)	C(2)-C(1)-C(6)-C(5)	-1.2(3)
C(3)-C(4)-C(5)-C(1)	8.5(3)	S(1)-C(1)-C(6)-C(5)	-178.21(15)
C(3)-C(4)-C(5)-C(6)	-170.8(3)	C(4)-C(5)-C(6)-C(1)	-6.4(3)
C(1)-C(5)-C(6)-C(14)	-1.1(3)	C(4)-C(5)-C(6)-C(7)	175.95(19)
C(4)-C(5)-C(6)-C(14)	178.2(3)	C(1)-C(6)-C(7)-C(8)	-0.6(2)
C(1)-C(5)-C(6)-C(7)	179.4(2)	C(5)-C(6)-C(7)-C(8)	177.26(19)
C(4)-C(5)-C(6)-C(7)	-1.3(4)	C(1)-C(6)-C(7)-C(19)	179.24(18)
C(14)-C(6)-C(7)-O(3)	170.9(2)	C(5)-C(6)-C(7)-C(19)	-2.9(3)
C(5)-C(6)-C(7)-O(3)	-9.7(3)	C(6)-C(7)-C(8)-N(1)	-176.46(18)
C(14)-C(6)-C(7)-N(1)	-9.8(4)	C(19)-C(7)-C(8)-N(1)	3.8(3)
C(5)-C(6)-C(7)-N(1)	169.5(2)	C(6)-C(7)-C(8)-S(1)	1.1(2)
C(13)-C(8)-C(9)-C(10)	-1.3(5)	C(19)-C(7)-C(8)-S(1)	-178.71(16)
N(1)-C(8)-C(9)-C(10)	-179.9(3)	N(1)-C(9)-C(10)-C(15)	0.8(3)
C(8)-C(9)-C(10)-C(11)	1.0(6)	N(1)-C(9)-C(10)-C(11)	178.92(19)
C(9)-C(10)-C(11)-C(12)	-0.3(6)	C(15)-C(10)-C(11)-C(12)	1.3(3)
C(10)-C(11)-C(12)-C(13)	0.0(5)	C(9)-C(10)-C(11)-C(12)	-176.91(18)
C(9)-C(8)-C(13)-F(1)	178.3(3)	C(10)-C(11)-C(12)-O(2)	179.61(19)
N(1)-C(8)-C(13)-F(1)	-3.0(4)	C(10)-C(11)-C(12)-C(13)	0.6(3)
C(9)-C(8)-C(13)-C(12)	1.1(5)	O(2)-C(12)-C(13)-O(3)	-4.3(3)
N(1)-C(8)-C(13)-C(12)	179.8(3)	C(11)-C(12)-C(13)-O(3)	174.83(18)
C(11)-C(12)-C(13)-C(8)	-0.4(5)	O(2)-C(12)-C(13)-C(14)	178.82(18)
C(11)-C(12)-C(13)-F(1)	-177.6(3)	C(11)-C(12)-C(13)-C(14)	-2.1(3)
C(5)-C(6)-C(14)-N(2)	-177.8(2)	O(3)-C(13)-C(14)-O(4)	4.3(3)
C(7)-C(6)-C(14)-N(2)	1.6(4)	C(12)-C(13)-C(14)-O(4)	-178.78(19)
C(5)-C(6)-C(14)-S(1)	2.2(2)	O(3)-C(13)-C(14)-C(15)	-175.20(18)
C(7)-C(6)-C(14)-S(1)	-178.42(19)	C(12)-C(13)-C(14)-C(15)	1.7(3)
N(2)-C(15)-C(16)-C(21)	-177.1(3)	O(4)-C(14)-C(15)-C(10)	-179.30(19)
N(2)-C(15)-C(16)-C(17)	3.2(4)	C(13)-C(14)-C(15)-C(10)	0.2(3)
C(21)-C(16)-C(17)-C(18)	0.9(4)	C(11)-C(10)-C(15)-C(14)	-1.7(3)
C(15)-C(16)-C(17)-C(18)	-179.4(2)	C(9)-C(10)-C(15)-C(14)	176.41(19)
C(16)-C(17)-C(18)-O(2)	179.5(3)	C(8)-C(7)-C(19)-O(5)	-178.9(2)
C(16)-C(17)-C(18)-C(19)	-1.0(4)	C(6)-C(7)-C(19)-O(5)	1.3(3)
O(2)-C(18)-C(19)-O(1)	0.5(4)	C(8)-C(7)-C(19)-N(2)	1.6(3)
C(17)-C(18)-C(19)-O(1)	-179.0(2)	C(6)-C(7)-C(19)-N(2)	-178.11(18)
O(2)-C(18)-C(19)-C(20)	-179.2(2)	C(25)-C(20)-C(21)-C(22)	1.2(3)
C(17)-C(18)-C(19)-C(20)	1.3(4)	N(2)-C(20)-C(21)-C(22)	-177.9(2)
O(1)-C(19)-C(20)-C(21)	178.8(3)	C(25)-C(20)-C(21)-F(1)	179.90(19)
C(18)-C(19)-C(20)-C(21)	-1.6(4)	N(2)-C(20)-C(21)-F(1)	0.9(3)
C(17)-C(16)-C(21)-C(20)	-1.2(4)	F(1)-C(21)-C(22)-C(23)	-179.0(2)
C(15)-C(16)-C(21)-C(20)	179.1(2)	C(20)-C(21)-C(22)-C(23)	-0.3(4)
C(19)-C(20)-C(21)-C(16)	1.5(4)	C(21)-C(22)-C(23)-C(24)	0.0(4)
O(3)-C(7)-N(1)-C(8)	1.8(4)	C(22)-C(23)-C(24)-C(25)	-0.5(5)
C(6)-C(7)-N(1)-C(8)	-177.5(2)	C(23)-C(24)-C(25)-C(20)	1.4(4)
C(13)-C(8)-N(1)-C(7)	174.5(3)	C(21)-C(20)-C(25)-C(24)	-1.7(3)
C(9)-C(8)-N(1)-C(7)	-7.0(4)	N(2)-C(20)-C(25)-C(24)	177.2(2)
C(16)-C(15)-N(2)-C(14)	179.0(2)	C(10)-C(9)-N(1)-C(8)	-176.51(18)
C(6)-C(14)-N(2)-C(15)	178.7(2)	C(7)-C(8)-N(1)-C(9)	170.39(19)

S(1)-C(14)-N(2)-C(15)	-1.3(3)	S(1)-C(8)-N(1)-C(9)	-6.9(2)
C(20)-C(19)-O(1)-C(22)	2.6(4)	O(5)-C(19)-N(2)-C(20)	-0.3(3)
C(18)-C(19)-O(1)-C(22)	-177.0(3)	C(7)-C(19)-N(2)-C(20)	179.11(19)
C(17)-C(18)-O(2)-C(23)	-5.7(4)	C(21)-C(20)-N(2)-C(19)	-163.6(2)
C(19)-C(18)-O(2)-C(23)	174.8(2)	C(25)-C(20)-N(2)-C(19)	17.4(3)
C(5)-C(1)-S(1)-C(14)	1.5(2)	C(11)-C(12)-O(2)-C(16)	19.5(3)
C(2)-C(1)-S(1)-C(14)	-176.1(3)	C(13)-C(12)-O(2)-C(16)	-161.4(2)
C(6)-C(14)-S(1)-C(1)	-2.09(18)	C(12)-C(13)-O(3)-C(17)	91.7(2)
N(2)-C(14)-S(1)-C(1)	177.85(19)	C(14)-C(13)-O(3)-C(17)	-91.4(2)
		C(15)-C(14)-O(4)-C(18)	-15.6(3)
		C(13)-C(14)-O(4)-C(18)	165.0(2)
		C(6)-C(1)-S(1)-C(8)	0.72(16)
		C(2)-C(1)-S(1)-C(8)	-176.50(18)
		C(7)-C(8)-S(1)-C(1)	-1.02(15)
		N(1)-C(8)-S(1)-C(1)	176.64(16)

5 Conclusion

Substituted thiophenes with electron withdrawing and methoxy groups play a vital role in their biological activity as antibacterial. The results of the present research indicate that the two molecules are nicely packed in the unit cell with extensive hydrogen bonding network. They exhibit a greater antibacterial activity. It may be interesting to see that more different substituted groups on the thiophene molecule could be a future investigation followed by their three-dimensional structure determination.

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