Crystal Structure of Emidazolidine-2-thione and Its Derivatives

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Abtract

Crystal structures of **emidazolidine-2-thione** or ethylenethiourea(etu) (1), 1-[4,5-dihydro-1*H*-imidazol-2-yl]imidazolidine-2-thione or Jaffe's base (2) and 1-[4,5-dihydro-1*H*-imidazol-2-yl]imidazolidine-2-thione hydrobromide or Jaffe's base HBr (3) have been determined by single crystal x-ray diffraction methods. Crystals of (1) are monoclinic, $P2_1/c$, *a* 5.794(1), *b* 14.509(5), *c* 5.773(2) Å, β 101.32(2)°, Z = 4; the structure was refined to a residual of 0.036 for 1193 independent 'observed' reflections. Crystals of (2) are monoclinic, $P2_1/c$, *a* 7.9079(8), *b* 12.480(2), *c* 7.7913(7) Å, β 92.89(1)°, Z = 4; R being 0.053 for 662 independent 'observed' reflections. The molecules of (1) and (2) are substantially planar. Crystals of (3) are orthorhombic, P_{nam}, *a* 15.295(3), *b* 9.063(2), *c* 6.895(7) Å, Z=4 . R was 0.034 for 1044 independent 'observed' reflections. The molecule is planar.

Introduction

During studies of complexes formed between ethylenethiourea and copper(I) halides(CuX, X = F, Cl, Br, I)[1] or oxyanions(X = NO_3, $1/2SO_4$),[2] we have purified the parent ligand by recrystallization of commercial ethylenethiourea twice from ethanol, obtaining well shaped pale yellow crystals and prepared desulfurated diethylenethiourea or Jaffe' base and also prepared desulfurated diethylene bromide from the reaction of copper(I) bromide and ethylenethiourea. The crystal structure of ethylenethiourea has been previously determined

the Computer Unit, Faculty of Science, Prince of Songkla University. Results are given in the Figures and Tables.

Material deposited comprises structure factor amplitudes, thermal parameters and hydrogen atom geometries (copies are available from the Australian Journal of Chemistry, P.O. Box 89, East Melbourne, Vic. 3002)

Imidazolididine-2-thione, [$C_3H_6N_2S$] , [1]

Crystal data. - $C_3H_6N_2S$, *M* 102.2, Monoclinic, space group $P2_1/c$ (C_{2h}^5 No.14), *a* 5.794(1), *b* 14.509(5), *c* 5.773(2) Å, *V* 475.9(2) Å^3, β 101.32(2)°, D_c(Z=4) 1.43 gcm^{-3}, *F*(000) 216. μ_{Mo} 4.6 cm^{-1}; specimen: 0.42 by 0.31 by 0.14 mm (no absorption correction), $2\theta_{max}$ 60°; *N* 1193, N_o 1193; *R* 0.036, R_w 0.042.

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione, [$C_6H_{10}N_4S$] , [2]

Crystal data. - $C_6H_{10}N_4S$, *M* 170.2. Monoclinic, space group $P2_1/c$ (C_{2h}^5 No.14), *a* 7.9079(8), *b* 12.480(2), *c* 7.7913(7) Å, β 92.89(1)°, *V* 768.0(2) Å^3, D_c(Z=4) 1.47 g cm^{-3}; *F*(000) 360. μ_{Mo} 3.1 cm^{-1}; specimen: 0.xx by 0.xx by 0.xx mm(no absorption correction), 2 θ_{max} 50°; *N* 662, N_o 662; *R* 0.052, R_w 0.053.

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione hydrobromide, [$C_6H_{11}BrN_4S$] , [3]

Crystal data. - $C_6H_{11}BrN_4S$, *M* 251.3. Orthorhombic, space group *Pnam* (D_{2h}^7, No. 53), *a* 15.295(3), *b* 9.063(2), *c* 6.895(7) Å, *V* 956(1) Å^3, D_c(Z=4) 1.75 g cm^{-3}; *F*(000) 504. μ_{Mo} 43.6 cm^{-1}; specimen: 0.59 by 0.58 by 0.37 mm; $A^*_{min,max}$ 2.76, 6.13. $2\theta_{max}$ 65°; *N* 1521, N_o 1044; *R* 0.034, R_w 0.038.

by film methods;[3] we have redetermined the crystal structure of ethylenethiourea by single crystal diffractometer data in order to establish the geometry of the parent ligand more precisely and we also determined the crystal structures of Jaffe's base and desulfurated diethylenethiourea bromide or Jaffe's base HBr which are the ethylenethiourea derivatives.

Experimental

Imidazolididine-2-thione [1]

Crystals of (1) obtained as pale yellow crystals by recrystallization of commercial ethylenethiourea twice from ethanol.

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione [2]

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione hydrobromide [3]

Ethylenethiourea (2.46 g, 0.024 mol) was dissolved in water (90 ml). CuBr (1.5 g, 0.01 mol) was added to the solution with continuous stirring at room temperature about 3 hours. The solution was filtered and allowed to cool. After the solvent evaporated the crystals formed under normal laboratory conditions.

Structure determination

A unique data set was measured within an appropriate $2\Theta_{max}$ limit as specified for each structure using an Enraf-Nonius four-circle diffractometer. Of the N reflections collected, N_o of those with $I > 3\sigma(I)$ being considered 'observed' and used in the refinement of the structure. The reflection intensities were corrected for Lorentz and polarization effects. The structures were solved by the direct methods. The hydrogen atoms were located in difference Fourier maps and refined in (x,y,z,U_{iso}) except the hydrogen atom on compound(2) were calculated and constrained in refinement. Anisotropic thermal parameters were refined for the non-hydrogen atoms. For compound(1), the $P2_1/c$ setting of the original $P2_1/a$ cell[3] was adopted. Neutral atom complex scattering factors were used;[4] computation used the XTAL3.2 program system[5] implemented on a PC Computer of the Department of Chemistry and XTAL3.4[5] implamented on a DEC Alpha Server computer of

Discussion

Imidazolididine-2-thione

The unit cell contents comprise discrete molecules of the ethylenethiourea with one molecule comprising the asymmetric unit. No short inter- or intramolecular hydrogen bonds are found. Unlike the suggestions of the earlier report, the molecule is almost planar; and the best plane of the six non hydrcgen atoms was calculated with the deviation of atoms S, N(1), N(2), C(1), C(2) and C(3) from the plane being 0.006(1), -0.017(2), -0.012(2), 0.020(2), 0.014(2) and -0.009(2) Å respectively. The H(N_1) and H(N_2) atoms are in this plane which the deviations from the plane are -0.02(2) and 0.06(2) Å. The geometry is a useful baseline for comparison with that of the molecule as a ligand in its complexes, e.g. in the recent studies of [Cu(etu)$_4$](NO_3) and [Cu(etu)$_3$]$_2$(SO_4), S-C_3 are 1.694(2), and 1.714(5), 1.698(6) Å respectively,[2] exhibiting surprisingly little change the present value of 1.688(2) Å.

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione

The structure consists of discrete Jaffe' base molecules held together by hydrogen bonds and van der Waals interactions. The N(3)—H(1') (-x, 1/2+y, 1/2-z) inter-hydrogen bond is 2.037(6) Å.

1-[4,5-Dihydro-1H-imidazol-2-yl]imidazolidine-2-thione hydrobromide

The structure of this compound consists of discrete desulfurated diethylenethiourea cations, [$C_6H_{11}N_4S$] and bromide ions. All non hydrogen atoms including the bromide ion, and the N-hydrogen atoms, lie in the same plane which is the mirror plane of the molecule at y = 1/4 and hydrogen atoms on CH_2 groups are related by this plane. The C-S distance 1.647(4) Å, is short compared with the parent ethylenethiourea molecule (1.688(2) Å) due the resonance effect.

Acknowledgement

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References

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Table 1. Atomic positional and isotropic displacement parameters

	x/a	y/b	z/c	U
S	0.22602(8)	0.11419(3)	0.04392(8)	0.0428(2)
N(1)	0.6472(3)	0.0675(1)	0.3059(3)	0.0491(5)
H(1)	0.668(3)	0.025(1)	0.204(3)	0.047(5)
N(2)	0.4717(3)	0.1767(1)	0.4573(3)	0.0431(5)
H(2)	0.367(4)	0.218(1)	0.459(3)	0.053(6)
C(1)	0.8167(3)	0.0907(1)	0.5194(3)	0.0416(6)
H(11)	0.848(4)	0.036(1)	0.625(3)	0.057(6)
H(12)	0.966(4)	0.113(1)	0.482(4)	0.057(6)
C(2)	0.6917(3)	0.1675(1)	0.6272(3)	0.0432(6)
H(21)	0.776(3)	0.227(1)	0.642(3)	0.059(6)
H(22)	0.661(4)	0.153(1)	0.780(4)	0.066(7)
C(3)	0.4551(3)	0.1192(1)	0.2748(3)	0.0324(4)

Table 2. Interatomic distances (Angstroms)

Atoms	Distance
S-C(3)	1.688(2)
N(1)-H(1)	.87(2)
N(1)-C(1)	1.456(2)
N(1)-C(3)	1.325(2)

N(2)-H(2)	.85(2)
N(2)-C(2)	1.454(2)
N(2)-C(3)	1.333(2)
C(1)-H(11)	1.00(2)
C(1)-H(12)	.99(2)
C(1)-C(2)	1.527(3)
C(2)-H(21)	.99(2)
C(2)-H(22)	.95(2)

Table 3. Interatomic angles (degrees)

Atoms	Distance
H(1)-N(1)-C(1)	125(1)
H(1)-N(1)-C(3)	122(1)
C(1)-N(1)-C(3)	113.1(2)
H(2)-N(2)-C(2)	126(1)
H(2)-N(2)-C(3)	120(1)
C(2)-N(2)-C(3)	113.2(1)
N(1)-C(1)-H(11)	110(1)
N(1)-C(1)-H(12)	112(1)
N(1)-C(1)-C(2)	102.6(1)
H(11)-C(1)-H(12)	110(2)
H(11)-C(1)-C(2)	112(1)
H(12)-C(1)-C(2)	111(1)
N(2)-C(2)-C(1)	102.4(1)

N(2)-C(2)-H(21)	109(1)
N(2)-C(2)-H(22)	110(1)
C(1)-C(2)-H(21)	114(1)
C(1)-C(2)-H(22)	114(1)
H(21)-C(2)-H(22)	107(2)
S-C(3)-N(1)	126.3(1)
S-C(3)-N(2)	125.1(1)
N(1)-C(3)-N(2)	108.6(1)

Table Sup-1 Atomic Displacement Parameters

	U11	U22	U33	U12	U13	U23
S	.0412(3)	.0459(3)	.0376(2)	-.0040(2)	-.0014(2)	-.0033(2)
N(1)	.0465(9)	.0554(9)	.0410(8)	.0149(7)	-.0024(7)	-.0193(7)
H(1)	.047(5)					
N(2)	.0420(8)	.0456(8)	.0387(8)	.0105(7)	.0008(6)	-.0122(6)
H(2)	.053(6)					
C(1)	.0393(9)	.047(1)	.0364(9)	.0068(8)	.0026(7)	-.0034(7)
H(11)	.057(6)					
H(12)	.057(6)					
C(2)	.045(1)	.047(1)	.0345(9)	.0040(8)	.0018(7)	-.0085(7)
H(21)	.059(6)					
H(22)	.066(7)					
C(3)	.0369(8)	.0308(7)	.0303(7)	-.0038(6)	.0084(6)	.0010(6)

Table Comparative SCN_2 geometries

Compound	S-C/ Å	C-N/ Å	S-C-N/ degrees	N-C-N/ degrees
tu[6]	1.720(9)	1.340(6)	120.5(5)	119.0(5)
etu	1.688(2)	1.325(2), 1.333(2)	125.1(1), 126.3(1)	108.6(1)
Jaffe's Base	1.671(8)	1.303(9), 1.394(9)	124.4(6), 126.0(6)	109.6(9)
Jaffe's Base HBr	1.648(4)	1.324(6), 1.412(5)	126.9(3), 127.3(3)	105.8(3)

Figure captions

Fig. 1 Molecular plot of ethylenethiourea normal to six non-hydrogen atoms.

Fig. 2 Molecular plot of ethylenethiourea through the plane of five ring atoms.

Fig. 3 Unit cell content of ethylenethiourea plot down *c*.

Atomic Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U(eq) A**2
N(1)	0.4717(3)	0.1767(1)	0.4573(3)	0.0431(5)
H(1)	0.367(4)	0.218(1)	0.459(3)	0.053(6)
C(2)	0.4551(3)	0.1192(1)	0.2748(3)	0.0324(4)
S(2)	0.22602(8)	0.11419(3)	0.04392(8)	0.0428(2)
N(3)	0.6472(3)	0.0675(1)	0.3059(3)	0.0491(5)
H(3)	0.668(3)	0.025(1)	0.204(3)	0.047(5)
C(4)	0.8167(3)	0.0907(1)	0.5194(3)	0.0416(6)
H(41)	0.848(4)	0.036(1)	0.625(3)	0.057(6)
H(42)	0.966(4)	0.113(1)	0.482(4)	0.057(6)
C(5)	0.6917(3)	0.1675(1)	0.6272(3)	0.0432(6)
H(51)	0.776(3)	0.227(1)	0.642(3)	0.059(6)
H(52)	0.661(4)	0.153(1)	0.780(4)	0.066(7)

Non-Hydrogen Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U(eq) A**2
N(1)	0.4717(3)	0.1767(1)	0.4573(3)	0.0431(5)
C(2)	0.4551(3)	0.1192(1)	0.2748(3)	0.0324(4)
S(2)	0.22602(8)	0.11419(3)	0.04392(8)	0.0428(2)
N(3)	0.6472(3)	0.0675(1)	0.3059(3)	0.0491(5)
C(4)	0.8167(3)	0.0907(1)	0.5194(3)	0.0416(6)
C(5)	0.6917(3)	0.1675(1)	0.6272(3)	0.0432(6)

Hydrogen Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U A**2
H(1)	0.367(4)	0.218(1)	0.459(3)	0.053(6)
H(3)	0.668(3)	0.025(1)	0.204(3)	0.047(5)
H(41)	0.848(4)	0.036(1)	0.625(3)	0.057(6)
H(42)	0.966(4)	0.113(1)	0.482(4)	0.057(6)
H(51)	0.776(3)	0.227(1)	0.642(3)	0.059(6)
H(52)	0.661(4)	0.153(1)	0.780(4)	0.066(7)

Atomic Anisotropic Displacement Parameters

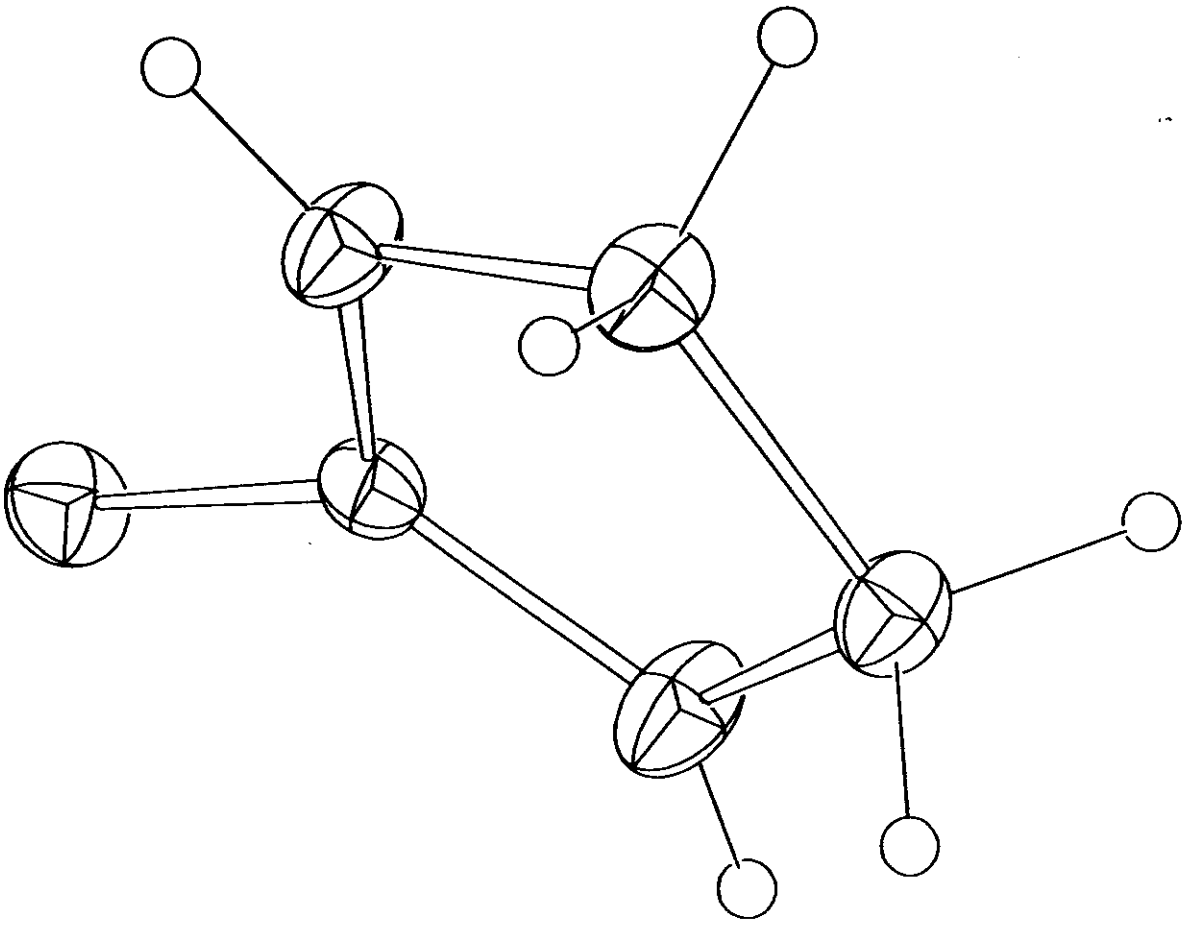
atom	U11	U22	U33	U12	U13	U23
N(1)	.0420(8)	.0456(8)	.0387(8)	.0105(7)	.0008(6)	-.0122(6)
C(2)	.0369(8)	.0308(7)	.0303(7)	-.0038(6)	.0084(6)	.0010(6)
S(2)	.0412(3)	.0459(3)	.0376(2)	-.0040(2)	-.0014(2)	-.0033(2)
N(3)	.0465(9)	.0554(9)	.0410(8)	.0149(7)	-.0024(7)	-.0193(7)
C(4)	.0393(9)	.047(1)	.0364(9)	.0068(8)	.0026(7)	-.0034(7)
C(5)	.045(1)	.047(1)	.0345(9)	.0040(8)	.0018(7)	-.0085(7)

Bond Distances (Angstroms)

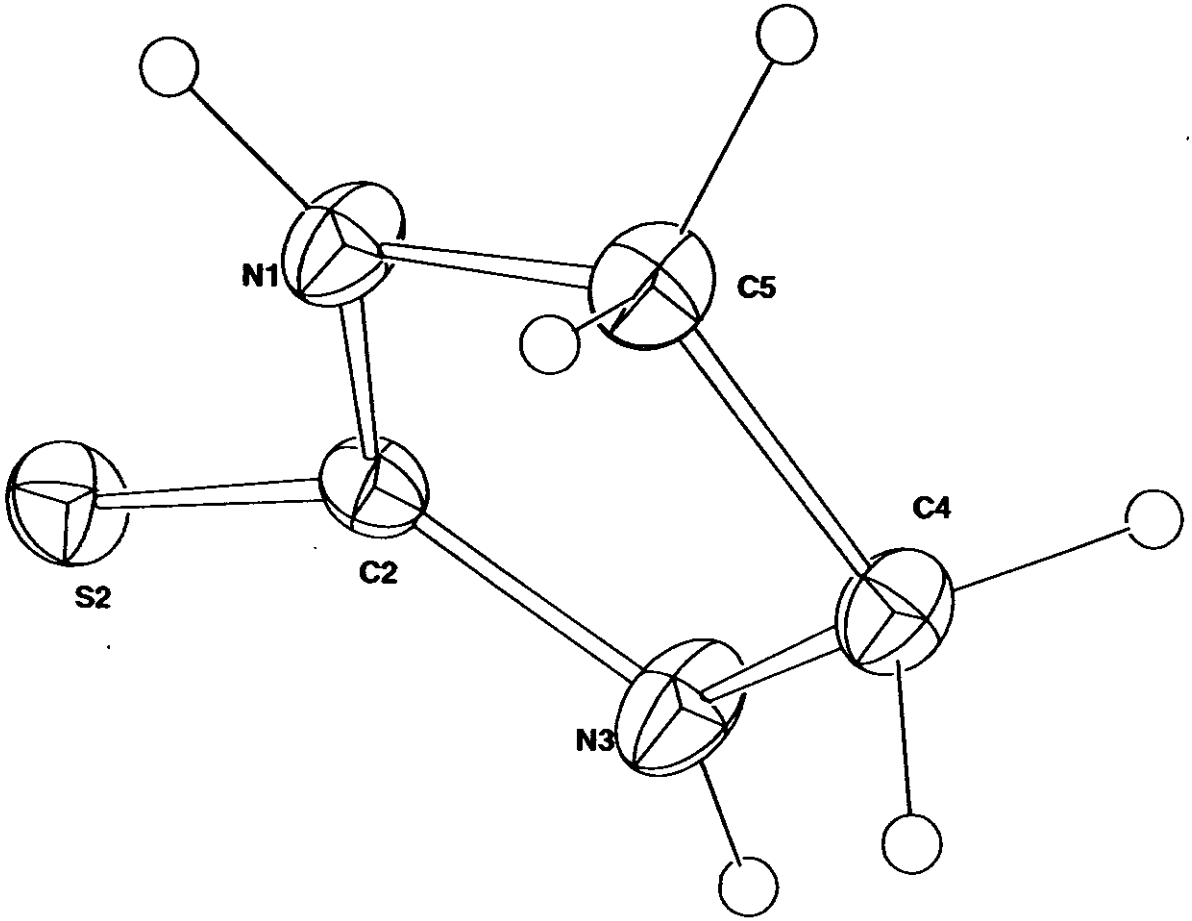
N(1)-C(2)	1.333(2)
N(1)-C(5)	1.454(2)
C(2)-S(2)	1.688(2)
C(2)-N(3)	1.325(2)
N(3)-C(4)	1.456(2)
C(4)-C(5)	1.527(3)

Bond Angles (degrees)

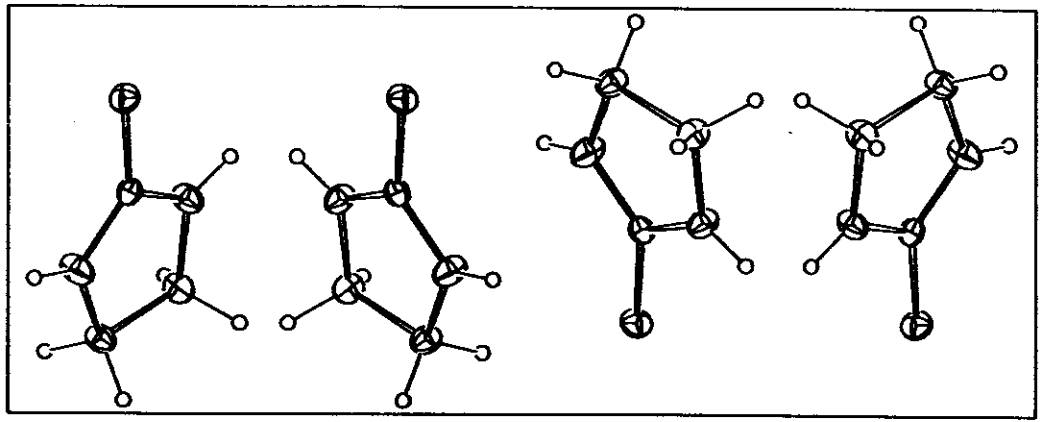
C(2)-N(1)-C(5)	113.2(1)
N(1)-C(2)-S(2)	125.1(1)
N(1)-C(2)-N(3)	108.6(1)
S(2)-C(2)-N(3)	126.3(1)
C(2)-N(3)-C(4)	113.1(2)
N(3)-C(4)-C(5)	102.6(1)
N(1)-C(5)-C(4)	102.4(1)



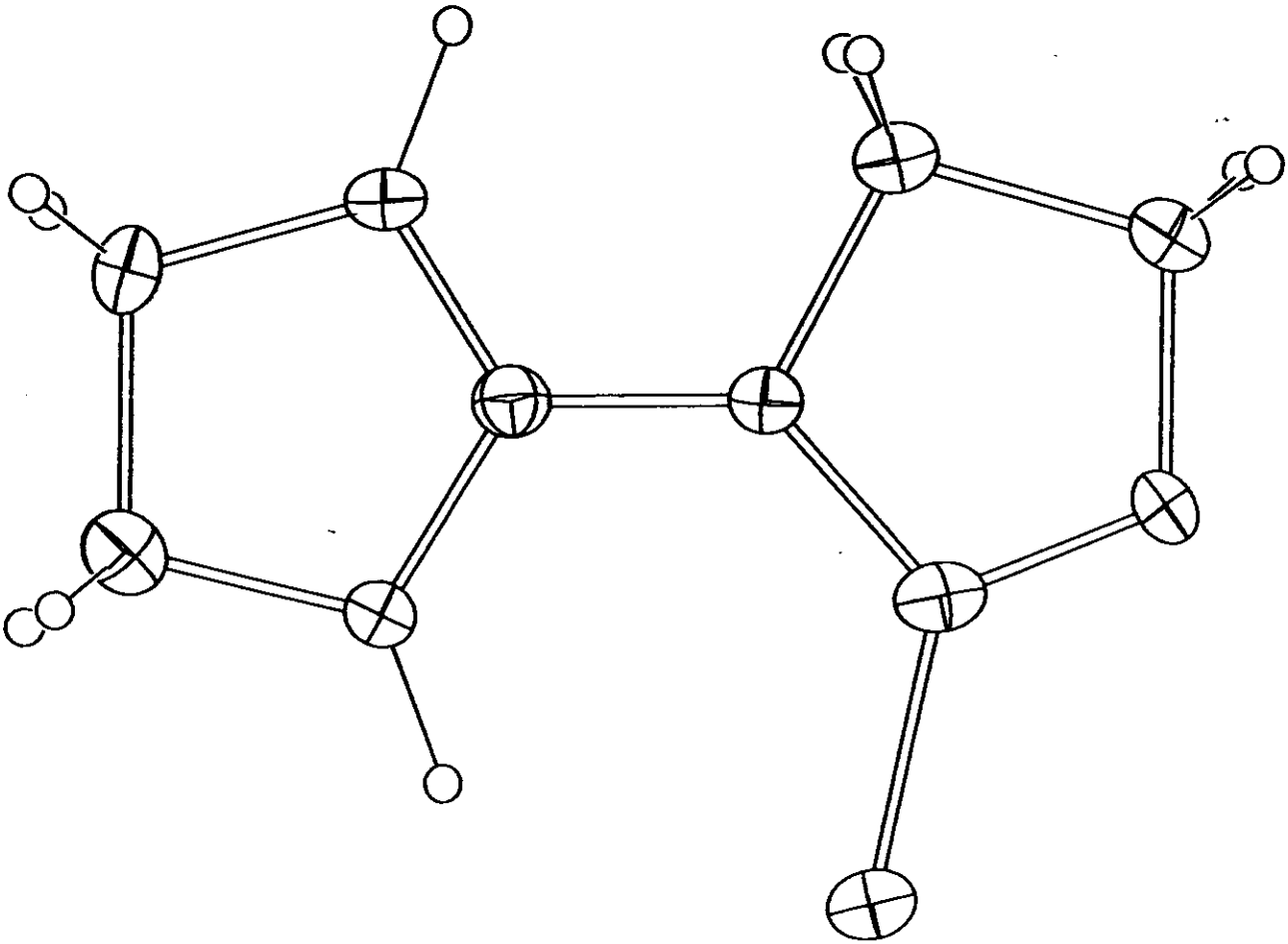
Ethylenethiourea



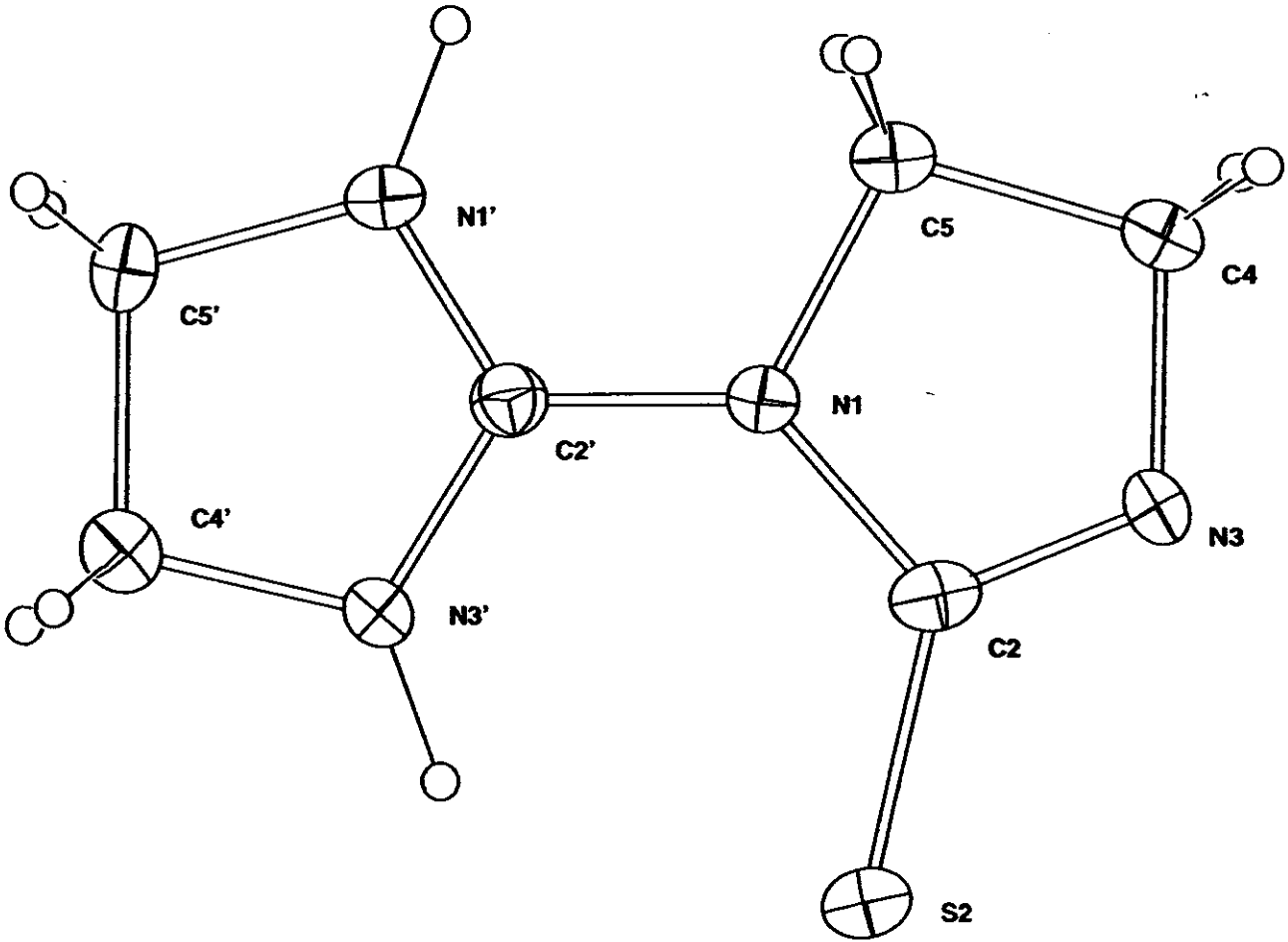
Ethylenethiourea



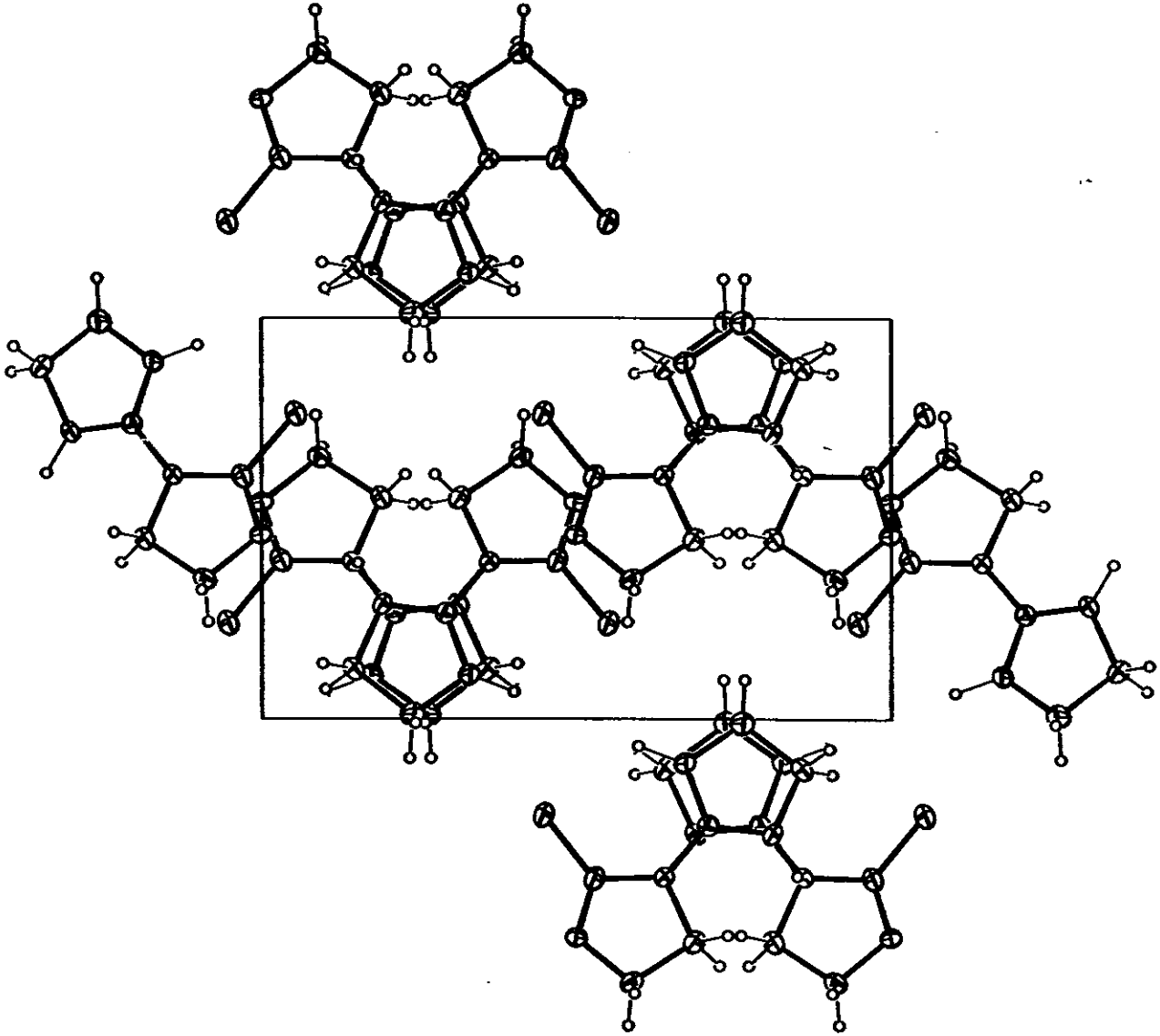
Ethylenethiourea: unit cell down c,b axis across



Jaffe's Base $[C_6H_{10}N_4S]$



Jaffe's Base



Jaffe's Base $C_6H_{10}N_4S$ unit cell down c axis,b axis across

Atomic Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U(eq) A**2
Br	0.30187(2)	0.49687(5)	1/4	0.0492(2)
N(1)	0.4457(2)	0.9443(3)	1/4	0.038(1)
C(2)	0.4601(3)	1.0981(5)	1/4	0.039(1)
S(2)	0.55494(8)	1.1844(1)	1/4	0.0539(4)
N(3)	0.3815(3)	1.1593(4)	1/4	0.052(1)
C(4)	0.3071(3)	1.0592(6)	1/4	0.052(2)
C(5)	0.3508(3)	0.9086(6)	1/4	0.049(2)
N(1')	0.4847(2)	0.6958(4)	1/4	0.046(1)
C(2')	0.5061(3)	0.8370(4)	1/4	0.036(1)
N(3')	0.5915(2)	0.8553(4)	1/4	0.047(1)
C(4')	0.6362(3)	0.7125(5)	1/4	0.050(2)
C(5')	0.5619(3)	0.6040(6)	1/4	0.064(2)
H(3)	0.367(3)	1.253(7)	1/4	0.09(2)
H(4)	0.266(2)	1.067(4)	0.364(5)	0.09(1)
H(1)	0.338(2)	0.851(3)	0.140(4)	0.049(9)
H(1')	0.436(2)	0.674(4)	1/4	0.03(1)
H(3')	0.615(3)	0.947(6)	1/4	0.06(1)
H(4')	0.670(2)	0.701(3)	0.141(4)	0.051(9)
H(5')	0.561(2)	0.540(3)	0.168(6)	0.06(1)

Non-Hydrogen Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U(eq) A**2
Br	0.30187(2)	0.49687(5)	1/4	0.0492(2)
N(1)	0.4457(2)	0.9443(3)	1/4	0.038(1)
C(2)	0.4601(3)	1.0981(5)	1/4	0.039(1)
S(2)	0.55494(8)	1.1844(1)	1/4	0.0539(4)
N(3)	0.3815(3)	1.1593(4)	1/4	0.052(1)
C(4)	0.3071(3)	1.0592(6)	1/4	0.052(2)
C(5)	0.3508(3)	0.9086(6)	1/4	0.049(2)
N(1')	0.4847(2)	0.6958(4)	1/4	0.046(1)
C(2')	0.5061(3)	0.8370(4)	1/4	0.036(1)
N(3')	0.5915(2)	0.8553(4)	1/4	0.047(1)
C(4')	0.6362(3)	0.7125(5)	1/4	0.050(2)
C(5')	0.5619(3)	0.6040(6)	1/4	0.064(2)

Hydrogen Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U A**2
H(3)	0.367(3)	1.253(7)	1/4	0.09(2)
H(4)	0.266(2)	1.067(4)	0.364(5)	0.09(1)
H(5)	0.338(2)	0.851(3)	0.140(4)	0.049(9)
H(1')	0.436(2)	0.674(4)	1/4	0.03(1)
H(3')	0.615(3)	0.947(6)	1/4	0.06(1)
H(4')	0.670(2)	0.701(3)	0.141(4)	0.051(9)
H(5')	0.561(2)	0.540(3)	0.168(6)	0.06(1)

Atomic Anisotropic Displacement Parameters

atom	U11	U22	U33	U12	U13	U23
Br	.0385(2)	.0340(2)	.0750(4)	.0049(2)	0	0
N(1)	.035(2)	.029(1)	.049(2)	.002(1)	0	0
C(2)	.049(2)	.031(2)	.036(3)	.002(2)	0	0
S(2)	.0582(7)	.0337(5)	.0698(9)	-.0088(6)	0	0
N(3)	.056(2)	.034(2)	.066(3)	.012(2)	0	0
C(4)	.047(3)	.048(3)	.062(4)	.007(2)	0	0
C(5)	.039(2)	.039(2)	.069(4)	.002(2)	0	0
N(1')	.037(2)	.031(2)	.070(3)	-.003(2)	0	0
C(2')	.039(2)	.030(2)	.040(3)	.001(2)	0	0
N(3')	.036(2)	.031(2)	.072(3)	-.000(1)	0	0
C(4')	.045(2)	.038(2)	.067(4)	.005(2)	0	0
C(5')	.052(3)	.029(2)	.109(5)	.004(2)	0	0

Bond Distances (Angstroms)

N(1)-C(2)	1.412(5)
N(1)-C(5)	1.487(5)
N(1)-C(2')	1.342(5)
C(2)-S(2)	1.648(4)
C(2)-N(3)	1.324(6)
N(3)-C(4)	1.455(6)
C(4)-C(5)	1.519(7)
N(1')-C(2')	1.321(5)
N(1')-C(5')	1.444(6)
C(2')-N(3')	1.316(5)
N(3')-C(4')	1.465(6)
C(4')-C(5')	1.503(7)

Bond Angles (degrees)

C(2)-N(1)-C(5)	111.6(3)
C(2)-N(1)-C(2')	127.4(3)
C(5)-N(1)-C(2')	121.0(3)
N(1)-C(2)-S(2)	127.3(3)
N(1)-C(2)-N(3)	105.8(3)
S(2)-C(2)-N(3)	126.9(3)
C(2)-N(3)-C(4)	116.7(4)
N(3)-C(4)-C(5)	102.5(4)
N(1)-C(5)-C(4)	103.5(4)
C(2')-N(1')-C(5')	110.8(4)
N(1)-C(2')-N(1')	122.1(4)
N(1)-C(2')-N(3')	126.3(4)
N(1')-C(2')-N(3')	111.6(4)
C(2')-N(3')-C(4')	110.6(3)
N(3')-C(4')-C(5')	103.0(4)
N(1')-C(5')-C(4')	104.0(4)

Hydrogen Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U A**2
H(3)	0.5702	0.5719	0.2961	0.063
H(41)	0.7547	0.4159	0.2581	0.087
H(42)	0.6767	0.4058	0.4361	0.087
H(51)	0.6086	0.2757	0.1650	0.080
H(52)	0.5340	0.2639	0.3444	0.080
H(1')	0.3866	0.1518	0.1547	0.069
H(41')	-0.0932	0.2335	0.0685	0.092
H(42')	-0.0100	0.2418	-0.1071	0.092
H(51')	0.0769	0.1025	0.1504	0.079
H(52')	0.1395	0.0994	-0.0350	0.079

Atomic Anisotropic Displacement Parameters

atom	U11	U22	J33	U12	U13	U23
N(1)	.039(3)	.032(3)	.068(4)	.003(2)	-.005(3)	.000(3)
C(2)	.048(4)	.037(4)	.054(5)	.004(3)	.004(3)	.002(3)
S(2)	.061(1)	.0399(9)	.101(2)	.0100(9)	-.012(1)	.003(1)
N(3)	.044(3)	.033(3)	.084(5)	-.005(3)	-.018(3)	-.006(3)
C(4)	.047(4)	.047(4)	.084(5)	.010(3)	-.013(4)	-.004(4)
C(5)	.048(4)	.043(4)	.072(5)	.009(3)	-.008(4)	.002(3)
N(1')	.042(3)	.038(3)	.087(5)	.006(3)	-.011(3)	-.001(3)
C(2')	.047(4)	.039(3)	.046(4)	-.002(3)	.005(3)	-.000(3)
N(3')	.036(3)	.050(3)	.105(5)	-.003(3)	-.029(3)	-.006(3)
C(4')	.048(4)	.059(4)	.077(5)	.003(3)	-.006(4)	-.003(4)
C(5')	.050(4)	.047(4)	.066(5)	-.009(3)	-.001(4)	-.007(3)

Atomic Positional and Isotropic Displacement Parameters

atom	x/a	y/b	z/c	U(eq)A**2
N(1)	0.3923(6)	0.3584(4)	0.1854(6)	* 0.046(2)
C(2)	0.3940(7)	0.4690(4)	0.2017(8)	* 0.046(2)
S(2)	0.2381(2)	0.5538(1)	0.1439(3)	* 0.0679(7)
N(3	0.5397(6)	0.4973(3)	0.2721(7)	* 0.055(2)
H(3	0.5702	0.5719	0.2961	0.063
C(4	0.6528(7)	0.4098(5)	0.3159(8)	* 0.060(2)
H(4)	0.7547	0.4159	0.2581	0.087
H(4 '	0.6767	0.4058	0.4361	0.087
C(5	0.5523(7)	0.3123(4)	0.2523(8)	* 0.055(2)
H(5	0.6086	0.2757	0.1650	0.080
H(5)	0.5340	0.2639	0.3444	0.080
N(1)	0.2851(5)	0.1902(4)	0.1234(6)	* 0.056(2)
H(1)	0.3866	0.1518	0.1547	0.069
C(2)	0.2632(7)	0.2913(4)	0.1270(8)	* 0.044(2)
N(3	0.1081(6)	0.3281(4)	0.0765(7)	* 0.065(2)
C(4	0.0114(7)	0.2380(5)	0.0133(8)	* 0.061(3)
H( )	-0.0932	0.2335	0.0685	0.092
H(4 ')	-0.0100	0.2418	-0.1071	0.092
C(5	0.1241(8)	0.1433(4)	0.0627(7)	* 0.055(2)
H(5)	0.0769	0.1025	0.1504	0.079
H(5	0.1395	0.0994	-0.0350	0.079

Non-hydrogen Positional and Isotropic Displacement Parameters

atc	x/a	y/b	z/c	U(eq) A**2
N(	0.3923(6)	0.3584(4)	0.1854(6)	* 0.046(2)
C(	0.3940(7)	0.4690(4)	0.2017(8)	* 0.046(2)
S(2	0.2381(2)	0.5538(1)	0.1439(3)	* 0.0679(7)
N(3	0.5397(6)	0.4973(3)	0.2721(7)	* 0.055(2)
C	0.6528(7)	0.4098(5)	0.3159(8)	* 0.060(2)
C(5	0.5523(7)	0.3123(4)	0.2523(8)	* 0.055(2)
N(1)	0.2851(5)	0.1902(4)	0.1234(6)	* 0.056(2)
C(2)	0.2632(7)	0.2913(4)	0.1270(8)	* 0.044(2)
N(3)	0.1081(6)	0.3281(4)	0.0765(7)	* 0.065(2)
C(4)	0.0114(7)	0.2380(5)	0.0133(8)	* 0.061(3)
C(5)	0.1241(8)	0.1433(4)	0.0627(7)	* 0.055(2)

Bond Distances	(Angstroms)
N(1)-C(2)	1.386(7)
N(1)-C(5)	1.462(7)
N(1)-C(2')	1.380(7)
C(2)-S(2)	1.669(6)
C(2)-N(3)	1.300(7)
N(3)-C(4)	1.441(7)
C(4)-C(5)	1.523(8)
N(1')-C(2')	1.275(7)
N(1')-C(5')	1.458(7)
C(2')-N(3')	1.350(7)
N(3')-C(4')	1.433(8)
C(4')-C(5')	1.518(8)

Bond Angles	(degrees)
C(2)-N(1)-C(5)	110.8(4)
C(2)-N(1)-C(2')	129.7(5)
C(5)-N(1)-C(2')	119.4(4)
N(1)-C(2)-S(2)	127.1(4)
N(1)-C(2)-N(3)	108.2(5)
S(2)-C(2)-N(3)	124.7(4)
C(2)-N(3)-C(4)	114.9(4)
N(3)-C(4)-C(5)	102.8(4)
N(1)-C(5)-C(4)	103.3(4)
C(2')-N(1')-C(5')	106.7(4)
N(1)-C(2')-N(1')	120.6(5)
N(1)-C(2')-N(3')	122.4(5)
N(1')-C(2')-N(3')	116.9(5)
C(2')-N(3')-C(4')	107.1(4)
N(3')-C(4')-C(5')	103.1(4)
N(1')-C(5')-C(4')	105.2(4)