3. Results

3.1 Preparation of Complexes

The condition of preparation of complexes for which X-ray crystal structures have been determined in the course of this study are shown in Table 1. And some of their physical properties are summarized in Table 2.

Table 1. The condition of preparation the studied complexes.

Complexes	**Reactants**	**Mole Ratio**	**Solvent**	**Temp. (°C)**
$[Cu(etu)_3]_2SO_4$	$Cu(CH_3COO)_2 \cdot H_2O$: etu	1 : 3	Distilled water	80
$[Cu_2(detu)_6](NO_3)_2$	$Cu(NO_3)_2 \cdot 3H_2O$: detu	1 : 3	Distilled water	60
$[Cu(detu)_3]_2SO_3$	$Cu(CH_3COO)_2 \cdot H_2O$: detu	1 : 3	Distilled water	55
$[Cu_2(detu)_6](ClO_4)_2$	$Cu(ClO_4)_2 \cdot 6H_2O$: detu	1 : 3	CH_3CN: EtOH	50

Table 2. The physical properties of ligands and the studied complexes.

Compounds	**Physical Properties**			
	Appearance	Color	Melting Point (°C)	Solubility
ligand etu	powder	white	198 – 200	soluble in H_2O, EtOH, CH_3CN, C_3H_6O and DMSO
$[Cu(etu)_3]_2SO_4$	prism	colorless	234 – 236	soluble in DMSO
ligand detu	powder	white	75 – 78	soluble in H_2O, EtOH, CH_3CN, C_3H_6O and DMSO
$[Cu_2(detu)_6](NO_3)_2$	prism	colorless	148 - 150	soluble in CH_3CN, C_3H_6O and DMSO
$[Cu(detu)_3]_2SO_3$	prism	colorless	193 – 195	insoluble in H_2O, EtOH, CH_3CN, C_3H_6O and DMSO
$[Cu_2(detu)_6](ClO_4)_2$	needle	colorless	138 - 139	soluble in H_2O, EtOH, CH_3CN, C_3H_6O and DMSO

3.2 X - ray Fluorescence Spectrometry

The X - ray fluorescence spectra of the studied complexes are shown in Figure 46. - 53. respectively.

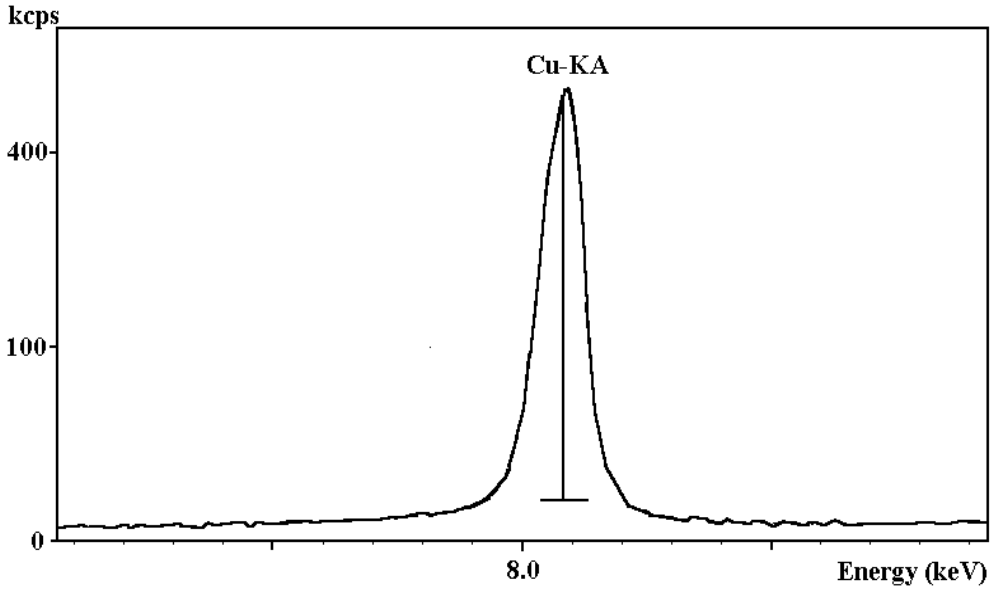

Figure 46. The Cu(K_α) spectrum of $[Cu(etu)_3]_2SO_4$.

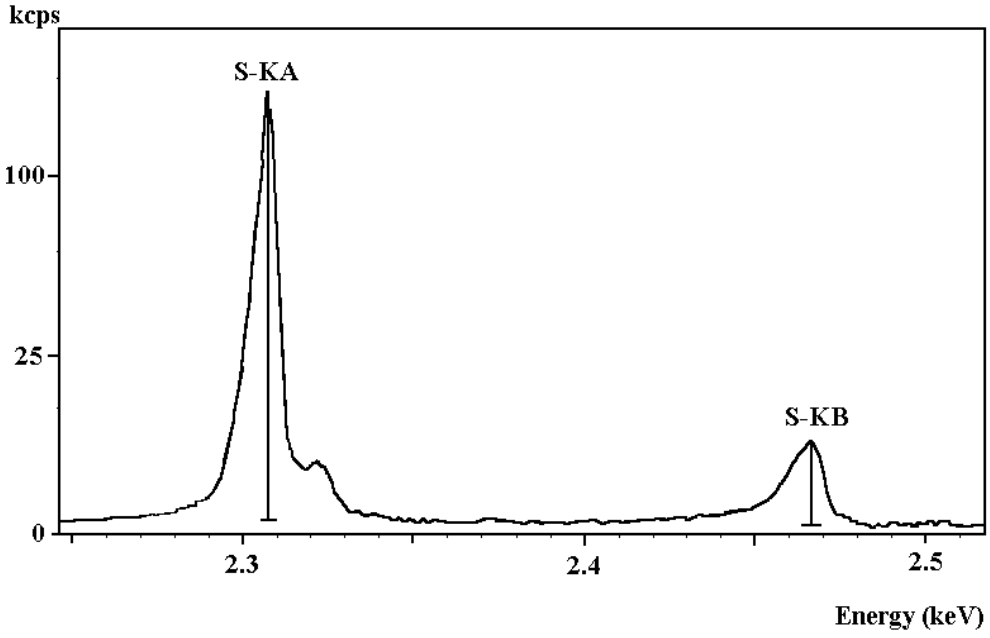

Figure 47. The S(K_α) and S(K_β) spectrum of $[Cu(etu)_3]_2SO_4$.

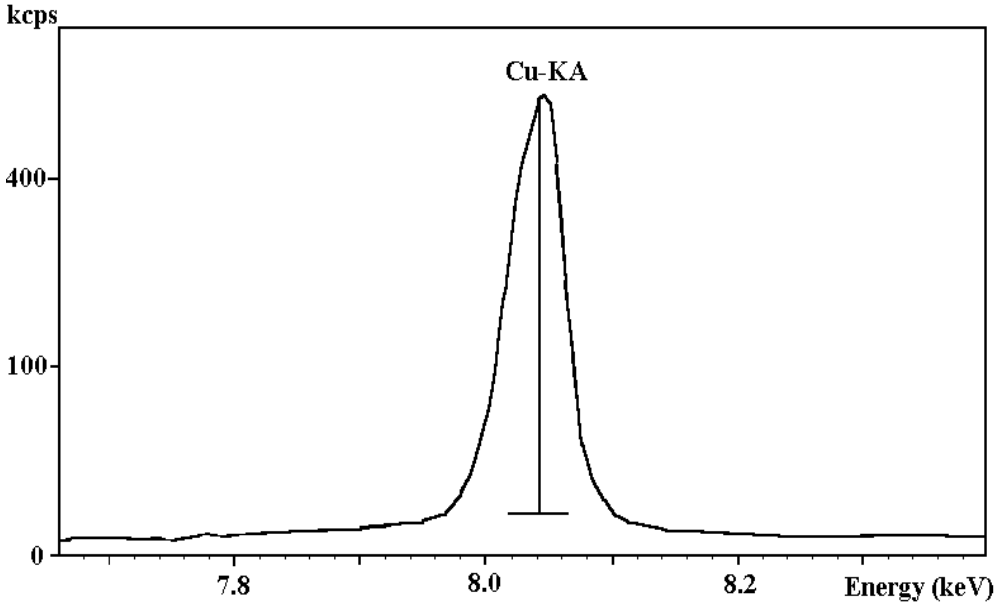

Figure 48. The Cu(K_α) spectrum of $[Cu_2(detu)_6](NO_3)_2$.

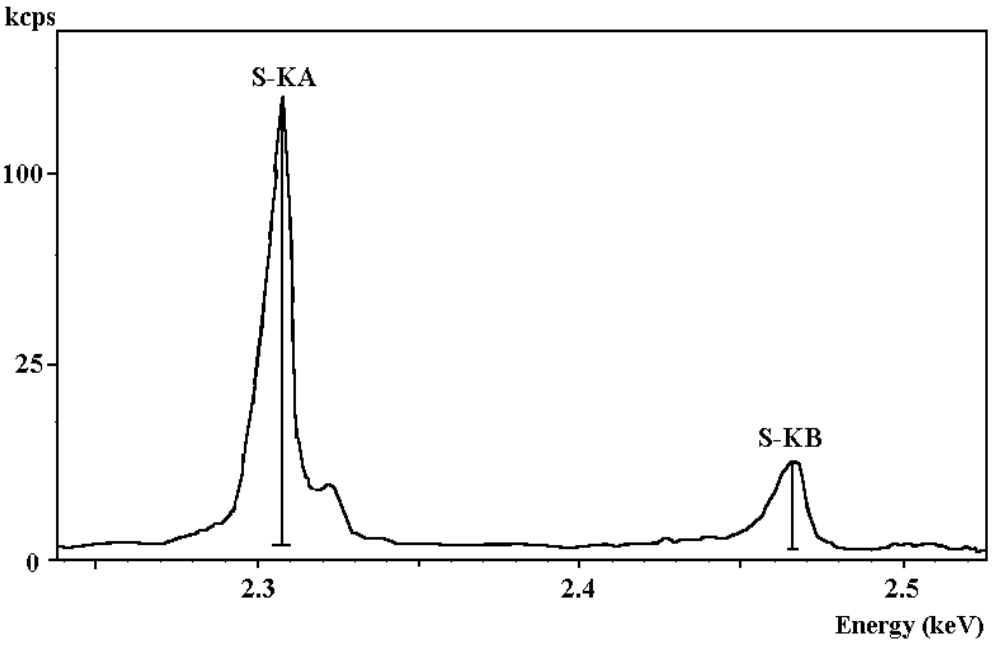

Figure 49. The S(K_α) and S(K_β) spectrum of $[Cu_2(detu)_6](NO_3)_2$.

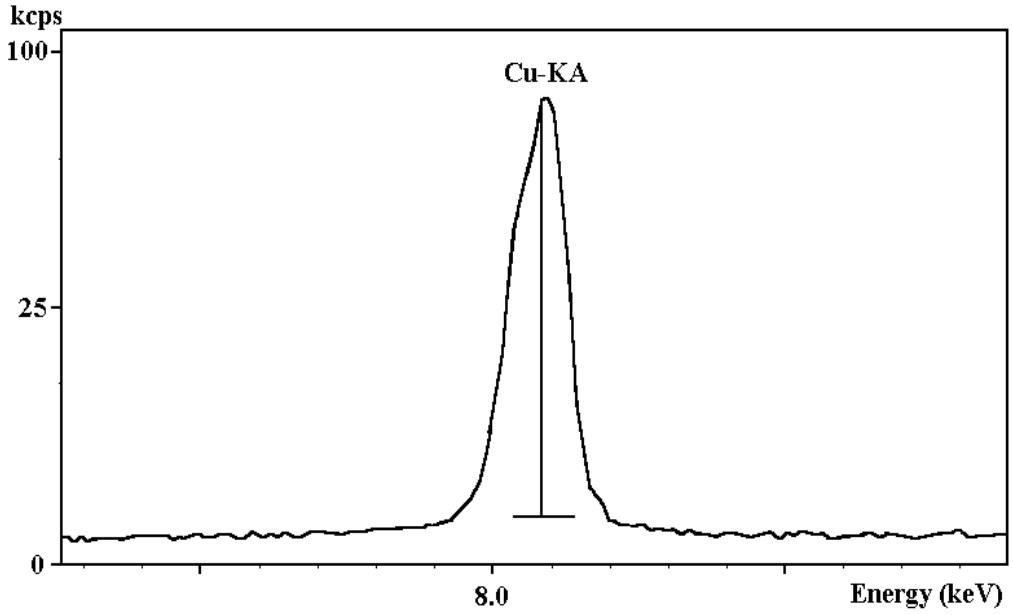

Figure 50. The Cu(K_α) spectrum of $[Cu(detu)_3]_2SO_3$.

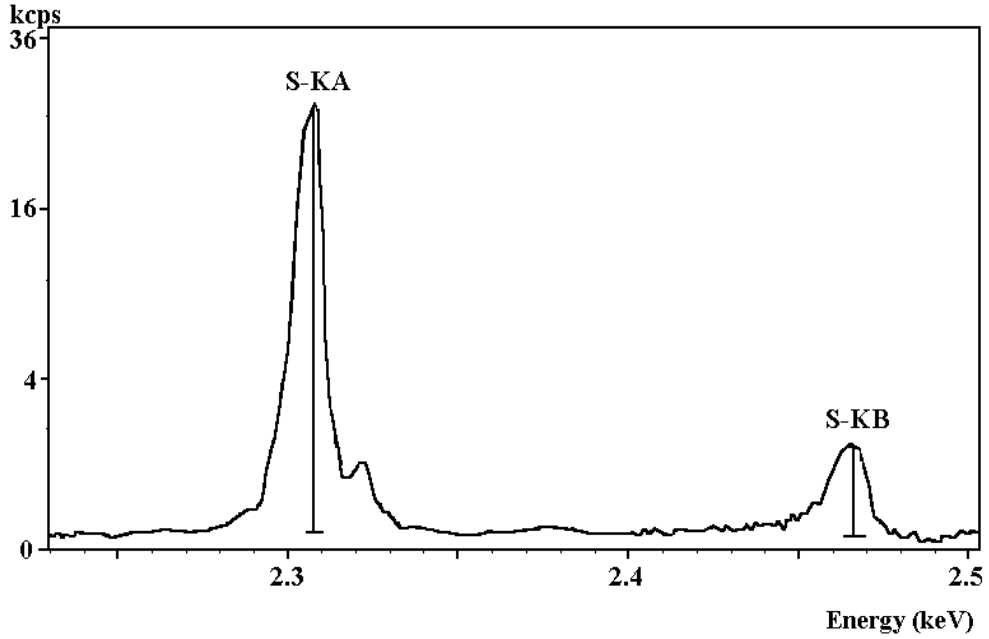

Figure 51. The S(K_α) and S(K_β) spectrum of $[Cu(detu)_3]_2SO_3$.

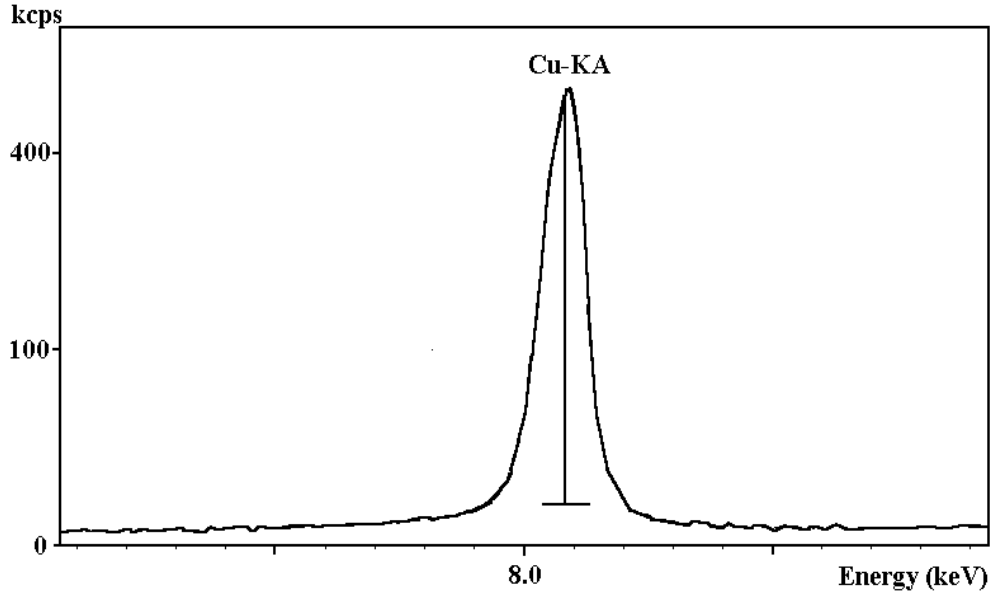

Figure 52. The Cu(K_α) spectrum of $[Cu_2(detu)_6](ClO_4)_2$.

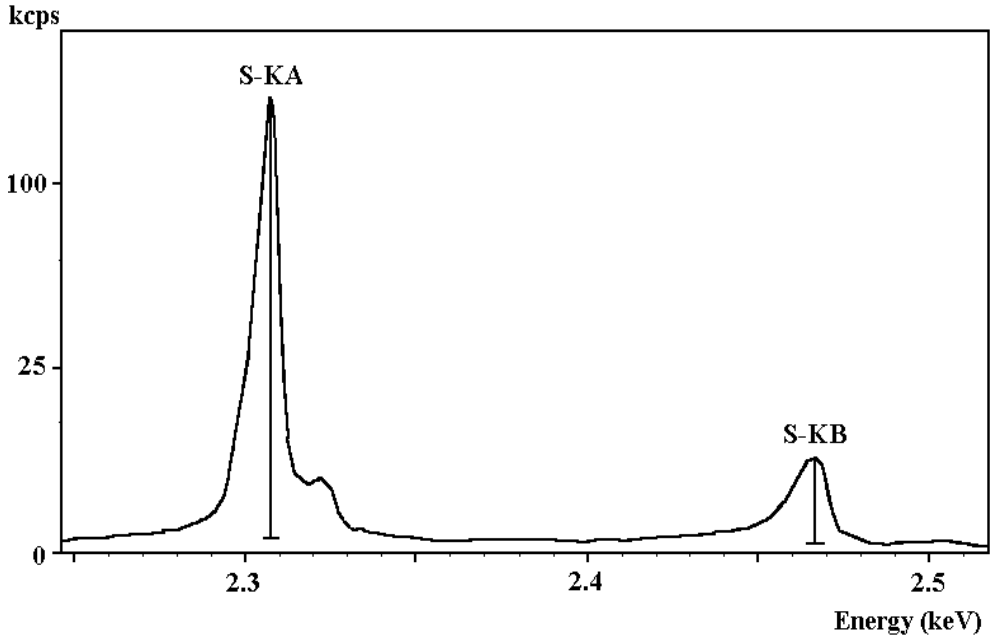

Figure 53. The S(K_α) and S(K_β) spectrum of $[Cu_2(detu)_6](ClO_4)_2$.

3.3 Infrared Spectroscopy

The infrared spectra of the ligands and complexes are shown in Figure 54. - 59.

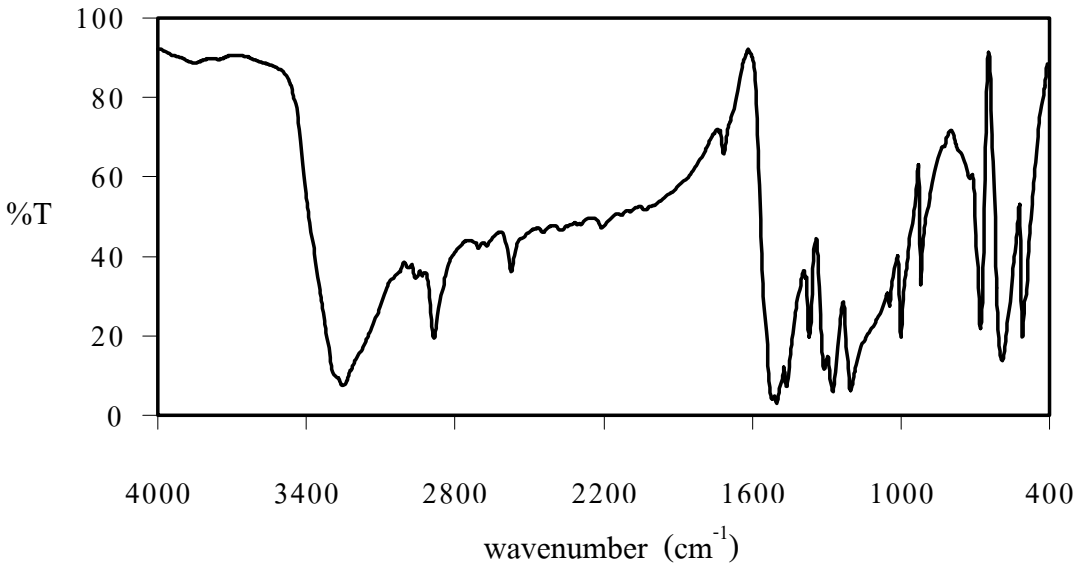

Figure 54. The infrared spectrum of etu.

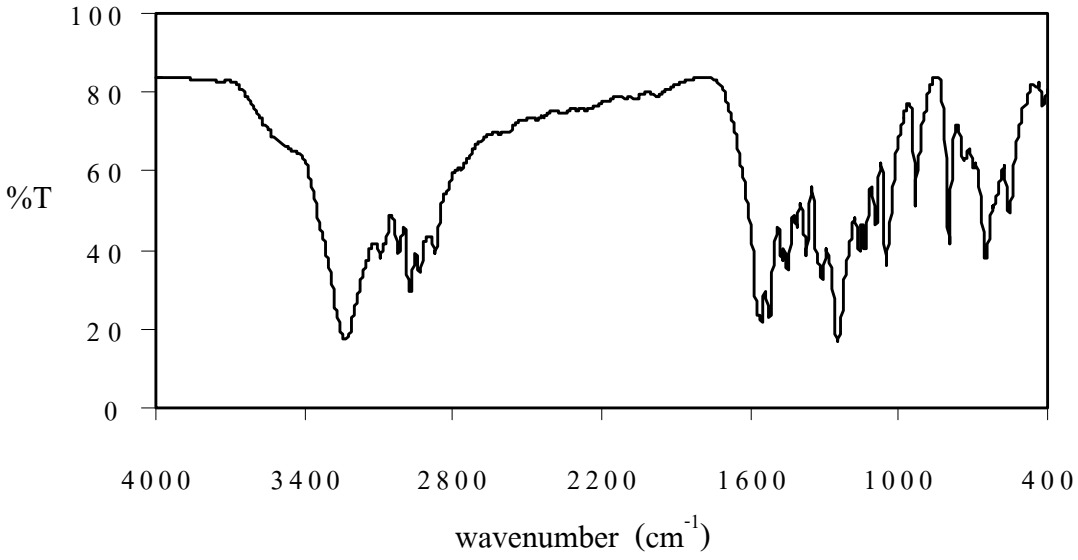

Figure 55. The infrared spectrum of detu.

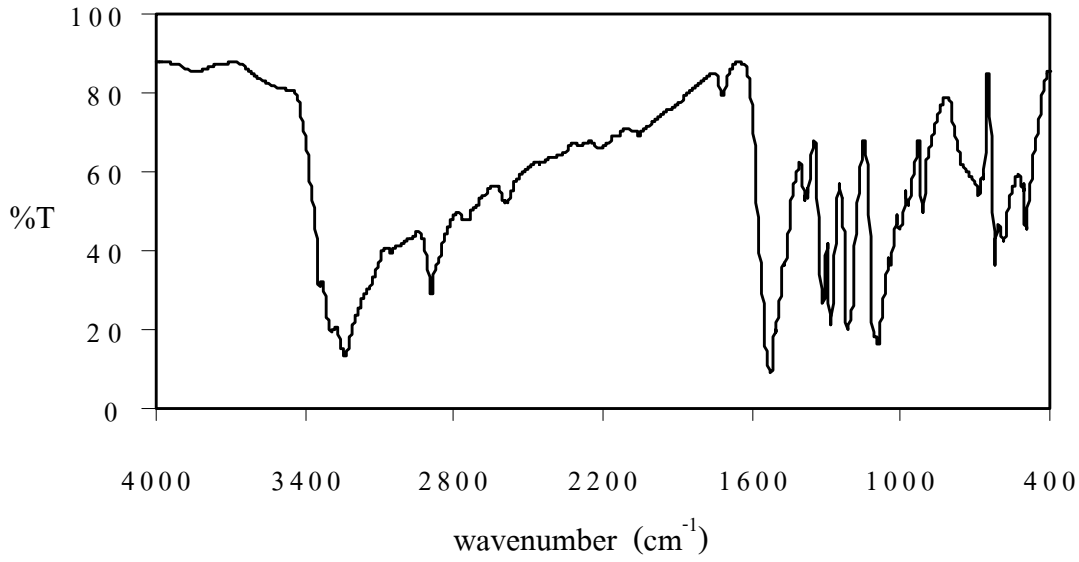

Figure 56. The infrared spectrum of $[Cu(etu)_3]_2SO_4$.

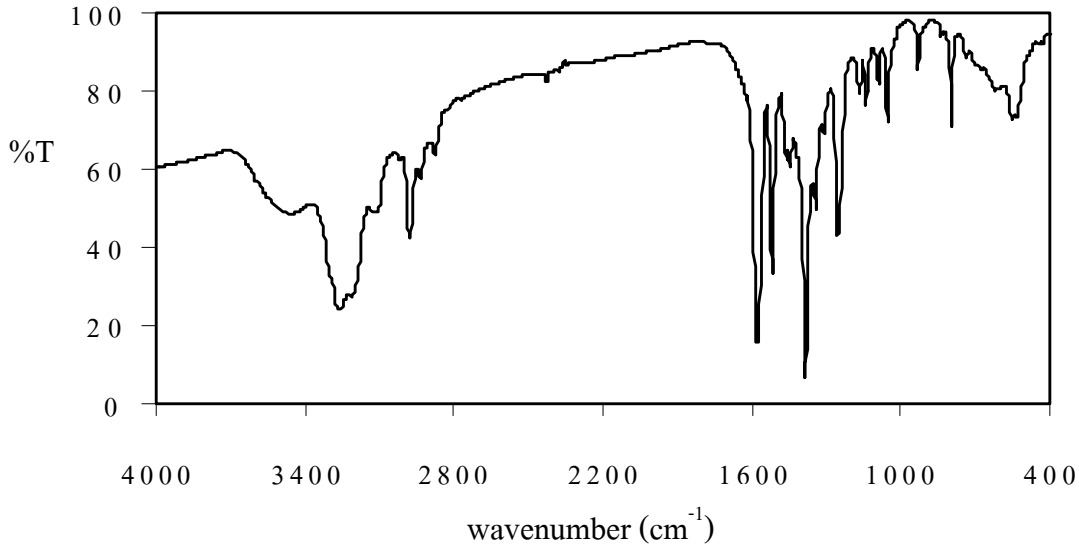

Figure 57. The infrared spectrum of $[Cu_2(detu)_6](NO_3)_2$.

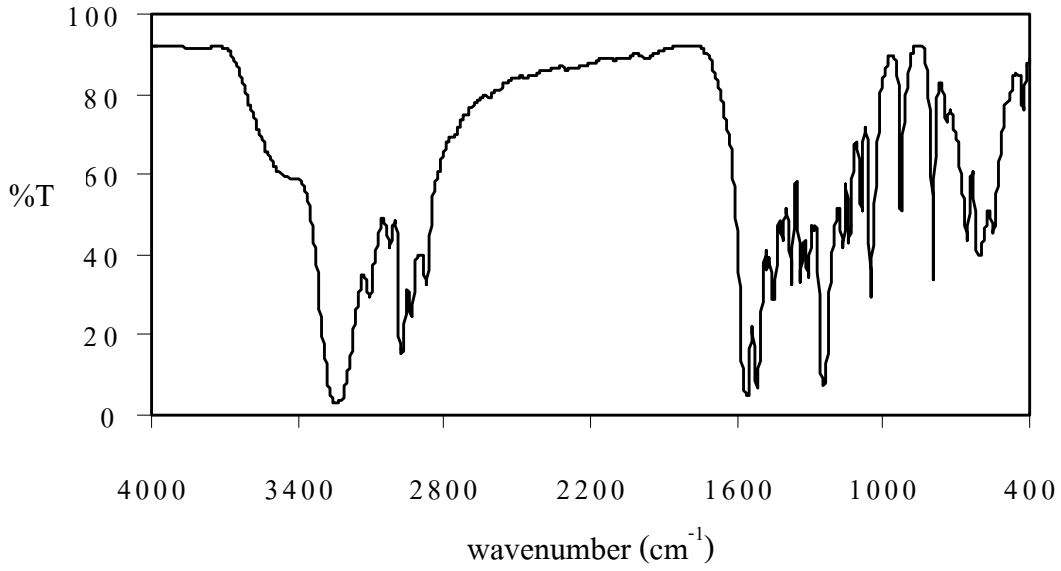

Figure 58. The infrared spectrum of $[Cu(detu)_3]_2SO_3$.

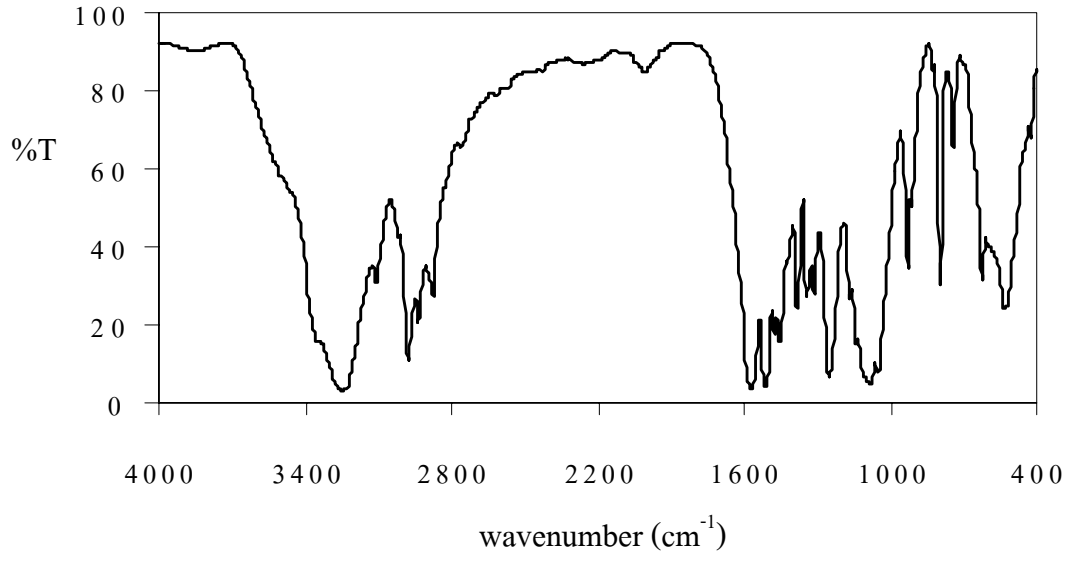

Figure 59. The infrared spectrum of $[Cu_2(detu)_6](ClO_4)_2$.

3.4 Elemental Analysis

The data of percentage carbon, hydrogen, nitrogen, and sulfur composition are given in Table 3.

Table 3. Elemental analysis data of complexes.

Complexes	Found (Calc.) %			
	%C	%H	%N	%S
$[Cu(etu)_3]_2SO_4$	25.06 (25.86)	4.34 (4.34)	19.92 (20.10)	26.36 (26.83)
$[Cu_2(detu)_6](NO_3)_2$	34.34 (34.49)	7.85 (6.95)	18.28 (18.77)	19.29 (18.42)
$[Cu(detu)_3]_2SO_3$	36.57 (36.01)	6.70 (7.25)	16.86 (16.80)	22.68 (22.43)
$[Cu_2(detu)_6](ClO_4)_2$	34.12 (34.72)	6.78 (6.99)	16.75 (16.20)	18.61 (18.54)

3.5 Single crystal X-ray diffractometry

3.5.1 X- ray Photography

$[Cu(etu)_3]_2SO_4$ was studied. The oscillation photograph is shown in Figure 60.

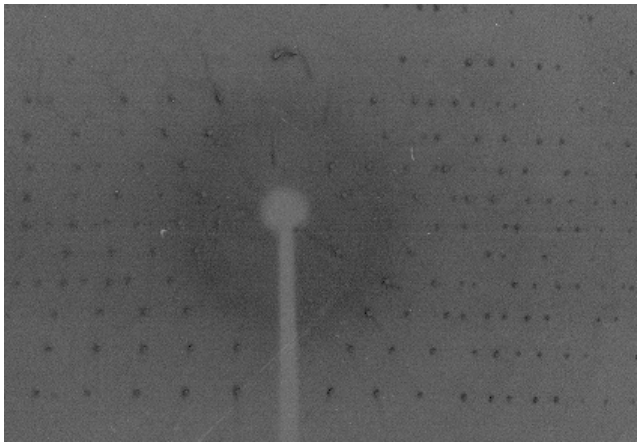

Figure 60. The oscillation photograph of $[Cu(etu)_3]_2SO_4$.

3.5.2 Crystal Structure

These results from crystal structure determination using Xtal 3.6 program system are shown in Table 4. - 18., Figure 61. - 70. and Appendix C.

Table 4. The crystallographic data for $[Cu(etu)_3]_2SO_4$.

Identification code	Cuetso
Empirical formula	$Cu_2S_7C_{18}N_{12}O_4H_{36}$
Formula weight	836.12
Measured temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Trigonal
Space group	*R*3*c* (No.161)
a (Å)	12.775(1)
b (Å)	12.775(1)
c (Å)	35.703(4)
α (°)	90.00
β (°)	90.00
γ (°)	120.00
V (Å^3)	5046.34(1)
Z	6
D_c (g/cm^3)	1.651
R	0.0201
R_W	0.0249
F(000)	2580
Measured reflections	1688
Condition for observed reflections	$F > 4\sigma(F)$
Observed reflections	1574

Table 5. Non - hydrogen interatomic distances of $[Cu(etu)_3]_2SO_4$.

Atom	Distance (Å)
CU(1) - S(1)	2.2513(6)
CU(1) - S(1')	2.2512(6)
CU(1) - S(1'')	2.2512(6)
CU(2) - S(2)	2.2753(6)
CU(2) - S(2')	2.2757(6)
CU(2) - S(2'')	2.2769(6)
CU(2) - - - O(2)	2.836(8)
S(1) - C(1)	1.717(5)
S(2) - C(2)	1.709(4)
C(1) - N(11)	1.332(4)
C(1) - N(12)	1.314(4)
C(2) - N(21)	1.321(6)
C(2) - N(22)	1.331(3)
N(11) - C(111)	1.461(5)
N(12) - C(121)	1.454(5)
N(21) - C(211)	1.462(4)
N(22) - C(221)	1.458(6)
C(111) - C(121)	1.531(4)
C(211) - C(221)	1.535(4)
S(3) - O(1)	1.477(3)
S(3) - O(1')	1.478(3)
S(3) - O(1'')	1.478(3)
S(3) - O(2)	1.468(8)

Table 6. Non - hydrogen interbond angles of $[Cu(etu)_3]_2SO_4$.

Atom	Angle (°)
S(1) - CU(1) - S(1')	120.00(2)
S(1) - CU(1) - S(1'')	120.00(2)
S(1') - CU(1) - S(1'')	120.00(3)
S(2) - CU(2) - S(2')	119.81(3)
S(2) - CU(2) - S(2'')	119.75(3)
S(2') - CU(2) - S(2'')	119.74(3)
CU(1) - S(1) - C(1)	107.7(2)
CU(2) - S(2) - C(2)	104.9(2)
S(1) - C(1) - N(11)	127.0(3)
S(1) - C(1) - N(12)	123.0(2)
S(2) - C(2) - N(21)	125.6(2)
S(2) - C(2) - N(22)	124.6(3)
C(1) - N(11) - C(111)	111.7(3)
C(1) - N(12) - C(121)	113.0(3)
C(2) - N(21) - C(211)	112.8(2)
C(2) - N(22) - C(221)	112.2(4)
N(11) - C(1) - N(12)	110.0(3)
N(21) - C(2) - N(22)	109.8(3)
N(11) - C(111) - C(121)	102.8(2)
N(12) - C(121) - C(111)	102.4(3)
N(22) - C(221) - C(211)	102.9(2)
N(21) - C(211) - C(221)	102.1(3)
O(1) - S(3) - O(2)	109.4(3)

Table 6. (continued).

Atom	Angle (°)
O(1) - S(3) - O(1')	109.6(2)
O(1) - S(3) - O(1'')	109.6(2)
O(1') - S(3) - O(1'')	109.6(2)
O(2) - S(3) - O(1')	109.3(3)
O(2) - S(3) - O(1'')	109.3(3)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

' = -y , +x-y , +z

'' = -x+y , -x , +z

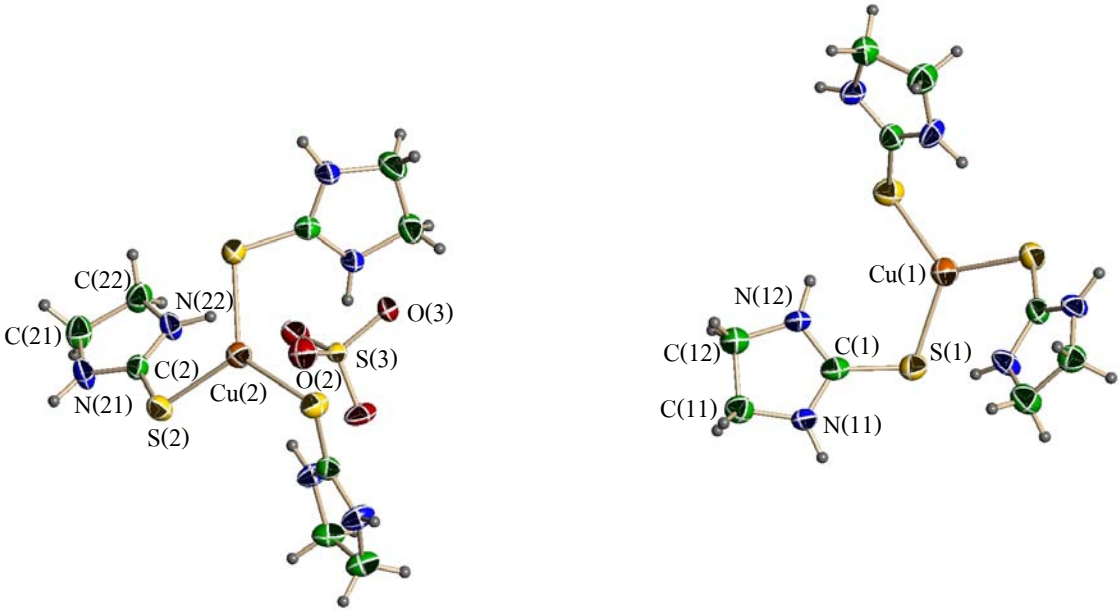

Figure 61. The structure of $[Cu(etu)_3]_2SO_4$. Ellipsoids are drawn at the 50 % probability level.

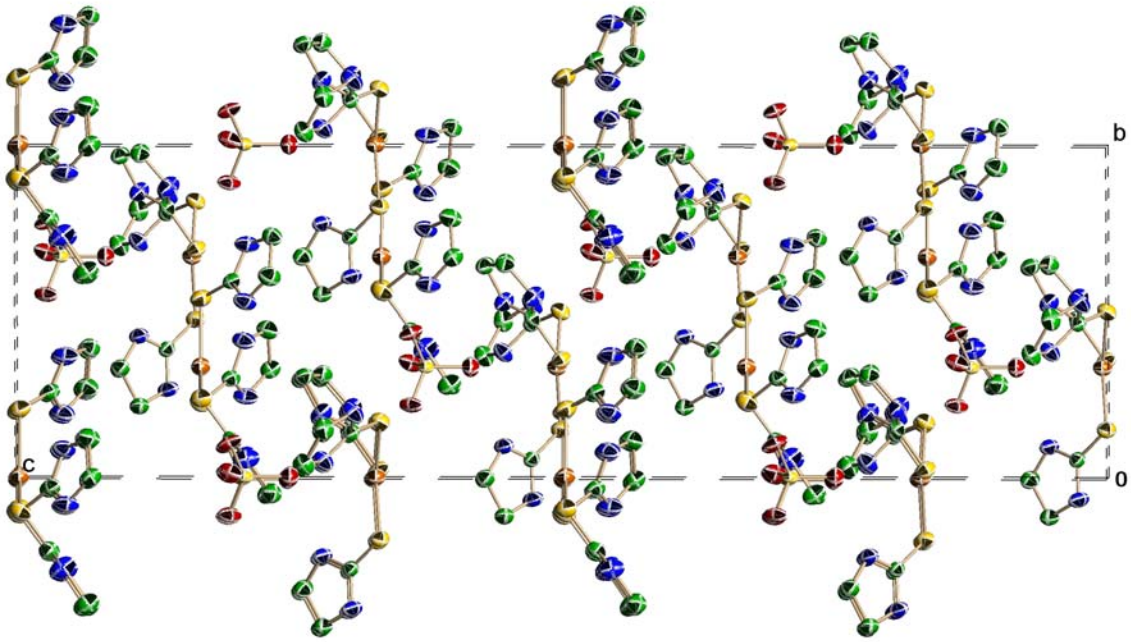

Figure 62. Unit cell contents of $[Cu(etu)_3]_2SO_4$ projected down *a*. The hydrogen atoms are omitted for clarity.

Table 7. The crystallographic data for $[Cu_2(detu)_6](NO_3)_2$.

Identification code	Cudeno
Empirical formula	$Cu_1S_3C_{15}N_7O_3H_{36}$
Formula weight	522.24
Measured temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$ (No.2)
a (Å)	9.099(2)
b (Å)	11.688(2)
c (Å)	13.201(3)
α (°)	111.34(3)
β (°)	104.52(3)
γ (°)	97.35(3)
V (Å^3)	1227.9(6)
Z	2
D_c (g/cm^3)	1.412
R	0.0353
R_W	0.0275
F(000)	5010
Measured reflections	12691
Condition for observed reflections	$F > 4\sigma(F)$
Observed reflections	9869

Table 8. Non - hydrogen interatomic distances of $[Cu_2(detu)_6](NO_3)_2$.

Atom	Distance (Å)
CU(1) - S(1)	2.2867(6)
CU(1) - S(2)	2.3419(6)
CU(1) - S(3)	2.3384(5)
CU(1) - S(3')	2.4593(6)
CU(1) - - - Cu(1')	2.9154(5)
S(1) - C(1)	1.722(1)
S(2) - C(2)	1.738(2)
S(3) - C(3)	1.735(2)
C(1) - N(11)	1.328(2)
C(1) - N(12)	1.339(2)
C(2) - N(21)	1.323(2)
C(2) - N(22)	1.326(2)
C(3) - N(31)	1.324(2)
C(3) - N(32)	1.323(1)
N(11) - C(111)	1.462(2)
N(12) - C(121)	1.459(2)
N(21) - C(211)	1.466(2)
N(22) - C(221)	1.455(2)
N(31) - C(311)	1.461(2)
N(32) - C(321)	1.460(2)
C(111) - C(112)	1.505(4)
C(121) - C(122)	1.436(4)

Table 8. (continued).

Atom	Distance (Å)
C(211) - C(212)	1.508(3)
C(221) - C(222)	1.509(2)
C(311) - C(312)	1.508(3)
C(321) - C(322)	1.519(2)
N(1) - O(1)	1.248(2)
N(1) - O(2)	1.246(1)
N(1) - O(3)	1.243(2)

Table 9. Non - hydrogen interbond angles of $[Cu_2(detu)_6](NO_3)_2$.

Atom	Angle (°)
S(1) - CU(1) - S(2)	112.10(2)
S(1) - CU(1) - S(3)	119.57(2)
S(1) - CU(1) - S(3')	103.24(2)
S(2) - CU(1) - S(3)	105.84(2)
S(2) - CU(1) - S(3')	110.55(2)
S(3) - CU(1) - S(3')	105.21(3)
CU(1) - S(1) - C(1)	108.00(6)
CU(1) - S(2) - C(2)	101.07(6)
CU(1) - S(3) - C(3)	127.00(3)
CU(1) - S(3') - C(3')	100.96(5)
CU(1) - S(3) - CU(1')	74.79(3)
S(1) - C(1) - N(11)	120.82(1)
S(1) - C(1) - N(12)	120.31(1)
S(2) - C(2) - N(21)	122.10(1)
S(2) - C(2) - N(22)	119.27(9)
S(3) - C(3) - N(31)	120.34(9)
S(3) - C(3) - N(32)	120.00(1)
C(1) - N(11) - C(111)	124.20(1)
C(1) - N(12) - C(121)	127.10(2)
C(2) - N(21) - C(211)	124.71(1)
C(2) - N(22) - C(221)	124.62(1)
C(3) - N(31) - C(311)	125.12(1)
C(3) - N(32) - C(321)	124.60(1)

Table 9. (continued).

Atom	Angle (°)
N(11) - C(1) - N(12)	119.0(1)
N(21) - C(2) - N(22)	118.7(1)
N(31) - C(3) - N(32)	119.6(1)
N(11) - C(111) - C(112)	113.7(1)
N(12) - C(121) - C(212)	114.3(2)
N(21) - C(211) - C(212)	113.1(1)
N(22) - C(221) - C(222)	111.2(1)
N(31) - C(311) - C(312)	110.2(1)
N(32) - C(321) - C(322)	112.4(2)
O(1) - N(1) - O(2)	120.0(1)
O(1) - N(1) - O(3)	118.9(1)
O(2) - N(1) - O(3)	121.1(1)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

' = +x , +y , +z

" = -x , -y , -z

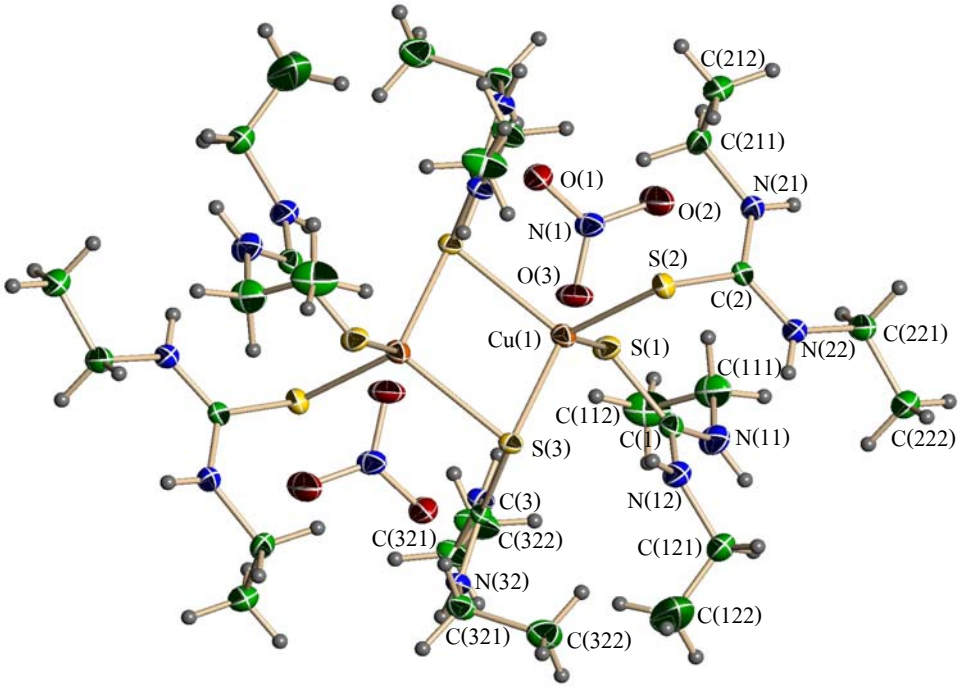

Figure 63. The structure of $[Cu_2(detu)_6](NO_3)_2$. Ellipsoids are drawn at the 50 % probability level.

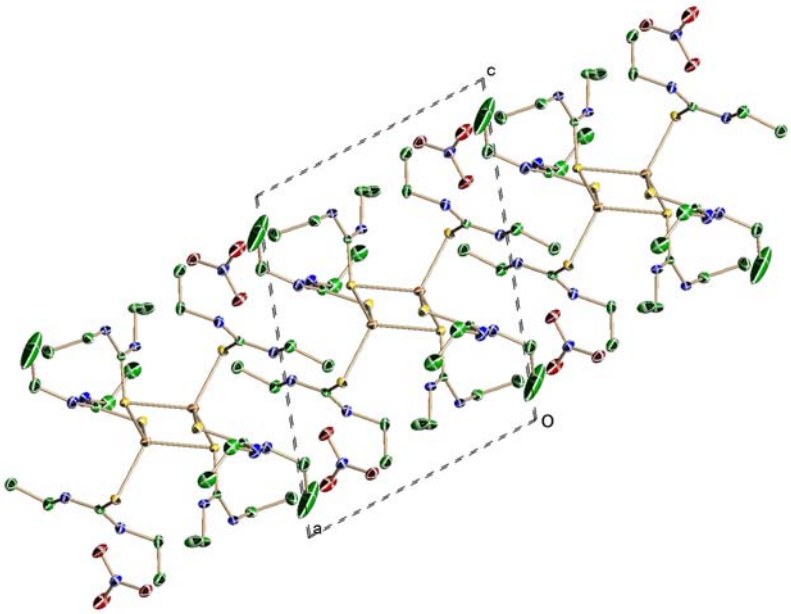

Figure 64. Unit cell contents of $[Cu_2(detu)_6](NO_3)_2$ projected down *c*. The hydrogen atoms are omitted for clarity.

Table 10. The crystallographic data for $[Cu(detu)_3]_2SO_3$.

Identification code	Cuhco
Empirical formula	$Cu_2S_7C_{30}N_{12}O_3H_{72}$
Formula weight	1000.54
Measured temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Trigonal
Space group	*R*3
a (Å)	12.335(1)
b (Å)	12.335(1)
c (Å)	27.919(5)
α (°)	90.00
β (°)	90.00
γ (°)	120.00
V (Å^3)	3678.5(9)
Z	3
D_c (g/cm^3)	1.355
R	0.0585
R_W	0.0683
F(000)	1590
Measured reflections	2568
Condition for observed reflections	$F > 4\sigma(F)$
Observed reflections	2283

Table 11. Non-hydrogen interatomic distances of $[Cu(detu)_3]_2SO_3$.

Atom	Distance (Å)
CU(1) - S(1)	2.238(3)
CU(1) - S(1')	2.238(3)
CU(1) - S(1'')	2.238(3)
CU(2) - S(2)	2.242(3)
CU(2) - S(2')	2.242(3)
CU(2) - S(2'')	2.242(3)
S(1) - C(1)	1.722(1)
S(2) - C(2)	1.714(8)
C(1) - N(11)	1.346(1)
C(1) - N(12)	1.299(1)
C(2) - N(21)	1.321(1)
C(2) - N(22)	1.299(1)
N(11) - C(111)	1.514(1)
N(12) - C(121)	1.510(1)
N(21) - C(211)	1.410(2)
N(22) - C(221)	1.240(1)
C(111) - C(112)	1.340(3)
C(121) - C(122)	1.591(2)
C(211) - C(212)	1.212(3)
C(221) - C(222)	1.371(8)
S(3) - O(1)	1.371(8)
S(3) - O(1')	1.371(8)
S(3) - O(1'')	1.371(8)

Table 12. Non - hydrogen interbond angles of $[Cu(detu)_3]_2SO_3$.

Atom	Angle (°)
S(1) - CU(1) - S(1')	119.37(3)
S(1) - CU(1) - S(1'')	119.37(3)
S(1') - CU(1) - S(1'')	119.37(3)
S(2) - CU(2) - S(2')	119.32(3)
S(2) - CU(2) - S(2'')	119.32(3)
S(2') - CU(2) - S(2'')	119.32(3)
CU(1) - S(1) - C(1)	107.30(3)
CU(2) - S(2) - C(2)	106.90(4)
S(1) - C(1) - N(11)	114.41(9)
S(1) - C(1) - N(12)	124.82(9)
S(2) - C(2) - N(21)	117.91(9)
S(2) - C(2) - N(22)	124.33(8)
C(1) - N(11) - C(111)	124.10(1)
C(1) - N(12) - C(121)	120.71(1)
C(2) - N(21) - C(211)	128.92(1)
C(2) - N(22) - C(221)	131.50(1)
N(11) - C(1) - N(12)	120.81(1)
N(21) - C(2) - N(22)	117.80(9)
N(11) - C(111) - C(112)	119.21(1)
N(12) - C(121) - C(122)	118.20(2)
N(21) - C(211) - C(212)	110.20(1)
N(22) - C(221) - C(222)	121.00(2)
O(1) - S(3) - O(1')	90.40(8)

Table 12. (continued).

Atom	Angle (°)
O(1) - S(3) - O(1$^{''}$)	91.40(8)
O(1$^{'}$) - S(3) - O(1$^{''}$)	91.40(8)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

$^{'}$ = +x , +y , +z

$^{''}$ = -y , +x-y , +z

$^{''}$ = -x+y , -x , +z

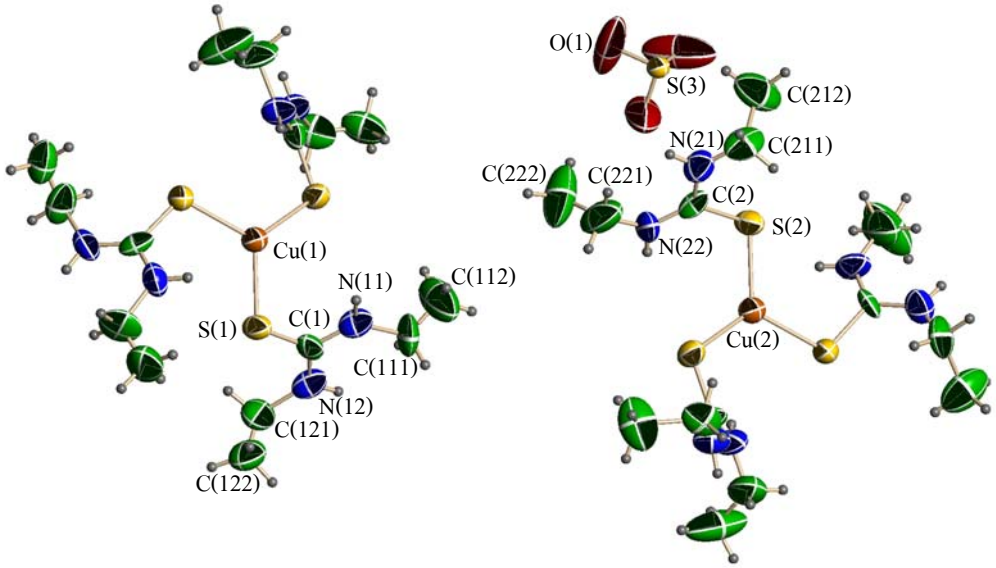

Figure 65. The structure of $[Cu(detu)_3]_2SO_3$. Ellipsoids are drawn at the 50 % probability level.

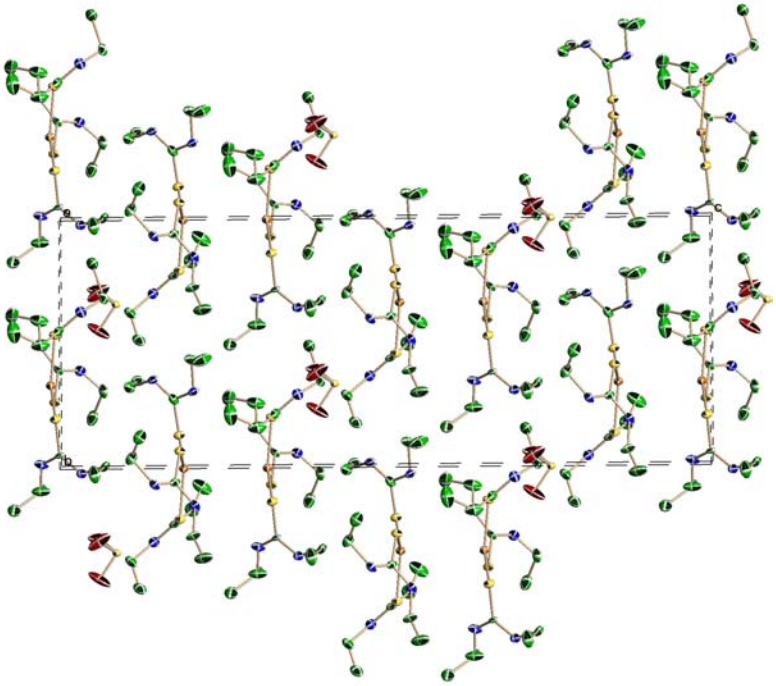

Figure 66. Unit cell contents of $[Cu(detu)_3]_2SO_3$ projected down *a*. The hydrogen atoms are omitted for clarity.

Table 13. The crystallographic data for $[Cu_2(detu)_6](ClO_4)_2$.

Identification code	Cuocl
Empirical formula	$Cu_1S_3C_{15}N_6O_4H_{36}Cl_1$
Formula weight	559.69
Measured temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$
a (Å)	9.293(2)
b (Å)	12.321(8)
c (Å)	13.622(9)
α (°)	113.50(1)
β (°)	105.18(1)
γ (°)	95.00(1)
V (Å^3)	1347.8(2)
Z	2
D_c (g/cm^3)	1.379
R	0.0601
R_W	0.0795
F(000)	588
Measured reflections	6237
Condition for observed reflections	$F > 4\sigma(F)$
Observed reflections	3229

Table 14. Non - hydrogen interatomic distances of $[Cu_2(detu)_6](ClO_4)_2$.

Atom	Distance (Å)
CU(1) - S(1)	2.283(2)
CU(1) - S(2)	2.344(2)
CU(1) - S(3)	2.364(1)
CU(1) - S(3')	2.447(1)
CU(1) - - - Cu(1')	2.904(1)
S(1) - C(1)	1.715(6)
S(2) - C(2)	1.719(7)
S(3) - C(3)	1.727(6)
C(1) - N(11)	1.303(9)
C(1) - N(12)	1.33(1)
C(2) - N(21)	1.311(8)
C(2) - N(22)	1.320(7)
C(3) - N(31)	1.307(9)
C(3) - N(32)	1.304(6)
N(11) - C(111)	1.440(6)
N(12) - C(121)	1.467(5)
N(21) - C(211)	1.498(9)
N(22) - C(221)	1.451(6)
N(31) - C(311)	1.456(6)
N(32) - C(321)	1.451(5)
C(111) - C(112)	1.522(9)
C(121) - C(122)	1.457(9)
C(211) - C(212)	1.355(2)

Table 14. (continued).

Atom	Distance (Å)
C(221) - C(222)	1.259(6)
C(311) - C(312)	1.304(9)
C(321) - C(322)	1.444(8)
Cl(1) - O(1)	1.356(6)
Cl(1) - O(2)	1.320(7)
Cl(1) - O(3)	1.320(8)
Cl(1) - O(4)	1.279(6)

Table 15. Non - hydrogen interbond angles of $[Cu_2(detu)_6](ClO_4)_2$.

Atom	Angle (°)
S(1) - CU(1) - S(2)	114.75(7)
S(1) - CU(1) - S(3)	118.73(6)
S(1) - CU(1) - S(3')	102.87(6)
S(2) - CU(1) - S(3)	102.74(6)
S(2) - CU(1) - S(3')	111.82(6)
S(3) - CU(1) - S(3')	105.78(5)
CU(1) - S(1) - C(1)	102.51(1)
CU(1) - S(2) - C(2)	107.46(2)
CU(1) - S(3) - C(3)	111.42(1)
CU(1) - S(3') - C(3')	103.10(1)
CU(1) - S(3) - CU(1')	74.19(3)
S(1) - C(1) - N(11)	121.70(3)
S(1) - C(1) - N(12)	119.02(3)
S(2) - C(2) - N(21)	119.22(4)
S(2) - C(2) - N(22)	120.33(3)
S(3) - C(3) - N(31)	120.65(3)
S(3) - C(3) - N(32)	120.41(3)
C(1) - N(11) - C(111)	125.62(4)
C(1) - N(12) - C(121)	125.44(4)
C(2) - N(21) - C(211)	125.61(5)
C(2) - N(22) - C(221)	128.31(5)
C(3) - N(31) - C(311)	125.62(4)
C(3) - N(32) - C(321)	127.14(4)

Table 15. (continued).

Atom	Angle (°)
N(11) - C(1) - N(12)	119.22(3)
N(21) - C(2) - N(22)	120.51(4)
N(31) - C(3) - N(32)	119.02(3)
N(11) - C(111) - C(112)	111.19(5)
N(12) - C(121) - C(122)	112.34(4)
N(21) - C(211) - C(212)	116.09(8)
N(22) - C(221) - C(222)	120.42(6)
N(31) - C(311) - C(312)	111.92(5)
N(32) - C(321) - C(322)	116.24(6)
O(1) - Cl(1) - O(2)	99.78(7)
O(1) - Cl(1) - O(3)	110.20(7)
O(1) - Cl(1) - O(4)	109.75(6)
O(2) - Cl(1) - O(3)	98.05(7)
O(2) - Cl(1) - O(4)	122.52(7)
O(3) - Cl(1) - O(4)	115.27(7)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

' = +x , +y , +z

'' = -x , -y , -z

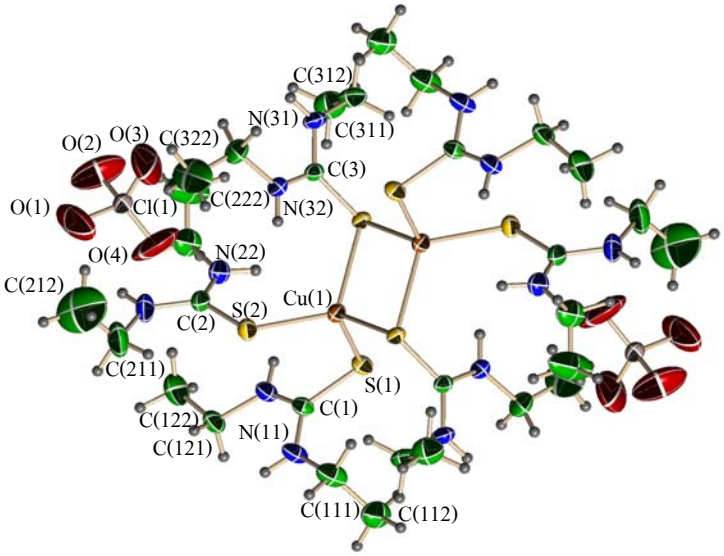

Figure 67. The structure of $[Cu_2(detu)_6](ClO_4)_2$. Ellipsoids are drawn at the 50 % probability level.

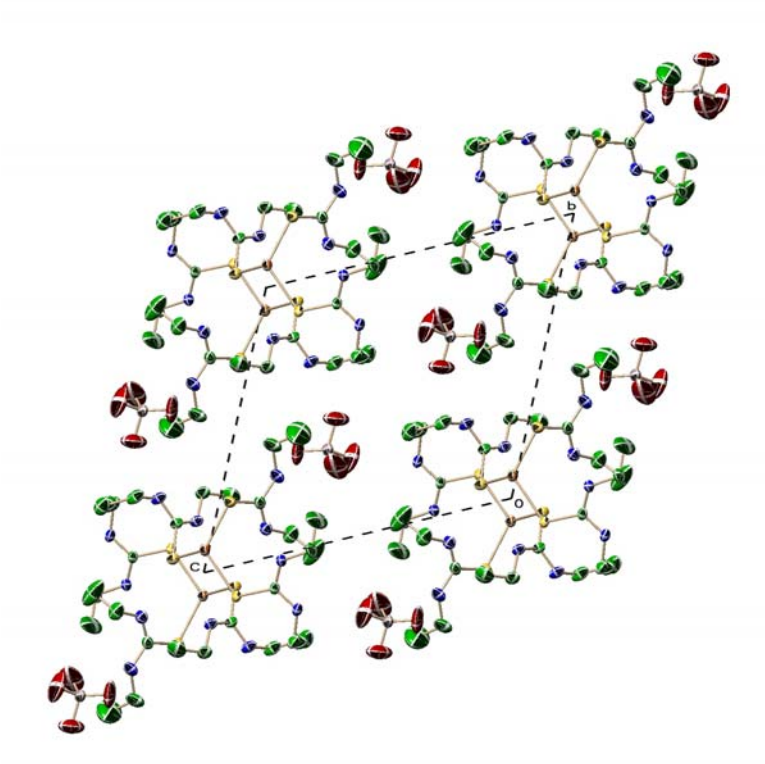

Figure 68. Unit cell contents of $[Cu_2(detu)_6](ClO_4)_2$ projected down *b*. The hydrogen atoms are omitted for clarity.

Table 16. The crystallographic data for S_8.

Identification code	S8
Empirical formula	S8
Formula weight	256.53
Measured temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	orthorhombic
Space group	*Fddd*
a (Å)	10.460(1)
b (Å)	12.865(1)
c (Å)	24.486(3)
α (°)	90.00
β (°)	90.00
γ (°)	90.00
V (Å^3)	3295.1(6)
Z	16
D_c (g/cm^3)	2.068
R	0.0303
R_W	0.0606
F(000)	2048
Measured reflections	978
Condition for observed reflections	$F > 4\sigma(F)$
Observed reflections	899

Table 17. Non-hydrogen interatomic distances of S_8.

Atom	Distance (Å)
S(1) - S(2)	2.044(7)
S(1) - S(1')	2.051(3)
S(2) - S(3)	2.048(5)
S(3) - S(4)	2.046(3)
S(4) - S(4')	2.042(2)
S(1') - S(2')	2.044(2)
S(2') - S(3')	2.048(2)
S(3') - S(4')	2.046(2)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

' = ¼ - x , ¼ - y , +z

Table 18. Non - hydrogen interbond angles of S_8.

Atom	Angle (°)
S(1) - S(2) - S(3)	107.96(5)
S(2) - S(3) - S(4)	107.31(5)
S(3) - S(4) - S(4')	108.42(5)
S(4) - S(4') - S(3')	108.42(5)
S(4') - S(3') - S(2')	107.31(5)
S(3') - S(2') - S(1')	107.93(5)
S(2') - S(1') - S(1)	108.97(5)
S(1') - S(1) - S(2)	108.97(5)

Superscript refers to the following symmetry operations, relative to the reference asymmetric unit at x , y , z :

' = ¼ - x , ¼ - y , +z

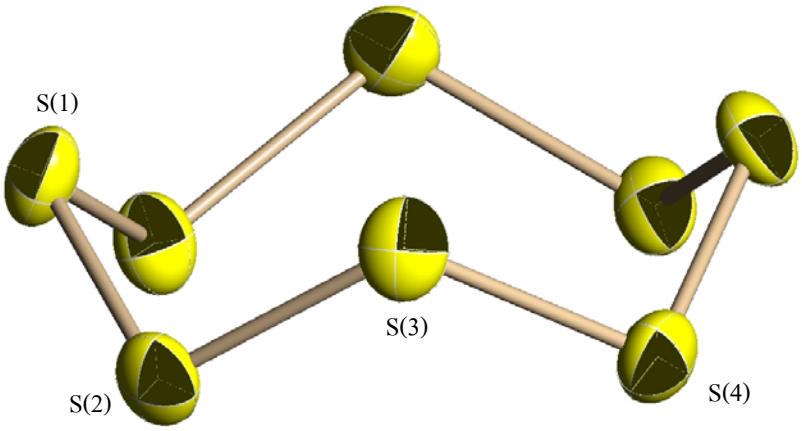

Figure 69. The structure of S_8. Ellipsoids are drawn at the 50 % probability level.

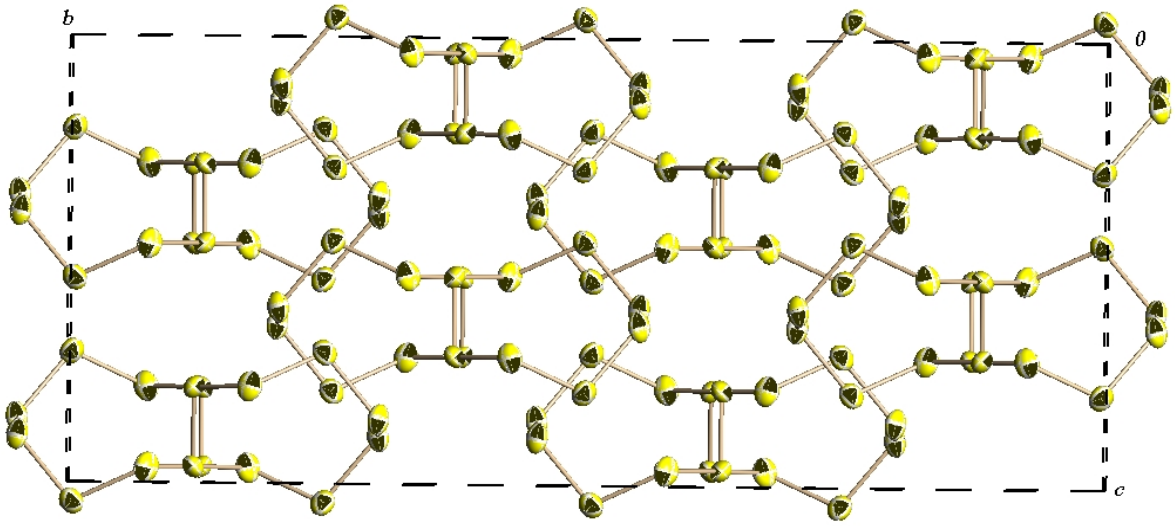

Figure 70. Unit cell contents of S_8 projected down *a*.