附錄 一

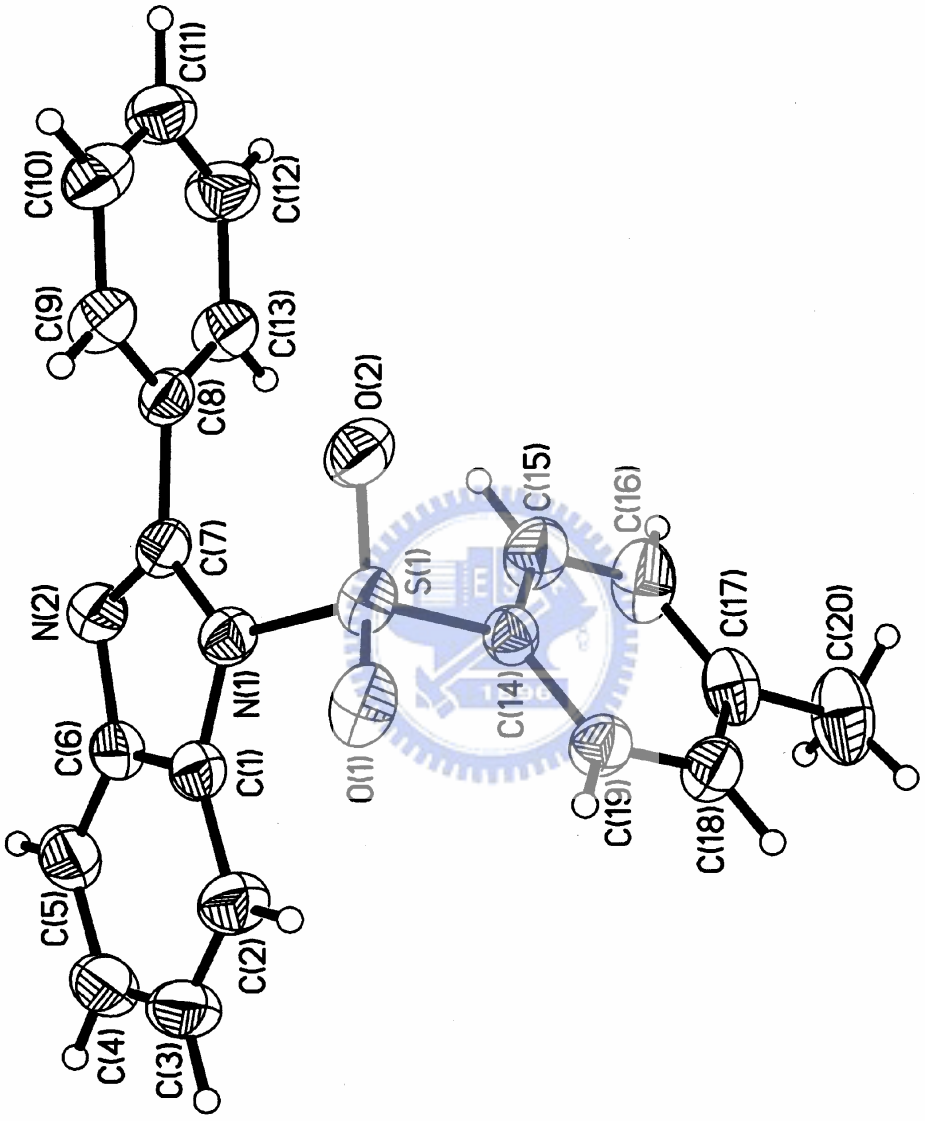

Fig. : The molecular structure of IC10918, thermal ellipsoids drawn at the 30% probability.

Table 1. Crystal data and structure refinement for ic10918.

Identification code	ic10918 (NTU structure analysis)
Empirical formula	$C_{20}H_{16}N_2O_2S$
Formula weight	348.41
Diffractometer used	NONIUS KappaCCD
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Fdd2
Unit cell dimensions	a = 33.8890(7) Å alpha = 90° b = 36.1413(7) Å beta = 90° c = 5.5735(1) Å gamma = 90°
Volume, Z	6826.4(2) $Å^3$, 16
Density (calculated)	1.356 Mg/m^3
Absorption coefficient	0.205 mm^{-1}
F(000)	2912
Crystal size	0.30 x 0.25 x 0.10 mm
θ range for data collection	1.65 to 27.50°
Limiting indices	$-43 \le h \le 44$, $-46 \le k \le 46$, $-7 \le l \le 7$
Reflections collected	17603
Independent reflections	3615 (R_{int} = 0.0382)
Completeness to θ = 27.50°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.982 and 0.927
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3615 / 1 / 228
Goodness-of-fit on F^2	1.006
Final R indices [I>2σ(I)]	R1 = 0.0371, wR2 = 0.0830
R indices (all data)	R1 = 0.0648, wR2 = 0.0925
Absolute structure parameter	0.00(7)
Extinction coefficient	0.00229(15)
Largest diff. peak and hole	0.238 and -0.243 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for ic10918.

S(1)-O(1)	1.4199(15)	S(1)-O(2)	1.4207(16)
S(1)-N(1)	1.6914(17)	S(1)-C(14)	1.743(2)
N(1)-C(7)	1.409(2)	N(1)-C(1)	1.418(3)
N(2)-C(7)	1.302(3)	N(2)-C(6)	1.404(3)
C(1)-C(6)	1.376(3)	C(1)-C(2)	1.391(3)
C(2)-C(3)	1.380(4)	C(3)-C(4)	1.372(4)
C(4)-C(5)	1.377(3)	C(5)-C(6)	1.392(3)
C(7)-C(8)	1.479(3)	C(8)-C(13)	1.380(3)
C(8)-C(9)	1.386(3)	C(9)-C(10)	1.383(3)
C(10)-C(11)	1.372(3)	C(11)-C(12)	1.365(4)
C(12)-C(13)	1.385(3)	C(14)-C(15)	1.369(3)
C(14)-C(19)	1.383(3)	C(15)-C(16)	1.367(4)
C(16)-C(17)	1.375(3)	C(17)-C(18)	1.375(3)
C(17)-C(20)	1.515(3)	C(18)-C(19)	1.379(3)

O(1)-S(1)-O(2)	121.51(11)	O(1)-S(1)-N(1)	105.80(9)
O(2)-S(1)-N(1)	105.76(8)	O(1)-S(1)-C(14)	108.78(8)
O(2)-S(1)-C(14)	109.64(10)	N(1)-S(1)-C(14)	103.83(9)
C(7)-N(1)-C(1)	104.76(16)	C(7)-N(1)-S(1)	127.82(14)
C(1)-N(1)-S(1)	123.20(13)	C(7)-N(2)-C(6)	105.64(18)
C(6)-C(1)-C(2)	121.7(2)	C(6)-C(1)-N(1)	105.97(17)
C(2)-C(1)-N(1)	132.3(2)	C(3)-C(2)-C(1)	116.3(2)
C(4)-C(3)-C(2)	122.3(2)	C(3)-C(4)-C(5)	121.4(3)
C(4)-C(5)-C(6)	117.1(3)	C(1)-C(6)-C(5)	121.1(2)
C(1)-C(6)-N(2)	110.61(19)	C(5)-C(6)-N(2)	128.3(2)
N(2)-C(7)-N(1)	112.98(17)	N(2)-C(7)-C(8)	122.34(18)
N(1)-C(7)-C(8)	124.64(18)	C(13)-C(8)-C(9)	119.50(19)
C(13)-C(8)-C(7)	118.69(19)	C(9)-C(8)-C(7)	121.69(19)
C(10)-C(9)-C(8)	120.0(2)	C(11)-C(10)-C(9)	120.2(2)
C(12)-C(11)-C(10)	119.9(2)	C(11)-C(12)-C(13)	120.7(2)
C(8)-C(13)-C(12)	119.7(2)	C(15)-C(14)-C(19)	119.79(19)
C(15)-C(14)-S(1)	120.27(16)	C(19)-C(14)-S(1)	119.92(15)
C(16)-C(15)-C(14)	119.7(2)	C(15)-C(16)-C(17)	121.6(2)
C(16)-C(17)-C(18)	118.4(2)	C(16)-C(17)-C(20)	121.2(2)
C(18)-C(17)-C(20)	120.3(2)	C(17)-C(18)-C(19)	120.7(2)
C(18)-C(19)-C(14)	119.7(2)		

Symmetry transformations used to generate equivalent atoms:

附錄 二

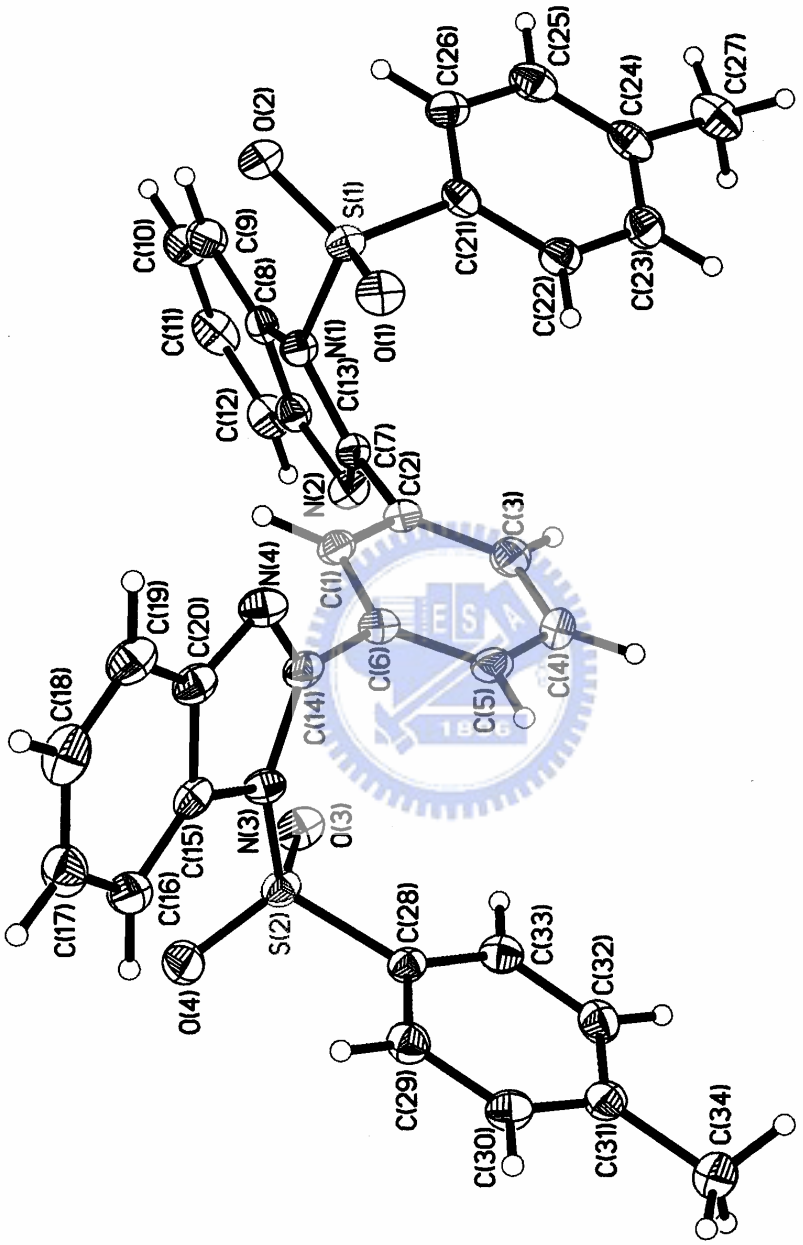

Fig. : The molecular structure of IC10755, thermal ellipsoids drawn at the 50% probability.

Table 1. Crystal data and structure refinement for ic10755.

Identification code	ic10755 (NTU structure analysis)
Empirical formula	$C_{34}H_{26}N_4O_4S_2$
Formula weight	618.71
Diffracometer used	BRUKER SMART APEXCCD
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 8.7601(4) Å alpha = 90° b = 19.8500(8) Å beta = 92.136(1)° c = 16.5776(7) Å gamma = 90°
Volume, Z	2880.6(2) $Å^3$, 4
Density (calculated)	1.427 Mg/m^3
Absorption coefficient	0.233 mm^{-1}
F(000)	1288
Crystal size	0.20 x 0.15 x 0.08 mm
θ range for data collection	1.60 to 27.50°
Limiting indices	$-9 \le h \le 11$, $-25 \le k \le 25$, $-21 \le l \le 21$
Reflections collected	24766
Independent reflections	6603 (R_{int} = 0.0563)
Completeness to θ = 27.50°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9816 and 0.9548
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6603 / 0 / 399
Goodness-of-fit on F^2	1.237
Final R indices [I>2σ(I)]	R1 = 0.0710, wR2 = 0.1404
R indices (all data)	R1 = 0.0865, wR2 = 0.1476
Largest diff. peak and hole	0.658 and -0.443 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for ic10755.

S(1)-O(1)	1.420(2)	S(1)-O(2)	1.421(2)
S(1)-N(1)	1.691(2)	S(1)-C(21)	1.750(3)
S(2)-O(3)	1.420(2)	S(2)-O(4)	1.425(2)
S(2)-N(3)	1.686(2)	S(2)-C(28)	1.754(3)
N(1)-C(7)	1.420(3)	N(1)-C(8)	1.423(4)
N(2)-C(7)	1.294(4)	N(2)-C(13)	1.397(4)
N(3)-C(15)	1.410(4)	N(3)-C(14)	1.417(3)
N(4)-C(14)	1.294(4)	N(4)-C(20)	1.394(4)
C(1)-C(2)	1.390(4)	C(1)-C(6)	1.390(4)
C(2)-C(3)	1.389(4)	C(2)-C(7)	1.476(4)
C(3)-C(4)	1.387(4)	C(4)-C(5)	1.382(4)
C(5)-C(6)	1.392(4)	C(6)-C(14)	1.473(4)
C(8)-C(9)	1.388(4)	C(8)-C(13)	1.392(4)
C(9)-C(10)	1.385(4)	C(10)-C(11)	1.390(5)
C(11)-C(12)	1.383(4)	C(12)-C(13)	1.384(4)
C(15)-C(16)	1.386(4)	C(15)-C(20)	1.397(4)
C(16)-C(17)	1.385(4)	C(17)-C(18)	1.393(5)
C(18)-C(19)	1.370(5)	C(19)-C(20)	1.387(4)
C(21)-C(22)	1.386(4)	C(21)-C(26)	1.388(4)
C(22)-C(23)	1.382(4)	C(23)-C(24)	1.390(4)
C(24)-C(25)	1.389(4)	C(24)-C(27)	1.500(4)
C(25)-C(26)	1.382(4)	C(28)-C(33)	1.381(4)
C(28)-C(29)	1.389(4)	C(29)-C(30)	1.383(4)
C(30)-C(31)	1.382(4)	C(31)-C(32)	1.390(4)
C(31)-C(34)	1.505(4)	C(32)-C(33)	1.386(4)

O(1)-S(1)-O(2)	120.55(13)	O(1)-S(1)-N(1)	105.84(12)
O(2)-S(1)-N(1)	106.23(12)	O(1)-S(1)-C(21)	110.94(13)
O(2)-S(1)-C(21)	109.43(13)	N(1)-S(1)-C(21)	102.06(13)
O(3)-S(2)-O(4)	120.85(13)	O(3)-S(2)-N(3)	106.64(12)
O(4)-S(2)-N(3)	104.83(13)	O(3)-S(2)-C(28)	109.28(13)
O(4)-S(2)-C(28)	108.80(13)	N(3)-S(2)-C(28)	105.29(12)
C(7)-N(1)-C(8)	104.2(2)	C(7)-N(1)-S(1)	123.64(19)
C(8)-N(1)-S(1)	119.72(19)	C(7)-N(2)-C(13)	106.2(2)
C(15)-N(3)-C(14)	106.0(2)	C(15)-N(3)-S(2)	125.5(2)
C(14)-N(3)-S(2)	128.2(2)	C(14)-N(4)-C(20)	106.3(2)
C(2)-C(1)-C(6)	119.8(3)	C(3)-C(2)-C(1)	120.0(3)
C(3)-C(2)-C(7)	119.1(3)	C(1)-C(2)-C(7)	120.4(2)
C(4)-C(3)-C(2)	120.2(3)	C(5)-C(4)-C(3)	119.7(3)
C(4)-C(5)-C(6)	120.5(3)	C(1)-C(6)-C(5)	119.6(3)
C(1)-C(6)-C(14)	119.6(2)	C(5)-C(6)-C(14)	120.8(2)
N(2)-C(7)-N(1)	113.3(2)	N(2)-C(7)-C(2)	122.0(2)
N(1)-C(7)-C(2)	124.5(3)	C(9)-C(8)-C(13)	122.2(3)
C(9)-C(8)-N(1)	131.9(3)	C(13)-C(8)-N(1)	105.9(2)
C(10)-C(9)-C(8)	116.0(3)	C(9)-C(10)-C(11)	122.0(3)
C(12)-C(11)-C(10)	121.7(3)	C(11)-C(12)-C(13)	116.8(3)
C(12)-C(13)-C(8)	121.2(3)	C(12)-C(13)-N(2)	128.4(3)
C(8)-C(13)-N(2)	110.4(2)	N(4)-C(14)-N(3)	112.2(3)
N(4)-C(14)-C(6)	125.0(3)	N(3)-C(14)-C(6)	122.8(2)
C(16)-C(15)-C(20)	122.1(3)	C(16)-C(15)-N(3)	133.3(3)
C(20)-C(15)-N(3)	104.6(2)	C(17)-C(16)-C(15)	116.5(3)
C(16)-C(17)-C(18)	121.6(3)	C(19)-C(18)-C(17)	121.6(3)
C(18)-C(19)-C(20)	117.9(3)	C(19)-C(20)-N(4)	128.7(3)
C(19)-C(20)-C(15)	120.4(3)	N(4)-C(20)-C(15)	110.9(3)
C(22)-C(21)-C(26)	120.9(3)	C(22)-C(21)-S(1)	119.8(2)

C(26)-C(21)-S(1)	119.1(2)	C(23)-C(22)-C(21)	119.1(3)
C(22)-C(23)-C(24)	121.0(3)	C(25)-C(24)-C(23)	118.8(3)
C(25)-C(24)-C(27)	121.0(3)	C(23)-C(24)-C(27)	120.2(3)
C(26)-C(25)-C(24)	121.1(3)	C(25)-C(26)-C(21)	119.0(3)
C(33)-C(28)-C(29)	121.5(3)	C(33)-C(28)-S(2)	118.6(2)
C(29)-C(28)-S(2)	119.7(2)	C(30)-C(29)-C(28)	118.3(3)
C(31)-C(30)-C(29)	121.6(3)	C(30)-C(31)-C(32)	118.8(3)
C(30)-C(31)-C(34)	121.0(3)	C(32)-C(31)-C(34)	120.1(3)
C(33)-C(32)-C(31)	120.7(3)	C(28)-C(33)-C(32)	119.0(3)

Symmetry transformations used to generate equivalent atoms:

附錄 三

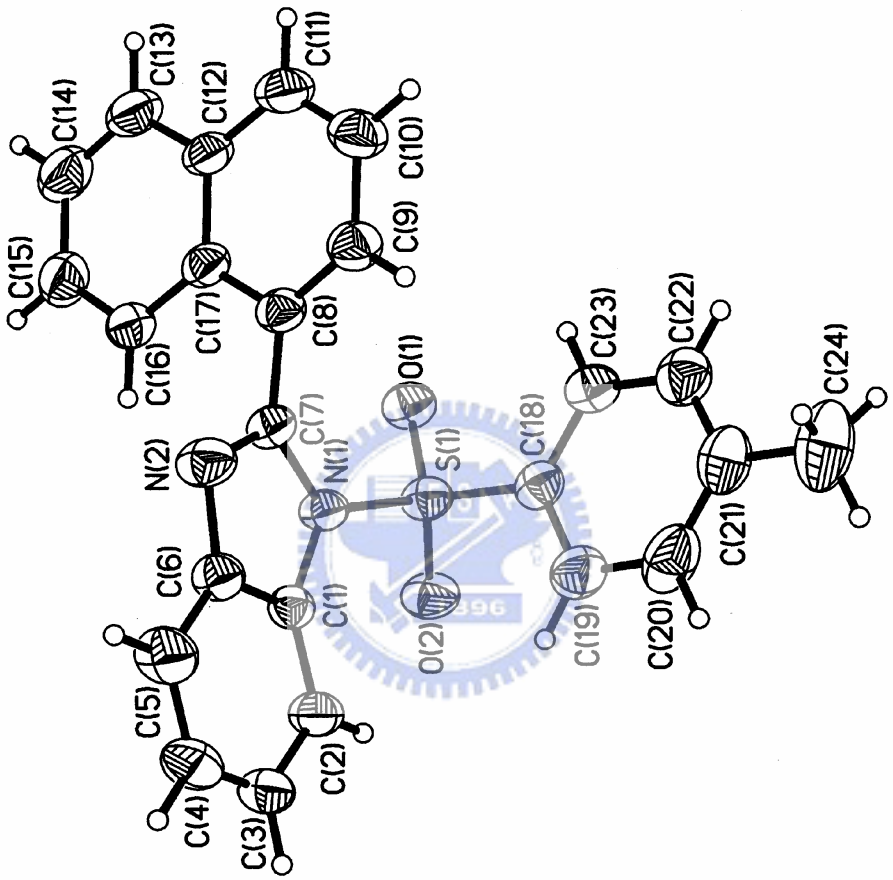

Fig. : The molecular structure of IC10917, thermal ellipsoids drawn at the 30% probability.

Table 1. Crystal data and structure refinement for ic10917.

Identification code	ic10917 (NTU structure analysis)
Empirical formula	$C_{24}H_{18}N_2O_2S$
Formula weight	398.46
Diffractometer used	$5 NONIUS KappaCCD
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.8390(1) Å alpha = 80.5325(9)° b = 10.9791(2) Å beta = 80.3051(9)° c = 21.2332(3) Å gamma = 81.7944(10)°
Volume, Z	1989.40(5) $Å^3$, 4
Density (calculated)	1.330 Mg/m^3
Absorption coefficient	0.186 mm^{-1}
F(000)	832
Crystal size	0.35 x 0.10 x 0.08 mm
θ range for data collection	1.89 to 27.50°
Limiting indices	$-11 \le h \le 11$, $-13 \le k \le 14$, $-27 \le l \le 27$
Reflections collected	38605
Independent reflections	9116 (R_{int} = 0.0496)
Completeness to θ = 27.50°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.993 and 0.924
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9116 / 0 / 526
Goodness-of-fit on F^2	1.010
Final R indices [I>2σ(I)]	R1 = 0.0471, wR2 = 0.1121
R indices (all data)	R1 = 0.1052, wR2 = 0.1333
Extinction coefficient	0.0238(18)
Largest diff. peak and hole	0.224 and -0.247 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for ic10917.

S(1)-O(1)	1.4199(13)	S(1)-O(2)	1.4253(13)
S(1)-N(1)	1.6813(15)	S(1)-C(18)	1.739(2)
N(1)-C(7)	1.407(2)	N(1)-C(1)	1.418(2)
N(2)-C(7)	1.292(2)	N(2)-C(6)	1.400(2)
C(1)-C(6)	1.378(3)	C(1)-C(2)	1.382(2)
C(2)-C(3)	1.377(3)	C(3)-C(4)	1.382(3)
C(4)-C(5)	1.361(3)	C(5)-C(6)	1.383(3)
C(7)-C(8)	1.485(2)	C(8)-C(9)	1.360(3)
C(8)-C(17)	1.418(3)	C(9)-C(10)	1.404(3)
C(10)-C(11)	1.365(3)	C(11)-C(12)	1.399(3)
C(12)-C(13)	1.409(3)	C(12)-C(17)	1.423(3)
C(13)-C(14)	1.351(3)	C(14)-C(15)	1.375(3)
C(15)-C(16)	1.362(3)	C(16)-C(17)	1.419(3)
C(18)-C(23)	1.384(3)	C(18)-C(19)	1.387(3)
C(19)-C(20)	1.383(4)	C(20)-C(21)	1.368(4)
C(21)-C(22)	1.368(3)	C(21)-C(24)	1.512(4)
C(22)-C(23)	1.367(3)	S(2)-O(3)	1.4189(14)
S(2)-O(4)	1.4234(13)	S(2)-N(3)	1.6857(15)
S(2)-C(42)	1.739(2)	N(3)-C(25)	1.408(2)
N(3)-C(31)	1.415(2)	N(4)-C(31)	1.291(2)
N(4)-C(30)	1.394(2)	C(25)-C(26)	1.384(3)
C(25)-C(30)	1.386(2)	C(26)-C(27)	1.377(3)
C(27)-C(28)	1.381(3)	C(28)-C(29)	1.357(3)
C(29)-C(30)	1.392(3)	C(31)-C(32)	1.484(3)
C(32)-C(33)	1.361(3)	C(32)-C(41)	1.416(3)
C(33)-C(34)	1.414(3)	C(34)-C(35)	1.354(3)
C(35)-C(36)	1.405(3)	C(36)-C(41)	1.416(3)
C(36)-C(37)	1.423(3)	C(37)-C(38)	1.357(4)
C(38)-C(39)	1.382(4)	C(39)-C(40)	1.356(3)
C(40)-C(41)	1.420(3)	C(42)-C(43)	1.381(3)
C(42)-C(47)	1.388(3)	C(43)-C(44)	1.376(3)
C(44)-C(45)	1.376(3)	C(45)-C(46)	1.380(4)
C(45)-C(48)	1.506(3)	C(46)-C(47)	1.374(3)

O(1)-S(1)-O(2)	120.27(9)	O(1)-S(1)-N(1)	106.15(8)
O(2)-S(1)-N(1)	104.77(8)	O(1)-S(1)-C(18)	110.11(9)
O(2)-S(1)-C(18)	110.07(9)	N(1)-S(1)-C(18)	104.02(9)
C(7)-N(1)-C(1)	105.76(14)	C(7)-N(1)-S(1)	127.13(12)
C(1)-N(1)-S(1)	124.93(12)	C(7)-N(2)-C(6)	106.44(16)
C(6)-C(1)-C(2)	121.45(17)	C(6)-C(1)-N(1)	105.00(15)
C(2)-C(1)-N(1)	133.55(18)	C(3)-C(2)-C(1)	116.9(2)
C(2)-C(3)-C(4)	121.8(2)	C(5)-C(4)-C(3)	120.9(2)
C(4)-C(5)-C(6)	118.2(2)	C(1)-C(6)-C(5)	120.76(19)
C(1)-C(6)-N(2)	110.65(16)	C(5)-C(6)-N(2)	128.59(19)
N(2)-C(7)-N(1)	112.08(16)	N(2)-C(7)-C(8)	121.99(17)
N(1)-C(7)-C(8)	125.88(17)	C(9)-C(8)-C(17)	119.92(18)
C(9)-C(8)-C(7)	120.73(19)	C(17)-C(8)-C(7)	119.02(18)
C(8)-C(9)-C(10)	121.3(2)	C(11)-C(10)-C(9)	119.6(2)
C(10)-C(11)-C(12)	121.3(2)	C(11)-C(12)-C(13)	123.1(2)
C(11)-C(12)-C(17)	119.0(2)	C(13)-C(12)-C(17)	117.9(2)
C(14)-C(13)-C(12)	122.2(2)	C(13)-C(14)-C(15)	120.0(2)
C(16)-C(15)-C(14)	121.1(2)	C(15)-C(16)-C(17)	120.6(2)
C(8)-C(17)-C(16)	122.87(17)	C(8)-C(17)-C(12)	118.88(19)
C(16)-C(17)-C(12)	118.25(19)	C(23)-C(18)-C(19)	119.5(2)
C(23)-C(18)-S(1)	120.25(16)	C(19)-C(18)-S(1)	120.21(17)

C(20)-C(19)-C(18)	118.6(2)	C(21)-C(20)-C(19)	122.4(2)
C(20)-C(21)-C(22)	117.7(3)	C(20)-C(21)-C(24)	120.2(3)
C(22)-C(21)-C(24)	122.0(3)	C(23)-C(22)-C(21)	122.0(2)
C(22)-C(23)-C(18)	119.7(2)	O(3)-S(2)-O(4)	120.61(9)
O(3)-S(2)-N(3)	106.06(8)	O(4)-S(2)-N(3)	104.40(8)
O(3)-S(2)-C(42)	110.25(9)	O(4)-S(2)-C(42)	110.13(9)
N(3)-S(2)-C(42)	103.79(8)	C(25)-N(3)-C(31)	105.90(14)
C(25)-N(3)-S(2)	125.12(12)	C(31)-N(3)-S(2)	126.91(13)
C(31)-N(4)-C(30)	106.74(15)	C(26)-C(25)-C(30)	121.09(18)
C(26)-C(25)-N(3)	133.87(17)	C(30)-C(25)-N(3)	105.03(15)
C(27)-C(26)-C(25)	116.92(19)	C(26)-C(27)-C(28)	122.2(2)
C(29)-C(28)-C(27)	120.9(2)	C(28)-C(29)-C(30)	118.2(2)
C(25)-C(30)-C(29)	120.72(19)	C(25)-C(30)-N(4)	110.52(17)
C(29)-C(30)-N(4)	128.76(19)	N(4)-C(31)-N(3)	111.75(16)
N(4)-C(31)-C(32)	122.18(15)	N(3)-C(31)-C(32)	126.05(16)
C(33)-C(32)-C(41)	120.55(19)	C(33)-C(32)-C(31)	119.76(18)
C(41)-C(32)-C(31)	119.21(18)	C(32)-C(33)-C(34)	120.5(2)
C(35)-C(34)-C(33)	120.0(2)	C(34)-C(35)-C(36)	121.1(2)
C(35)-C(36)-C(41)	119.2(2)	C(35)-C(36)-C(37)	122.5(2)
C(41)-C(36)-C(37)	118.3(2)	C(38)-C(37)-C(36)	121.0(2)
C(37)-C(38)-C(39)	120.6(2)	C(40)-C(39)-C(38)	120.8(3)
C(39)-C(40)-C(41)	120.9(2)	C(32)-C(41)-C(36)	118.65(19)
C(32)-C(41)-C(40)	122.86(18)	C(36)-C(41)-C(40)	118.48(19)
C(43)-C(42)-C(47)	121.0(2)	C(43)-C(42)-S(2)	120.02(16)
C(47)-C(42)-S(2)	119.00(18)	C(44)-C(43)-C(42)	118.8(2)
C(45)-C(44)-C(43)	121.6(2)	C(44)-C(45)-C(46)	118.3(2)
C(44)-C(45)-C(48)	120.7(3)	C(46)-C(45)-C(48)	121.0(3)
C(47)-C(46)-C(45)	121.8(2)	C(46)-C(47)-C(42)	118.4(2)

Symmetry transformations used to generate equivalent atoms: