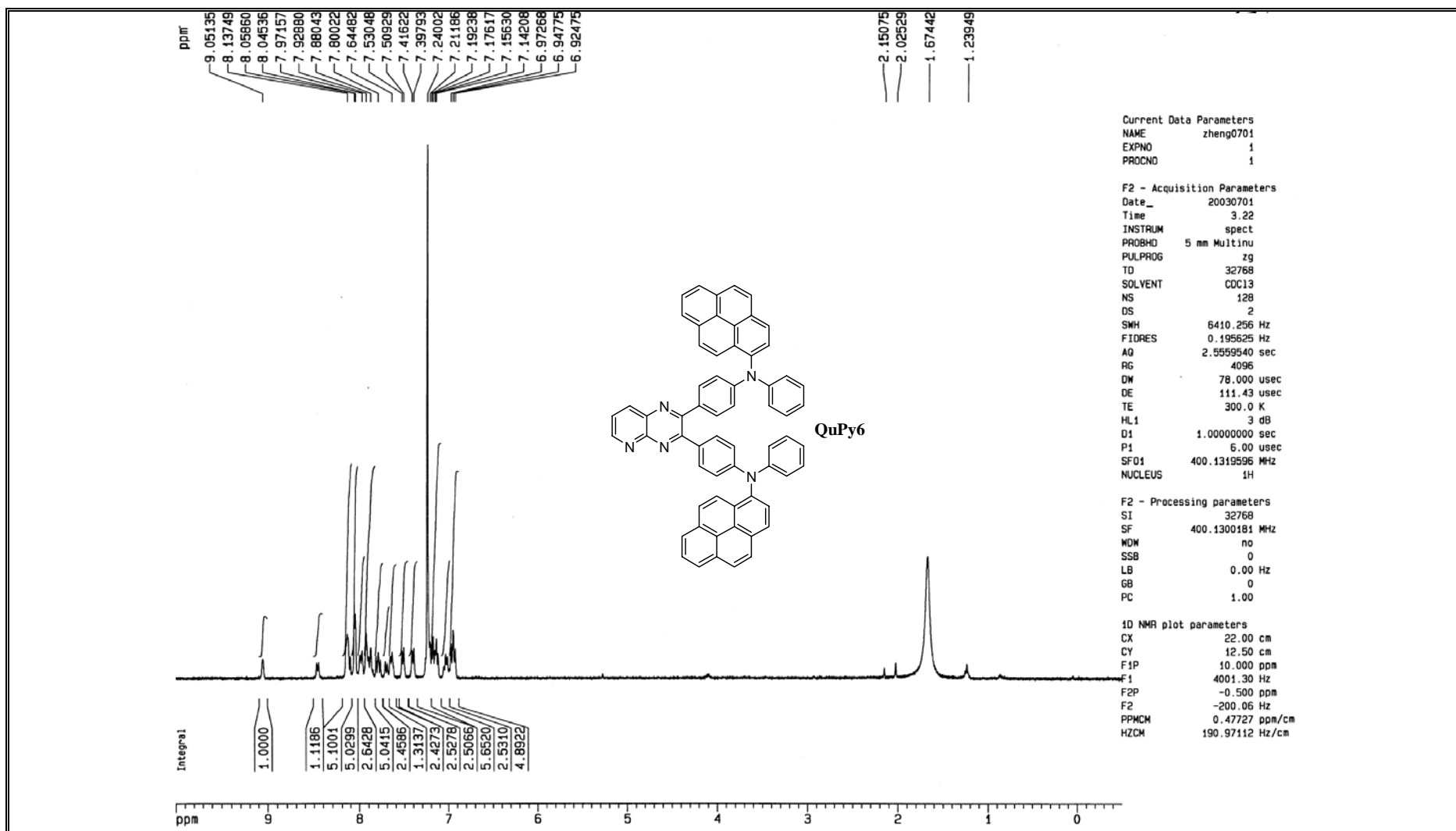
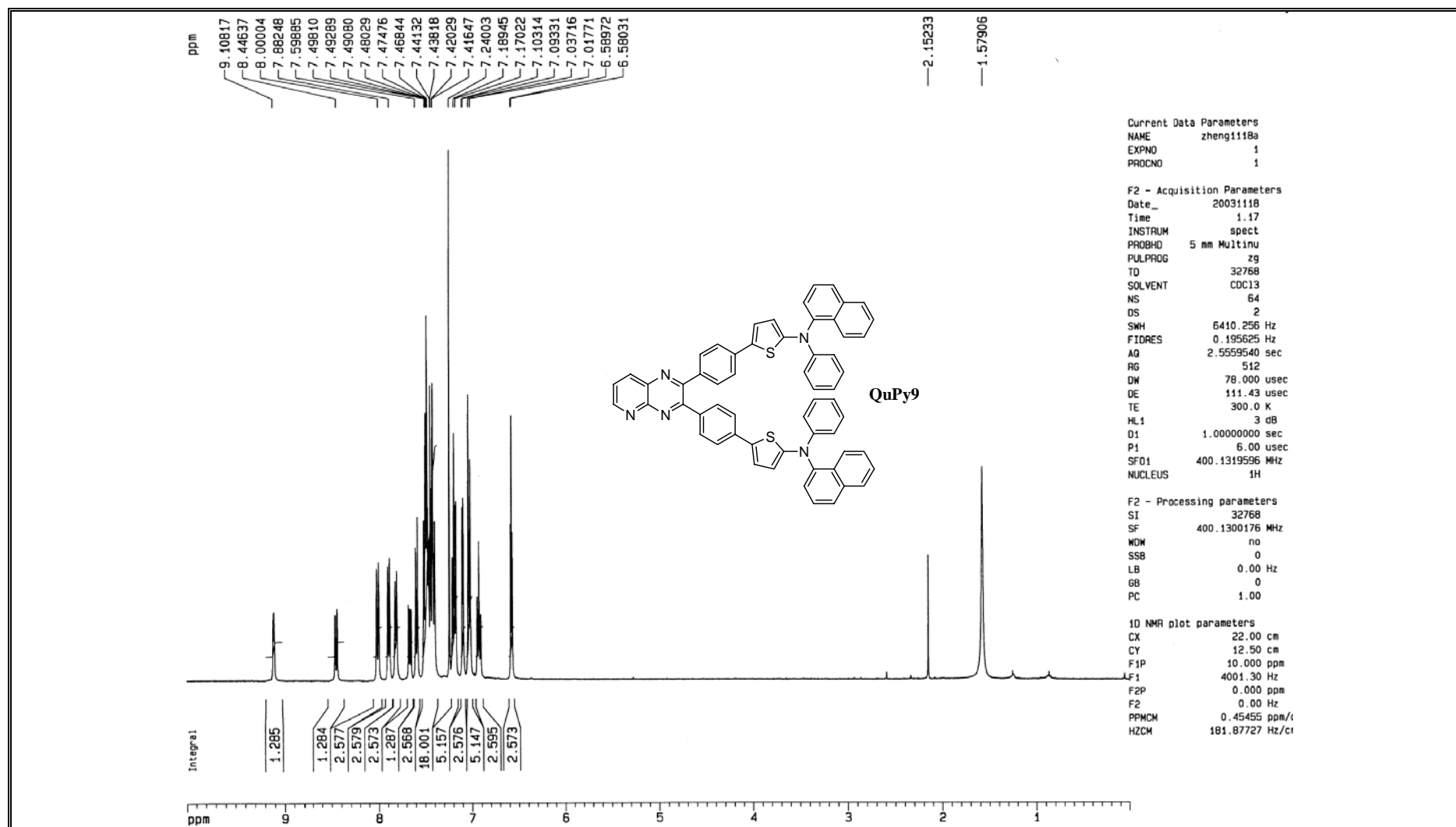
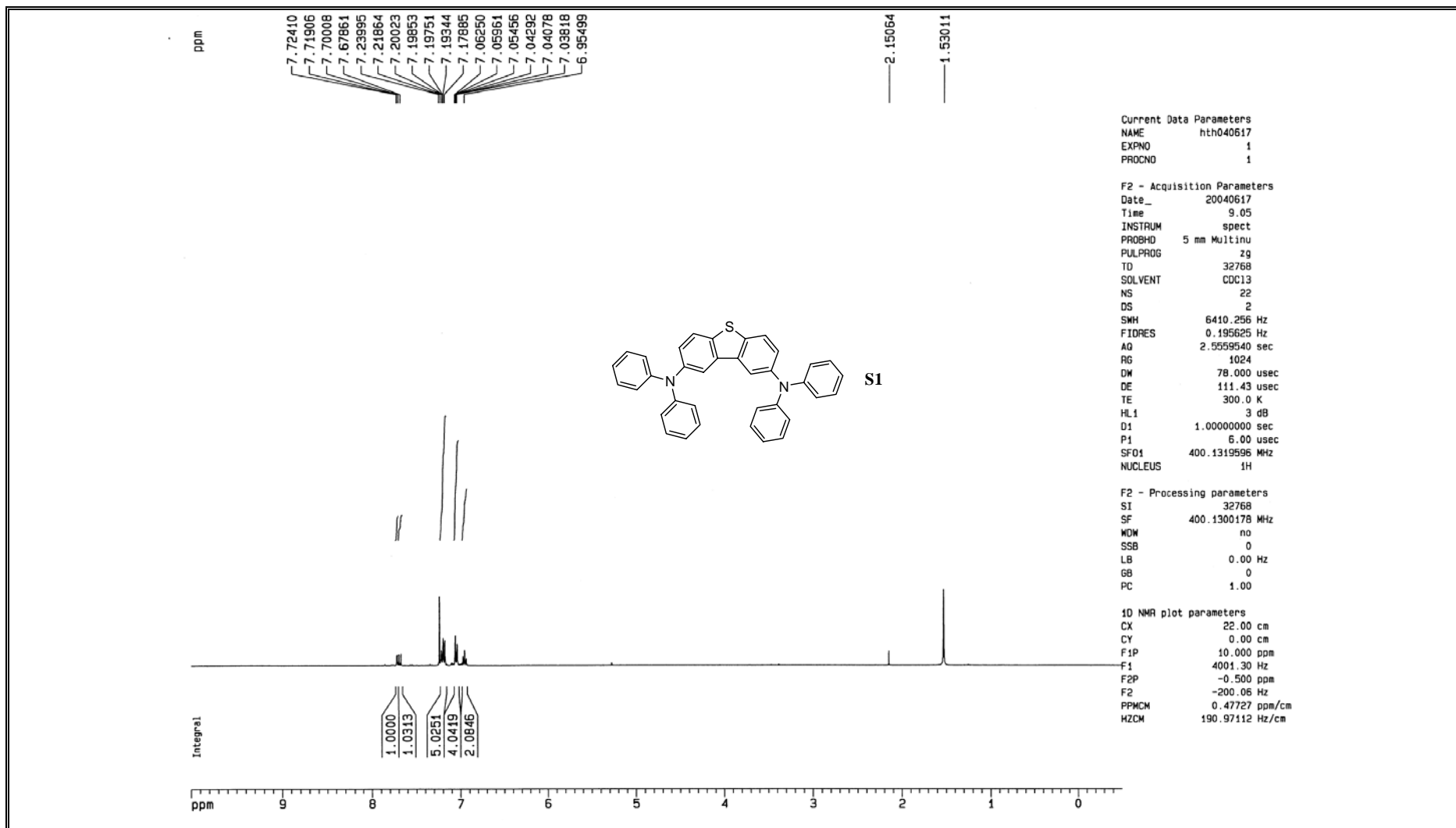
化合物QuPy3之¹H NMR光譜

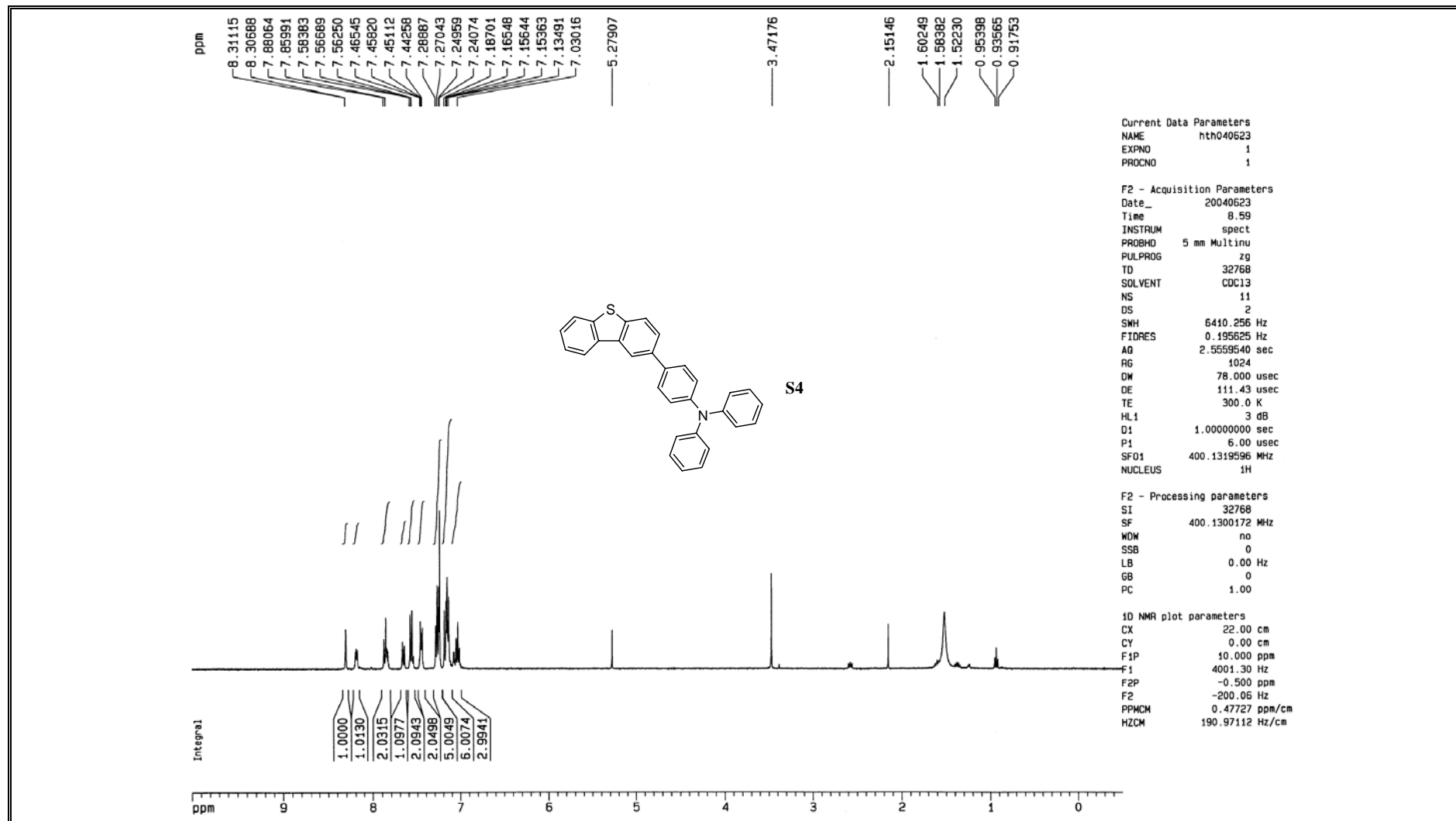


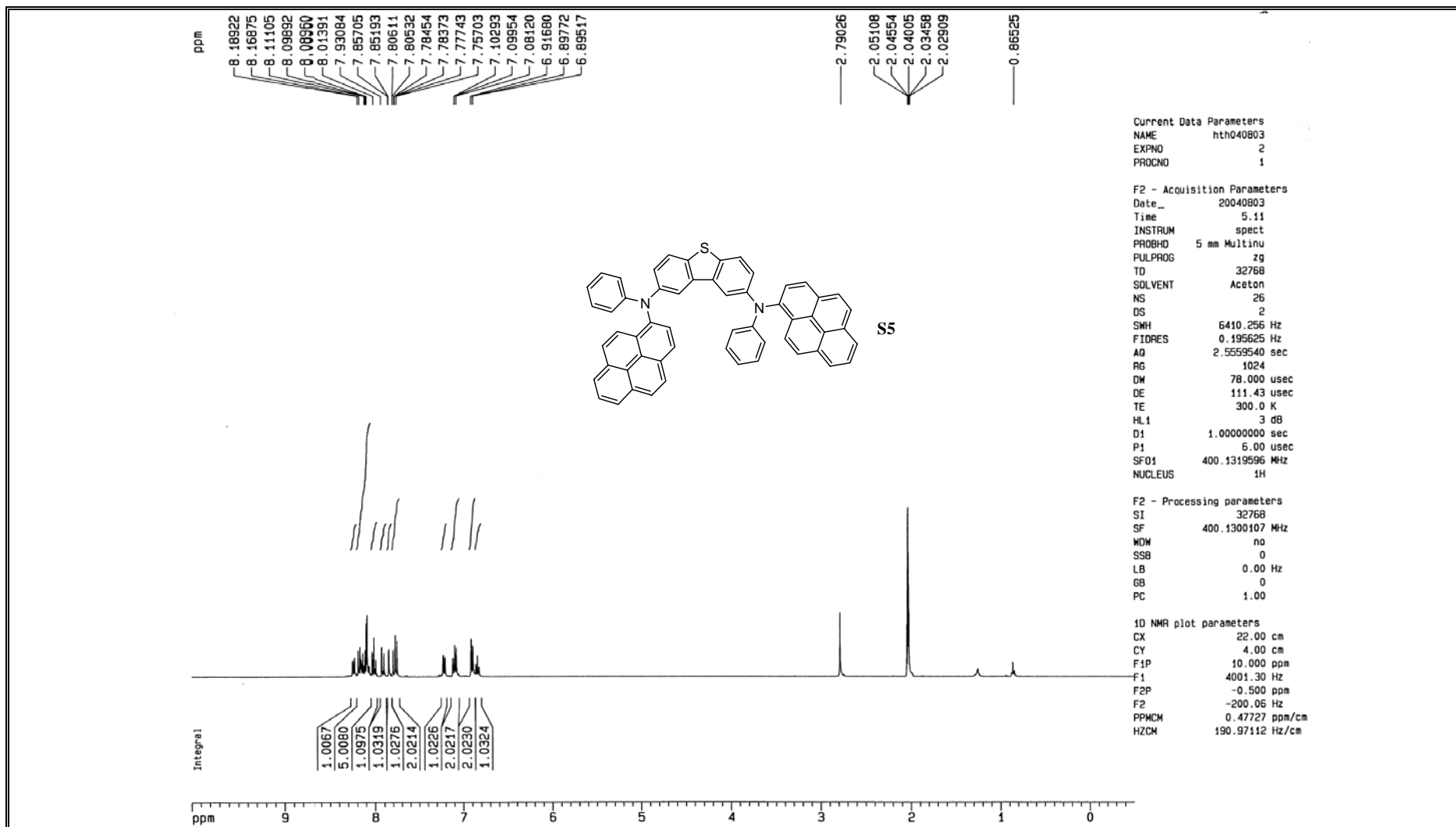
化合物QuPy6之¹H NMR光譜

化合物QuPy9之¹H NMR光譜

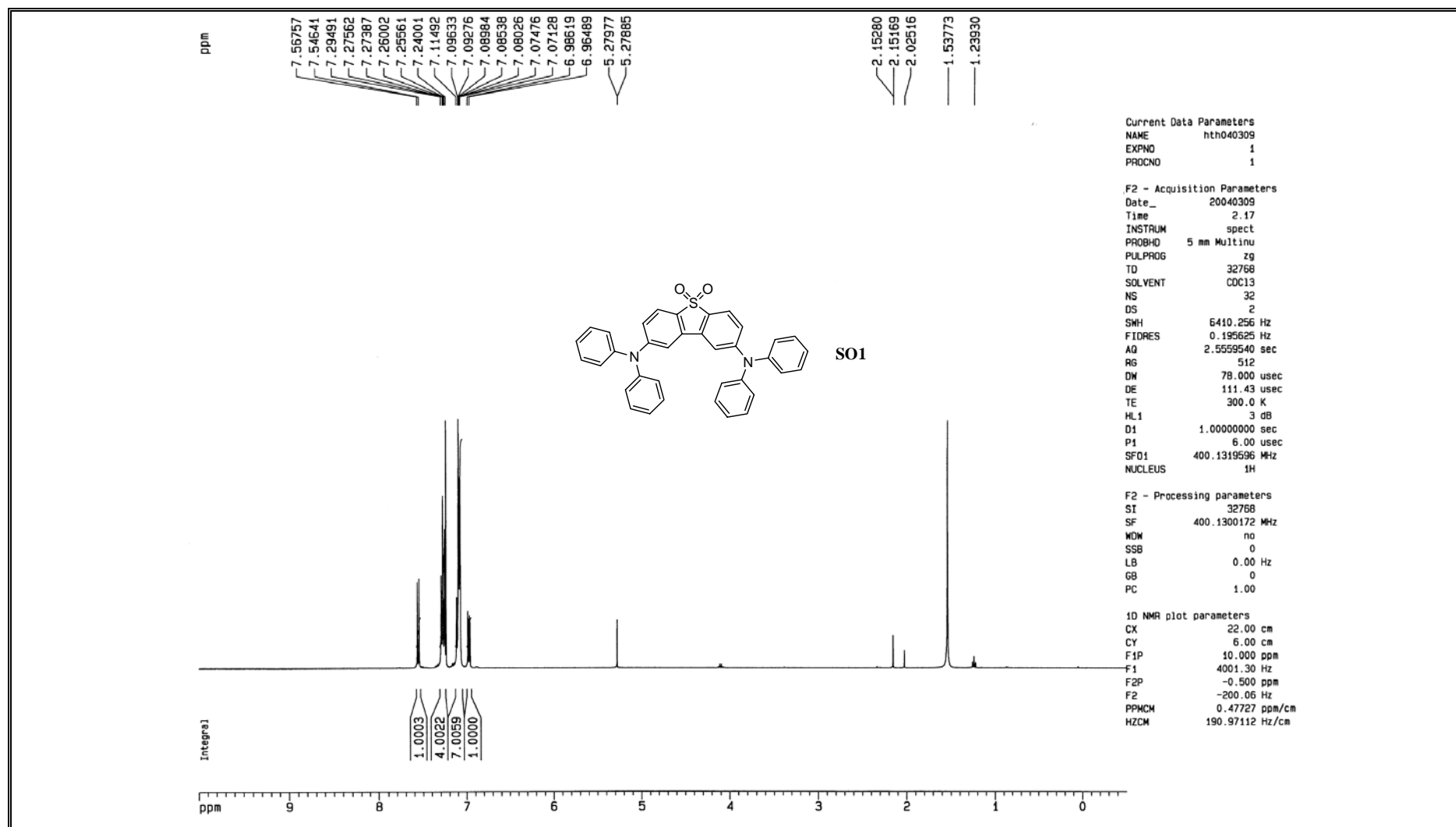


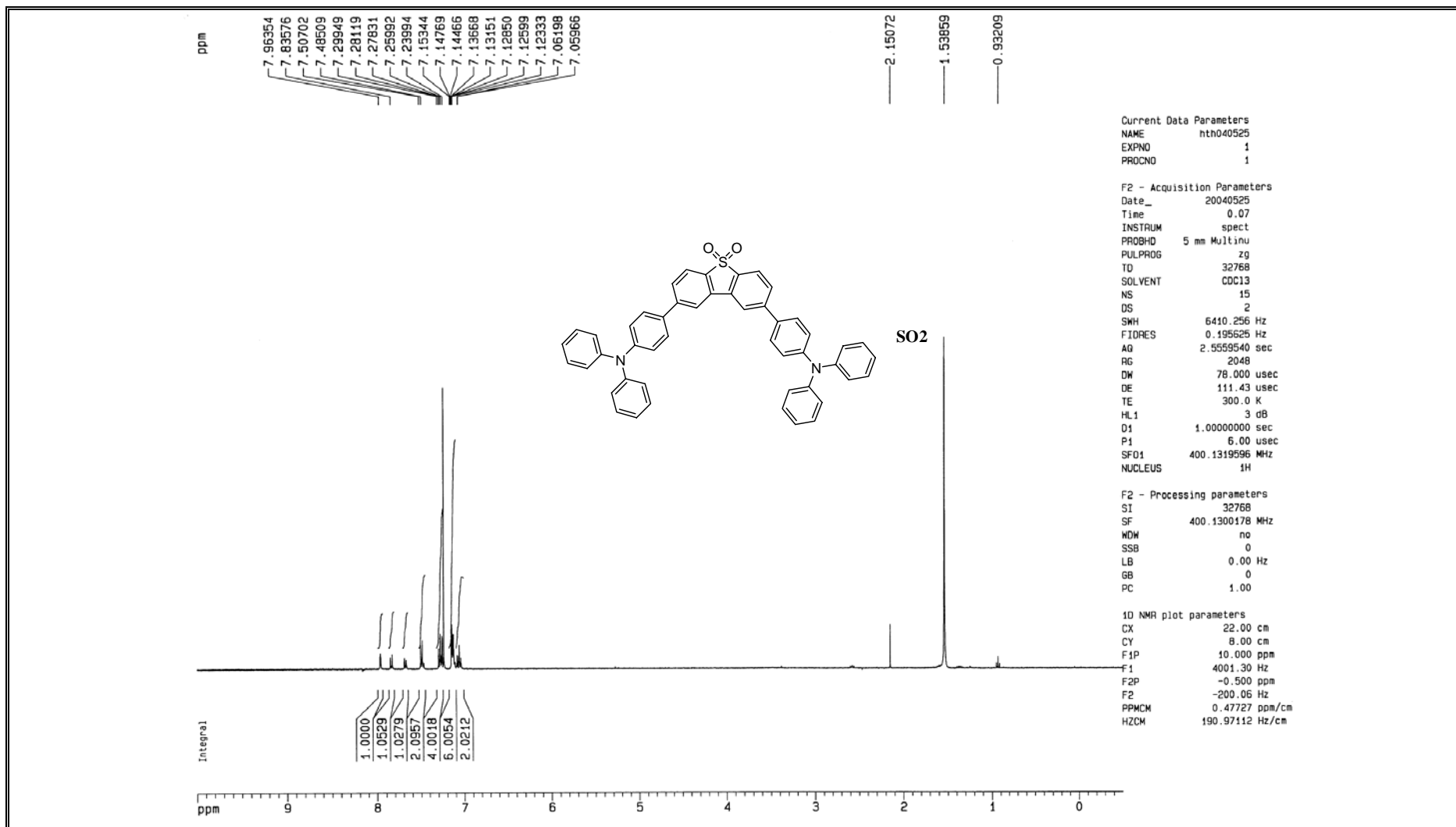
化合物S1之¹H NMR光譜

化合物S4之¹H NMR光譜

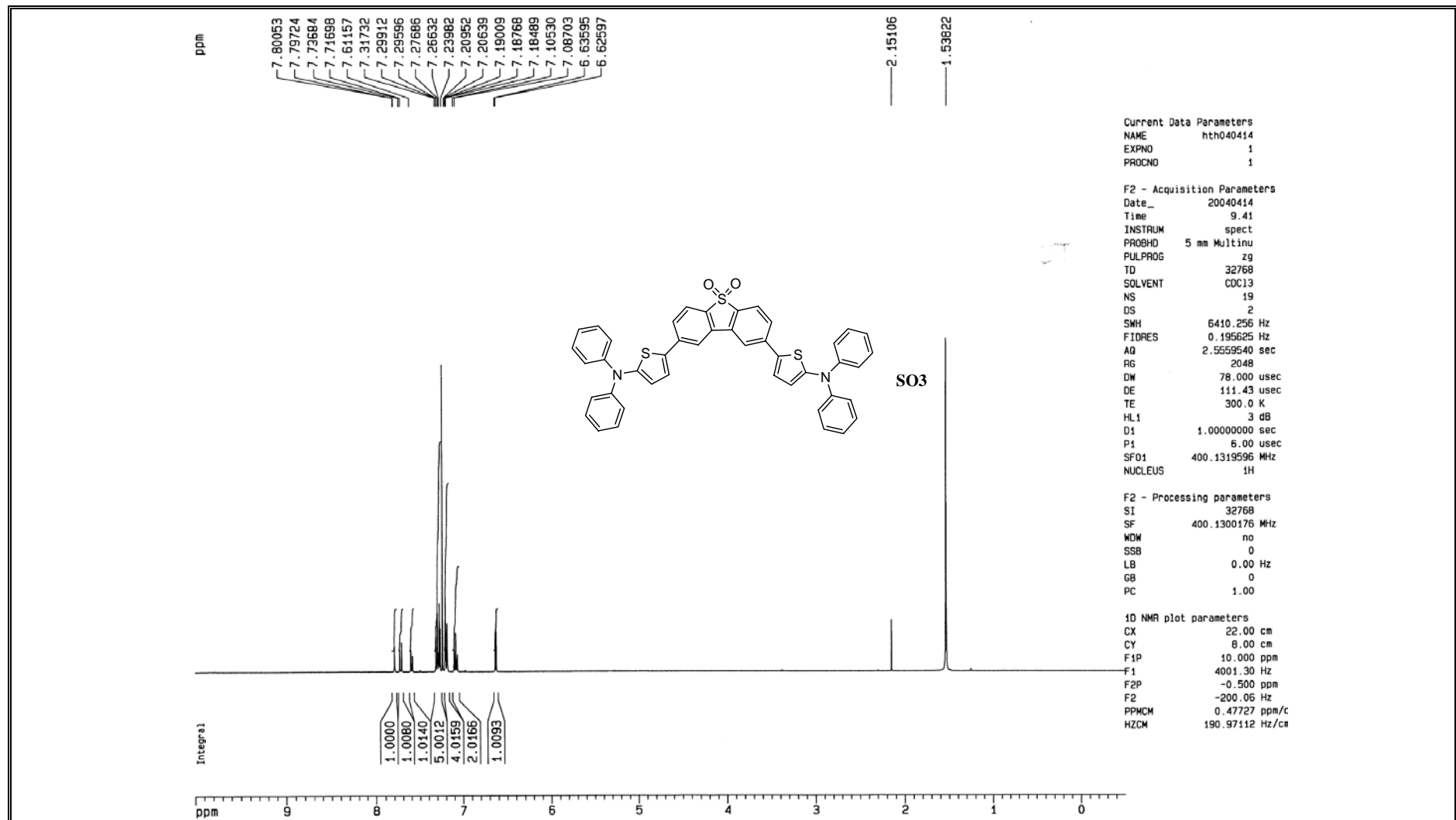


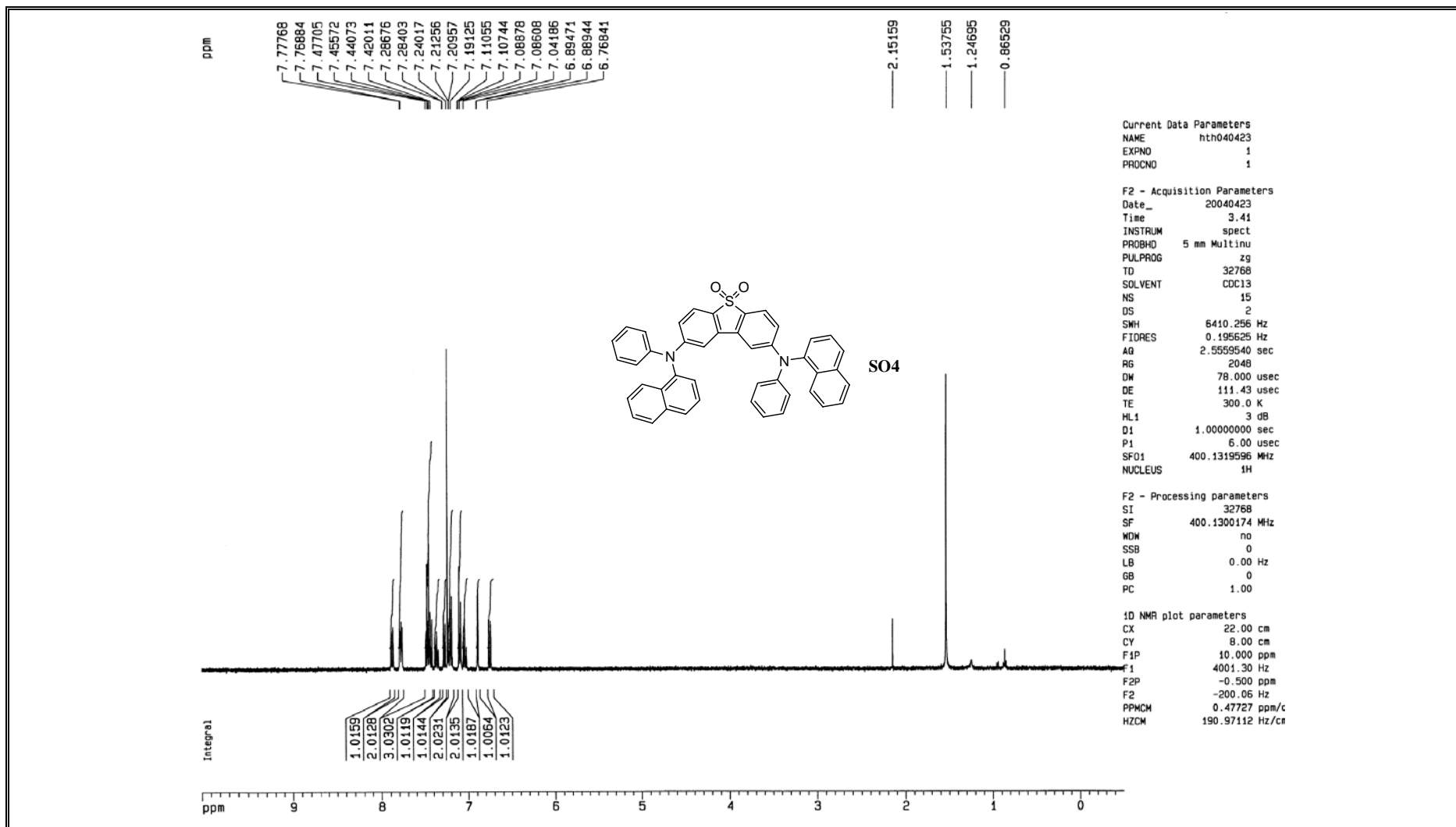
化合物S5之¹H NMR光譜

化合物SO1之 ^1H NMR光譜

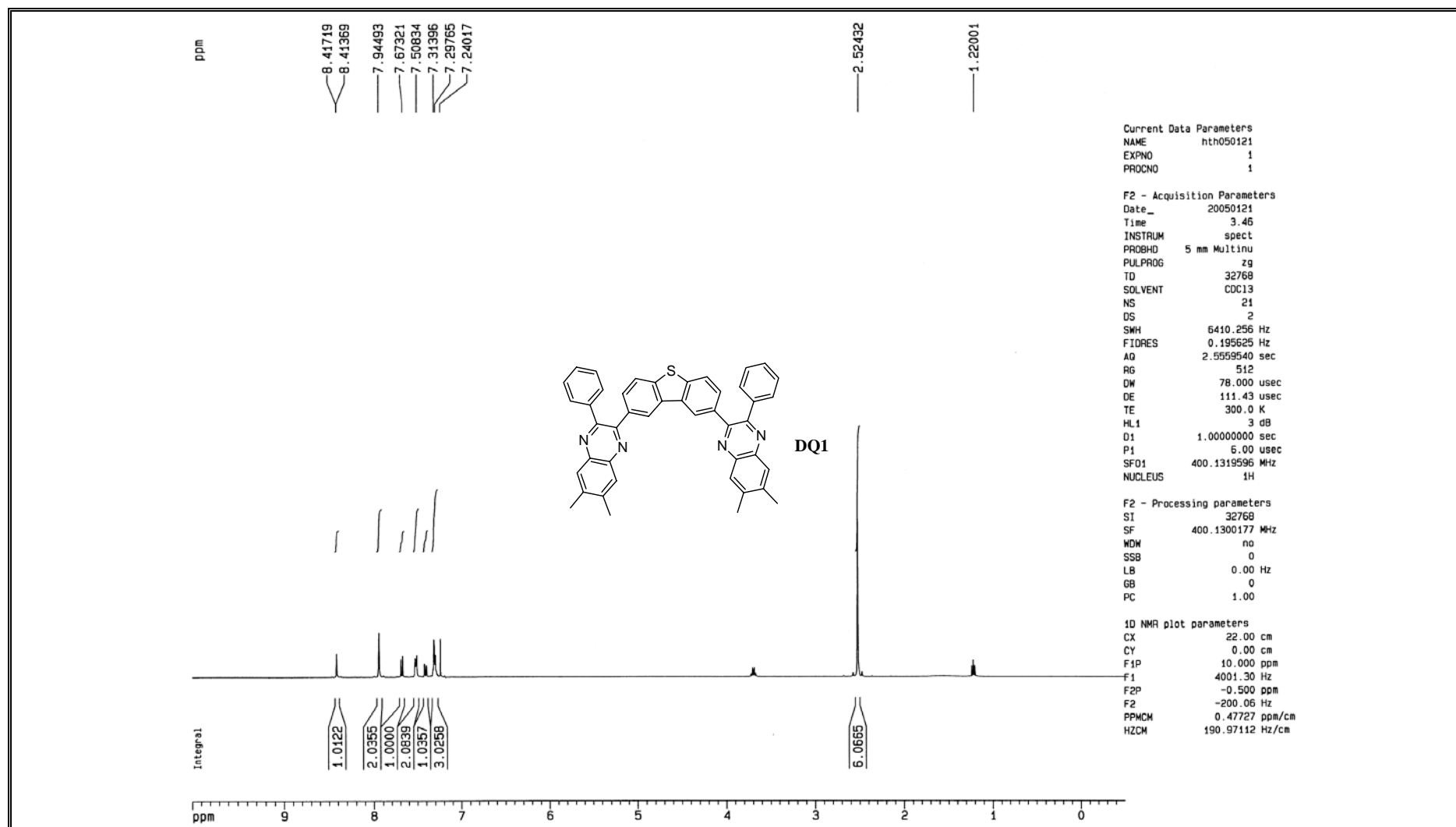


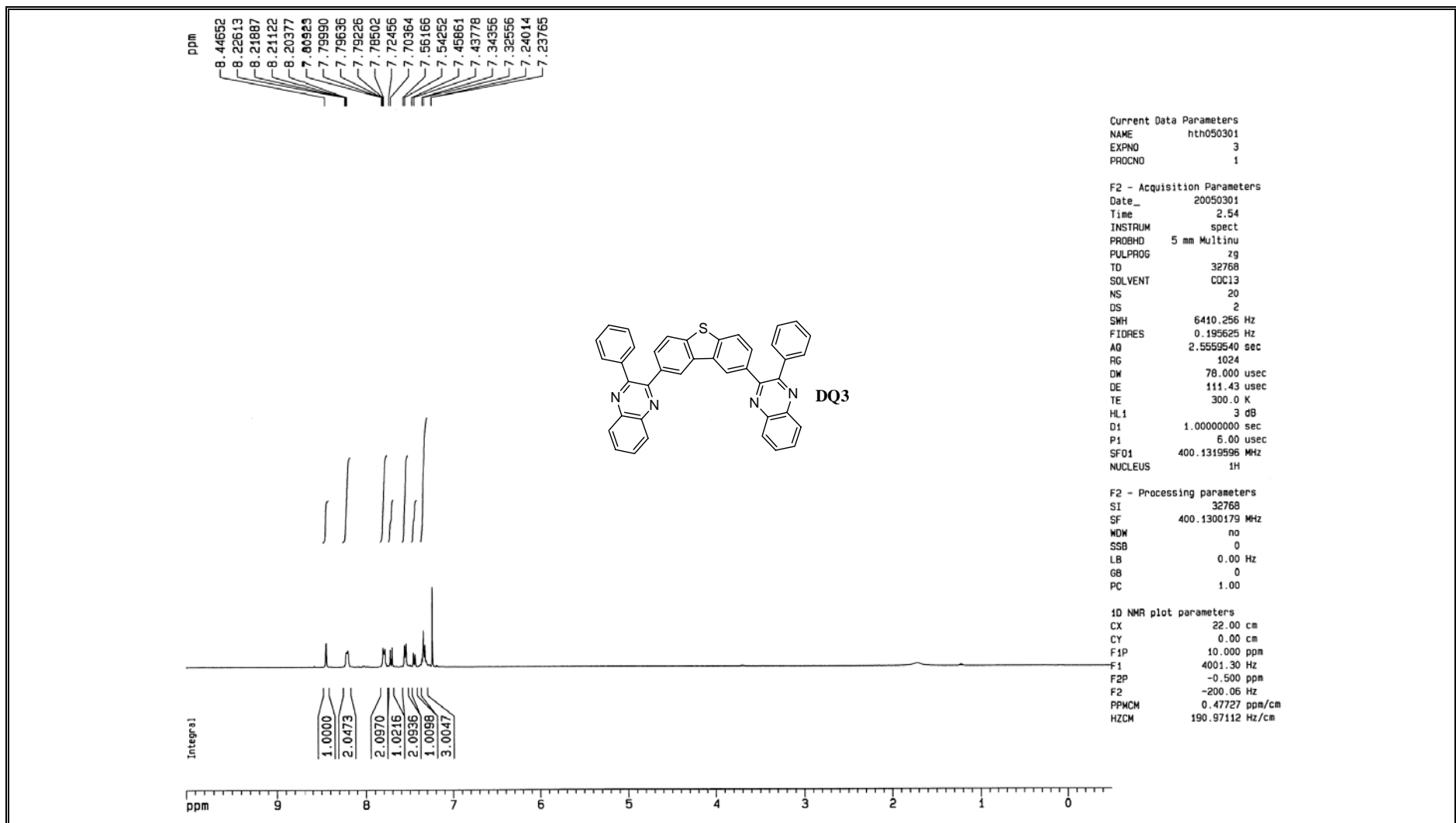
化合物SO2之¹H NMR光譜

化合物SO3之¹H NMR光譜

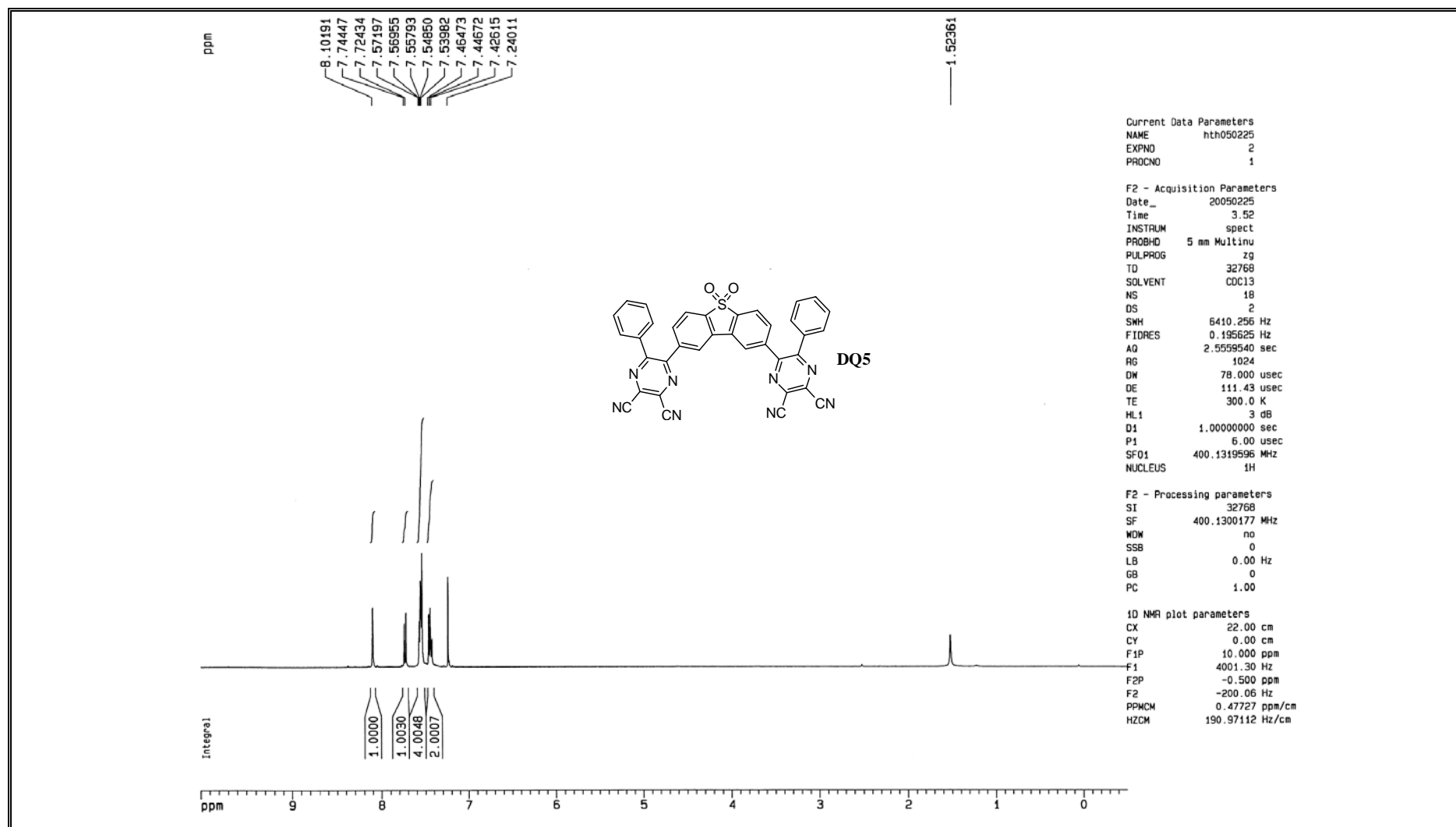


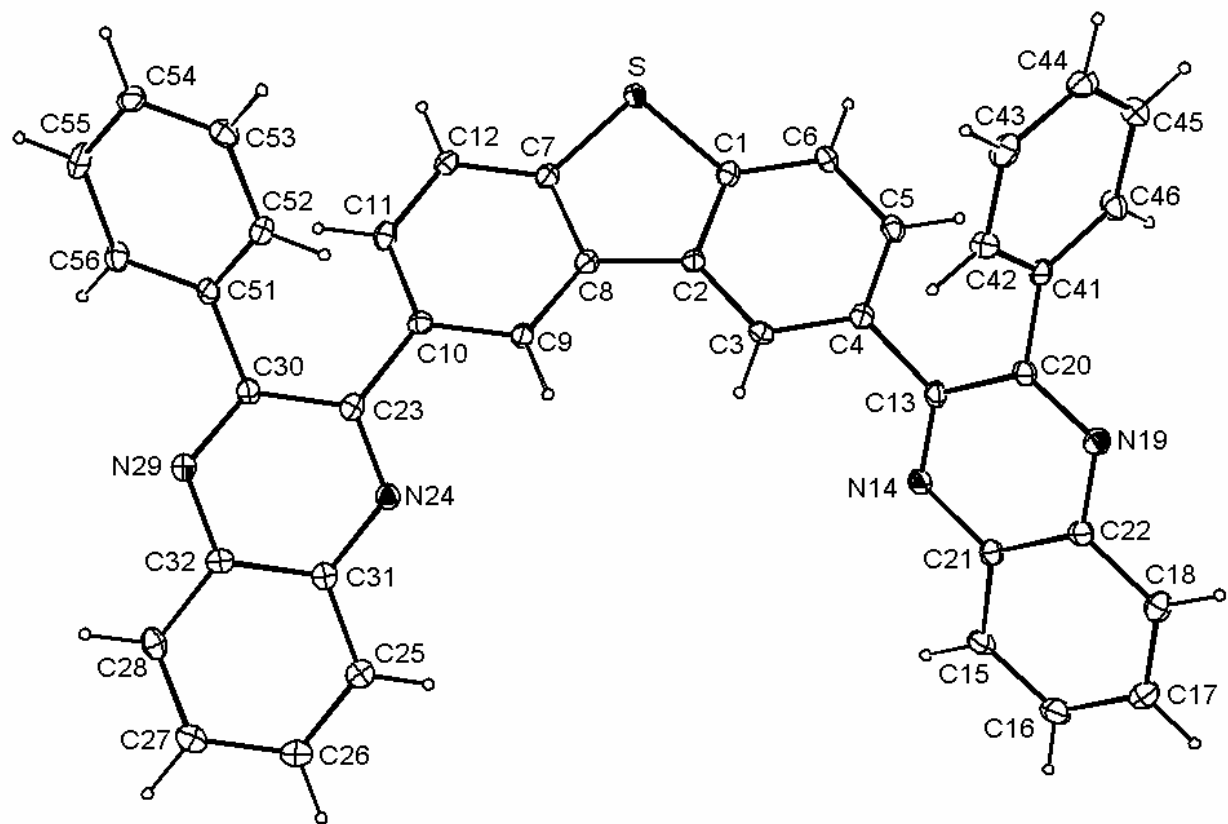
化合物SO4之¹H NMR光譜

化合物DQ1之¹H NMR光譜



化合物DQ3之¹H NMR光譜

化合物**DQ5**之¹H NMR光譜



化合物 **DQ3** 之 ORTEP 圖

化合物 **DQ3** 之 X-ray 繞射數據

Table 1. Crystal data and structure refinement for DQ3.

Identification code	DQ3	
Empirical formula	C ₄₀ H ₂₄ N ₄ S	
Formula weight	592.69	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9452(7) Å	α = 90.480(3)°.
	b = 11.6962(9) Å	β = 102.645(3)°.
	c = 12.7037(9) Å	γ = 102.501(2)°.
Volume	1405.27(18) Å ³	
Z	2	
Density (calculated)	1.401 Mg/m ³	
Absorption coefficient	0.154 mm ⁻¹	
F(000)	616	
Crystal size	0.12 x 0.10 x 0.04 mm ³	
Theta range for data collection	1.65 to 25.03°	
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -15 ≤ l ≤ 15	
Reflections collected	21681	
Independent reflections	4945 [R(int) = 0.0720]	
Completeness to theta = 25.03°	100.0 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.9938 and 0.9817	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4945 / 0 / 407	
Goodness-of-fit on F ²	1.092	
Final R indices [I > 2σ(I)]	R1 = 0.0593, wR2 = 0.1692	
R indices (all data)	R1 = 0.0886, wR2 = 0.1785	
Extinction coefficient	0.010(2)	
Largest diff. peak and hole	0.464 and -0.356 e.Å ⁻³	

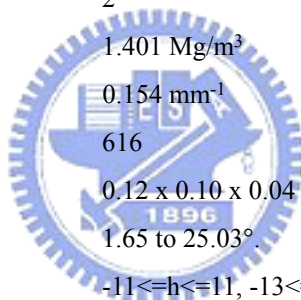


Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ3. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S	2170(1)	5017(1)	9068(1)	20(1)
N(14)	-4232(3)	2036(3)	9384(2)	21(1)
N(19)	-5487(3)	331(3)	7658(3)	21(1)
N(24)	1765(3)	3151(3)	13924(2)	19(1)
N(29)	4381(3)	3182(3)	15333(3)	19(1)
C(1)	472(4)	4122(3)	8836(3)	18(1)
C(2)	209(4)	3497(3)	9738(3)	16(1)
C(3)	-1112(4)	2749(3)	9668(3)	18(1)
C(4)	-2134(4)	2605(3)	8712(3)	17(1)
C(5)	-1852(4)	3245(3)	7824(3)	20(1)
C(6)	-567(4)	4011(3)	7879(3)	19(1)
C(7)	2549(4)	4595(3)	10387(3)	18(1)
C(8)	1426(4)	3776(3)	10648(3)	17(1)
C(9)	1581(4)	3366(3)	11690(3)	18(1)
C(10)	2837(4)	3776(3)	12463(3)	17(1)
C(11)	3928(4)	4602(3)	12175(3)	20(1)
C(12)	3814(4)	5014(3)	11156(3)	19(1)
C(13)	-3553(4)	1843(4)	8639(3)	19(1)
C(15)	-6401(4)	1631(4)	9996(3)	24(1)
C(16)	-7780(4)	1049(4)	9847(3)	27(1)
C(17)	-8404(4)	201(4)	8988(3)	25(1)
C(18)	-7643(4)	-40(4)	8274(3)	24(1)
C(20)	-4179(4)	953(3)	7772(3)	18(1)
C(21)	-5589(4)	1397(3)	9272(3)	19(1)
C(22)	-6217(4)	554(3)	8400(3)	19(1)
C(23)	2947(4)	3384(3)	13582(3)	18(1)
C(25)	612(4)	2562(3)	15370(3)	21(1)
C(26)	687(4)	2385(3)	16436(3)	22(1)
C(27)	2014(4)	2553(3)	17168(3)	23(1)
C(28)	3233(4)	2846(3)	16806(3)	22(1)
C(30)	4279(4)	3306(3)	14289(3)	17(1)

C(31)	1846(4)	2901(3)	14980(3)	18(1)
C(32)	3177(4)	3002(3)	15708(3)	18(1)
C(41)	-3381(4)	660(3)	6980(3)	18(1)
C(42)	-2323(4)	42(4)	7287(3)	22(1)
C(43)	-1650(4)	-303(4)	6543(3)	25(1)
C(44)	-2019(4)	-26(4)	5472(3)	24(1)
C(45)	-3034(4)	603(4)	5159(3)	27(1)
C(46)	-3715(4)	944(4)	5915(3)	23(1)
C(51)	5579(4)	3330(3)	13890(3)	17(1)
C(52)	5531(4)	2647(3)	12981(3)	20(1)
C(53)	6736(4)	2677(4)	12605(3)	21(1)
C(54)	8011(4)	3384(4)	13145(3)	25(1)
C(55)	8074(4)	4060(4)	14050(3)	26(1)
C(56)	6862(4)	4035(4)	14439(3)	21(1)



Table 3. Bond lengths [\AA] and angles [$^\circ$] for DQ3.

S-C(7)	1.735(4)
S-C(1)	1.745(4)
N(14)-C(13)	1.320(5)
N(14)-C(21)	1.370(5)
N(19)-C(20)	1.323(5)
N(19)-C(22)	1.365(5)
N(24)-C(23)	1.316(5)
N(24)-C(31)	1.364(5)
N(29)-C(30)	1.320(5)
N(29)-C(32)	1.359(5)
C(1)-C(6)	1.396(5)
C(1)-C(2)	1.407(5)
C(2)-C(3)	1.396(5)
C(2)-C(8)	1.456(5)
C(3)-C(4)	1.385(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.404(5)
C(4)-C(13)	1.480(5)
C(5)-C(6)	1.380(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.401(5)
C(7)-C(8)	1.406(5)
C(8)-C(9)	1.399(5)
C(9)-C(10)	1.396(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.404(5)
C(10)-C(23)	1.486(5)
C(11)-C(12)	1.375(5)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(20)	1.444(5)
C(15)-C(16)	1.364(6)
C(15)-C(21)	1.411(5)



C(15)-H(15)	0.9500
C(16)-C(17)	1.407(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.365(6)
C(17)-H(17)	0.9500
C(18)-C(22)	1.411(5)
C(18)-H(18)	0.9500
C(20)-C(41)	1.490(5)
C(21)-C(22)	1.414(5)
C(23)-C(30)	1.450(5)
C(25)-C(26)	1.360(5)
C(25)-C(31)	1.403(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.412(6)
C(26)-H(26)	0.9500
C(27)-C(28)	1.366(6)
C(27)-H(27)	0.9500
C(28)-C(32)	1.398(5)
C(28)-H(28)	0.9500
C(30)-C(51)	1.483(5)
C(31)-C(32)	1.420(5)
C(41)-C(46)	1.382(5)
C(41)-C(42)	1.392(6)
C(42)-C(43)	1.375(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.390(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.368(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.392(6)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(51)-C(52)	1.385(5)
C(51)-C(56)	1.393(5)
C(52)-C(53)	1.378(5)
C(52)-H(52)	0.9500



C(53)-C(54)	1.385(6)
C(53)-H(53)	0.9500
C(54)-C(55)	1.372(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.394(6)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(7)-S-C(1)	91.00(19)
C(13)-N(14)-C(21)	117.3(3)
C(20)-N(19)-C(22)	117.3(3)
C(23)-N(24)-C(31)	117.9(3)
C(30)-N(29)-C(32)	118.2(3)
C(6)-C(1)-C(2)	121.1(4)
C(6)-C(1)-S	126.0(3)
C(2)-C(1)-S	112.9(3)
C(3)-C(2)-C(1)	119.1(3)
C(3)-C(2)-C(8)	129.5(4)
C(1)-C(2)-C(8)	111.4(3)
C(4)-C(3)-C(2)	120.2(4)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	119.7(4)
C(3)-C(4)-C(13)	120.6(4)
C(5)-C(4)-C(13)	119.6(3)
C(6)-C(5)-C(4)	121.3(4)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(1)	118.5(4)
C(5)-C(6)-H(6)	120.7
C(1)-C(6)-H(6)	120.7
C(12)-C(7)-C(8)	121.1(4)
C(12)-C(7)-S	125.7(3)
C(8)-C(7)-S	113.3(3)
C(9)-C(8)-C(7)	119.5(3)
C(9)-C(8)-C(2)	129.1(4)



C(7)-C(8)-C(2)	111.4(3)
C(10)-C(9)-C(8)	120.0(4)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	118.9(3)
C(9)-C(10)-C(23)	119.2(3)
C(11)-C(10)-C(23)	121.9(3)
C(12)-C(11)-C(10)	122.5(4)
C(12)-C(11)-H(11)	118.8
C(10)-C(11)-H(11)	118.8
C(11)-C(12)-C(7)	118.1(4)
C(11)-C(12)-H(12)	120.9
C(7)-C(12)-H(12)	120.9
N(14)-C(13)-C(20)	121.7(4)
N(14)-C(13)-C(4)	117.0(3)
C(20)-C(13)-C(4)	121.2(3)
C(16)-C(15)-C(21)	119.9(4)
C(16)-C(15)-H(15)	120.1
C(21)-C(15)-H(15)	120.1
C(15)-C(16)-C(17)	120.9(4)
C(15)-C(16)-H(16)	119.5
C(17)-C(16)-H(16)	119.5
C(18)-C(17)-C(16)	120.4(4)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(17)-C(18)-C(22)	120.1(4)
C(17)-C(18)-H(18)	120.0
C(22)-C(18)-H(18)	120.0
N(19)-C(20)-C(13)	121.3(4)
N(19)-C(20)-C(41)	116.4(3)
C(13)-C(20)-C(41)	122.2(3)
N(14)-C(21)-C(15)	119.7(4)
N(14)-C(21)-C(22)	120.8(4)
C(15)-C(21)-C(22)	119.4(4)
N(19)-C(22)-C(18)	119.2(4)
N(19)-C(22)-C(21)	121.4(4)



C(18)-C(22)-C(21)	119.4(4)
N(24)-C(23)-C(30)	120.9(3)
N(24)-C(23)-C(10)	116.2(3)
C(30)-C(23)-C(10)	122.8(3)
C(26)-C(25)-C(31)	120.7(4)
C(26)-C(25)-H(25)	119.7
C(31)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	120.2(4)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(28)-C(27)-C(26)	120.3(4)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(32)	120.3(4)
C(27)-C(28)-H(28)	119.9
C(32)-C(28)-H(28)	119.9
N(29)-C(30)-C(23)	120.8(4)
N(29)-C(30)-C(51)	116.4(3)
C(23)-C(30)-C(51)	122.8(3)
N(24)-C(31)-C(25)	120.4(3)
N(24)-C(31)-C(32)	120.7(4)
C(25)-C(31)-C(32)	118.9(4)
N(29)-C(32)-C(28)	120.1(3)
N(29)-C(32)-C(31)	120.3(3)
C(28)-C(32)-C(31)	119.5(4)
C(46)-C(41)-C(42)	118.4(4)
C(46)-C(41)-C(20)	121.0(4)
C(42)-C(41)-C(20)	120.5(3)
C(43)-C(42)-C(41)	120.8(4)
C(43)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(42)-C(43)-C(44)	119.9(4)
C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0
C(45)-C(44)-C(43)	120.2(4)
C(45)-C(44)-H(44)	119.9



C(43)-C(44)-H(44)	119.9
C(44)-C(45)-C(46)	119.5(4)
C(44)-C(45)-H(45)	120.2
C(46)-C(45)-H(45)	120.2
C(41)-C(46)-C(45)	121.1(4)
C(41)-C(46)-H(46)	119.4
C(45)-C(46)-H(46)	119.4
C(52)-C(51)-C(56)	119.6(4)
C(52)-C(51)-C(30)	120.5(3)
C(56)-C(51)-C(30)	119.9(3)
C(53)-C(52)-C(51)	120.5(4)
C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7
C(52)-C(53)-C(54)	119.9(4)
C(52)-C(53)-H(53)	120.0
C(54)-C(53)-H(53)	120.0
C(55)-C(54)-C(53)	120.1(4)
C(55)-C(54)-H(54)	119.9
C(53)-C(54)-H(54)	119.9
C(54)-C(55)-C(56)	120.5(4)
C(54)-C(55)-H(55)	119.8
C(56)-C(55)-H(55)	119.8
C(51)-C(56)-C(55)	119.3(4)
C(51)-C(56)-H(56)	120.3
C(55)-C(56)-H(56)	120.3



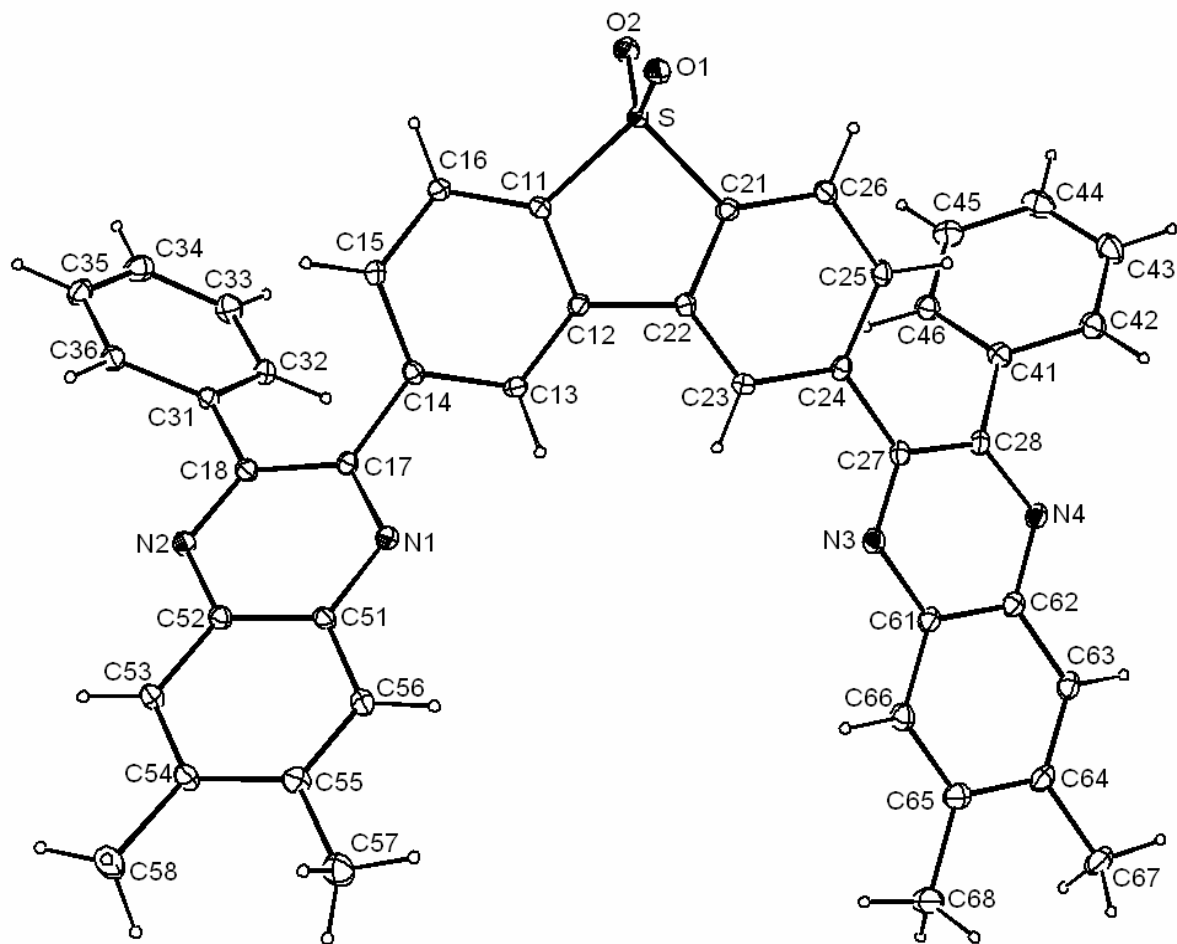
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S	19(1)	22(1)	16(1)	1(1)	3(1)	2(1)
N(14)	19(2)	26(2)	17(2)	3(2)	3(2)	7(2)
N(19)	19(2)	22(2)	23(2)	2(2)	5(2)	6(2)
N(24)	20(2)	21(2)	17(2)	4(1)	3(1)	5(2)
N(29)	19(2)	17(2)	21(2)	0(1)	2(2)	5(1)
C(1)	18(2)	16(2)	21(2)	0(2)	4(2)	5(2)
C(2)	16(2)	16(2)	16(2)	-1(2)	5(2)	5(2)
C(3)	21(2)	19(2)	16(2)	0(2)	6(2)	5(2)
C(4)	17(2)	17(2)	18(2)	-3(2)	4(2)	7(2)
C(5)	21(2)	23(2)	16(2)	-4(2)	2(2)	6(2)
C(6)	22(2)	20(2)	14(2)	3(2)	2(2)	6(2)
C(7)	15(2)	19(2)	21(2)	-4(2)	5(2)	4(2)
C(8)	18(2)	16(2)	18(2)	-1(2)	5(2)	3(2)
C(9)	16(2)	20(2)	18(2)	0(2)	2(2)	3(2)
C(10)	16(2)	18(2)	18(2)	3(2)	5(2)	6(2)
C(11)	20(2)	17(2)	20(2)	-4(2)	0(2)	1(2)
C(12)	16(2)	18(2)	22(2)	2(2)	4(2)	1(2)
C(13)	18(2)	24(2)	15(2)	2(2)	0(2)	6(2)
C(15)	26(2)	32(3)	17(2)	2(2)	7(2)	7(2)
C(16)	26(2)	35(3)	23(2)	7(2)	10(2)	11(2)
C(17)	20(2)	26(2)	30(2)	7(2)	7(2)	6(2)
C(18)	23(2)	18(2)	28(2)	0(2)	3(2)	2(2)
C(20)	17(2)	21(2)	15(2)	5(2)	2(2)	7(2)
C(21)	16(2)	23(2)	19(2)	5(2)	4(2)	5(2)
C(22)	18(2)	22(2)	20(2)	7(2)	6(2)	8(2)
C(23)	17(2)	14(2)	22(2)	-4(2)	3(2)	3(2)
C(25)	22(2)	18(2)	24(2)	1(2)	7(2)	6(2)
C(26)	27(2)	16(2)	26(2)	2(2)	11(2)	6(2)
C(27)	33(3)	17(2)	21(2)	0(2)	9(2)	7(2)
C(28)	27(2)	17(2)	18(2)	0(2)	0(2)	5(2)
C(30)	18(2)	14(2)	17(2)	2(2)	2(2)	2(2)

C(31)	21(2)	13(2)	21(2)	0(2)	4(2)	6(2)
C(32)	21(2)	13(2)	21(2)	1(2)	7(2)	5(2)
C(41)	15(2)	15(2)	19(2)	-3(2)	2(2)	-2(2)
C(42)	23(2)	25(2)	20(2)	2(2)	6(2)	3(2)
C(43)	18(2)	25(2)	34(3)	-1(2)	4(2)	9(2)
C(44)	22(2)	22(2)	28(2)	-3(2)	10(2)	4(2)
C(45)	26(2)	33(3)	20(2)	0(2)	5(2)	4(2)
C(46)	23(2)	29(2)	20(2)	1(2)	3(2)	11(2)
C(51)	16(2)	17(2)	18(2)	5(2)	2(2)	6(2)
C(52)	16(2)	22(2)	20(2)	0(2)	2(2)	4(2)
C(53)	26(2)	22(2)	18(2)	5(2)	6(2)	9(2)
C(54)	17(2)	34(3)	29(2)	13(2)	7(2)	11(2)
C(55)	15(2)	25(2)	32(3)	2(2)	-5(2)	1(2)
C(56)	20(2)	21(2)	22(2)	-2(2)	1(2)	7(2)





化合物 **DQ4** 之 ORTEP 圖

化合物 **DQ4** 之 X-ray 繞射數據

Table 2. Crystal data and structure refinement for DQ4.

Identification code	DQ4	
Empirical formula	C ₄₅ H ₃₄ Cl ₂ N ₄ O ₂ S	
Formula weight	765.72	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9170(2) Å	= 68.236(2)°.
	b = 14.0969(4) Å	= 75.3130(10)°.
	c = 15.0742(4) Å	= 76.9500(10)°.
Volume	1872.71(8) Å ³	
Z	2	
Density (calculated)	1.358 Mg/m ³	
Absorption coefficient	0.274 mm ⁻¹	
F(000)	796	
Crystal size	0.16 x 0.1 x 0.1 mm ³	
Theta range for data collection	1.48 to 25.03°	
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 16, 0 ≤ l ≤ 17	
Reflections collected	6485	
Independent reflections	6485 [R(int) = 0.0397]	
Completeness to theta = 25.03°	97.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6485 / 12 / 536	
Goodness-of-fit on F ²	1.039	
Final R indices [I > 2σ(I)]	R1 = 0.0454, wR2 = 0.1128	
R indices (all data)	R1 = 0.0639, wR2 = 0.1229	
Extinction coefficient	0.0004(7)	
Largest diff. peak and hole	0.305 and -0.563 e.Å ⁻³	

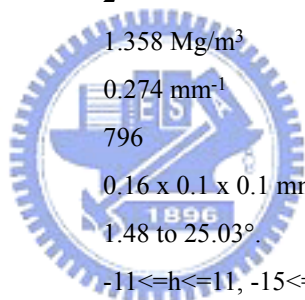


Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S	6475(1)	5312(1)	3669(1)	16(1)
Cl(1)	13738(1)	-455(1)	1977(1)	44(1)
Cl(2)	16668(1)	-1160(1)	1294(1)	58(1)
O(1)	6808(2)	5220(1)	4573(1)	21(1)
O(2)	5300(2)	6068(1)	3350(1)	23(1)
N(1)	8450(2)	637(2)	3503(1)	17(1)
N(2)	6370(2)	-535(2)	3730(1)	17(1)
N(3)	12173(2)	4622(2)	423(1)	18(1)
N(4)	13065(2)	6444(2)	-967(1)	18(1)
C(1)	15271(3)	-1311(2)	2295(2)	36(1)
C(11)	6412(2)	4078(2)	3641(2)	15(1)
C(12)	7562(2)	3797(2)	2988(2)	15(1)
C(13)	7769(2)	2818(2)	2925(2)	15(1)
C(14)	6805(2)	2143(2)	3493(2)	15(1)
C(15)	5630(3)	2458(2)	4120(2)	18(1)
C(16)	5436(3)	3426(2)	4209(2)	17(1)
C(17)	7122(2)	1060(2)	3485(2)	16(1)
C(18)	6073(2)	475(2)	3535(2)	16(1)
C(21)	7981(2)	5486(2)	2738(2)	16(1)
C(22)	8433(2)	4628(2)	2436(2)	16(1)
C(23)	9565(2)	4655(2)	1672(2)	16(1)
C(24)	10231(2)	5531(2)	1223(2)	16(1)
C(25)	9777(3)	6365(2)	1570(2)	19(1)
C(26)	8650(3)	6350(2)	2334(2)	18(1)
C(27)	11453(2)	5536(2)	405(2)	16(1)
C(28)	11859(2)	6469(2)	-348(2)	17(1)
C(31)	4625(2)	963(2)	3370(2)	16(1)
C(32)	4390(3)	1865(2)	2595(2)	20(1)
C(33)	3034(3)	2309(2)	2454(2)	24(1)
C(34)	1894(3)	1868(2)	3090(2)	26(1)
C(35)	2114(3)	967(2)	3858(2)	23(1)

C(36)	3466(3)	509(2)	3988(2)	20(1)
C(41)	10962(3)	7496(2)	-550(2)	19(1)
C(42)	11571(3)	8386(2)	-797(2)	24(1)
C(43)	10752(3)	9348(2)	-1022(2)	30(1)
C(44)	9348(3)	9445(2)	-1031(2)	32(1)
C(45)	8739(3)	8572(2)	-816(2)	28(1)
C(46)	9536(3)	7602(2)	-568(2)	21(1)
C(51)	8774(3)	-392(2)	3656(2)	17(1)
C(52)	7712(3)	-990(2)	3827(2)	17(1)
C(53)	8058(3)	-2074(2)	4108(2)	20(1)
C(54)	9406(3)	-2553(2)	4216(2)	20(1)
C(55)	10491(3)	-1942(2)	4012(2)	21(1)
C(56)	10168(3)	-892(2)	3723(2)	20(1)
C(57)	11962(3)	-2456(2)	4146(3)	31(1)
C(58)	9745(3)	-3710(2)	4566(2)	31(1)
C(61)	13358(3)	4587(2)	-270(2)	18(1)
C(62)	13831(3)	5508(2)	-935(2)	18(1)
C(63)	15076(3)	5449(2)	-1633(2)	21(1)
C(64)	15801(3)	4526(2)	-1695(2)	21(1)
C(65)	15320(3)	3587(2)	-1020(2)	23(1)
C(66)	14124(3)	3634(2)	-330(2)	21(1)
C(67)	17052(3)	4507(3)	-2502(2)	29(1)
C(68)	16123(3)	2573(2)	-1085(2)	30(1)

Table 4. Bond lengths [\AA] and angles [$^\circ$] for DQ4.

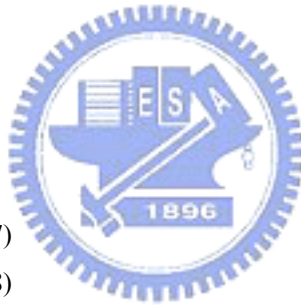
S-O(1)	1.4363(18)
S-O(2)	1.4381(18)
S-C(21)	1.763(2)
S-C(11)	1.770(2)
Cl(1)-C(1)	1.763(3)
Cl(2)-C(1)	1.754(3)
N(1)-C(17)	1.319(3)
N(1)-C(51)	1.356(3)
N(2)-C(18)	1.321(3)
N(2)-C(52)	1.359(3)
N(3)-C(27)	1.319(3)
N(3)-C(61)	1.366(3)
N(4)-C(28)	1.320(3)
N(4)-C(62)	1.356(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(11)-C(16)	1.383(3)
C(11)-C(12)	1.395(3)
C(12)-C(13)	1.383(3)
C(12)-C(22)	1.477(3)
C(13)-C(14)	1.394(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.403(3)
C(14)-C(17)	1.490(3)
C(15)-C(16)	1.386(3)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-C(18)	1.439(3)
C(18)-C(31)	1.484(3)
C(21)-C(26)	1.379(3)
C(21)-C(22)	1.390(3)
C(22)-C(23)	1.385(3)
C(23)-C(24)	1.394(3)
C(23)-H(23)	0.9300



C(24)-C(25)	1.399(3)
C(24)-C(27)	1.492(3)
C(25)-C(26)	1.384(3)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-C(28)	1.443(3)
C(28)-C(41)	1.487(3)
C(31)-C(32)	1.392(4)
C(31)-C(36)	1.396(3)
C(32)-C(33)	1.383(4)
C(32)-H(32)	0.9300
C(33)-C(34)	1.382(4)
C(33)-H(33)	0.9300
C(34)-C(35)	1.384(4)
C(34)-H(34)	0.9300
C(35)-C(36)	1.379(4)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(41)-C(46)	1.394(4)
C(41)-C(42)	1.398(4)
C(42)-C(43)	1.384(4)
C(42)-H(42)	0.9300
C(43)-C(44)	1.371(4)
C(43)-H(43)	0.9300
C(44)-C(45)	1.387(4)
C(44)-H(44)	0.9300
C(45)-C(46)	1.384(4)
C(45)-H(45)	0.9300
C(46)-H(46)	0.9300
C(51)-C(52)	1.410(3)
C(51)-C(56)	1.412(3)
C(52)-C(53)	1.410(3)
C(53)-C(54)	1.375(4)
C(53)-H(53)	0.9300
C(54)-C(55)	1.431(4)
C(54)-C(58)	1.502(4)



C(55)-C(56)	1.365(4)
C(55)-C(57)	1.502(4)
C(56)-H(56)	0.9300
C(57)-H(57A)	0.964(17)
C(57)-H(57B)	0.960(18)
C(57)-H(57C)	0.951(18)
C(58)-H(58A)	0.960(17)
C(58)-H(58B)	0.952(18)
C(58)-H(58C)	0.962(18)
C(61)-C(62)	1.408(4)
C(61)-C(66)	1.409(3)
C(62)-C(63)	1.413(3)
C(63)-C(64)	1.361(4)
C(63)-H(63)	0.9300
C(64)-C(65)	1.434(4)
C(64)-C(67)	1.505(3)
C(65)-C(66)	1.372(3)
C(65)-C(68)	1.495(4)
C(66)-H(66)	0.9300
C(67)-H(67A)	0.954(17)
C(67)-H(67B)	0.961(18)
C(67)-H(67C)	0.971(18)
C(68)-H(68A)	0.976(18)
C(68)-H(68B)	0.964(17)
C(68)-H(68C)	0.979(18)
O(1)-S-O(2)	117.25(10)
O(1)-S-C(21)	110.44(11)
O(2)-S-C(21)	110.23(11)
O(1)-S-C(11)	110.27(11)
O(2)-S-C(11)	113.28(11)
C(21)-S-C(11)	92.68(11)
C(17)-N(1)-C(51)	117.8(2)
C(18)-N(2)-C(52)	117.9(2)
C(27)-N(3)-C(61)	117.9(2)
C(28)-N(4)-C(62)	117.9(2)



Cl(2)-C(1)-Cl(1)	111.28(17)
Cl(2)-C(1)-H(1A)	109.4
Cl(1)-C(1)-H(1A)	109.4
Cl(2)-C(1)-H(1B)	109.4
Cl(1)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	108.0
C(16)-C(11)-C(12)	122.4(2)
C(16)-C(11)-S	127.08(18)
C(12)-C(11)-S	110.45(18)
C(13)-C(12)-C(11)	119.2(2)
C(13)-C(12)-C(22)	127.9(2)
C(11)-C(12)-C(22)	112.9(2)
C(12)-C(13)-C(14)	119.7(2)
C(12)-C(13)-H(13)	120.2
C(14)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	120.0(2)
C(13)-C(14)-C(17)	118.6(2)
C(15)-C(14)-C(17)	121.1(2)
C(16)-C(15)-C(14)	120.7(2)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(11)-C(16)-C(15)	118.0(2)
C(11)-C(16)-H(16)	121.0
C(15)-C(16)-H(16)	121.0
N(1)-C(17)-C(18)	121.3(2)
N(1)-C(17)-C(14)	114.5(2)
C(18)-C(17)-C(14)	124.0(2)
N(2)-C(18)-C(17)	120.6(2)
N(2)-C(18)-C(31)	116.9(2)
C(17)-C(18)-C(31)	122.5(2)
C(26)-C(21)-C(22)	122.6(2)
C(26)-C(21)-S	126.23(18)
C(22)-C(21)-S	111.16(18)
C(23)-C(22)-C(21)	118.9(2)
C(23)-C(22)-C(12)	128.5(2)
C(21)-C(22)-C(12)	112.6(2)



C(22)-C(23)-C(24)	119.9(2)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	119.5(2)
C(23)-C(24)-C(27)	118.8(2)
C(25)-C(24)-C(27)	121.7(2)
C(26)-C(25)-C(24)	121.2(2)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(21)-C(26)-C(25)	117.8(2)
C(21)-C(26)-H(26)	121.1
C(25)-C(26)-H(26)	121.1
N(3)-C(27)-C(28)	121.3(2)
N(3)-C(27)-C(24)	115.5(2)
C(28)-C(27)-C(24)	123.2(2)
N(4)-C(28)-C(27)	120.6(2)
N(4)-C(28)-C(41)	114.4(2)
C(27)-C(28)-C(41)	124.9(2)
C(32)-C(31)-C(36)	118.6(2)
C(32)-C(31)-C(18)	121.4(2)
C(36)-C(31)-C(18)	120.1(2)
C(33)-C(32)-C(31)	120.5(2)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(34)-C(33)-C(32)	120.2(3)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	119.8(2)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(36)-C(35)-C(34)	120.1(2)
C(36)-C(35)-H(35)	119.9
C(34)-C(35)-H(35)	119.9
C(35)-C(36)-C(31)	120.7(2)
C(35)-C(36)-H(36)	119.6
C(31)-C(36)-H(36)	119.6



C(46)-C(41)-C(42)	118.8(2)
C(46)-C(41)-C(28)	121.2(2)
C(42)-C(41)-C(28)	119.8(2)
C(43)-C(42)-C(41)	120.1(3)
C(43)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(44)-C(43)-C(42)	120.6(3)
C(44)-C(43)-H(43)	119.7
C(42)-C(43)-H(43)	119.7
C(43)-C(44)-C(45)	119.9(3)
C(43)-C(44)-H(44)	120.1
C(45)-C(44)-H(44)	120.1
C(46)-C(45)-C(44)	120.2(3)
C(46)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(45)-C(46)-C(41)	120.3(3)
C(45)-C(46)-H(46)	119.8
C(41)-C(46)-H(46)	119.8
N(1)-C(51)-C(52)	120.6(2)
N(1)-C(51)-C(56)	120.1(2)
C(52)-C(51)-C(56)	119.1(2)
N(2)-C(52)-C(51)	120.9(2)
N(2)-C(52)-C(53)	120.1(2)
C(51)-C(52)-C(53)	119.0(2)
C(54)-C(53)-C(52)	121.3(2)
C(54)-C(53)-H(53)	119.4
C(52)-C(53)-H(53)	119.4
C(53)-C(54)-C(55)	119.6(2)
C(53)-C(54)-C(58)	120.7(2)
C(55)-C(54)-C(58)	119.7(2)
C(56)-C(55)-C(54)	119.4(2)
C(56)-C(55)-C(57)	120.4(2)
C(54)-C(55)-C(57)	120.1(2)
C(55)-C(56)-C(51)	121.6(2)
C(55)-C(56)-H(56)	119.2
C(51)-C(56)-H(56)	119.2



C(55)-C(57)-H(57A)	111.0(18)
C(55)-C(57)-H(57B)	109(2)
H(57A)-C(57)-H(57B)	111(3)
C(55)-C(57)-H(57C)	108(2)
H(57A)-C(57)-H(57C)	108(3)
H(57B)-C(57)-H(57C)	110(3)
C(54)-C(58)-H(58A)	109.1(18)
C(54)-C(58)-H(58B)	109(2)
H(58A)-C(58)-H(58B)	113(3)
C(54)-C(58)-H(58C)	107.8(19)
H(58A)-C(58)-H(58C)	109(3)
H(58B)-C(58)-H(58C)	109(3)
N(3)-C(61)-C(62)	120.2(2)
N(3)-C(61)-C(66)	120.7(2)
C(62)-C(61)-C(66)	119.1(2)
N(4)-C(62)-C(61)	121.5(2)
N(4)-C(62)-C(63)	119.4(2)
C(61)-C(62)-C(63)	119.0(2)
C(64)-C(63)-C(62)	121.6(2)
C(64)-C(63)-H(63)	119.2
C(62)-C(63)-H(63)	119.2
C(63)-C(64)-C(65)	119.5(2)
C(63)-C(64)-C(67)	119.5(3)
C(65)-C(64)-C(67)	120.9(2)
C(66)-C(65)-C(64)	119.4(2)
C(66)-C(65)-C(68)	121.1(3)
C(64)-C(65)-C(68)	119.5(2)
C(65)-C(66)-C(61)	121.4(2)
C(65)-C(66)-H(66)	119.3
C(61)-C(66)-H(66)	119.3
C(64)-C(67)-H(67A)	110.2(17)
C(64)-C(67)-H(67B)	111.5(19)
H(67A)-C(67)-H(67B)	107(3)
C(64)-C(67)-H(67C)	110.2(18)
H(67A)-C(67)-H(67C)	109(3)
H(67B)-C(67)-H(67C)	109(3)



C(65)-C(68)-H(68A)	113.1(18)
C(65)-C(68)-H(68B)	111.0(18)
H(68A)-C(68)-H(68B)	109(3)
C(65)-C(68)-H(68C)	109.6(18)
H(68A)-C(68)-H(68C)	105(3)
H(68B)-C(68)-H(68C)	108(3)

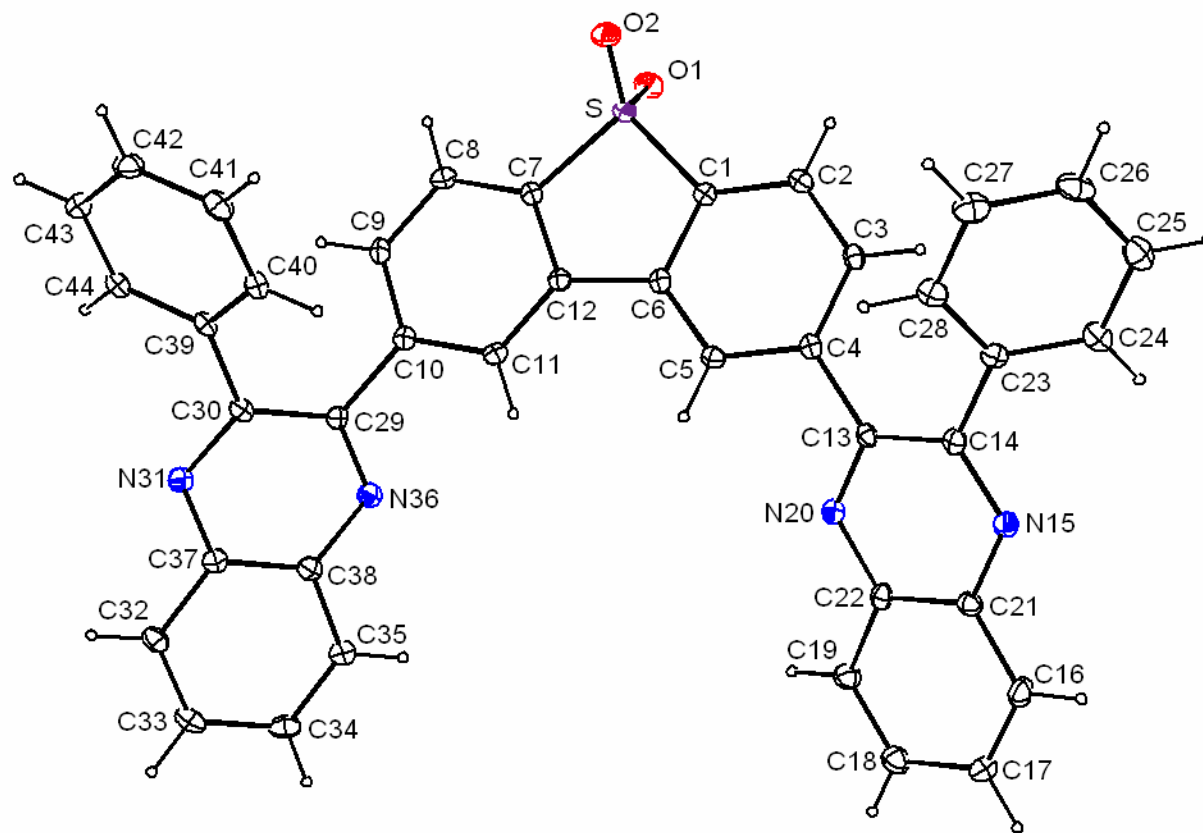
Symmetry transformations used to generate equivalent atoms:



Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ4. The anisotropic displacement factor exponent takes the form: $-2 \sum [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
S	16(1)	13(1)	19(1)	-7(1)	2(1)	-4(1)
Cl(1)	44(1)	38(1)	52(1)	-21(1)	-18(1)	9(1)
Cl(2)	37(1)	62(1)	70(1)	-19(1)	-4(1)	-8(1)
O(1)	25(1)	22(1)	18(1)	-10(1)	2(1)	-7(1)
O(2)	20(1)	16(1)	29(1)	-7(1)	-1(1)	-1(1)
N(1)	17(1)	15(1)	17(1)	-5(1)	1(1)	-3(1)
N(2)	19(1)	16(1)	17(1)	-6(1)	-2(1)	-4(1)
N(3)	19(1)	18(1)	17(1)	-5(1)	-1(1)	-5(1)
N(4)	17(1)	21(1)	17(1)	-6(1)	0(1)	-7(1)
C(1)	41(2)	31(2)	41(2)	-11(2)	-18(2)	-7(1)
C(11)	17(1)	12(1)	16(1)	-5(1)	-4(1)	-1(1)
C(12)	14(1)	15(1)	13(1)	-4(1)	0(1)	-3(1)
C(13)	14(1)	15(1)	14(1)	-5(1)	-1(1)	0(1)
C(14)	16(1)	12(1)	16(1)	-4(1)	-4(1)	-2(1)
C(15)	18(1)	15(1)	19(1)	-4(1)	0(1)	-5(1)
C(16)	17(1)	16(1)	18(1)	-6(1)	2(1)	-3(1)
C(17)	18(1)	14(1)	12(1)	-3(1)	1(1)	-4(1)
C(18)	20(1)	14(1)	13(1)	-5(1)	1(1)	-5(1)
C(21)	17(1)	16(1)	14(1)	-5(1)	-1(1)	-2(1)
C(22)	17(1)	14(1)	16(1)	-4(1)	-2(1)	-3(1)
C(23)	16(1)	15(1)	17(1)	-7(1)	-2(1)	-1(1)
C(24)	15(1)	16(1)	14(1)	-3(1)	-3(1)	-3(1)
C(25)	21(1)	15(1)	18(1)	-3(1)	-1(1)	-7(1)
C(26)	21(1)	16(1)	19(1)	-7(1)	-2(1)	-4(1)
C(27)	16(1)	17(1)	16(1)	-5(1)	-3(1)	-6(1)
C(28)	17(1)	19(1)	16(1)	-5(1)	-2(1)	-7(1)
C(31)	18(1)	16(1)	16(1)	-8(1)	-1(1)	-5(1)
C(32)	20(1)	18(1)	20(1)	-6(1)	1(1)	-7(1)
C(33)	27(2)	20(2)	23(1)	-3(1)	-8(1)	-2(1)
C(34)	18(1)	33(2)	32(2)	-16(1)	-7(1)	0(1)
C(35)	18(1)	30(2)	24(1)	-14(1)	1(1)	-8(1)

C(36)	25(1)	19(1)	17(1)	-7(1)	0(1)	-7(1)
C(41)	25(1)	18(1)	12(1)	-3(1)	-1(1)	-6(1)
C(42)	27(1)	22(2)	21(1)	-6(1)	0(1)	-7(1)
C(43)	38(2)	20(2)	32(2)	-6(1)	-3(1)	-10(1)
C(44)	41(2)	17(2)	33(2)	-6(1)	-10(1)	3(1)
C(45)	27(2)	26(2)	30(2)	-11(1)	-5(1)	1(1)
C(46)	24(1)	19(1)	20(1)	-6(1)	-1(1)	-5(1)
C(51)	21(1)	11(1)	16(1)	-4(1)	0(1)	-3(1)
C(52)	20(1)	15(1)	15(1)	-5(1)	-1(1)	-4(1)
C(53)	22(1)	15(1)	23(1)	-7(1)	-1(1)	-5(1)
C(54)	24(1)	13(1)	23(1)	-5(1)	-3(1)	-3(1)
C(55)	22(1)	18(1)	23(1)	-7(1)	-3(1)	-2(1)
C(56)	19(1)	15(1)	25(1)	-7(1)	-3(1)	-4(1)
C(57)	25(2)	21(2)	45(2)	-9(2)	-10(1)	0(1)
C(58)	28(2)	18(2)	46(2)	-8(1)	-9(2)	-3(1)
C(61)	17(1)	21(1)	16(1)	-6(1)	-1(1)	-6(1)
C(62)	17(1)	23(2)	17(1)	-7(1)	-3(1)	-5(1)
C(63)	20(1)	25(2)	19(1)	-6(1)	0(1)	-9(1)
C(64)	14(1)	32(2)	21(1)	-13(1)	-2(1)	-5(1)
C(65)	20(1)	27(2)	24(1)	-12(1)	-7(1)	-1(1)
C(66)	22(1)	20(1)	20(1)	-5(1)	-2(1)	-5(1)
C(67)	17(1)	39(2)	29(2)	-16(2)	3(1)	-6(1)
C(68)	27(2)	29(2)	34(2)	-17(2)	-3(1)	2(1)



化合物 **DQ6** 之 ORTEP 圖

化合物 DQ6 之 X-ray 繞射數據

Table 1. Crystal data and structure refinement for DQ6.

Identification code	DQ6	
Empirical formula	C ₄₀ H ₂₄ N ₄ O ₂ S	
Formula weight	624.69	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.7261(3) Å	= 107.719(2)°.
	b = 12.0606(4) Å	= 103.656(2)°.
	c = 13.4213(4) Å	= 108.751(2)°.
Volume	1454.81(8) Å ³	
Z	2	
Density (calculated)	1.426 Mg/m ³	
Absorption coefficient	0.158 mm ⁻¹	
F(000)	648	
Crystal size	0.16 x 0.15 x 0.14 mm ³	
Theta range for data collection	1.71 to 25.03°	
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 13, -15 ≤ l ≤ 14	
Reflections collected	10660	
Independent reflections	5107 [R(int) = 0.0424]	
Completeness to theta = 25.03°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9803 and 0.8731	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5107 / 0 / 425	
Goodness-of-fit on F ²	0.817	
Final R indices [I > 2σ(I)]	R1 = 0.0372, wR2 = 0.0629	
R indices (all data)	R1 = 0.0627, wR2 = 0.0660	
Extinction coefficient	0.0012(4)	
Largest diff. peak and hole	0.309 and -0.376 e.Å ⁻³	

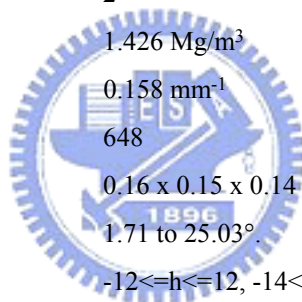


Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ6. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
S	6504(1)	2736(1)	1265(1)	19(1)
O(1)	7636(1)	2431(1)	1724(1)	24(1)
O(2)	6801(1)	4078(1)	1626(1)	25(1)
N(15)	-1070(2)	-1346(2)	1698(1)	20(1)
N(20)	400(2)	-1722(2)	249(1)	20(1)
N(31)	2753(2)	-410(2)	-5622(1)	19(1)
N(36)	2736(2)	-1489(2)	-4030(1)	20(1)
C(1)	4914(2)	1876(2)	1393(2)	16(1)
C(2)	4673(2)	1949(2)	2371(2)	20(1)
C(3)	3345(2)	1182(2)	2289(2)	18(1)
C(4)	2265(2)	340(2)	1238(2)	16(1)
C(5)	2536(2)	276(2)	264(2)	17(1)
C(6)	3859(2)	1045(2)	333(2)	16(1)
C(7)	5770(2)	1931(2)	-226(2)	17(1)
C(8)	6462(2)	2094(2)	-950(2)	19(1)
C(9)	5678(2)	1390(2)	-2096(2)	19(1)
C(10)	4259(2)	531(2)	-2499(2)	17(1)
C(11)	3600(2)	361(2)	-1747(2)	18(1)
C(12)	4359(2)	1080(2)	-600(2)	16(1)
C(13)	869(2)	-605(2)	1100(2)	16(1)
C(14)	91(2)	-398(2)	1828(2)	18(1)
C(16)	-2768(2)	-3543(2)	655(2)	26(1)
C(17)	-3249(2)	-4702(2)	-232(2)	26(1)
C(18)	-2533(2)	-4876(2)	-980(2)	26(1)
C(19)	-1342(2)	-3892(2)	-819(2)	24(1)
C(21)	-1550(2)	-2515(2)	826(2)	19(1)
C(22)	-825(2)	-2691(2)	81(2)	19(1)
C(23)	521(2)	866(2)	2751(2)	19(1)
C(24)	451(2)	919(2)	3789(2)	24(1)
C(25)	885(2)	2094(2)	4667(2)	30(1)
C(26)	1370(2)	3215(2)	4519(2)	32(1)

C(27)	1393(2)	3170(2)	3483(2)	30(1)
C(28)	961(2)	2002(2)	2605(2)	24(1)
C(29)	3435(2)	-243(2)	-3728(2)	15(1)
C(30)	3412(2)	315(2)	-4526(2)	16(1)
C(32)	1202(2)	-2509(2)	-7106(2)	22(1)
C(33)	377(2)	-3768(2)	-7429(2)	25(1)
C(34)	342(2)	-4310(2)	-6633(2)	25(1)
C(35)	1143(2)	-3571(2)	-5519(2)	22(1)
C(37)	2015(2)	-1699(2)	-5953(2)	19(1)
C(38)	1975(2)	-2238(2)	-5156(2)	19(1)
C(39)	4042(2)	1726(2)	-4186(2)	18(1)
C(40)	3745(2)	2529(2)	-3367(2)	22(1)
C(41)	4253(2)	3833(2)	-3106(2)	25(1)
C(42)	5071(2)	4352(2)	-3646(2)	27(1)
C(43)	5377(2)	3576(2)	-4453(2)	24(1)
C(44)	4857(2)	2266(2)	-4721(2)	20(1)

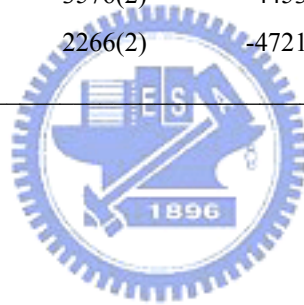


Table 3. Bond lengths [\AA] and angles [$^\circ$] for DQ6.

S-O(1)	1.4353(13)
S-O(2)	1.4407(13)
S-C(1)	1.7669(19)
S-C(7)	1.7747(19)
N(15)-C(14)	1.322(2)
N(15)-C(21)	1.366(2)
N(20)-C(13)	1.315(2)
N(20)-C(22)	1.362(2)
N(31)-C(30)	1.325(2)
N(31)-C(37)	1.365(2)
N(36)-C(29)	1.320(2)
N(36)-C(38)	1.370(2)
C(1)-C(2)	1.380(2)
C(1)-C(6)	1.397(2)
C(2)-C(3)	1.383(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.401(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.391(2)
C(4)-C(13)	1.489(2)
C(5)-C(6)	1.386(2)
C(5)-H(5)	0.9300
C(6)-C(12)	1.480(3)
C(7)-C(8)	1.377(2)
C(7)-C(12)	1.388(2)
C(8)-C(9)	1.389(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.393(2)
C(9)-H(9)	0.9300
C(10)-C(11)	1.389(2)
C(10)-C(29)	1.489(2)
C(11)-C(12)	1.389(2)
C(11)-H(11)	0.9300
C(13)-C(14)	1.444(2)



C(14)-C(23)	1.483(3)
C(16)-C(17)	1.368(3)
C(16)-C(21)	1.393(2)
C(16)-H(16)	0.9300
C(17)-C(18)	1.408(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.351(3)
C(18)-H(18)	0.9300
C(19)-C(22)	1.402(3)
C(19)-H(19)	0.9300
C(21)-C(22)	1.413(2)
C(23)-C(28)	1.389(3)
C(23)-C(24)	1.396(3)
C(24)-C(25)	1.384(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.378(3)
C(25)-H(25)	0.9300
C(26)-C(27)	1.381(3)
C(26)-H(26)	0.9300
C(27)-C(28)	1.378(3)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-C(30)	1.428(3)
C(30)-C(39)	1.484(3)
C(32)-C(33)	1.353(3)
C(32)-C(37)	1.416(2)
C(32)-H(32)	0.9300
C(33)-C(34)	1.413(3)
C(33)-H(33)	0.9300
C(34)-C(35)	1.363(2)
C(34)-H(34)	0.9300
C(35)-C(38)	1.419(3)
C(35)-H(35)	0.9300
C(37)-C(38)	1.413(3)
C(39)-C(44)	1.385(2)
C(39)-C(40)	1.401(2)



C(40)-C(41)	1.384(3)
C(40)-H(40)	0.9300
C(41)-C(42)	1.382(3)
C(41)-H(41)	0.9300
C(42)-C(43)	1.381(3)
C(42)-H(42)	0.9300
C(43)-C(44)	1.389(3)
C(43)-H(43)	0.9300
C(44)-H(44)	0.9300
O(1)-S-O(2)	117.01(8)
O(1)-S-C(1)	112.40(9)
O(2)-S-C(1)	110.57(8)
O(1)-S-C(7)	110.72(8)
O(2)-S-C(7)	110.94(9)
C(1)-S-C(7)	92.60(9)
C(14)-N(15)-C(21)	118.26(17)
C(13)-N(20)-C(22)	118.56(17)
C(30)-N(31)-C(37)	117.41(17)
C(29)-N(36)-C(38)	117.08(17)
C(2)-C(1)-C(6)	121.64(18)
C(2)-C(1)-S	127.57(15)
C(6)-C(1)-S	110.78(14)
C(1)-C(2)-C(3)	118.62(18)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	121.04(18)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	119.36(18)
C(5)-C(4)-C(13)	117.04(16)
C(3)-C(4)-C(13)	123.28(17)
C(6)-C(5)-C(4)	120.22(17)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	119.12(17)



C(5)-C(6)-C(12)	128.05(17)
C(1)-C(6)-C(12)	112.79(17)
C(8)-C(7)-C(12)	122.64(17)
C(8)-C(7)-S	126.47(15)
C(12)-C(7)-S	110.89(14)
C(7)-C(8)-C(9)	117.29(17)
C(7)-C(8)-H(8)	121.4
C(9)-C(8)-H(8)	121.4
C(8)-C(9)-C(10)	121.48(18)
C(8)-C(9)-H(9)	119.3
C(10)-C(9)-H(9)	119.3
C(11)-C(10)-C(9)	119.90(17)
C(11)-C(10)-C(29)	118.88(17)
C(9)-C(10)-C(29)	121.20(17)
C(12)-C(11)-C(10)	119.33(17)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3
C(7)-C(12)-C(11)	119.31(17)
C(7)-C(12)-C(6)	112.89(16)
C(11)-C(12)-C(6)	127.79(17)
N(20)-C(13)-C(14)	120.87(17)
N(20)-C(13)-C(4)	113.17(17)
C(14)-C(13)-C(4)	125.89(17)
N(15)-C(14)-C(13)	121.05(17)
N(15)-C(14)-C(23)	115.88(17)
C(13)-C(14)-C(23)	123.07(17)
C(17)-C(16)-C(21)	119.78(19)
C(17)-C(16)-H(16)	120.1
C(21)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	121.02(19)
C(16)-C(17)-H(17)	119.5
C(18)-C(17)-H(17)	119.5
C(19)-C(18)-C(17)	119.9(2)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(22)	120.36(19)



C(18)-C(19)-H(19)	119.8
C(22)-C(19)-H(19)	119.8
N(15)-C(21)-C(16)	120.41(18)
N(15)-C(21)-C(22)	120.37(17)
C(16)-C(21)-C(22)	119.22(18)
N(20)-C(22)-C(19)	119.53(18)
N(20)-C(22)-C(21)	120.76(18)
C(19)-C(22)-C(21)	119.67(18)
C(28)-C(23)-C(24)	118.77(18)
C(28)-C(23)-C(14)	121.84(18)
C(24)-C(23)-C(14)	119.37(18)
C(25)-C(24)-C(23)	120.0(2)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(26)-C(25)-C(24)	120.3(2)
C(26)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	120.1(2)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(28)-C(27)-C(26)	119.8(2)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(23)	120.92(19)
C(27)-C(28)-H(28)	119.5
C(23)-C(28)-H(28)	119.5
N(36)-C(29)-C(30)	122.23(17)
N(36)-C(29)-C(10)	115.19(17)
C(30)-C(29)-C(10)	122.58(17)
N(31)-C(30)-C(29)	121.18(18)
N(31)-C(30)-C(39)	116.14(17)
C(29)-C(30)-C(39)	122.59(17)
C(33)-C(32)-C(37)	120.3(2)
C(33)-C(32)-H(32)	119.9
C(37)-C(32)-H(32)	119.9
C(32)-C(33)-C(34)	120.98(19)



C(32)-C(33)-H(33)	119.5
C(34)-C(33)-H(33)	119.5
C(35)-C(34)-C(33)	120.49(19)
C(35)-C(34)-H(34)	119.8
C(33)-C(34)-H(34)	119.8
C(34)-C(35)-C(38)	119.5(2)
C(34)-C(35)-H(35)	120.3
C(38)-C(35)-H(35)	120.3
N(31)-C(37)-C(38)	121.13(17)
N(31)-C(37)-C(32)	119.99(18)
C(38)-C(37)-C(32)	118.77(18)
N(36)-C(38)-C(37)	120.74(18)
N(36)-C(38)-C(35)	119.35(18)
C(37)-C(38)-C(35)	119.91(17)
C(44)-C(39)-C(40)	118.60(18)
C(44)-C(39)-C(30)	120.81(17)
C(40)-C(39)-C(30)	120.46(18)
C(41)-C(40)-C(39)	120.45(19)
C(41)-C(40)-H(40)	119.8
C(39)-C(40)-H(40)	119.8
C(42)-C(41)-C(40)	119.95(19)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(43)-C(42)-C(41)	120.4(2)
C(43)-C(42)-H(42)	119.8
C(41)-C(42)-H(42)	119.8
C(42)-C(43)-C(44)	119.54(19)
C(42)-C(43)-H(43)	120.2
C(44)-C(43)-H(43)	120.2
C(39)-C(44)-C(43)	121.04(18)
C(39)-C(44)-H(44)	119.5
C(43)-C(44)-H(44)	119.5

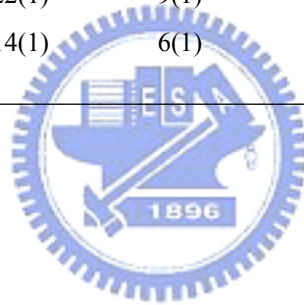


Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for DQ6. The anisotropic displacement factor exponent takes the form: $-2 \left[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} \right]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S	19(1)	18(1)	17(1)	6(1)	6(1)	6(1)
O(1)	15(1)	30(1)	24(1)	10(1)	2(1)	10(1)
O(2)	29(1)	14(1)	26(1)	4(1)	9(1)	7(1)
N(15)	21(1)	20(1)	20(1)	8(1)	8(1)	9(1)
N(20)	21(1)	21(1)	19(1)	10(1)	8(1)	8(1)
N(31)	20(1)	20(1)	20(1)	7(1)	9(1)	10(1)
N(36)	18(1)	22(1)	19(1)	7(1)	8(1)	9(1)
C(1)	16(1)	16(1)	17(1)	7(1)	6(1)	9(1)
C(2)	21(1)	18(1)	16(1)	4(1)	4(1)	9(1)
C(3)	21(1)	20(1)	16(1)	7(1)	9(1)	11(1)
C(4)	20(1)	17(1)	17(1)	8(1)	8(1)	12(1)
C(5)	17(1)	16(1)	16(1)	6(1)	3(1)	8(1)
C(6)	20(1)	16(1)	18(1)	9(1)	8(1)	12(1)
C(7)	19(1)	16(1)	17(1)	7(1)	7(1)	10(1)
C(8)	17(1)	16(1)	24(1)	7(1)	7(1)	7(1)
C(9)	23(1)	21(1)	18(1)	10(1)	11(1)	12(1)
C(10)	19(1)	17(1)	19(1)	9(1)	9(1)	11(1)
C(11)	17(1)	15(1)	21(1)	7(1)	8(1)	8(1)
C(12)	19(1)	13(1)	18(1)	7(1)	7(1)	8(1)
C(13)	20(1)	16(1)	14(1)	8(1)	6(1)	10(1)
C(14)	19(1)	22(1)	18(1)	13(1)	7(1)	12(1)
C(16)	22(1)	32(1)	28(1)	15(1)	14(1)	11(1)
C(17)	22(1)	24(1)	28(1)	11(1)	9(1)	5(1)
C(18)	31(1)	22(1)	22(1)	7(1)	7(1)	10(1)
C(19)	23(1)	23(1)	22(1)	4(1)	10(1)	8(1)
C(21)	19(1)	19(1)	18(1)	8(1)	4(1)	8(1)
C(22)	20(1)	22(1)	20(1)	12(1)	9(1)	11(1)
C(23)	15(1)	20(1)	20(1)	6(1)	6(1)	9(1)
C(24)	23(1)	28(1)	21(1)	7(1)	6(1)	14(1)
C(25)	26(1)	39(2)	25(1)	10(1)	11(1)	18(1)
C(26)	24(1)	27(1)	31(1)	-2(1)	7(1)	12(1)

C(27)	28(1)	24(1)	37(2)	10(1)	11(1)	13(1)
C(28)	23(1)	24(1)	24(1)	9(1)	5(1)	12(1)
C(29)	14(1)	17(1)	17(1)	6(1)	9(1)	8(1)
C(30)	15(1)	20(1)	16(1)	5(1)	7(1)	11(1)
C(32)	20(1)	27(1)	18(1)	7(1)	5(1)	13(1)
C(33)	25(1)	25(1)	18(1)	1(1)	1(1)	13(1)
C(34)	22(1)	15(1)	31(1)	3(1)	7(1)	7(1)
C(35)	20(1)	20(1)	25(1)	9(1)	9(1)	10(1)
C(37)	17(1)	20(1)	22(1)	8(1)	8(1)	10(1)
C(38)	15(1)	23(1)	20(1)	7(1)	7(1)	9(1)
C(39)	18(1)	22(1)	12(1)	6(1)	3(1)	10(1)
C(40)	24(1)	26(1)	18(1)	10(1)	9(1)	13(1)
C(41)	29(1)	26(1)	20(1)	6(1)	8(1)	17(1)
C(42)	30(1)	17(1)	25(1)	7(1)	2(1)	6(1)
C(43)	23(1)	22(1)	22(1)	9(1)	8(1)	5(1)
C(44)	22(1)	24(1)	14(1)	6(1)	5(1)	11(1)



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