Sulfur-based protecting groups for pyrroles and the facile deprotection of 2-(2,4-dinitrobenzene)sulfinyl and sulfonyl pyrroles

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Supplementary Information

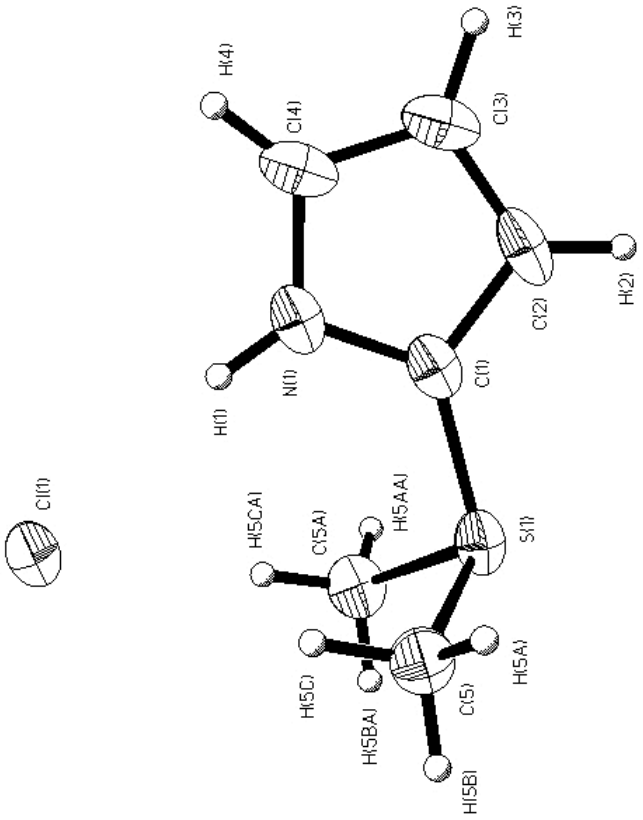
Table of Contents

General Experimental Procedures

Proton and carbon nuclear magnetic resonance (NMR) spectra were recorded at 250 or 500 and 63 or 125 MHz, respectively. Chemical shifts (δ_H and δ_C) are quoted in parts per million (ppm), referenced to the appropriate residual solvent peak, and all coupling constants are reported in hertz (Hz). Mass spectra are reported in units of mass over charge (*m/z*) for all values between 50 and the molecular ion, if over 10% of the base peak. Intensities are reported in parentheses as a percentage of the base peak. Melting points were collected on a hot-stage apparatus and are uncorrected. Nitrogen-purged dichloromethane was dried by passing it through two columns of activated alumina using an Innovative Technology solvent purification system. All other reagents and solvents were used as received.

Crystallographic Data

Dimethyl(2-pyrrolyl)sulphonium chloride (1)



Crystal data and structure refinement. CCDC 244774

Empirical formula	C6 H10 Cl N S	
Formula weight	163.66	
Temperature	143(2) K	
Wavelength	0.7107 Å	
Crystal system	Orthorhombic	
Space group	*Pnma*	
Unit cell dimensions	a = 10.792(4) Å	α= 90°
	b = 7.052(2) Å	β= 90°
	c = 10.863(2) Å	γ = 90°
Volume	826.8(4) Å^3	
Z	4 Density (calculated)	1.315 Mg/m^3
Absorption coefficient	0.631 mm^{-1}	
F(000)	344	
Crystal size	0.22 x 0.11 x 0.08 mm^3	

Theta range for data collection	2.66 to 30.05°
Index ranges	-15<=h<=12, -6<=k<=8, -12<=l<=0
Reflections collected	1750
Independent reflections	806 [R(int) = 0.0490]
Completeness to theta = 30.05°	61.8 %.
Absorption correction	None
Max. and min. transmission	0.951 and 0.874
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	806 / 0 / 53
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0389, wR2 = 0.0999
R indices (all data)	R1 = 0.1071, wR2 = 0.1198
Largest diff. peak and hole	0.962 and -0.278 e.$Å^{-3}$

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3).
U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8532(1)	2500	6545(1)	41(1)
S(1)	6763(1)	2500	9941(1)	31(1)
N(1)	9250(4)	2500	9385(4)	31(1)
C(1)	8336(5)	2500	10247(4)	30(1)
C(2)	8894(6)	2500	11392(5)	37(1)
C(3)	10166(5)	2500	11194(5)	41(1)
C(4)	10370(5)	2500	9948(5)	36(1)
C(5)	6536(3)	4463(5)	8918(3)	34(1)

Table 2. Bond lengths [Å].

S(1)-C(1)	1.730(6)
S(1)-C(5)#1	1.792(4)
S(1)-C(5)	1.792(4)
N(1)-C(4)	1.354(7)
N(1)-C(1)	1.360(7)
N(1)-H(1)	0.8800
C(1)-C(2)	1.382(7)
C(2)-C(3)	1.389(8)

C(2)-H(2)	0.9500
C(3)-C(4)	1.372(8)
C(3)-H(3)	0.9500
C(4)-H(4)	0.9500
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800

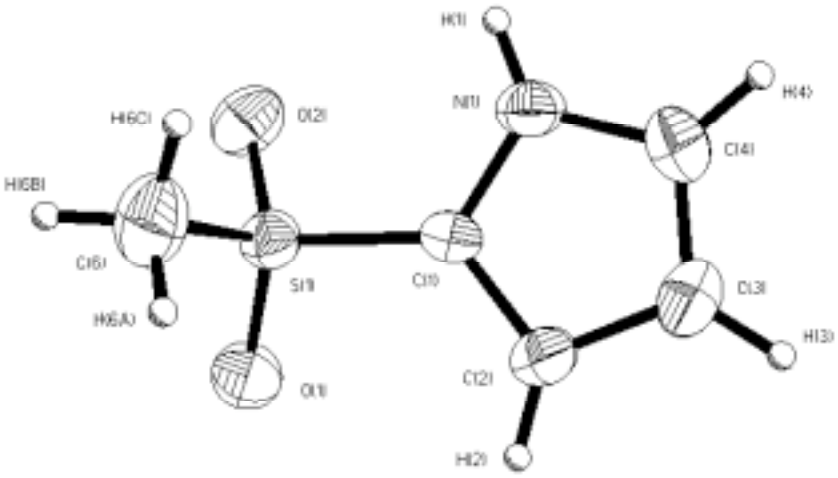
Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z

Table 3. Bond angles [°].

C(1)-S(1)-C(5)#1	104.68(16)
C(1)-S(1)-C(5)	104.68(16)
C(5)#1-S(1)-C(5)	101.1(2)
C(4)-N(1)-C(1)	109.6(4)
C(4)-N(1)-H(1)	125.2
C(1)-N(1)-H(1)	125.2
N(1)-C(1)-C(2)	107.7(5)
N(1)-C(1)-S(1)	125.4(4)
C(2)-C(1)-S(1)	126.9(4)
C(1)-C(2)-C(3)	106.9(5)
C(1)-C(2)-H(2)	126.5
C(3)-C(2)-H(2)	126.5
C(4)-C(3)-C(2)	108.1(5)
C(4)-C(3)-H(3)	125.9
C(2)-C(3)-H(3)	125.9
N(1)-C(4)-C(3)	107.6(5)
N(1)-C(4)-H(4)	126.2
C(3)-C(4)-H(4)	126.2
S(1)-C(5)-H(5A)	109.5
S(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
S(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z

2-(Methylsulfonyl)pyrrole (4)



Crystal data and structure refinement. CCDC 244775

Empirical formula	C5 H7 N1 O2 S1	
Formula weight	145.18	
Temperature	296(2) K	
Wavelength	0.7107 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 8.201(2) Å	α= 90°
	b = 10.060(3) Å	β= 90°
	c = 7.764(2) Å	γ = 90°
Volume	640.6(3) Å^3	
Z	4	
Density (calculated)	1.505 Mg/m^3	
Absorption coefficient	0.423 mm^{-1}	
F(000)	304	
Crystal size	0.42 x 0.23 x 0.18 mm^3	
Theta range for data collection	2.63 to 30.05°	
Index ranges	0<=h<=11, 0<=k<=14, 0<=l<=10	
Reflections collected	1118	
Independent reflections	1102 [R(int) = 0.0000]	
Completeness to theta = 30.05°	100.0 %	
Absorption correction	Psi scan	
Max. and min. transmission	0.928 and 0.842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1102 / 0 / 82	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0294, wR2 = 0.0812	

R indices (all data)	R1 = 0.0925, wR2 = 0.0982
Absolute structure parameter	0.20(18)
Largest diff. peak and hole	0.259 and -0.240 e.Å^{-3}

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3).
U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5017(1)	1615(1)	1883(1)	34(1)
O(1)	5204(4)	2965(2)	1308(3)	53(1)
O(2)	3623(3)	885(3)	1307(3)	49(1)
N(1)	4338(3)	668(2)	5085(4)	37(1)
C(1)	5001(5)	1653(2)	4104(3)	32(1)
C(2)	5615(4)	2616(3)	5169(5)	40(1)
C(3)	5300(4)	2205(3)	6855(4)	43(1)
C(4)	4511(4)	1018(3)	6766(4)	42(1)
C(6)	6757(4)	714(4)	1292(5)	53(1)

Table 2. Bond lengths [Å].

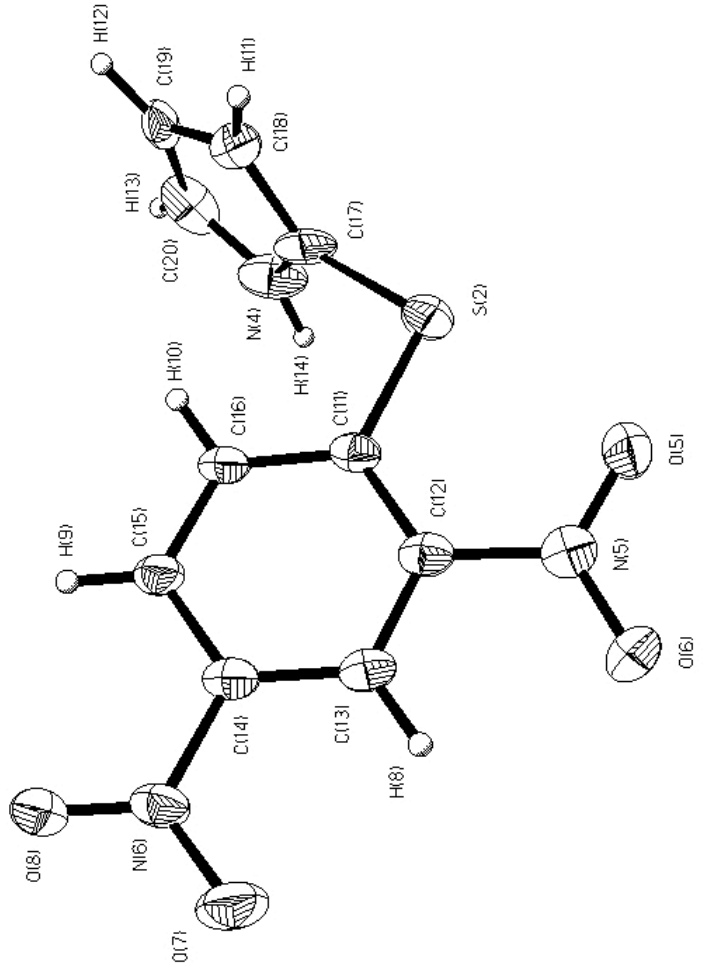
S(1)-O(2)	1.431(2)
S(1)-O(1)	1.438(2)
S(1)-C(1)	1.725(3)
S(1)-C(6)	1.752(4)
N(1)-C(4)	1.360(4)
N(1)-C(1)	1.363(4)
N(1)-H(1)	0.8600
C(1)-C(2)	1.370(4)
C(2)-C(3)	1.397(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.360(4)
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600

Table 2. Bond angles [°].

O(2)-S(1)-O(1)	118.26(19)
O(2)-S(1)-C(1)	108.52(19)
O(1)-S(1)-C(1)	106.91(14)
O(2)-S(1)-C(6)	107.65(15)
O(1)-S(1)-C(6)	108.7(2)

C(1)-S(1)-C(6)	106.2(2)
C(4)-N(1)-C(1)	107.9(3)
C(4)-N(1)-H(1)	126.1
C(1)-N(1)-H(1)	126.1
N(1)-C(1)-C(2)	108.9(3)
N(1)-C(1)-S(1)	123.1(2)
C(2)-C(1)-S(1)	128.0(3)
C(1)-C(2)-C(3)	106.8(3)
C(1)-C(2)-H(2)	126.6
C(3)-C(2)-H(2)	126.6
C(4)-C(3)-C(2)	107.5(3)
C(4)-C(3)-H(3)	126.3
C(2)-C(3)-H(3)	126.3
C(3)-C(4)-N(1)	109.0(3)
C(3)-C(4)-H(4)	125.5
N(1)-C(4)-H(4)	125.5
S(1)-C(6)-H(6A)	109.5
S(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
S(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5

2-(2,4-Dinitrobenzenesulfenyl)pyrrole (5)



Crystal data and structure refinement. CCDC 244776

Empirical Formula	$C_{10}H_7N_3O_4S$	
Formula Weight	265.24	
Crystal Color, Habit	Orange, needle	
Crystal Dimensions	0.06 X 0.16 X 0.32 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
No. of Reflections Used for Unit Cell Determination (2θ range)	22 (36.2 - 39.5°)	
Omega Scan Peak Width at Half-height	0.27°	
Lattice Parameters	a = 10.343(5) Å	β = 100.40(2) °
	b = 7.963(4) Å	V = 2194(1) Å^3
	c = 27.085(3) Å	

Space Group	$P2_1/c$ (#14)
Z value	8
D_{calc}	1.606 g/cm^3
F_{000}	1088.00
μ(MoKα)	3.06 cm^{-1}
Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.66, 13.02, 47.26)
Take-off Angle	6.0^o
Detector Aperture	9.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Voltage, Current	54kV, 170mA
Temperature	-150.0^{o}C
Scan Type	ω-2θ
Scan Rate	16.0^o/min (in ω) (up to 6 scans)
Scan Width	(0.79 + 0.35 tan θ)^o
$2\theta_{max}$	60.9^o
No. of Reflections Measured	Total: 7265 Unique: 6487 (R_{int} = 0.106)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8745 - 1.0000)
Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1
p-factor	0.0083
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	1985
No. Variables	325
Reflection/Parameter Ratio	6.11
Residuals: R; Rw	0.061 ; 0.068
Goodness of Fit Indicator	1.30
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.37 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.38 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
S(1)	0.5464(2)	0.8167(2)	0.25549(7)	1.87(4)
S(2)	0.4050(2)	0.2686(2)	0.49700(7)	2.42(5)
O(1)	0.8031(6)	0.8077(6)	0.2582(2)	3.0(1)
O(2)	0.9577(7)	0.7216(7)	0.3177(2)	3.6(1)
O(3)	0.8751(7)	0.3469(6)	0.4415(2)	3.2(1)
O(4)	0.6743(6)	0.3021(5)	0.4531(2)	2.8(1)
O(5)	0.5351(6)	0.0983(6)	0.5764(2)	3.0(2)
O(6)	0.4560(7)	-0.0601(6)	0.6290(2)	2.9(2)
O(7)	0.0090(7)	-0.0752(6)	0.6391(2)	3.4(2)
O(8)	-0.1354(7)	0.0581(5)	0.5858(2)	2.8(1)
N(1)	0.3244(7)	0.9297(6)	0.2876(2)	2.5(1)
N(2)	0.8422(7)	0.7310(6)	0.2975(2)	2.1(1)
N(3)	0.7550(8)	0.3682(6)	0.4301(2)	2.1(1)
N(4)	0.2686(9)	0.2810(7)	0.4009(3)	3.3(2)
N(5)	0.4393(7)	0.0393(6)	0.5926(2)	2.3(1)
N(6)	-0.0245(8)	0.0167(6)	0.6015(3)	2.3(1)
C(1)	0.6083(6)	0.6844(6)	0.3067(2)	1.6(1)
C(2)	0.7408(6)	0.6515(6)	0.3217(2)	1.8(1)
C(3)	0.7914(6)	0.5479(6)	0.3613(2)	1.9(2)
C(4)	0.7024(6)	0.4747(6)	0.3874(2)	1.9(1)
C(5)	0.5691(6)	0.5012(7)	0.3741(2)	2.0(1)
C(6)	0.5234(7)	0.6064(6)	0.3341(2)	2.2(2)
C(7)	0.3772(8)	0.8222(7)	0.2576(3)	2.0(1)
C(8)	0.2807(9)	0.7320(8)	0.2301(3)	2.4(1)
C(9)	0.1634(9)	0.7864(8)	0.2439(3)	2.4(2)
C(10)	0.1925(9)	0.9052(8)	0.2790(3)	2.8(1)
C(11)	0.2796(6)	0.1941(6)	0.5287(2)	1.9(1)
C(12)	0.3063(7)	0.0908(6)	0.5707(2)	2.0(1)
C(13)	0.2089(6)	0.0326(6)	0.5951(2)	1.9(1)
C(14)	0.0810(6)	0.0773(7)	0.5764(2)	2.1(1)
C(15)	0.0492(6)	0.1802(7)	0.5348(2)	2.1(2)
C(16)	0.1496(6)	0.2367(7)	0.5112(2)	2.0(1)
C(17)	0.3152(9)	0.3643(7)	0.4445(3)	2.5(1)
C(18)	0.2870(8)	0.5328(7)	0.4358(3)	2.2(2)
C(19)	0.2191(9)	0.5479(9)	0.3861(3)	2.8(2)
C(20)	0.212(1)	0.392(1)	0.3656(3)	3.3(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
S(1)	C(1)	1.768(7)	S(1)	C(7)	1.762(9)
S(2)	C(11)	1.781(6)	S(2)	C(17)	1.73(1)
O(1)	N(2)	1.23(1)	O(2)	N(2)	1.22(1)
O(3)	N(3)	1.24(1)	O(4)	N(3)	1.246(8)
O(5)	N(5)	1.246(8)	O(6)	N(5)	1.251(8)
O(7)	N(6)	1.252(9)	O(8)	N(6)	1.20(1)
N(1)	C(7)	1.361(8)	N(1)	C(10)	1.36(1)
N(2)	C(2)	1.477(8)	N(3)	C(4)	1.46(1)
N(4)	C(17)	1.36(1)	N(4)	C(20)	1.36(1)
N(5)	C(12)	1.45(1)	N(6)	C(14)	1.467(9)
C(1)	C(2)	1.382(5)*	C(1)	C(6)	1.394(5)*
C(2)	C(3)	1.380(5)*	C(3)	C(4)	1.386(5)*
C(4)	C(5)	1.377(5)*	C(5)	C(6)	1.383(5)*
C(7)	C(8)	1.34(1)	C(8)	C(9)	1.40(1)
C(9)	C(10)	1.34(1)	C(11)	C(12)	1.391(5)*
C(11)	C(16)	1.385(5)*	C(12)	C(13)	1.382(5)*
C(13)	C(14)	1.375(5)*	C(14)	C(15)	1.385(5)*
C(15)	C(16)	1.388(5)*	C(17)	C(18)	1.38(1)
C(18)	C(19)	1.41(1)	C(19)	C(20)	1.35(1)

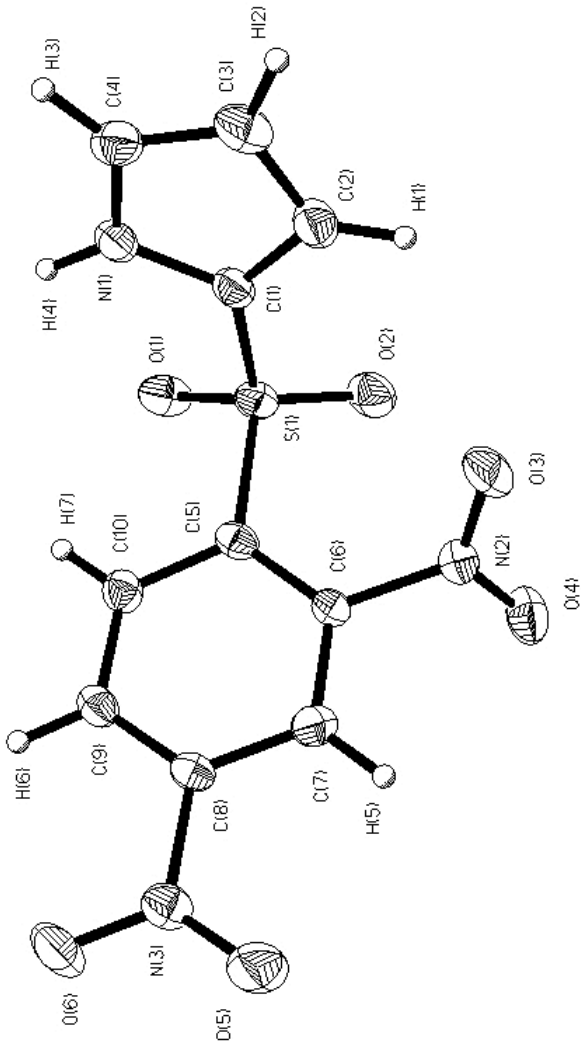
* restrained during refinement

Table 3. Bond Angles(^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	S(1)	C(7)	102.2(3)	C(11)	S(2)	C(17)	102.3(4)
C(7)	N(1)	C(10)	107.9(7)	O(1)	N(2)	O(2)	124.1(6)
O(1)	N(2)	C(2)	116.6(8)	O(2)	N(2)	C(2)	119.3(7)
O(3)	N(3)	O(4)	123.3(7)	O(3)	N(3)	C(4)	119.6(6)
O(4)	N(3)	C(4)	117.1(8)	C(17)	N(4)	C(20)	109.4(7)
O(5)	N(5)	O(6)	120.7(8)	O(5)	N(5)	C(12)	120.2(6)
O(6)	N(5)	C(12)	119.1(6)	O(7)	N(6)	O(8)	123.9(6)
O(7)	N(6)	C(14)	116.7(8)	O(8)	N(6)	C(14)	119.4(6)
S(1)	C(1)	C(2)	122.8(4)	S(1)	C(1)	C(6)	120.6(5)
C(2)	C(1)	C(6)	116.5(6)	N(2)	C(2)	C(1)	122.3(5)
N(2)	C(2)	C(3)	113.7(6)	C(1)	C(2)	C(3)	123.9(6)
C(2)	C(3)	C(4)	117.0(6)	N(3)	C(4)	C(3)	117.5(6)
N(3)	C(4)	C(5)	120.6(5)	C(3)	C(4)	C(5)	121.9(6)
C(4)	C(5)	C(6)	118.8(6)	C(1)	C(6)	C(5)	121.8(6)
S(1)	C(7)	N(1)	122.9(7)	S(1)	C(7)	C(8)	127.8(6)
N(1)	C(7)	C(8)	109.3(8)	C(7)	C(8)	C(9)	106.2(7)
C(8)	C(9)	C(10)	108.3(9)	N(1)	C(10)	C(9)	108.3(6)

S(2)	C(11)	C(12)	122.5(5)	S(2)	C(11)	C(16)	120.1(4)
C(12)	C(11)	C(16)	117.5(6)	N(5)	C(12)	C(11)	122.3(5)
N(5)	C(12)	C(13)	115.3(6)	C(11)	C(12)	C(13)	122.4(7)
C(12)	C(13)	C(14)	118.3(6)	N(6)	C(14)	C(13)	119.4(6)
N(6)	C(14)	C(15)	119.0(6)	C(13)	C(14)	C(15)	121.6(6)
C(14)	C(15)	C(16)	118.6(6)	C(11)	C(16)	C(15)	121.7(6)
S(2)	C(17)	N(4)	123.4(6)	S(2)	C(17)	C(18)	129.2(7)
N(4)	C(17)	C(18)	107.1(8)	C(17)	C(18)	C(19)	107.4(7)
C(18)	C(19)	C(20)	107.1(7)	N(4)	C(20)	C(19)	109.0(9)

2-(2,4-Dinitrobenzenesulfonyl)pyrrole (7)



Crystal data and structure refinement CCDC 744777

Empirical Formula	$C_{10}H_7N_3O_6S_1$
Formula Weight	297.24
Crystal Color, Habit	Yellow orange, needle
Crystal Dimensions	0.07 X 0.18 X 0.27 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (36.7 - 39.8°)
Omega Scan Peak Width at Half-height	0.37°
Lattice Parameters	a = 7.810(3) Å b = 14.752(5) Å c = 10.283(4) Å β = 94.08(3) ° V = 1181.7(7) Å^3

Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.671 g/cm^3
F_{000}	608.00
μ(MoKα)	3.06 cm^{-1}
Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.66, 13.02, 47.26)
Take-off Angle	6.0^o
Detector Aperture	9.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Voltage, Current	54kV, 160mA
Temperature	-90.0^{o}C
Scan Type	ω-2θ
Scan Rate	16.0^o/min (in ω) (up to 6 scans)
Scan Width	(1.78 + 0.35 tan θ)^o
$2\theta_{max}$	60.2^o
No. of Reflections Measured	Total: 3833 Unique: 3464 (R_{int} = 0.039 (5σ))
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9401 - 1.0000)
Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [σ^2(Fo^2) + (0.0388 · P)^2 + 0.0000 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
p-factor	0.0072
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	3464
No. Variables	181
Reflection/Parameter Ratio	19.1
Residuals: R1; wR2	0.0399 ; 0.129
Goodness of Fit Indicator	0.98
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.34 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.64 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
S(1)	-0.0009(1)	0.24370(5)	0.1988(1)	1.84(2)
O(1)	-0.1329(3)	0.1878(2)	0.2473(2)	2.43(8)
O(2)	0.1455(3)	0.2034(2)	0.1474(2)	2.53(8)
O(3)	0.3333(3)	0.3755(2)	0.1459(2)	3.13(9)
O(4)	0.4900(3)	0.2960(2)	0.2854(2)	2.68(8)

O(5)	0.3592(3)	0.5160(2)	0.6591(2)	3.14(9)
O(6)	0.1209(3)	0.4863(2)	0.7439(2)	2.91(8)
N(1)	-0.2668(3)	0.3375(2)	0.0876(2)	1.91(8)
N(2)	0.3616(3)	0.3390(2)	0.2521(2)	1.97(8)
N(3)	0.2215(4)	0.4772(2)	0.6599(2)	2.01(8)
C(1)	-0.0955(4)	0.3165(2)	0.0856(3)	1.8(1)
C(2)	-0.0293(4)	0.3639(2)	-0.0143(3)	2.3(1)
C(3)	-0.1642(5)	0.4133(2)	-0.0743(3)	2.5(1)
C(4)	-0.3086(5)	0.3960(2)	-0.0100(3)	2.2(1)
C(5)	0.0725(4)	0.3127(2)	0.3351(3)	1.6(1)
C(6)	0.2339(4)	0.3521(2)	0.3491(3)	1.59(9)
C(7)	0.2863(4)	0.4047(2)	0.4549(3)	1.8(1)
C(8)	0.1694(4)	0.4180(2)	0.5471(3)	1.52(9)
C(9)	0.0105(4)	0.3787(2)	0.5405(3)	1.7(1)
C(10)	-0.0381(4)	0.3253(2)	0.4340(3)	1.8(1)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
S1	O2	1.423(2)	S1	O1	1.437(2)
S1	C1	1.712(3)	S1	C5	1.793(3)
O3	N2	1.223(3)	O4	N2	1.216(3)
O5	N3	1.219(3)	O6	N3	1.216(3)
N1	C4	1.347(4)	N1	C1	1.374(4)
N2	C6	1.472(4)	N3	C8	1.485(4)
C1	C2	1.374(4)	C2	C3	1.389(5)
C3	C4	1.372(5)	C5	C6	1.386(4)
C5	C10	1.393(4)	C6	C7	1.375(4)
C7	C8	1.376(4)	C8	C9	1.367(4)
C9	C10	1.380(4)			

Table 3. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O2	S1	O1	120.30(15)	O2	S1	C1	109.19(15)
O1	S1	C1	108.06(15)	O2	S1	C5	107.86(15)
O1	S1	C5	104.61(14)	C1	S1	C5	105.88(14)
C4	N1	C1	108.5(3)	O4	N2	O3	125.0(3)
O4	N2	C6	117.6(2)	O3	N2	C6	117.4(3)
O6	N3	O5	124.6(3)	O6	N3	C8	117.7(3)
O5	N3	C8	117.6(3)	C2	C1	N1	108.4(3)
C2	C1	S1	131.3(3)	N1	C1	S1	120.3(2)
C1	C2	C3	106.6(3)	C4	C3	C2	108.2(3)
N1	C4	C3	108.3(3)	C6	C5	C10	118.4(3)
C6	C5	S1	123.8(2)	C10	C5	S1	117.8(2)
C7	C6	C5	122.4(3)	C7	C6	N2	115.6(3)
C5	C6	N2	122.0(3)	C6	C7	C8	116.8(3)
C9	C8	C7	123.3(3)	C9	C8	N3	119.1(3)
C7	C8	N3	117.6(3)	C8	C9	C10	118.7(3)
C9	C10	C5	120.3(3)				