Lattice Parameters	a = 9.378(4)Å b = 10.758(8)Å c = 12.753(3)Å V = 1204.7(9)Å^3	β = 101.56(2)°
formula	$C_{13}H_{13}NOS$	
formula weight	231.31	
Z value	4	
D_{calc}	1.275 g/cm^3	
Crystal System	Monoclinic	
Space Group	$P2_1/a$ (#14)	
Radiation	Cu K_α(λ = 1.54178 Å)	
Number of Reflections ($I > 3.0\sigma(I)$)	1186	
Number of Weak Reflections ($I < 3.0\sigma(I)$)	432	
Instrument	Rigaku AFC5	
Scan Type	ω - 2 Θ	
Structure Solution	"Mithril" - Gilmore, C.J. ; Mithril - an integrated direct methods computer program. J. Appl. Cryst. 17, 42-46, Univ. of Glasgow, Scotland (1984).	
Structure Refinement	"TEXSAN - TEXRAY" Structure Analysis Package, Molecular Structure Corporation (1985)	
Number of Variables	145	
Reflections/Parameter Ratio	8.18	
Residuals: R;R_w	0.054; 0.067	

There were no significant features present in the final difference Fourier map

Positional parameters and B(eq) for xray234

atom	x	y	z	B(eq)
S(1)	0.1038(2)	0.6444(2)	0.0402(1)	4.33(7)
O(1)	0.3353(4)	0.5537(4)	-0.0160(3)	4.5(2)
N(1)	0.4214(5)	0.4945(4)	0.0835(4)	3.8(2)
C(1)	0.5750(7)	0.5105(7)	0.3403(6)	4.9(3)
C(2)	0.6660(8)	0.4602(8)	0.4406(6)	6.4(4)
C(3)	0.6334(9)	0.3411(8)	0.4693(6)	6.4(4)
C(4)	0.5182(8)	0.2734(7)	0.4006(6)	5.7(4)
C(5)	0.4267(7)	0.3240(7)	0.2982(6)	4.5(3)
C(6)	0.4553(7)	0.4397(6)	0.2685(5)	3.7(3)
C(7)	0.3621(6)	0.4972(6)	0.1605(5)	3.5(3)
C(8)	0.2163(6)	0.5569(5)	0.1504(5)	3.5(3)
C(9)	0.1543(7)	0.5521(6)	0.2350(5)	4.1(3)
C(10)	0.0166(7)	0.6192(6)	0.2075(5)	4.4(3)
C(11)	-0.0229(6)	0.6745(6)	0.1077(6)	4.7(3)
C(12)	-0.0738(7)	0.6274(7)	0.2850(6)	6.6(4)
C(13)	0.3041(8)	0.2468(7)	0.2240(6)	6.6(4)
H(1)	0.5923	0.5978	0.3185	5.5
H(2)	0.7548	0.5051	0.4941	6.7
H(3)	0.6984	0.3083	0.5400	6.3
H(4)	0.4989	0.1905	0.4265	5.9
H(5)	0.2013	0.5091	0.3068	4.3
H(6)	-0.1159	0.7280	0.0782	4.9
H(7)	-0.0792	0.7137	0.3077	6.1
H(8)	-0.1759	0.5992	0.2506	6.1
H(9)	-0.0276	0.5812	0.3532	6.1
H(10)	0.2045	0.2845	0.2090	6.3
H(11)	0.3137	0.2310	0.1529	6.3
H(12)	0.2981	0.1655	0.2567	6.3
H(13)	0.4081	0.5594	-0.0631	6.6

U values for xray234

atom	U11	U22	U33	U12	U13	U23
S(1)	0.038(1)	0.072(1)	0.061(1)	0.010(1)	0.0244(8)	0.011(1)
O(1)	0.042(2)	0.090(3)	0.049(3)	0.019(2)	0.031(2)	0.015(2)
N(1)	0.034(3)	0.074(4)	0.046(3)	0.012(3)	0.023(3)	0.010(3)
C(1)	0.039(4)	0.098(6)	0.052(5)	0.008(4)	0.017(4)	0.008(5)
C(2)	0.049(5)	0.129(8)	0.067(6)	-0.004(5)	0.021(4)	-0.008(6)
C(3)	0.070(6)	0.115(8)	0.064(5)	0.017(6)	0.032(5)	0.019(6)
C(4)	0.062(5)	0.098(7)	0.058(5)	0.007(5)	0.025(4)	0.015(5)
C(5)	0.046(4)	0.078(6)	0.055(5)	0.005(4)	0.027(4)	-0.005(4)
C(6)	0.040(4)	0.062(5)	0.052(4)	0.011(4)	0.035(4)	0.010(4)
C(7)	0.035(4)	0.057(4)	0.046(4)	0.006(3)	0.021(3)	0.005(3)
C(8)	0.036(4)	0.054(4)	0.047(4)	0.000(3)	0.021(3)	0.002(3)
C(9)	0.045(4)	0.070(5)	0.047(4)	0.005(4)	0.024(3)	0.002(4)
C(10)	0.041(4)	0.076(5)	0.061(5)	0.009(4)	0.033(4)	0.002(4)
C(11)	0.036(4)	0.077(5)	0.077(5)	0.018(4)	0.037(4)	-0.001(4)
C(12)	0.066(5)	0.106(6)	0.103(6)	0.017(5)	0.060(5)	0.001(5)
C(13)	0.099(6)	0.084(5)	0.079(5)	-0.001(5)	0.044(5)	-0.001(5)
H(1)	0.0696					
H(2)	0.0851					
H(3)	0.0804					
H(4)	0.0747					
H(5)	0.0539					
H(6)	0.0619					
H(7)	0.0770					
H(8)	0.0770					
H(9)	0.0770					
H(10)	0.0804					
H(11)	0.0804					
H(12)	0.0804					
H(13)	0.0836					

Intramolecular Bond Angles

atom	atom	atom	angle	atom	atom	atom	angle
C(8)	S(1)	C(11)	91.6(3)	S(1)	C(8)	C(7)	126.6(5)
N(1)	O(1)	H(13)	105.01	S(1)	C(8)	C(9)	110.5(4)
O(1)	N(1)	C(7)	114.6(4)	C(7)	C(8)	C(9)	122.8(5)
C(2)	C(1)	C(6)	119.2(7)	C(8)	C(9)	C(10)	112.5(5)
C(2)	C(1)	H(1)	120.99	C(8)	C(9)	H(5)	124.51
C(6)	C(1)	H(1)	119.76	C(10)	C(9)	H(5)	122.98
C(1)	C(2)	C(3)	118.9(6)	C(9)	C(10)	C(11)	112.8(7)
C(1)	C(2)	H(2)	122.85	C(9)	C(10)	C(12)	122.7(6)
C(3)	C(2)	H(2)	118.25	C(11)	C(10)	C(12)	124.4(6)
C(2)	C(3)	C(4)	121.9(7)	S(1)	C(11)	C(10)	112.5(5)
C(2)	C(3)	H(3)	117.28	S(1)	C(11)	H(6)	125.55
C(4)	C(3)	H(3)	120.84	C(10)	C(11)	H(6)	121.92
C(3)	C(4)	C(5)	119.2(7)	C(10)	C(12)	H(7)	110.32
C(3)	C(4)	H(4)	118.14	C(10)	C(12)	H(8)	112.60
C(5)	C(4)	H(4)	122.60	C(10)	C(12)	H(9)	112.46
C(4)	C(5)	C(6)	120.2(6)	H(7)	C(12)	H(8)	106.89
C(4)	C(5)	C(13)	117.9(7)	H(7)	C(12)	H(9)	106.00
C(6)	C(5)	C(13)	121.9(6)	H(8)	C(12)	H(9)	108.21
C(1)	C(6)	C(5)	120.6(6)	C(5)	C(13)	H(10)	111.92
C(1)	C(6)	C(7)	117.2(6)	C(5)	C(13)	H(11)	113.49
C(5)	C(6)	C(7)	122.2(5)	C(5)	C(13)	H(12)	112.40
N(1)	C(7)	C(6)	115.3(5)	H(10)	C(13)	H(11)	106.89
N(1)	C(7)	C(8)	125.3(5)	H(10)	C(13)	H(12)	105.15
C(6)	C(7)	C(8)	119.3(6)	H(11)	C(13)	H(12)	106.44

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances

atom	atom	distance	atom	atom	distance
S(1)	C(8)	1.712(5)	C(5)	C(13)	1.464(9)
S(1)	C(11)	1.726(8)	C(6)	C(7)	1.482(8)
O(1)	N(1)	1.396(6)	C(7)	C(8)	1.474(8)
O(1)	H(13)	1.058	C(8)	C(9)	1.39(1)
N(1)	C(7)	1.288(9)	C(9)	C(10)	1.412(9)
C(1)	C(2)	1.375(9)	C(9)	H(5)	0.981
C(1)	C(6)	1.399(8)	C(10)	C(11)	1.334(9)
C(1)	H(1)	1.009	C(10)	C(12)	1.51(1)
C(2)	C(3)	1.40(1)	C(11)	H(6)	1.001
C(2)	H(2)	0.996	C(12)	H(7)	0.979
C(3)	C(4)	1.34(1)	C(12)	H(8)	0.952
C(3)	H(3)	0.961	C(12)	H(9)	0.963
C(4)	C(5)	1.397(9)	C(13)	H(10)	0.974
C(4)	H(4)	0.989	C(13)	H(11)	0.957
C(5)	C(6)	1.35(1)	C(13)	H(12)	0.980

Distances are in angstroms. Estimated standard deviations in