References

SMART (Ver 5.611). Software for data collection on CCD Detector System. Bruker X-ray Analytical Instruments, Madison, WI, 1995.

SAINT+(Ver 5.6). Software for data reduction for CCD Detector System. Bruker X-ray Analytical Instruments, Madison, WI, 1995.

SHELXTL-PC.(Ver 5.1) G.M.Sheldrick, Buker X-ray Analytical Instruments Inc. Madison, WI. (1990).

SADABS. G.M.Sheldrick, Bruker X-ray Analytical Instrument, Inc. Madison, WI (1999).

H.D.Flack. Acta Crystallographica, A39, 876-881(1983).

Table 1. Crystal data and structure refinement for HOS2lm.

Empirical formula	$C_{14}H_{12}N_2O_2S_2$
Formula weight	304.38
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 11.958(5) Å alpha = 90° b = 5.025(2) Å beta = 114.393(7)° c = 13.114(5) Å gamma = 90°
Volume, Z	717.7(5) $Å^3$, 2
Density (calculated)	1.408 Mg/m^3
Absorption coefficient	0.372 mm^{-1}
F(000)	316
Crystal size	0.08 x 0.16 x 0.32 mm
Θ range for data collection	1.87 to 23.40°
Limiting indices	$-13 \le h \le 11$, $-5 \le k \le 5$, $-10 \le l \le 14$
Reflections collected	3214
Independent reflections	2010 (R_{int} = 0.0673)
Completeness to Θ = 23.40°	99.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2010 / 1 / 181
Goodness-of-fit on F^2	0.906
Final R indices [I>2σ(I)]	R1 = 0.0480, wR2 = 0.0913
R indices (all data)	R1 = 0.0683, wR2 = 0.0967
Absolute structure parameter	-0.04(14)
Largest diff. peak and hole	0.219 and -0.233 $eÅ^{-3}$

$R1=(\sum \| \|F_o\| - \|F_c\| \| / \sum |F_o|)$, $wR2=\sum w(F_o^2-F_c^2)^2 / \sum w[(F_o^2)^2]^{1/2}$,

$S=[\sum w(F_o^2-F_c^2)^2/(n-p)]^{1/2}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for HOS21m. U(eq) is defined as

$$U_{eq}=1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U(eq)
S(1)	6608(1)	2970(3)	1769(1)	60(1)
S(2)	8730(1)	8217(3)	-333(1)	59(1)
O(1)	4847(3)	11106(12)	-3154(4)	122(2)
O(2)	6269(5)	8730(20)	-3332(5)	205(4)
N(1)	8278(3)	4335(8)	1131(3)	44(1)
N(2)	6414(3)	9251(8)	-868(3)	47(1)
C(1)	8674(5)	-1037(10)	3188(4)	59(2)
C(2)	9554(6)	-2760(10)	3887(5)	77(2)
C(3)	10740(6)	-2656(12)	3985(5)	76(2)
C(4)	11024(5)	-853(12)	3359(5)	67(2)
C(5)	10172(4)	895(11)	2658(4)	59(2)
C(6)	8970(4)	828(10)	2562(4)	48(1)
C(7)	8069(4)	2697(12)	1807(4)	45(1)
C(8)	6287(4)	5403(10)	800(4)	52(1)
C(9)	7265(4)	5884(10)	557(4)	43(1)
C(10)	7305(4)	7802(11)	-248(4)	43(1)
C(11)	8105(3)	10832(11)	-1321(4)	64(2)
C(12)	6715(4)	11001(11)	-1606(4)	52(1)
C(13)	5954(6)	10062(18)	-2777(5)	90(2)
C(14)	3992(5)	10300(30)	-4273(6)	217(6)

Table 3. Bond lengths [Å] and angles [°] for HOS21m.

S(1)-C(8)	1.689(5)	S(1)-C(7)	1.732(4)
S(2)-C(10)	1.766(4)	S(2)-C(11)	1.779(5)
O(1)-C(13)	1.315(7)	O(1)-C(14)	1.457(8)
O(2)-C(13)	1.159(8)	N(1)-C(7)	1.307(6)
N(1)-C(9)	1.373(5)	N(2)-C(10)	1.269(5)
N(2)-C(12)	1.459(6)	C(1)-C(2)	1.379(6)
C(1)-C(6)	1.384(6)	C(2)-C(3)	1.372(7)
C(3)-C(4)	1.356(7)	C(4)-C(5)	1.372(6)
C(5)-C(6)	1.391(6)	C(6)-C(7)	1.464(7)
C(8)-C(9)	1.356(5)	C(9)-C(10)	1.444(6)
C(11)-C(12)	1.549(5)	C(12)-C(13)	1.502(8)
C(8)-S(1)-C(7)	89.5(3)	C(10)-S(2)-C(11)	90.4(2)
C(13)-O(1)-C(14)	116.5(7)	C(7)-N(1)-C(9)	110.9(4)
C(10)-N(2)-C(12)	113.5(3)	C(2)-C(1)-C(6)	120.5(5)
C(3)-C(2)-C(1)	120.9(5)	C(4)-C(3)-C(2)	118.5(5)
C(3)-C(4)-C(5)	122.1(5)	C(4)-C(5)-C(6)	119.9(5)
C(1)-C(6)-C(5)	118.1(5)	C(1)-C(6)-C(7)	122.6(5)
C(5)-C(6)-C(7)	119.3(5)	N(1)-C(7)-C(6)	124.7(4)
N(1)-C(7)-S(1)	113.8(4)	C(6)-C(7)-S(1)	121.5(4)
C(9)-C(8)-S(1)	110.8(4)	C(8)-C(9)-N(1)	114.9(5)
C(8)-C(9)-C(10)	125.7(4)	N(1)-C(9)-C(10)	119.5(4)
N(2)-C(10)-C(9)	125.3(4)	N(2)-C(10)-S(2)	118.0(4)
C(9)-C(10)-S(2)	116.7(4)	C(12)-C(11)-S(2)	107.6(3)
N(2)-C(12)-C(13)	106.2(4)	N(2)-C(12)-C(11)	110.0(4)
C(13)-C(12)-C(11)	111.5(4)	O(2)-C(13)-O(1)	122.1(7)
O(2)-C(13)-C(12)	127.3(7)	O(1)-C(13)-C(12)	110.4(6)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for HOS21m.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23}]$

	U11	U22	U33	U23	U13	U12
S(1)	48(1)	70(1)	71(1)	7(1)	33(1)	-4(1)
S(2)	34(1)	71(1)	74(1)	14(1)	26(1)	5(1)
O(1)	54(2)	203(5)	86(3)	21(4)	7(2)	-4(3)
O(2)	130(4)	356(12)	108(5)	-116(7)	29(3)	3(6)
N(1)	40(2)	47(3)	44(2)	-4(2)	17(2)	0(2)
N(2)	31(2)	61(3)	48(3)	9(2)	17(2)	8(2)
C(1)	69(3)	52(4)	52(4)	3(3)	20(3)	-4(3)
C(2)	106(4)	54(4)	63(4)	0(3)	28(4)	-6(4)
C(3)	93(5)	63(5)	56(4)	-2(3)	14(4)	16(4)
C(4)	64(3)	69(4)	64(4)	-7(3)	21(3)	15(3)
C(5)	57(3)	72(4)	50(4)	10(3)	23(3)	10(3)
C(6)	55(3)	45(3)	44(3)	-7(3)	21(3)	-1(3)
C(7)	41(3)	51(4)	45(3)	-3(3)	18(2)	-4(3)
C(8)	42(3)	55(3)	58(4)	-3(3)	21(3)	-4(3)
C(9)	35(3)	46(3)	44(3)	-1(3)	14(3)	-4(2)
C(10)	34(2)	50(3)	44(3)	-11(3)	16(2)	-2(3)
C(11)	41(3)	76(4)	79(4)	11(4)	29(3)	1(3)
C(12)	46(3)	63(4)	44(3)	3(3)	16(3)	7(3)
C(13)	65(4)	158(7)	53(4)	-1(5)	31(4)	-3(4)
C(14)	88(5)	437(18)	75(6)	16(8)	-17(4)	-78(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for HOS21m.

	x	y	z	U(eq)
H(1B)	7858	-1131	3134	71
H(2B)	9335	-4036	4308	92
H(3A)	11349	-3820	4479	92
H(4A)	11839	-801	3407	81
H(5A)	10403	2151	2238	71
H(8A)	5523	6311	470	62
H(11A)	8512	12539	-1000	77
H(11B)	8234	10459	-2006	77
H(12A)	6490	12875	-1516	62
H(14A)	3206	11210	-4469	260
H(14B)	3867	8371	-4288	260
H(14C)	4330	10778	-4813	260

Table 6. Torsion angles [°] for HOS21m.

C(6)-C(1)-C(2)-C(3)	0.4(8)	C(1)-C(2)-C(3)-C(4)	-1.3(8)
C(2)-C(3)-C(4)-C(5)	1.6(8)	C(3)-C(4)-C(5)-C(6)	-0.9(8)
C(2)-C(1)-C(6)-C(5)	0.4(7)	C(2)-C(1)-C(6)-C(7)	179.9(5)
C(4)-C(5)-C(6)-C(1)	-0.1(7)	C(4)-C(5)-C(6)-C(7)	-179.7(5)
C(9)-N(1)-C(7)-C(6)	-178.2(4)	C(9)-N(1)-C(7)-S(1)	0.2(5)
C(1)-C(6)-C(7)-N(1)	-173.9(5)	C(5)-C(6)-C(7)-N(1)	5.6(7)
C(1)-C(6)-C(7)-S(1)	7.9(7)	C(5)-C(6)-C(7)-S(1)	-172.6(4)
C(8)-S(1)-C(7)-N(1)	-0.1(4)	C(8)-S(1)-C(7)-C(6)	178.3(4)
C(7)-S(1)-C(8)-C(9)	0.0(4)	S(1)-C(8)-C(9)-N(1)	0.1(5)
S(1)-C(8)-C(9)-C(10)	178.9(4)	C(7)-N(1)-C(9)-C(8)	-0.2(6)
C(7)-N(1)-C(9)-C(10)	-179.1(4)	C(12)-N(2)-C(10)-C(9)	-179.7(4)
C(12)-N(2)-C(10)-S(2)	2.5(5)	C(8)-C(9)-C(10)-N(2)	-2.4(8)
N(1)-C(9)-C(10)-N(2)	176.3(4)	C(8)-C(9)-C(10)-S(2)	175.4(4)
N(1)-C(9)-C(10)-S(2)	-5.8(6)	C(11)-S(2)-C(10)-N(2)	2.2(4)
C(11)-S(2)-C(10)-C(9)	-175.8(4)	C(10)-S(2)-C(11)-C(12)	-5.6(4)
C(10)-N(2)-C(12)-C(13)	114.0(5)	C(10)-N(2)-C(12)-C(11)	-6.8(5)
S(2)-C(11)-C(12)-N(2)	7.9(5)	S(2)-C(11)-C(12)-C(13)	-109.6(5)
C(14)-O(1)-C(13)-O(2)	5.7(12)	C(14)-O(1)-C(13)-C(12)	-178.1(6)
N(2)-C(12)-C(13)-O(2)	-100.0(10)	C(11)-C(12)-C(13)-O(2)	19.7(12)
N(2)-C(12)-C(13)-O(1)	84.0(6)	C(11)-C(12)-C(13)-O(1)	-156.2(5)