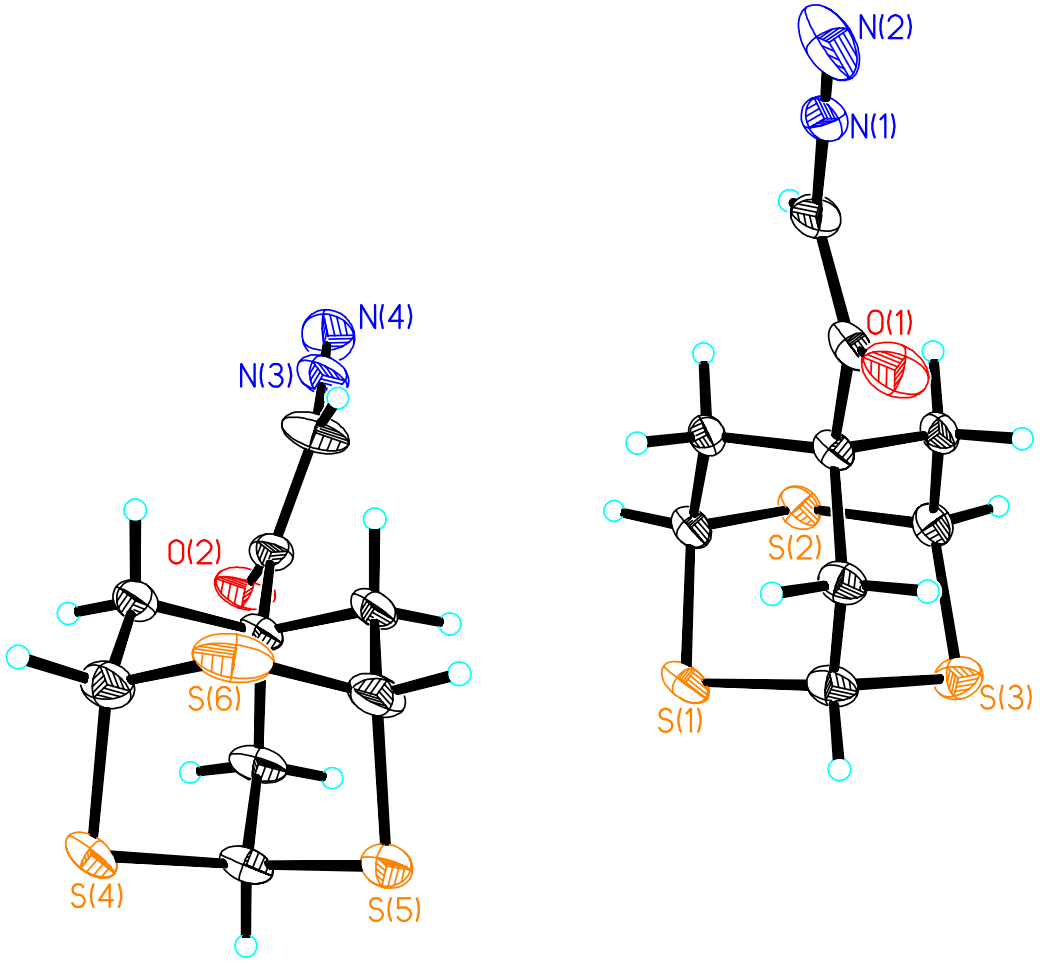
Asymmetric Unit



One Molecule

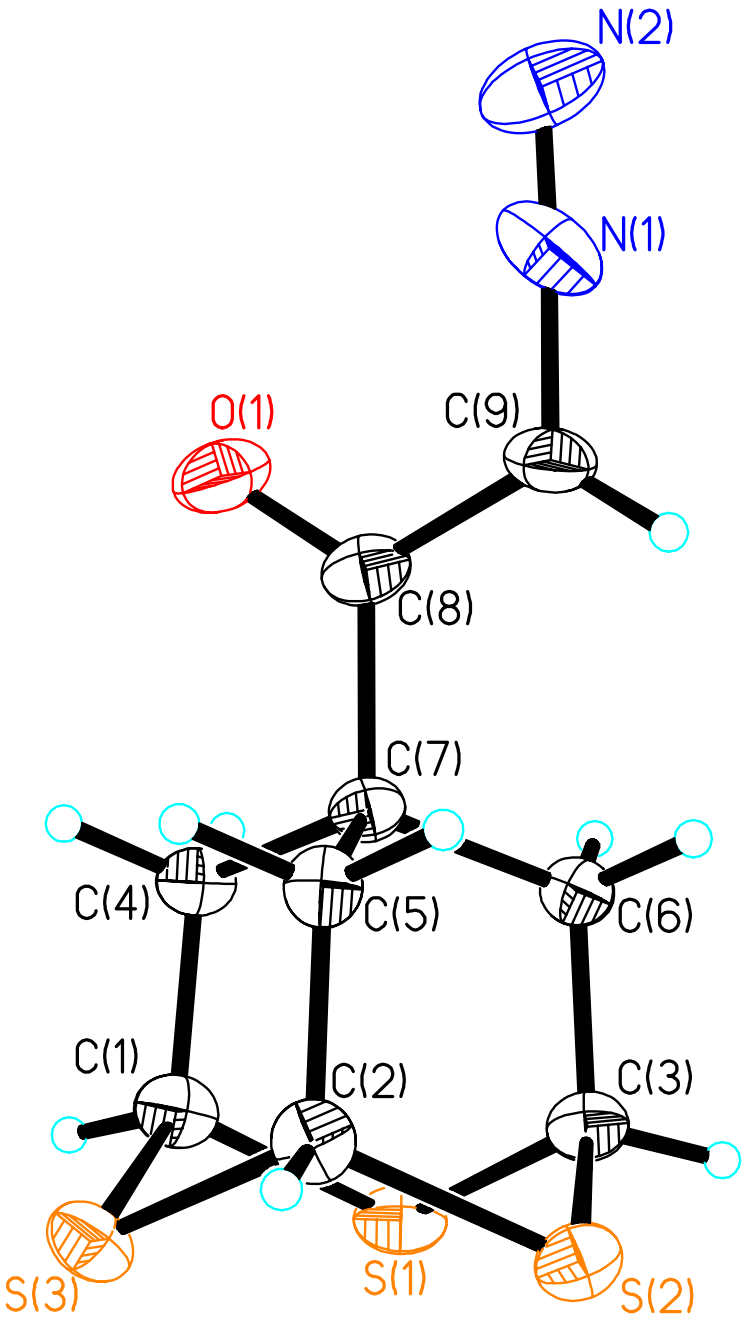


Table 1. Crystal data and structure refinement for **$C_9H_{10}N_2OS_3$**.

Identification code	**$C_9H_{10}N_2OS_3$**	
Empirical formula	C9 H10 N2 O S3	
Formula weight	258.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.3568(14) Å	α= 87.701(3)°.
	b = 9.8242(18) Å	β= 87.867(3)°.
	c = 15.334(3) Å	γ = 87.491(3)°.
Volume	1105.6(4) $Å^3$	
Z	4	
Density (calculated)	1.552 Mg/m^3	
Absorption coefficient	0.643 mm^{-1}	
F(000)	536	
Crystal size	0.48 x 0.21 x 0.15 mm^3	
Theta range for data collection	1.33 to 27.56°.	
Index ranges	$-9 \leq h \leq 9$, $-12 \leq k \leq 12$, $-19 \leq l \leq 19$	
Reflections collected	9429	
Independent reflections	4892 [R(int) = 0.0401]	
Completeness to theta = 27.56°	95.5 %	
Max. and min. transmission	0.9097 and 0.7477	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4892 / 0 / 271	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1380	
R indices (all data)	R1 = 0.0642, wR2 = 0.1438	
Largest diff. peak and hole	0.855 and -0.460 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **$C_9H_{10}N_2OS_3$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1658(1)	5753(1)	2475(1)	27(1)
S(2)	1045(1)	2816(1)	2037(1)	25(1)
S(3)	-1261(1)	4186(1)	3489(1)	28(1)
S(4)	7381(1)	10997(1)	1507(1)	30(1)
S(5)	4324(1)	9566(1)	2532(1)	33(1)
S(6)	8297(1)	8949(1)	2990(1)	38(1)
O(1)	4309(3)	3301(2)	5290(1)	37(1)
O(2)	6530(3)	6839(2)	-227(1)	37(1)
N(1)	6859(3)	1358(2)	4924(2)	35(1)
N(2)	7827(5)	1139(3)	5414(2)	48(1)
N(3)	7771(4)	4334(2)	236(2)	34(1)
N(4)	7756(4)	3583(3)	-279(2)	41(1)
C(1)	657(4)	5306(3)	3550(2)	26(1)
C(2)	67(4)	2668(3)	3155(2)	24(1)
C(3)	2718(4)	4074(3)	2246(2)	24(1)
C(4)	2084(4)	4707(3)	4172(2)	23(1)
C(5)	1531(4)	2253(3)	3811(2)	22(1)
C(6)	3998(4)	3564(3)	2966(2)	21(1)
C(7)	2985(4)	3347(2)	3867(2)	21(1)
C(8)	4332(4)	2825(3)	4562(2)	25(1)
C(9)	5629(4)	1739(3)	4319(2)	29(1)
C(10)	8839(4)	9537(3)	1867(2)	30(1)
C(11)	6087(5)	8255(3)	2796(2)	34(1)
C(12)	5277(4)	10096(3)	1463(2)	25(1)
C(13)	8811(4)	8366(3)	1229(2)	24(1)
C(14)	6287(4)	7177(3)	2101(2)	30(1)
C(15)	5520(4)	8883(3)	860(2)	28(1)
C(16)	6896(4)	7769(2)	1197(2)	21(1)
C(17)	7013(4)	6629(3)	524(2)	24(1)
C(18)	7716(5)	5299(3)	826(2)	37(1)

Table 3. Bond lengths [Å] and angles [°] for **$C_9H_{10}N_2OS_3$**.

S(1)-C(1)	1.826(3)
S(1)-C(3)	1.834(3)
S(2)-C(3)	1.827(3)
S(2)-C(2)	1.837(3)
S(3)-C(2)	1.827(3)
S(3)-C(1)	1.834(3)
S(4)-C(12)	1.821(3)
S(4)-C(10)	1.832(3)
S(5)-C(12)	1.824(3)
S(5)-C(11)	1.832(3)
S(6)-C(11)	1.830(4)
S(6)-C(10)	1.831(3)
O(1)-C(8)	1.227(3)
O(2)-C(17)	1.225(3)
N(1)-N(2)	1.063(4)
N(1)-C(9)	1.352(4)
N(3)-N(4)	1.102(3)
N(3)-C(18)	1.335(4)
C(1)-C(4)	1.528(4)
C(2)-C(5)	1.533(4)
C(3)-C(6)	1.532(4)
C(4)-C(7)	1.546(3)
C(5)-C(7)	1.557(4)
C(6)-C(7)	1.557(3)
C(7)-C(8)	1.539(4)
C(8)-C(9)	1.451(4)
C(10)-C(13)	1.541(4)
C(11)-C(14)	1.531(4)
C(12)-C(15)	1.538(3)
C(13)-C(16)	1.553(4)
C(14)-C(16)	1.540(4)
C(15)-C(16)	1.545(4)
C(16)-C(17)	1.550(3)
C(17)-C(18)	1.450(4)

C(1)-S(1)-C(3)	97.48(12)
C(3)-S(2)-C(2)	96.99(12)
C(2)-S(3)-C(1)	96.98(12)
C(12)-S(4)-C(10)	97.25(13)
C(12)-S(5)-C(11)	97.02(13)
C(11)-S(6)-C(10)	97.56(13)
N(2)-N(1)-C(9)	175.5(3)
N(4)-N(3)-C(18)	176.1(3)
C(4)-C(1)-S(1)	111.83(19)
C(4)-C(1)-S(3)	111.60(19)
S(1)-C(1)-S(3)	112.37(14)
C(5)-C(2)-S(3)	111.40(17)
C(5)-C(2)-S(2)	111.33(18)
S(3)-C(2)-S(2)	113.67(14)
C(6)-C(3)-S(2)	111.54(17)
C(6)-C(3)-S(1)	111.76(18)
S(2)-C(3)-S(1)	112.53(15)
C(1)-C(4)-C(7)	113.0(2)
C(2)-C(5)-C(7)	112.6(2)
C(3)-C(6)-C(7)	112.7(2)
C(8)-C(7)-C(4)	108.0(2)
C(8)-C(7)-C(6)	110.4(2)
C(4)-C(7)-C(6)	110.4(2)
C(8)-C(7)-C(5)	107.3(2)
C(4)-C(7)-C(5)	110.4(2)
C(6)-C(7)-C(5)	110.3(2)
O(1)-C(8)-C(9)	121.3(3)
O(1)-C(8)-C(7)	121.7(3)
C(9)-C(8)-C(7)	117.0(2)
N(1)-C(9)-C(8)	115.5(3)
C(13)-C(10)-S(6)	111.52(19)
C(13)-C(10)-S(4)	111.4(2)
S(6)-C(10)-S(4)	112.77(16)
C(14)-C(11)-S(6)	110.4(2)
C(14)-C(11)-S(5)	111.9(2)

S(6)-C(11)-S(5)	113.44(16)
C(15)-C(12)-S(4)	111.0(2)
C(15)-C(12)-S(5)	111.16(19)
S(4)-C(12)-S(5)	113.96(15)
C(10)-C(13)-C(16)	112.1(2)
C(11)-C(14)-C(16)	112.9(2)
C(12)-C(15)-C(16)	113.1(2)
C(14)-C(16)-C(15)	111.3(2)
C(14)-C(16)-C(17)	110.0(2)
C(15)-C(16)-C(17)	107.2(2)
C(14)-C(16)-C(13)	110.8(2)
C(15)-C(16)-C(13)	109.6(2)
C(17)-C(16)-C(13)	107.7(2)
O(2)-C(17)-C(18)	121.5(2)
O(2)-C(17)-C(16)	121.8(2)
C(18)-C(17)-C(16)	116.8(2)
N(3)-C(18)-C(17)	115.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for $\mathbf{C_9H_{10}N_2OS_3}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	32(1)	17(1)	33(1)	7(1)	-9(1)	-3(1)
S(2)	29(1)	21(1)	25(1)	-2(1)	-5(1)	-5(1)
S(3)	21(1)	26(1)	36(1)	-5(1)	-4(1)	-1(1)
S(4)	39(1)	13(1)	37(1)	1(1)	-3(1)	-4(1)
S(5)	38(1)	21(1)	38(1)	0(1)	8(1)	3(1)
S(6)	55(1)	32(1)	28(1)	-6(1)	-17(1)	15(1)
O(1)	50(1)	34(1)	26(1)	3(1)	-10(1)	5(1)
O(2)	57(2)	26(1)	26(1)	-2(1)	-4(1)	9(1)
N(1)	23(1)	20(1)	62(2)	14(1)	3(1)	-3(1)
N(2)	62(2)	45(2)	37(2)	17(1)	-9(2)	-16(2)
N(3)	38(2)	18(1)	45(2)	-2(1)	-8(1)	0(1)
N(4)	49(2)	32(1)	43(2)	-9(1)	5(1)	-2(1)
C(1)	28(2)	18(1)	32(1)	-4(1)	-6(1)	-1(1)
C(2)	25(1)	19(1)	28(1)	-2(1)	-1(1)	-6(1)
C(3)	26(1)	19(1)	25(1)	4(1)	-3(1)	-3(1)
C(4)	26(1)	19(1)	26(1)	-1(1)	-6(1)	-2(1)
C(5)	25(1)	16(1)	25(1)	1(1)	1(1)	-4(1)
C(6)	21(1)	20(1)	24(1)	4(1)	0(1)	-3(1)
C(7)	24(1)	17(1)	21(1)	3(1)	-3(1)	-1(1)
C(8)	31(2)	20(1)	25(1)	7(1)	-4(1)	-6(1)
C(9)	26(2)	31(2)	30(1)	9(1)	-6(1)	3(1)
C(10)	30(2)	21(1)	39(2)	-3(1)	-8(1)	-2(1)
C(11)	49(2)	23(1)	27(1)	7(1)	7(1)	10(1)
C(12)	33(2)	15(1)	28(1)	0(1)	-8(1)	3(1)
C(13)	26(1)	18(1)	29(1)	1(1)	-2(1)	-1(1)
C(14)	38(2)	14(1)	36(2)	3(1)	6(1)	1(1)
C(15)	37(2)	17(1)	32(1)	-5(1)	-13(1)	5(1)
C(16)	27(1)	12(1)	26(1)	1(1)	-3(1)	0(1)
C(17)	25(1)	17(1)	31(1)	-3(1)	-2(1)	1(1)
C(18)	57(2)	19(1)	36(2)	-7(1)	-18(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **$C_9H_{10}N_2OS_3$**.

	x	y	z	U(eq)
H(1)	159	6174	3802	31
H(2)	-794	1907	3165	28
H(3)	3485	4190	1698	28
H(4A)	1502	4554	4758	28
H(4B)	3039	5375	4224	28
H(5A)	2142	1381	3639	26
H(5B)	941	2100	4396	26
H(6A)	4950	4233	3021	26
H(6B)	4608	2691	2796	26
H(9)	5615	1323	3770	35
H(10)	10114	9852	1854	36
H(11)	5676	7778	3352	41
H(12)	4361	10749	1192	30
H(13A)	9700	7633	1411	29
H(13B)	9190	8707	636	29
H(14A)	5105	6746	2052	35
H(14B)	7189	6458	2291	35
H(15A)	5939	9219	273	34
H(15B)	4326	8475	802	34
H(18)	8109	5125	1405	44