

Table 1. Crystal data and structure refinement for structure10.

Identification code	structure10
Empirical formula	C12 H8.67 Cu N2 O8.33 S
Formula weight	409.81
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	R32
Unit cell dimensions	a = 23.060(7) Å $\alpha = 90^\circ$. b = 23.060(7) Å $\beta = 90^\circ$. c = 7.053(2) Å $\gamma = 120^\circ$.
Volume	3248.1(17) Å ³
Z	9
Calculated density	1.886 Mg/m ³
Absorption coefficient	1.708 mm ⁻¹
F(000)	1857
Crystal size	0.43 x 0.38 x 0.38 mm ³
Theta range for data collection	1.77 to 28.33°.
Limiting indices	-30 ≤ h ≤ 30, -30 ≤ k ≤ 30, -9 ≤ l ≤ 9
Reflections collected	17801
Independent reflections	6366 [R(int) = 0.0604]
Completeness to theta = 28.33°	96.7%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.676
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10929 / 1 / 121
Goodness-of-fit on F ²	1.043
Final R indices [I > 2σ(I)]	R1 = 0.0465, wR2 = 0.1313
R indices (all data)	R1 = 0.0528, wR2 = 0.1406
Absolute structure parameter	0.000(16)
Largest diff. peak and hole	1.098 and -0.521 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct10. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	-2774(1)	559(1)	1667	13(1)
S(1)	-3333	-905(1)	3333	13(1)
O(1)	-3059(1)	-399(1)	1781(2)	15(1)
O(2)	-3868(1)	-1523(1)	2560(3)	25(1)
O(3)	598(1)	2390(1)	2937(3)	27(1)
O(4)	550(1)	1406(1)	2618(3)	37(1)
N(1)	-1812(1)	874(1)	1821(3)	13(1)
C(1)	-1543(1)	488(1)	2079(4)	17(1)
C(2)	-859(1)	759(2)	2323(4)	19(1)
C(3)	-451(1)	1447(1)	2296(4)	17(1)
C(4)	-737(1)	1842(1)	2033(4)	17(1)
C(5)	-1420(1)	1545(1)	1792(4)	14(1)
C(6)	290(1)	1741(2)	2625(4)	22(1)
O(5)	0	3160(4)	5000	50(3)

Table 3. Bond lengths [Å] and angles [°] for struct10.

Cu(1)-N(1)	1.963(2)
Cu(1)-N(1)#1	1.963(2)
Cu(1)-O(1)	1.9673(19)
Cu(1)-O(1)#1	1.9673(19)
S(1)-O(2)	1.4455(18)
S(1)-O(2)#2	1.4456(18)
S(1)-O(1)#2	1.4908(18)
S(1)-O(1)	1.4909(18)
O(3)-C(6)	1.315(3)
O(4)-C(6)	1.189(4)
N(1)-C(1)	1.325(3)
N(1)-C(5)	1.347(3)
C(1)-C(2)	1.388(4)
C(2)-C(3)	1.381(4)
C(3)-C(6)	1.510(4)
C(4)-C(5)	1.378(3)
C(5)-C(5)#1	1.481(5)
N(1)-Cu(1)-N(1)#1	82.82(12)
N(1)-Cu(1)-O(1)	95.36(8)
N(1)#1-Cu(1)-O(1)	177.95(8)
N(1)-Cu(1)-O(1)#1	177.95(8)
N(1)#1-Cu(1)-O(1)#1	95.36(8)
O(1)-Cu(1)-O(1)#1	86.48(11)
O(2)-S(1)-O(2)#2	112.18(19)
O(2)-S(1)-O(1)#2	108.88(11)
O(2)#2-S(1)-O(1)#2	108.24(10)
O(2)-S(1)-O(1)	108.24(10)
O(2)#2-S(1)-O(1)	108.88(11)
O(1)#2-S(1)-O(1)	110.42(15)
S(1)-O(1)-Cu(1)	133.01(11)
C(1)-N(1)-C(5)	120.2(2)
C(1)-N(1)-Cu(1)	125.52(18)
C(5)-N(1)-Cu(1)	114.12(16)
N(1)-C(1)-C(2)	121.6(2)

C (3) -C (2) -C (1)	118.8 (3)
C (4) -C (3) -C (2)	119.0 (2)
C (4) -C (3) -C (6)	122.2 (3)
C (2) -C (3) -C (6)	118.8 (2)
C (5) -C (4) -C (3)	119.5 (2)
N (1) -C (5) -C (4)	120.8 (2)
N (1) -C (5) -C (5) #1	114.41 (13)
C (4) -C (5) -C (5) #1	124.73 (16)
O (4) -C (6) -O (3)	125.3 (3)
O (4) -C (6) -C (3)	122.2 (3)
O (3) -C (6) -C (3)	112.5 (3)

Symmetry transformations used to generate equivalent atoms:

#1 $y-1/3, x+1/3, -z+1/3$ #2 $-x-2/3, -x+y-1/3, -z+2/3$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct10.

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}
Cu (1)	8 (1)	8 (1)	21 (1)	0 (1)	0 (1)	2 (1)
S (1)	15 (1)	9 (1)	16 (1)	0 (1)	0 (1)	7 (1)
O (1)	15 (1)	9 (1)	19 (1)	1 (1)	4 (1)	5 (1)
O (2)	32 (1)	8 (1)	22 (1)	2 (1)	0 (1)	0 (1)
O (3)	8 (1)	23 (1)	45 (2)	-4 (1)	-5 (1)	3 (1)
O (4)	16 (1)	31 (1)	69 (2)	-10 (1)	-10 (1)	16 (1)
N (1)	10 (1)	16 (1)	15 (1)	-1 (1)	-1 (1)	7 (1)
C (1)	17 (1)	10 (1)	22 (2)	0 (1)	1 (1)	6 (1)
C (2)	15 (1)	19 (2)	28 (2)	-3 (1)	-2 (1)	12 (1)
C (3)	11 (1)	20 (2)	18 (1)	-1 (1)	2 (1)	6 (1)
C (4)	11 (1)	14 (1)	21 (2)	-1 (1)	-2 (1)	3 (1)
C (5)	13 (1)	13 (1)	10 (1)	2 (1)	0 (1)	2 (1)
C (6)	14 (2)	27 (2)	21 (2)	3 (1)	2 (1)	6 (1)
O (5)	27 (6)	26 (4)	98 (11)	0 (3)	0 (6)	14 (3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct10.

	x	y	z	U(eq)
H(3)	1008	2533	3107	41
H(1)	-1826	16	2096	20
H(2)	-674	476	2507	23
H(4)	-465	2316	2017	20
H(5)	200(60)	3050(60)	4200(130)	76

